Electronic Supplementary Material (ESI) for Polymer Chemistry.

Supporting Information

Effect of conjugation pathway on electronic structures in p-π* conjugated polymers with fused borepin units

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Supporting Figures and Tables

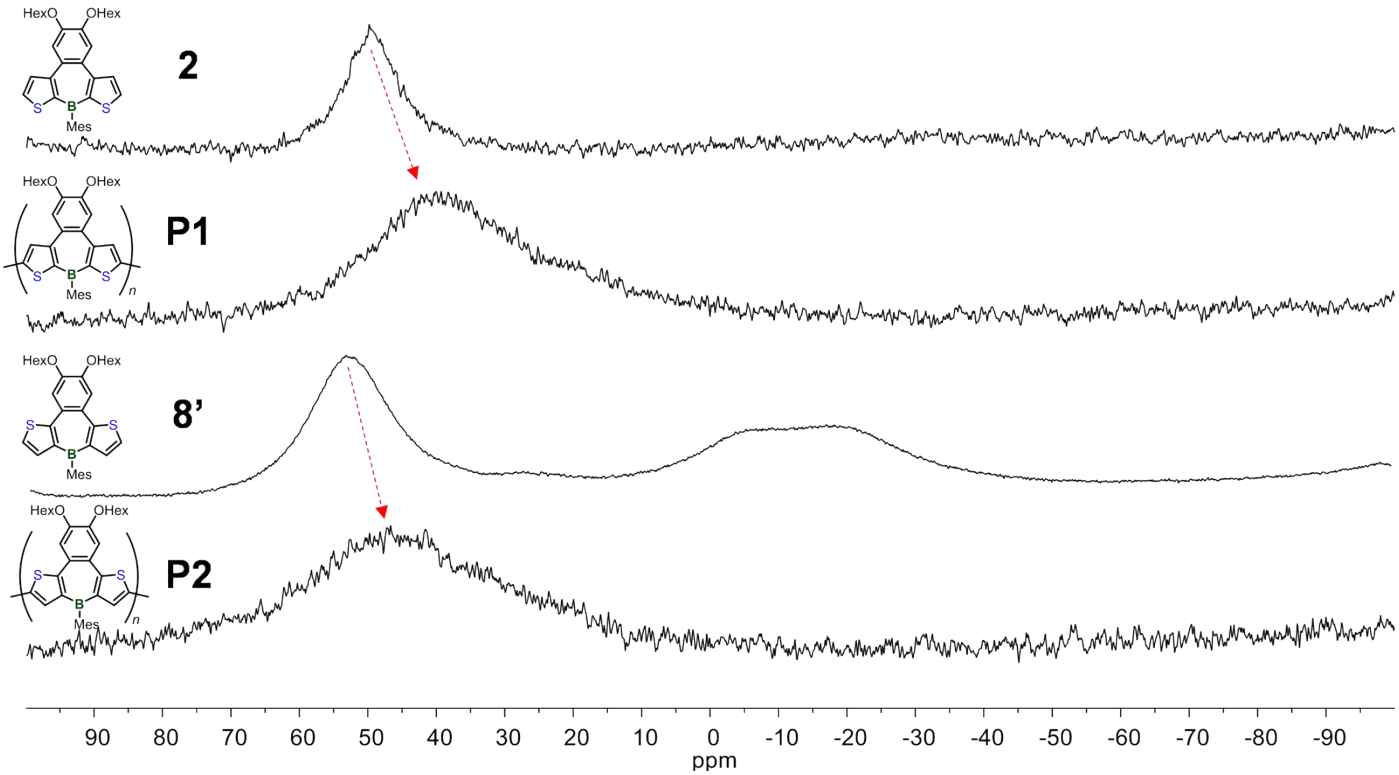


Figure S1. ^{11}B NMR spectra of **2**, **P1**, **8'**, and **P2** in $CDCl_3$ at room temperature.

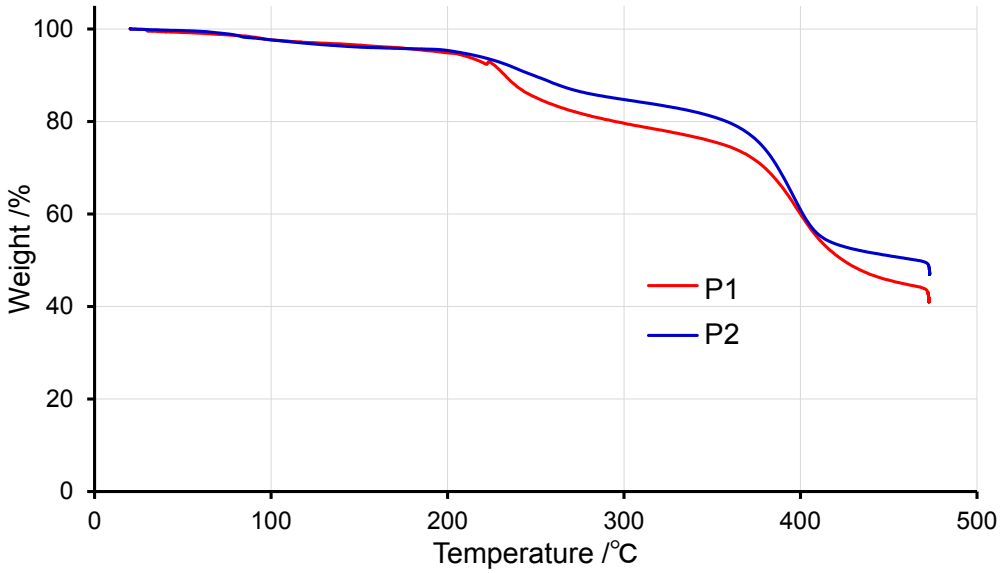


Figure S2. TGA curves of **P1** and **P2** under nitrogen atmosphere at the heating rate of 10 °C min^{-1}.

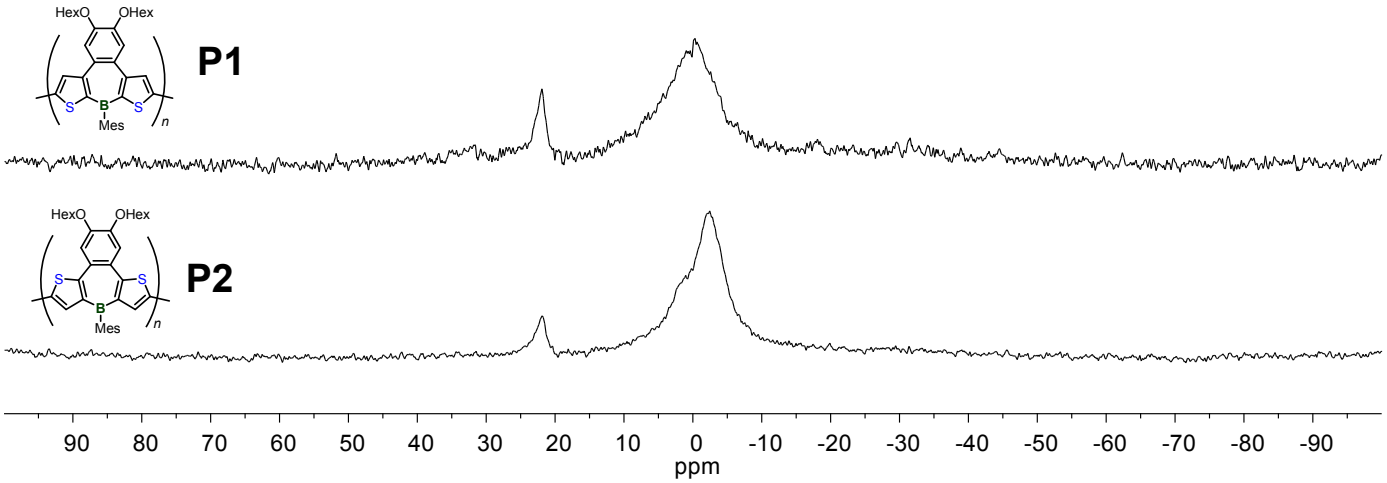


Figure S3. ^{11}B NMR spectra of **P1** and **P2** in pyridine-d_5 at room temperature.

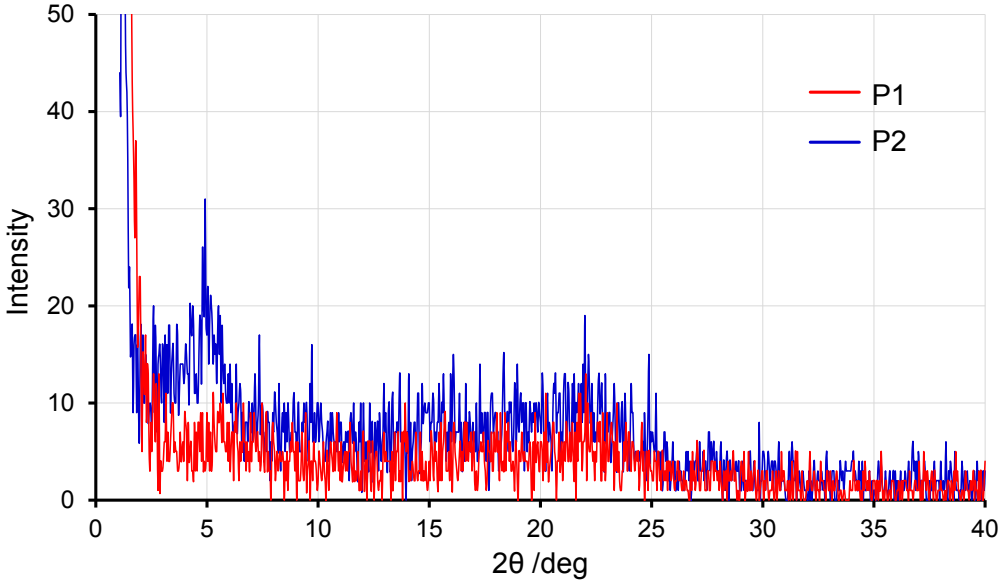


Figure S4. Powder X-ray diffraction patterns of **P1** and **P2**.

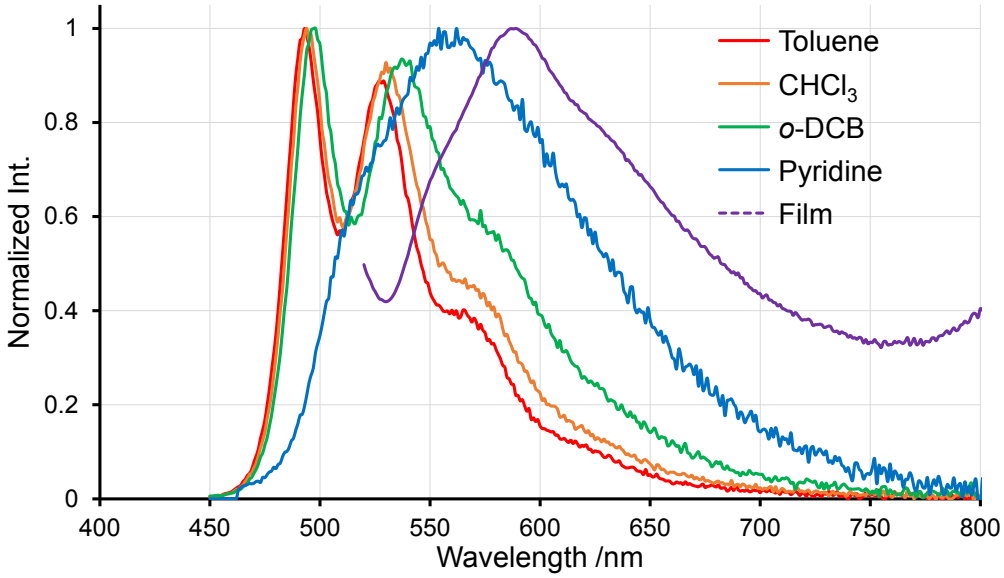


Figure S5. Fluorescence spectra of **P1** in various solvents and in cast film.

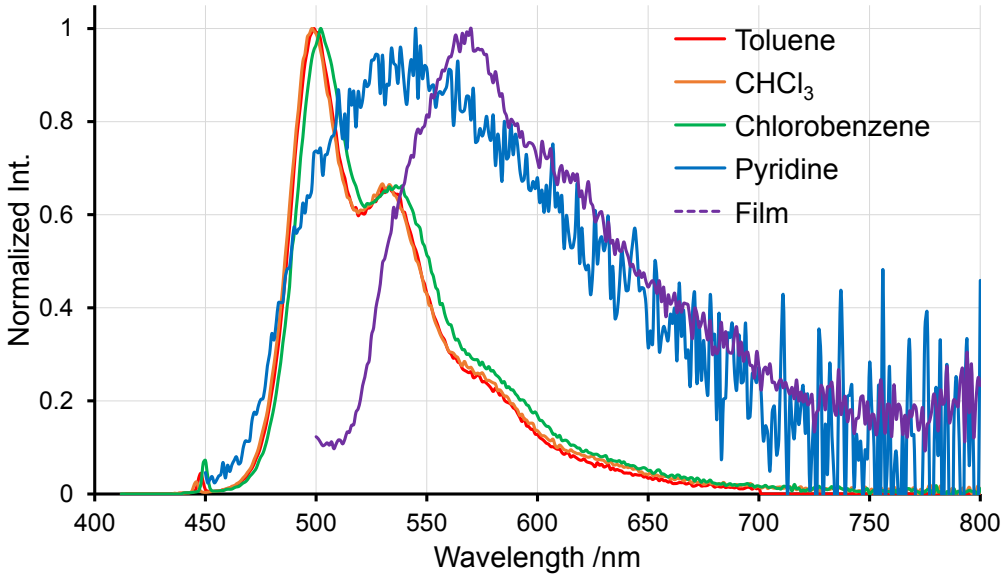


Figure S6. Fluorescence spectra of **P2** in various solvents and in cast film.

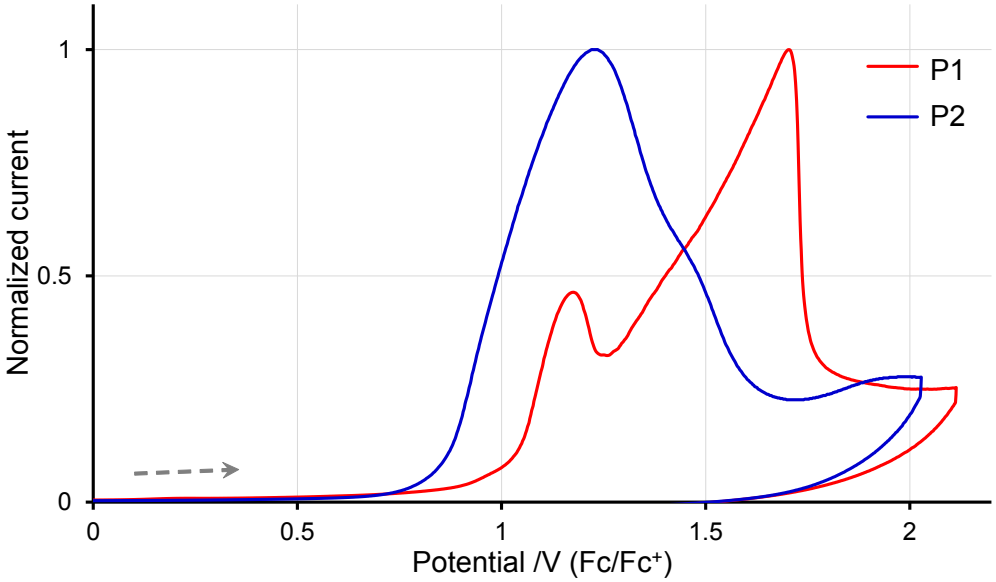


Figure S7. Anodic cyclic voltammetry data for **P1** and **P2** films in acetonitrile with 0.1 M $TBAPF_6$ at the scan rate of 100 mV/s.

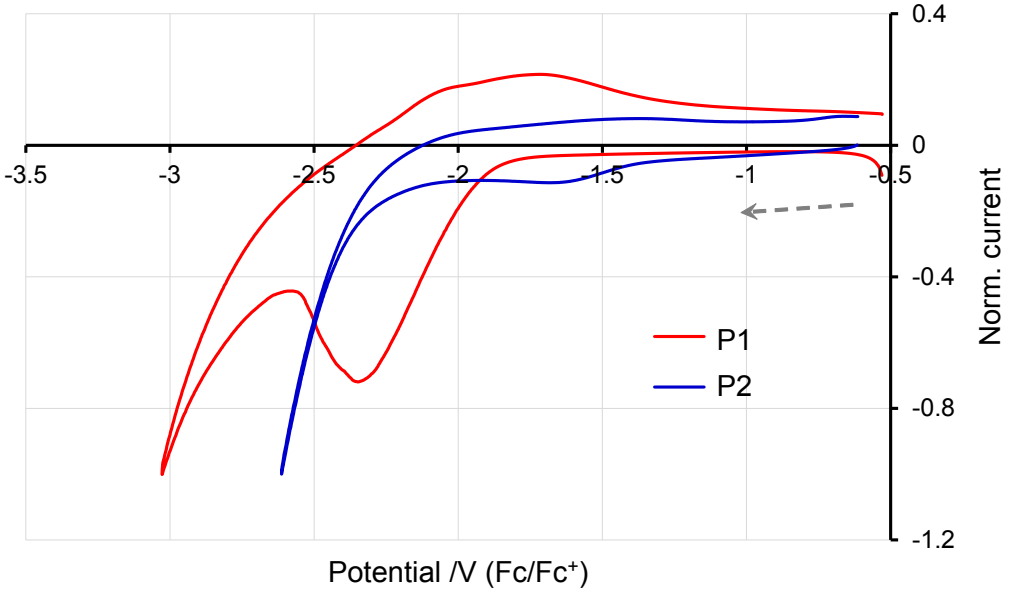


Figure S8. Cathodic cyclic voltammetry data for **P1** and **P2** films in acetonitrile with 0.1 M $TBAPF_6$ at the scan rate of 100 mV/s.

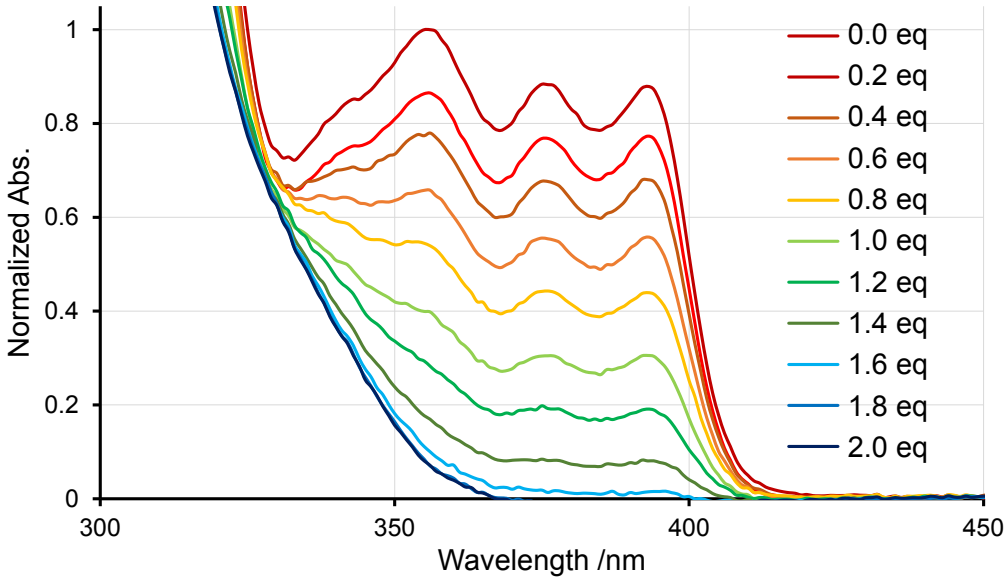


Figure S9. UV-Vis absorption data for titrations of **8'** with TBACN aliquots in toluene.

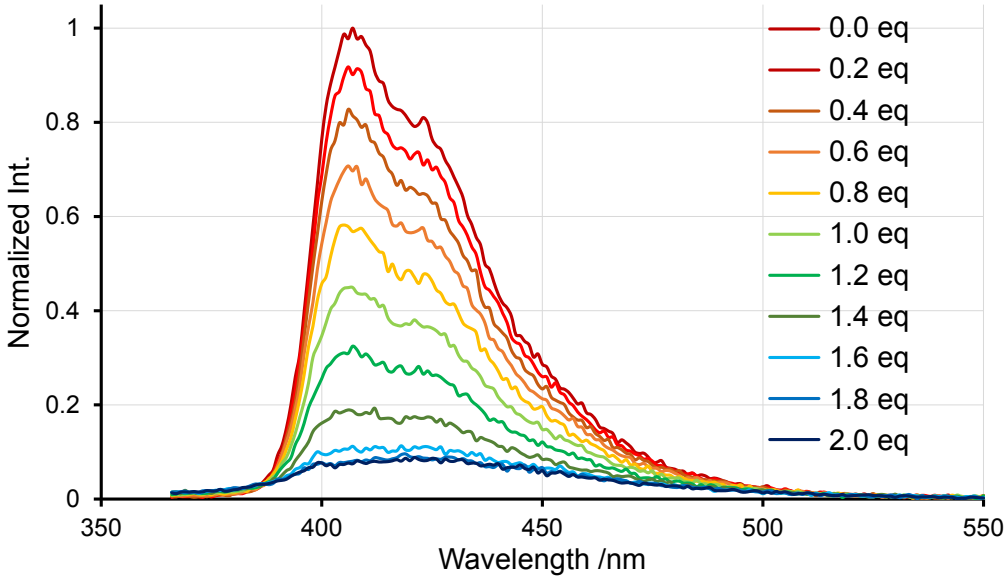


Figure S10. Fluorescence data for titrations of **8'** with TBACN aliquots in toluene.

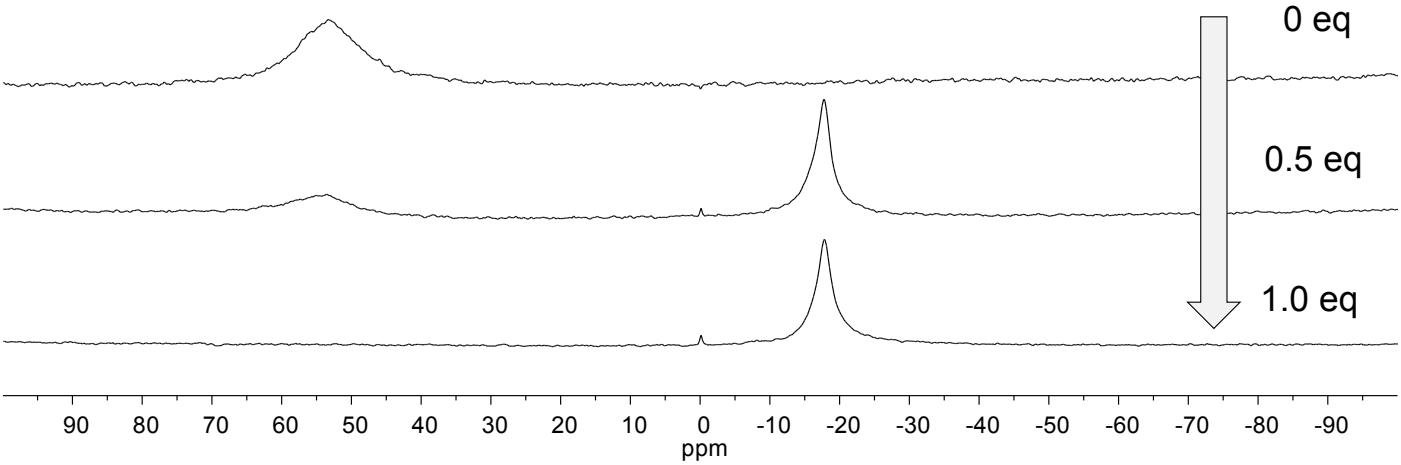


Figure S11. ^{11}B NMR spectra of **8'** before and after the addition of TBACN in benzene-d_6.

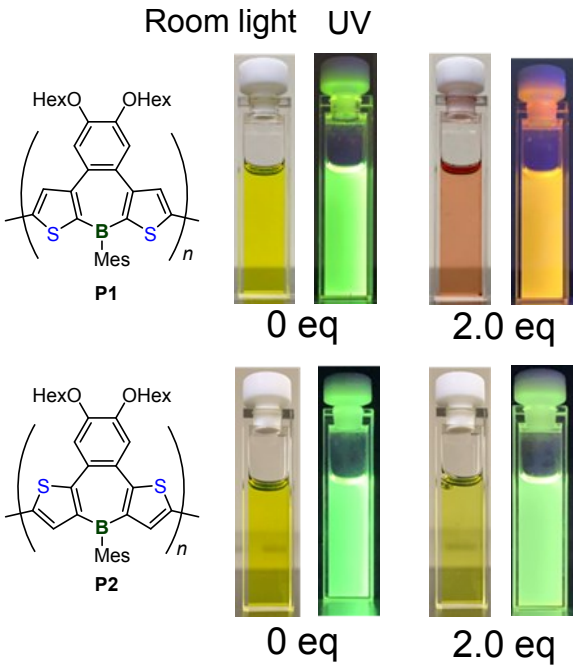


Figure S12. Photographs of diluted solutions of **P1** and **P2** before and after the addition of TBACN in toluene.

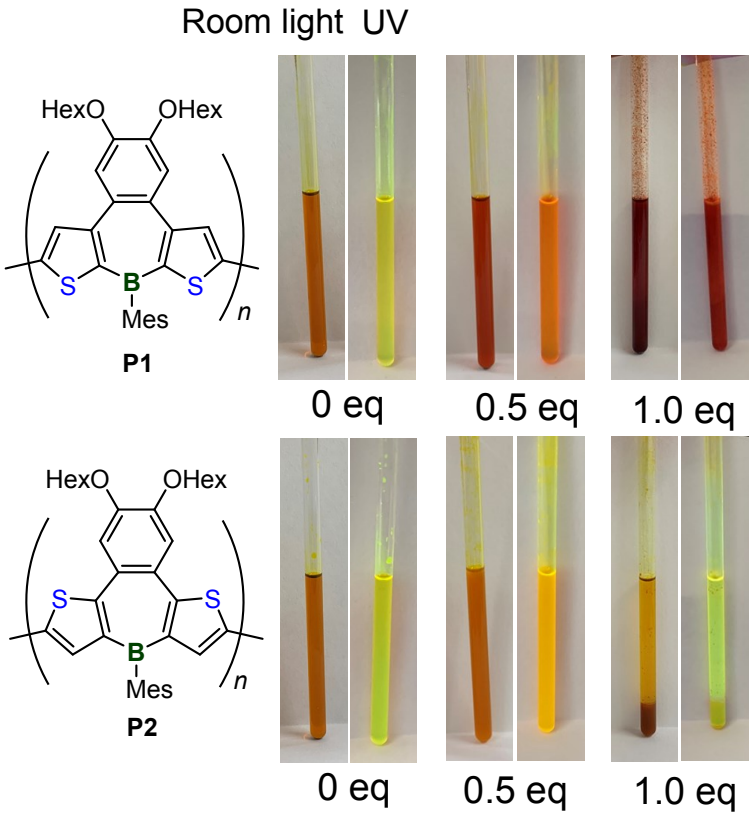


Figure S13. Photographs of NMR samples of **P1** and **P2** before and after the addition of TBACN in benzene-d_6.

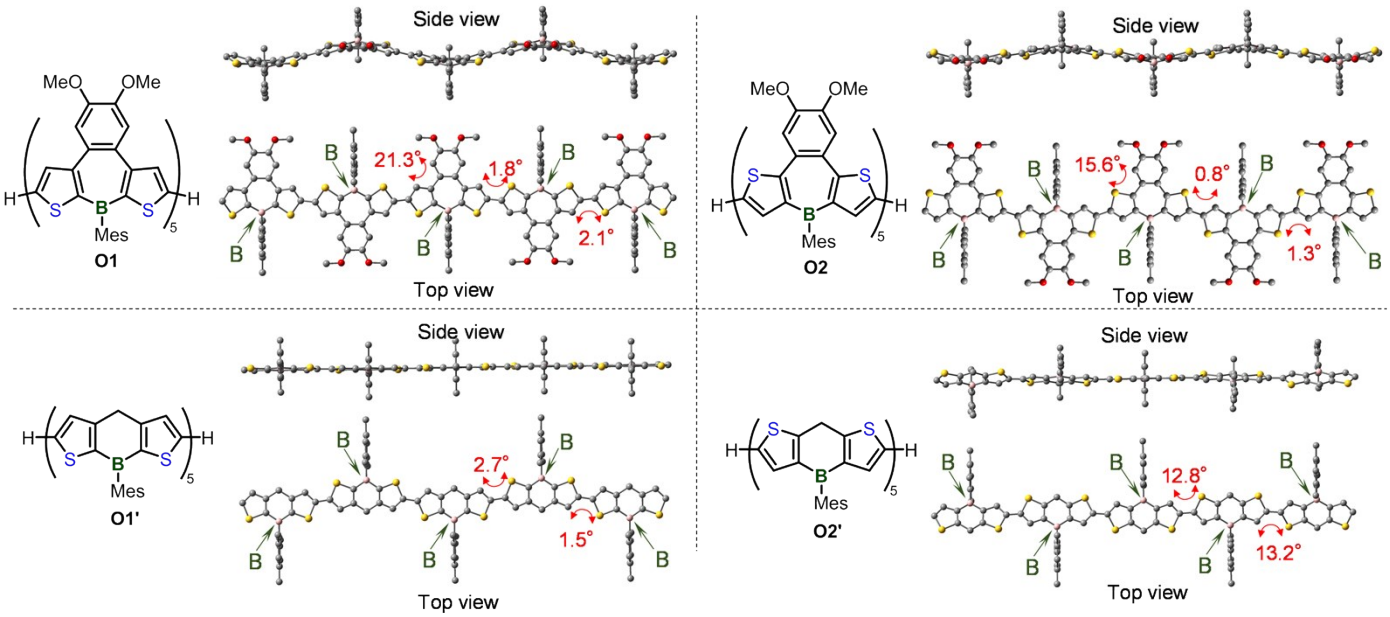


Figure S14. DFT-optimized geomerties of **O1**, **O1'**, **O2**, and **O2'** calculated at the B3LYP/6-31G(d) level. Hydrogen atoms are omitted for clarity.

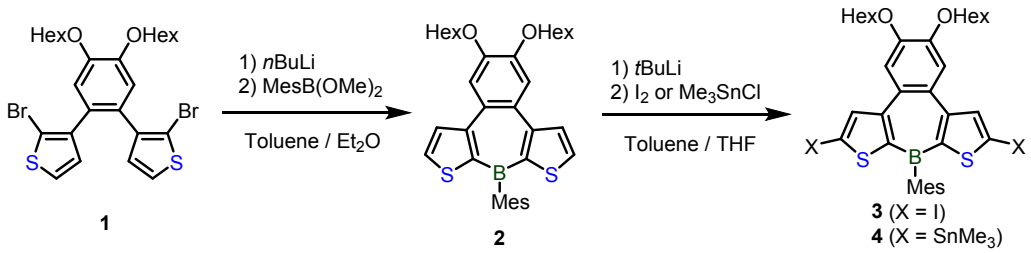
Table S1. TD-DFT data of the model compounds at the CAM-B3LYP/6-31G(d) level.

Compound	Excited state	Composition [a]	CI	Excitation energy /eV	Wavelength /nm	Oscillator strength
O1	S0→S1	H-7→L+2	-0.17341	2.97	417	3.67
		H-6→L+1	-0.22909			
		H-4→L	0.12022			
		H-1→L+1	0.19301			
		H→L	0.54444			
O2	S0→S1	H-3→L+3	0.15332	2.92	425	3.78
		H-2→L+2	0.21493			
		H-1→L+1	-0.31471			
		H→L	0.52265			
O1'	S0→S1	H-2→L+2	-0.18811	2.87	432	3.84
		H-1→L+1	0.30349			
		H→L	0.56696			
O2'	S0→S1	H-3→L+1	0.10309	3.90	318	1.19
		H-3→L+3	-0.11048			
		H-3→L+5	0.23747			
		H-2→L	0.13239			
		H-2→L+2	-0.21319			
		H-2→L+6	0.1459			
		H-1→L+1	-0.30924			
		H→L	0.44322			
	S0→S14	H-3→L+1	0.10651	4.31	287	3.27
		H-3→L+5	-0.27623			
		H-2→L	0.10007			
		H-2→L+6	-0.26293			
		H-1→L+7	0.27386			
		H→L	0.17071			
		H→L+8	0.32307			

[a] H and L denote HOMO and LUMO, respectively.

Experimental

All reactions were carried out under dry argon. For the reaction solvents, toluene, diethyl ether, and THF were purchased from Kanto Chemical Co., Ltd. and were distilled from calcium hydride and stored over activated molecular sieves under argon until use, whereas chloroform was distilled from calcium hydride immediately before use. All other chemicals were purchased from FUJIFILM Wako Pure Chemical Industries, Ltd. and TCI Co., Ltd. Starting materials **1** and **5** were prepared according to the literature.[S1] Dimethoxy(mesityl)borane was prepared by a method similar to the synthesis of dimethoxy(triply)borane, using mesityl bromide instead of tripyl bromide.[S2] Microwave-assisted reactions were carried out using a Biotage Initiator+. TGA was carried out on a SII TG/DTA-6200 analyzer under a gentle nitrogen flow (30 mL/min) at a heating rate of 10 ºC/min. Powder XRD patterns were obtained on a Rigaku Ultima IV multipurpose X-ray diffraction system. NMR spectra were recorded on Varian System 500 and 400MR spectrometers. High-resolution mass spectra were obtained on a Thermo Fisher Scientific LTQ Orbitrap XL spectrometer at N-BARD, Hiroshima University. Several compounds were purified by preparative gel permeation chromatography (GPC) using toluene as an eluent and serially connected Shodex KF2001 and KF2002 columns. UV–vis absorption spectra were measured with a Shimadzu UV-3600 plus spectrometer. Photoluminescence (PL) spectra were measured with a HORIBA FluoroMax-4 spectrophotometer. The absolute PL quantum yields were determined by using a HORIBA FluoroMax-4 spectrophotometer attached to an integration sphere. Titration experiments with TBACN were performed in ca. 0.1 mM toluene solutions for absorption and fluorescence measurements, whereas ca. 10 mM of benzene-d_6 solutions were used for the NMR experiments. The concentration of the polymer solutions was calculated based on the molecular weight of the monomer. In all the measurements, the samples were left for 3 minutes to equilibrate after each addition of cyanide. CVs were measured with an AMETEK VersaSTAT 4 potentiostat/galvanostat in a solution of 0.1 M tetrabutylammonium hexafluorophosphate in acetonitrile using a three-electrode system with a Pt plate counter electrode, a Pt wire working electrode, and an Ag/Ag^+ reference electrode. For the DFT calculations, all geometrical optimizations were performed on a Gaussian 16 program at the B3LYP/6-31G(d) level of theory. TD-DFT calculations of the optimized structures were carried out at the CAM-B3LYP/6-31G(d) level of theory.

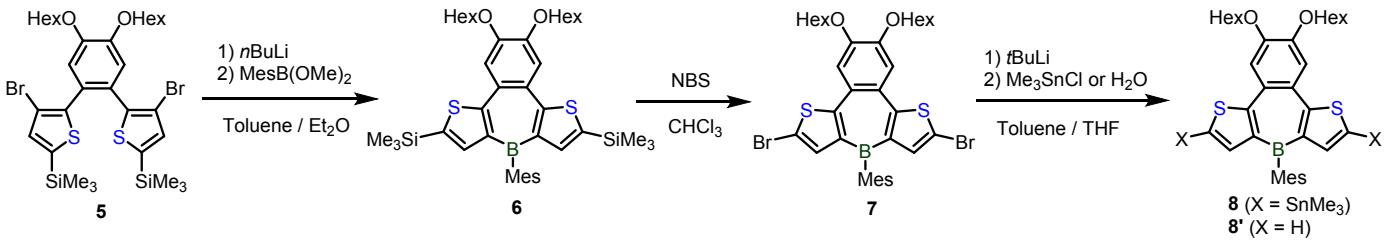


Synthesis of 2. To a solution of 4.90 g (8.16 mmol) of **1** in a mixed solvent of toluene (60 mL) and diethyl ether (15 mL) was slowly added 10.8 mL (16.7 mmol) of 1.55 M *n*BuLi in hexane at −80 °C over 20 min, and the mixture was stirred at this temperature for 30 min. To this was added 1.72 g (8.96 mmol) of dimethoxy(mesityl)borane at this temperature, and the mixture was stirred at room temperature overnight. The resulting mixture was hydrolyzed with saturated ammonium chloride aqueous solution, and the organic layer was separated. The aqueous layer was extracted with toluene, and the combined organic layers were washed with saturated ammonium chloride solution then with brine. After drying over anhydrous magnesium sulfate, the solvent was evaporated. The residue was purified by silica gel chromatography (hexane/CH_2Cl_2 = 2/1) to afford **2** in 63% yield (2.92 g, 5.12 mmol) as an off-white powder. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.06 (2H, d, J = 5.2 Hz, Th), 7.92 (2H, d, J = 5.2 Hz, Th), 7.83 (2H, s, Bz), 6.93 (2H, s, Mes), 4.21 (4H, t, J = 6.6 Hz, OHex), 2.39 (3H, s, Mes), 2.10 (6H, s), 1.98–1.89 (4H, m, OHex), 1.61–1.52 (4H, m, OHex), 1.44–1.35 (8H, m, OHex), 0.94 (6H, t, J = 7.0 Hz, OHex). ^{11}B NMR (160 MHz, $CDCl_3$) δ: 49.8. ^{13}C NMR (100 MHz, $CDCl_3$) δ: 150.6, 148.5, 138.9, 137.4, 135.2, 130.9, 127.6, 127.1, 115.5, 69.3, 31.6, 29.3, 25.8, 22.8, 22.7, 21.4, 14.1. Two signals for B−C were not detected, probably due to their low intensity as a result of quadrupolar broadening. m.p. 108.8–110.6 ℃. HR-MS(APCI) Calculated for $C_{35}H_{44}O_2BS_2$ $[M+H]^+$: 571.28703, Found: 571.28705.

Synthesis of 3. To a solution of 289 mg (0.506 mmol) of **2** in a mixed solvent of toluene (16 mL) and diethyl ether (4 mL) was slowly added 1.24 mL (2.00 mmol) of 1.61 M *t*BuLi in pentane at −80 °C over 10 min, and the mixture was stirred at this temperature for 30 min. To this was added 8 mL of a toluene solution of elemental iodine (I_2, 533 mg, 2.10 mmol) at this temperature, and the mixture was stirred at room temperature

overnight. The resulting mixture was hydrolyzed with sodium thiosulfate aqueous solution, and the organic layer was separated. The aqueous layer was extracted with toluene, and the combined organic layers were washed with water then with brine. After drying over anhydrous magnesium sulfate, the solvent was evaporated. The residue was purified by silica gel chromatography (hexane/CH_2Cl_2 = 3/1) to afford **3** in 55% yield (228 mg, 0.277 mmol) as an off-white powder. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.12 (2H, s, Th), 7.69 (2H, s, Bz), 6.92 (2H, s, Mes), 4.22 (4H, t, J = 6.5 Hz, OHex), 2.38 (3H, s, Mes), 2.09 (6H, s, Mes), 2.00–1.90 (4H, m, OHex), 1.62–1.54 (4H, m, OHex), 1.45–1.38 (8H, m, OHex), 0.95 (6H, t, J = 7.1 Hz, OHex). ^{11}B NMR (128 MHz, $CDCl_3$) δ: 47.3. ^{13}C NMR (100 MHz, $CDCl_3$) δ: 151.7, 149.8 (br, B–C), 148.9, 140.6, 138.9, 137.9, 127.2, 126.2, 115.0, 88.1, 69.3, 31.6, 29.2, 25.8, 22.8, 22.6, 21.4, 14.1. One signal for B−C was not detected, probably due to its low intensity as a result of quadrupolar broadening. m.p. 184.5–186.0 ℃. HR-MS(APCI) Calculated for $C_{35}H_{41}O_2BI_2S_2$ $[M]^+$: 822.07249, Found: 822.07330.

Synthesis of 4. Compound **4** was prepared from 295 mg (0.517 mmol) of **2**, 1.3 mL (2.1 mmol) of 1.61 M *t*BuLi in pentane, 443 mg (2.22 mmol) of trimethyltin chloride, 16 mL of toluene, and 4 mL of THF in a manner similar to that above. The crude product was purified by preparative GPC with toluene as the eluent to afford **4** as a light yellowish solid (327 mg, 0.365 mmol, 71% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.11 (2H, s, Th), 7.92 (2H, s, Bz), 6.99 (2H, s, Mes), 4.28 (4H, t, J = 6.6 Hz, OHex), 2.45 (3H, s, Mes), 2.17 (6H, s, Mes), 2.04–1.93 (4H, m, OHex), 1.66–1.58 (4H, m, OHex), 1.50–1.39 (8H, m, OHex), 0.99 (6H, t, J = 7.1 Hz, OHex), 0.46 (18H, s, $SnMe_3$). ^{11}B NMR (128 MHz, $CDCl_3$) δ: 50.1. ^{13}C NMR (100 MHz, $CDCl_3$) δ: 150.8, 150.2, 148.8 (br, B–C), 148.3, 141.8 (br, B–C), 138.7, 138.5, 137.0, 127.7, 127.0, 116.0, 69.5, 31.6, 29.3, 25.8, 22.9, 22.7, 21.5, 14.1, -8.1. m.p. 177.0–178.2 ℃. HR-MS(APCI) Calculated for $C_{41}H_{60}O_2BS_2Sn_2$ $[M+H]^+$: 899.21662, Found: 899.21869.



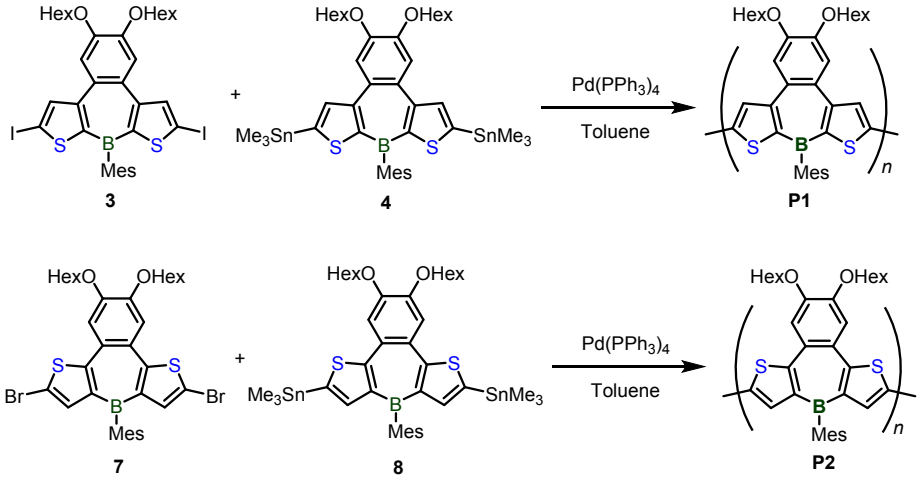
Synthesis of 6. Compound **6** was prepared from 3.61 g (4.85 mmol) of **5**, 6.34 mL (9.95 mmol) of 1.57 M *n*BuLi in hexane, 1.02 g (5.31 mmol) of dimethoxy(mesityl)borane, 20 mL of toluene, and 5 mL of diethyl ether in a manner similar to that of **2**. The crude product was purified by silica gel chromatography (hexane/CH_2Cl_2 = 3/1) to afford **6** as a light yellowish solid (2.64 g, 3.69 mmol, 76% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.85 (2H, s, Bz), 7.34 (2H, s, Th), 6.89 (2H, s, Mes), 4.22 (4H, t, *J* = 6.5 Hz, OHex), 2.39 (3H, s, Mes), 1.98 (6H, s, Mes), 1.99–1.88 (4H, m, OHex), 1.63–1.51 (4H, m, OHex), 1.44–1.36 (8H, m, OHex), 0.94 (6H, t, *J* = 7.1 Hz), 0.30 (18H, s, $SiMe_3$). ^{11}B NMR (160 MHz, $CDCl_3$) δ: 53.8. ^{13}C NMR (100 MHz, $CDCl_3$) δ: 162.2, 149.3, 145.4 (br, B–C), 145.0, 144.2 (br, B–C), 137.5, 137.3, 135.8, 127.0, 125.0, 114.8, 69.1, 31.6, 29.1, 25.8, 22.7, 22.6, 21.2, 14.0, -0.1. HR-MS(APCI) Calculated for $C_{41}H_{60}O_2BS_2Si_2$ $[M+H]^+$: 715.36608, Found: 715.36761.

Synthesis of 7. To a solution of 545 mg (0.762 mmol) of **6** in 70 mL of $CHCl_3$ was added 299.6 mg (1.68 mmol) of NBS in several portions at 0 °C, and the reaction mixture was stirred for 2 hours at room temperature. The resulting mixture was hydrolyzed, and the organic layer was separated. The aqueous layer was extracted with chloroform and the combined organic layers were washed with saturated ammonium chloride aqueous solution, water, then with brine. After drying over anhydrous magnesium sulfate, the solvent was evaporated. The residue was purified by silica gel chromatography (hexane/CH_2Cl_2 = 1/1) to afford **7** in 48% yield (266 mg, 0.365 mmol) as a light yellowish powder. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.63 (2H, s, Bz), 7.14 (2H, s, Th), 6.91 (2H, s, Mes), 4.18 (4H, t, *J* = 6.6 Hz, OHex), 2.38 (3H, s, Mes), 1.97 (6H, s, Mes), 1.97–1.88 (4H, m, OHex), 1.58–1.51 (4H, m, OHex), 1.42–1.37 (8H, m, OHex), 0.94 (6H, t, *J* = 7.1 Hz, OHex). ^{11}B NMR (160 MHz, $CDCl_3$) δ: 51.4. ^{13}C NMR (100 MHz, $CDCl_3$) δ: 159.2, 149.8, 145.4 (br, B–C), 143.2(br, B–C), 139.7, 137.4, 136.7, 127.2, 124.6, 113.6, 110.9, 69.3, 31.6, 29.0, 25.7, 22.7, 22.6, 21.2, 14.0. m.p. 165.4–166.1 ℃. HR-MS(APCI) Calculated for $C_{35}H_{41}O_2BBr_2S_2$ $[M]^+$: 726.10023, Found: 726.10089.

Synthesis of 8. To a solution of 147 mg (0.202 mmol) of **7** in a mixed solvent of toluene (8 mL) and THF (2 mL) was slowly added 0.27 mL (0.42 mmol) of 1.55 M *n*BuLi in hexane at −80 °C, and the mixture was

stirred at this temperature for 30 min. To this was added 88.2 mg (0.443 mmol) of trimethyltin chloride at this temperature, and the mixture was stirred at room temperature for 1 hour. The resulting mixture was hydrolyzed, and the organic layer was separated. The aqueous layer was extracted with toluene, and the combined organic layers were washed with saturated ammonium chloride aqueous solution, water, then with brine. After drying over anhydrous magnesium sulfate, the solvent was evaporated. The residue was purified by preparative GPC with toluene as the eluent to afford **8** in 33% yield (60.4 mg, 67.4 μmol) as a light yellowish solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.91 (2H, s, Bz), 7.34 (2H, s, Th), 6.93 (2H, s, Mes), 4.24 (4H, t, J = 6.6 Hz, OHex), 2.42 (3H, s, Mes), 2.02 (6H, s, Mes), 2.00–1.91 (4H, m, OHex), 1.64–1.54 (4H, m, OHex), 1.46–1.38 (8H, m, OHex), 0.96 (6H, t, J = 7.0 Hz, OHex), 0.38 (18H, s, $SnMe_3$). ^{11}B NMR (128 MHz, $CDCl_3$) δ: 55.2. ^{13}C NMR (100 MHz, $CDCl_3$) δ: 162.8, 149.1, 146.2, 137.6, 135.8, 135.4, 126.9, 124.8, 114.8, 69.2, 31.6, 29.1, 25.8, 22.8, 22.6, 21.3, 14.0, -8.1. Two signals for B−C were not detected, probably due to their low intensity as a result of quadrupolar broadening. m.p. 156.8–157.5 ℃. HR-MS(APCI) Calculated for $C_{41}H_{59}O_2BS_2Sn_2$ $[M]^+$: 898.20880, Found: 898.20972.

Synthesis of 8'. Compound **8'** was prepared from 364 mg (0.500 mmol) of **7**, 0.68 mL (1.0 mmol) of 1.55 M *n*BuLi in hexane, 20 mL of toluene, and 5 mL of THF in a manner similar to that of **8**. The lithiated solution was quenched with a few drops of saturated ammonium chloride aqueous solution instead of trimethyltin chloride. The crude product was purified by silica gel chromatography (hexane/CH_2Cl_2 = 4/1) to afford **8'** as a light yellowish solid (247 mg, 0.433 mmol, 87% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.92 (2H, s, Bz), 7.30 (2H, d, J = 5.3 Hz, Th), 7.28 (2H, d, J = 5.3 Hz, Th), 6.93 (2H, s, Mes), 4.24 (4H, t, J = 6.6 Hz, OHex), 2.41 (3H, s, Mes), 2.02 (6H, s, Mes), 2.00–1.91 (4H, m, OHex), 1.64–1.54 (4H, m, OHex), 1.46–1.39 (8H, m, OHex), 0.97 (6H, t, J = 7.1 Hz, OHex). ^{11}B NMR (128 MHz, $CDCl_3$) δ: 53.2. ^{13}C NMR (100 MHz, $CDCl_3$) δ: 158.0, 149.3, 144.3 (br, B–C), 144.0 (br, B–C), 137.9, 137.5, 136.1, 127.0, 125.3, 122.7, 114.5, 69.2, 31.6, 29.1, 25.7, 22.6, 22.6, 21.2, 14.0. m.p. 131.8–132.6 ℃. HR-MS(APCI) Calculated for $C_{35}H_{44}O_2BS_2$ $[M+H]^+$: 571.28703, Found: 571.28778.



Polymer Synthesis

A mixture of 100 mg (0.122 mmol) of **3**, 109 mg (0.122 mmol) of **4**, 10.0 mg (7 mol%) of $Pd(PPh_3)_4$, and 20 mL of toluene was heated to 140 °C for 1 hour in a microwave reactor. The mixture was cooled to room temperature and hydrolyzed, then the organic layer was separated. The organic layer was washed with water then brine. The residue was reprecipitated from 3 mL of chloroform into 100 mL of a 1:1 mixture of ethanol and acetone to give 71.3 mg (51% yield) of **P1** as a red powder: ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.18 (2H, br s, Th), 7.74 (2H, br s, Bz), 6.99 (2H, br s, Mes), 4.23 (4H, t, J = 6.0 Hz, OHex), 2.44 (3H, br s, Mes), 2.15 (6H, br s, Mes), 1.97–1.87 (4H, m, OHex), 1.61–1.52 (4H, m, OHex), 1.44–1.33 (8H, m, OHex), 0.92 (6H, t, J = 6.7 Hz, OHex). ^{11}B NMR (160 MHz, $CDCl_3$) δ: 39.3. T_d^5: 196 ℃.

Polymer **P2** was prepared from 73.3 mg (0.101 mmol) of **7** and 90.2 mg (0.101 mmol) of **8**, 5.8 mg (5 mol%) of $Pd(PPh_3)_4$, and 16 mL of toluene as an orangish powder (88.2 mg, 77% yield) in a manner similar to that above. The polymer was purified by reprecipitating from 3 mL of chloroform into 100 mL of a 1:1 mixture of hexane and ethanol: ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.78 (2H, br s, Bz), 7.32 (2H, br s, Th), 6.99 (2H, br s, Mes), 4.26 (4H, br s, OHex), 2.48 (3H, br s, Mes), 2.08 (6H, br s, Mes), 2.04–1.87 (4H, m, OHex), 1.72–1.51 (4H, m, OHex), 1.53–1.28 (8H, m, OHex), 1.06–0.87 (6H, m, OHex). ^{11}B NMR (160 MHz, $CDCl_3$) δ: 46.0. T_d^5: 206 ℃.

References

[S1] J. G. Weis and T. M. Swager, *ACS Macro Lett.*, 2015, **4**, 138.

[S2] W.-M. Wan, F. Cheng and F. Jäkle, *Angew. Chem. Int. Ed.*, 2014, **53**, 8934.

NMR spectra

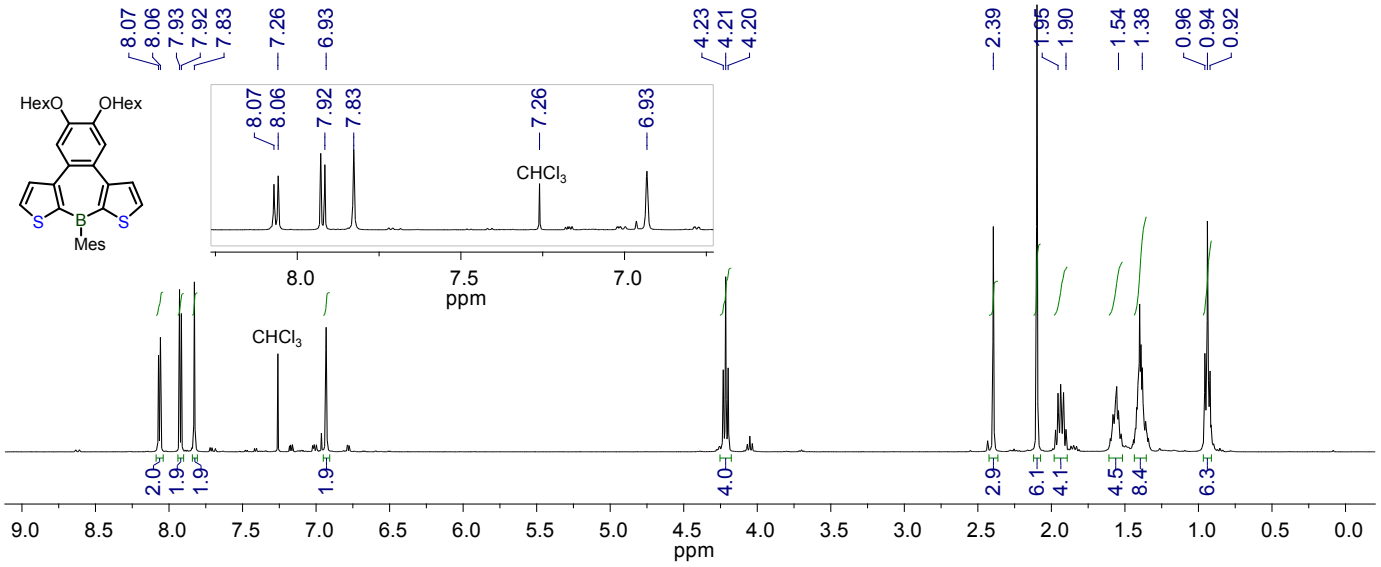


Figure S15. ^{1}H NMR spectrum of **2** in $CDCl_3$ at room temperature (400 MHz).

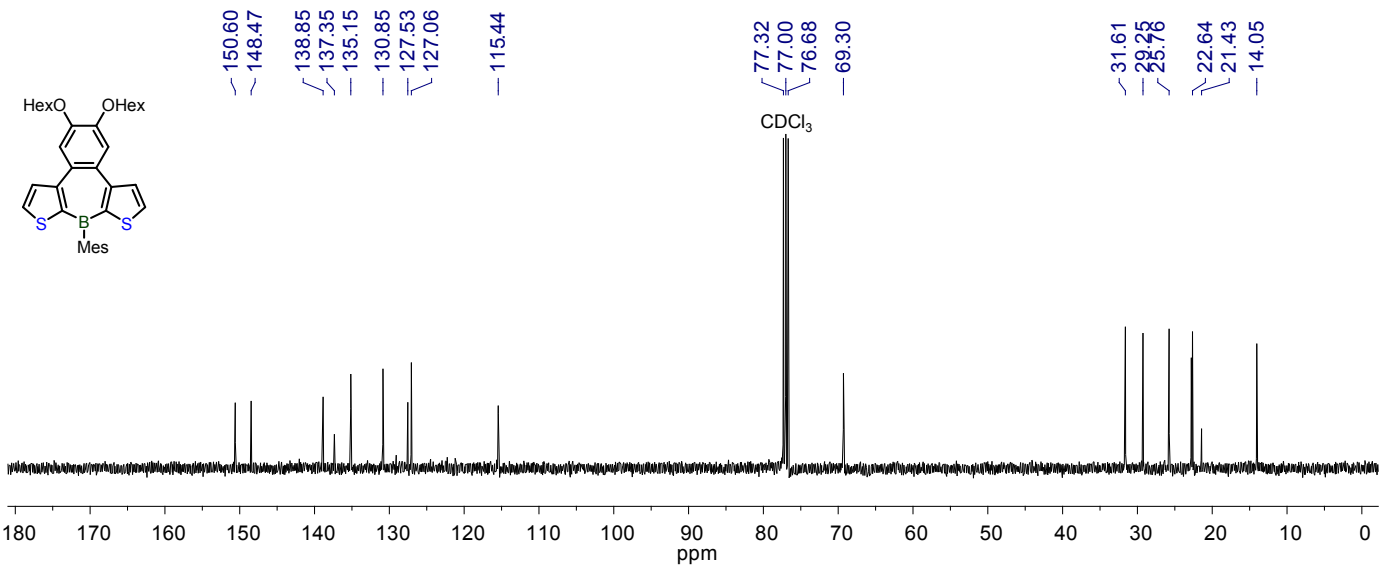


Figure S16. ^{13}C NMR spectrum of **2** in $CDCl_3$ at room temperature (100 MHz).

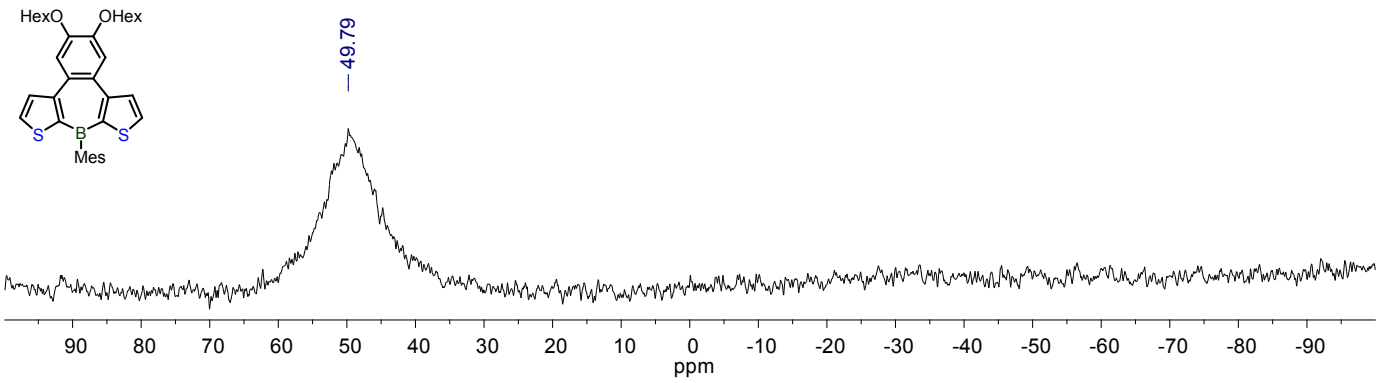


Figure S17. ^{11}B NMR spectrum of **2** in $CDCl_3$ at room temperature (160 MHz).

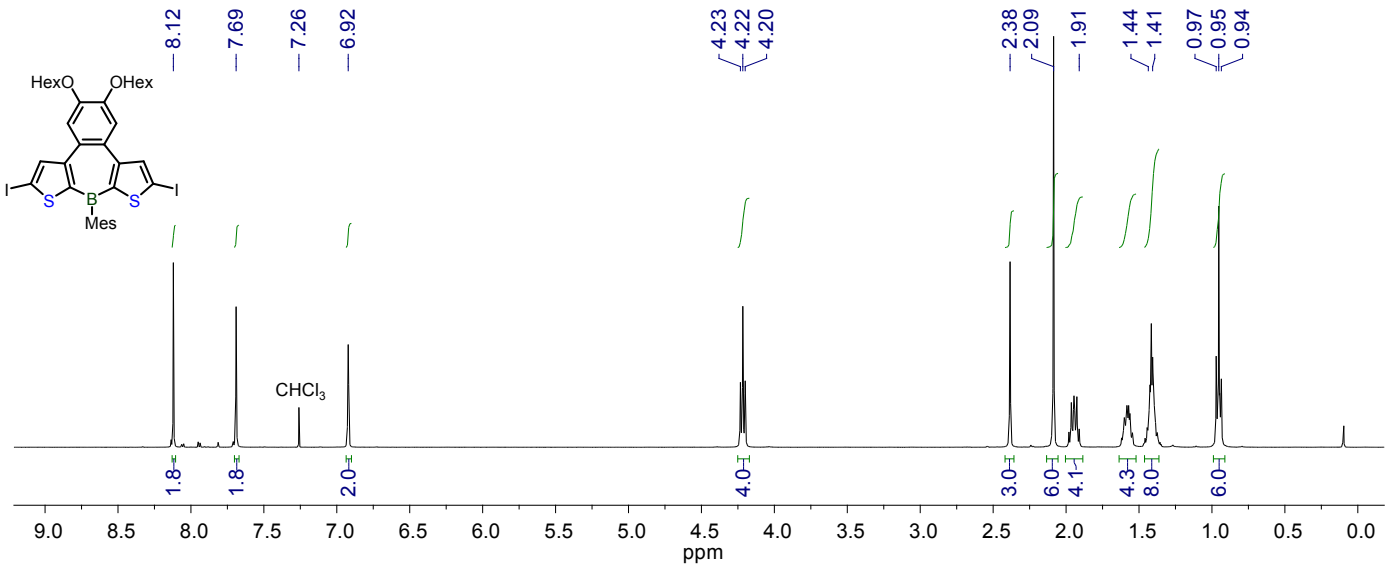


Figure S18. ^{1}H NMR spectrum of **3** in $CDCl_3$ at room temperature (400 MHz).

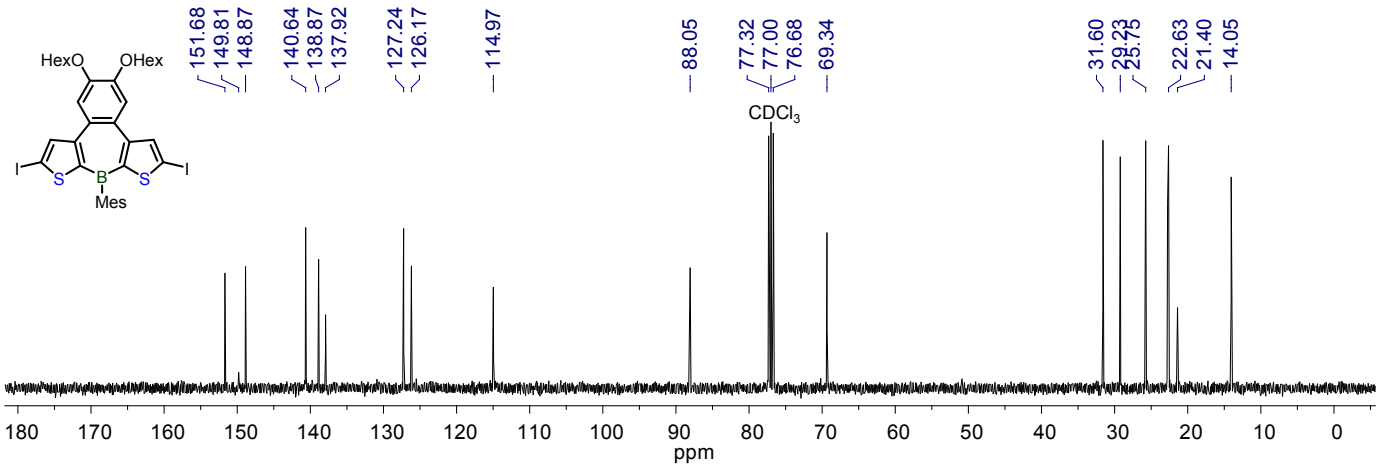


Figure S19. ^{13}C NMR spectrum of **3** in $CDCl_3$ at room temperature (100 MHz).

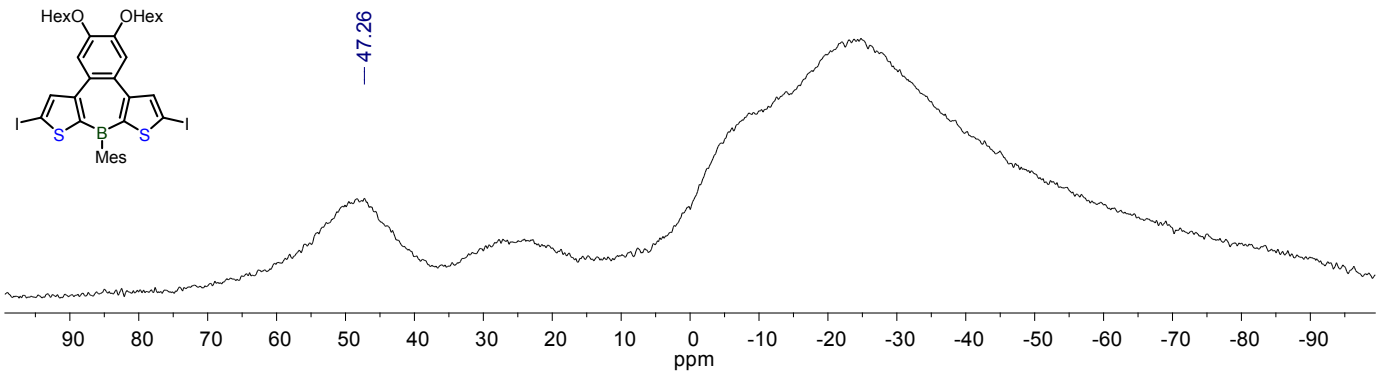


Figure S20. ^{11}B NMR spectrum of **3** in $CDCl_3$ at room temperature (128 MHz).

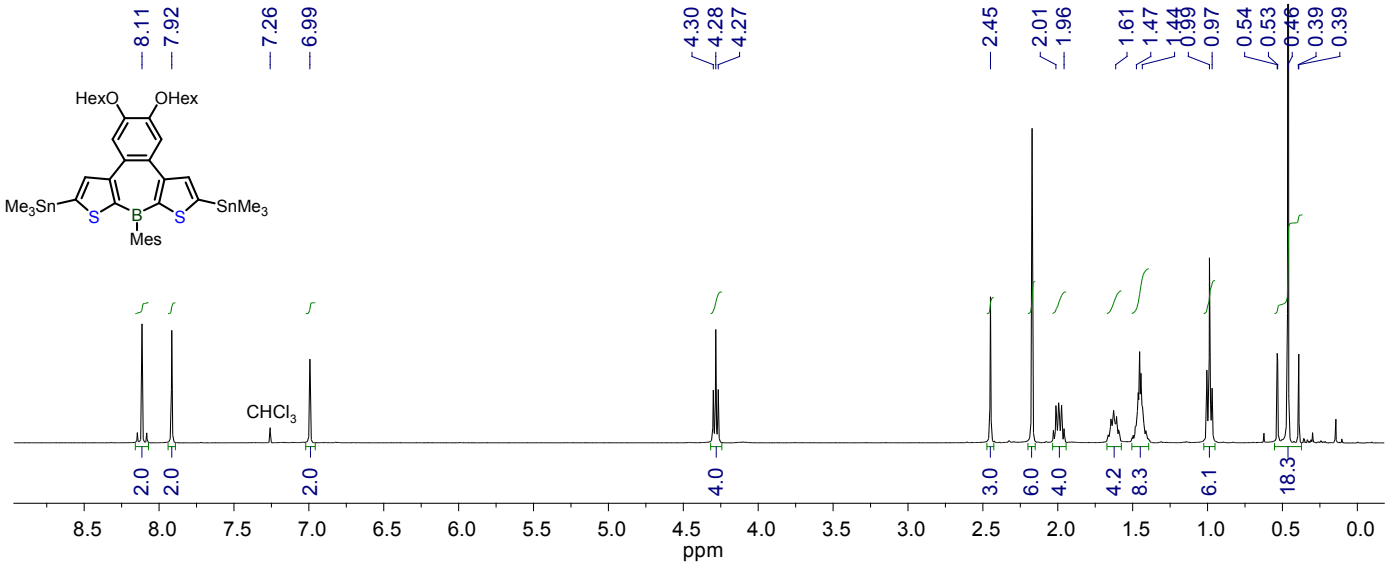


Figure S21. ^{1}H NMR spectrum of **4** in $CDCl_3$ at room temperature (400 MHz).

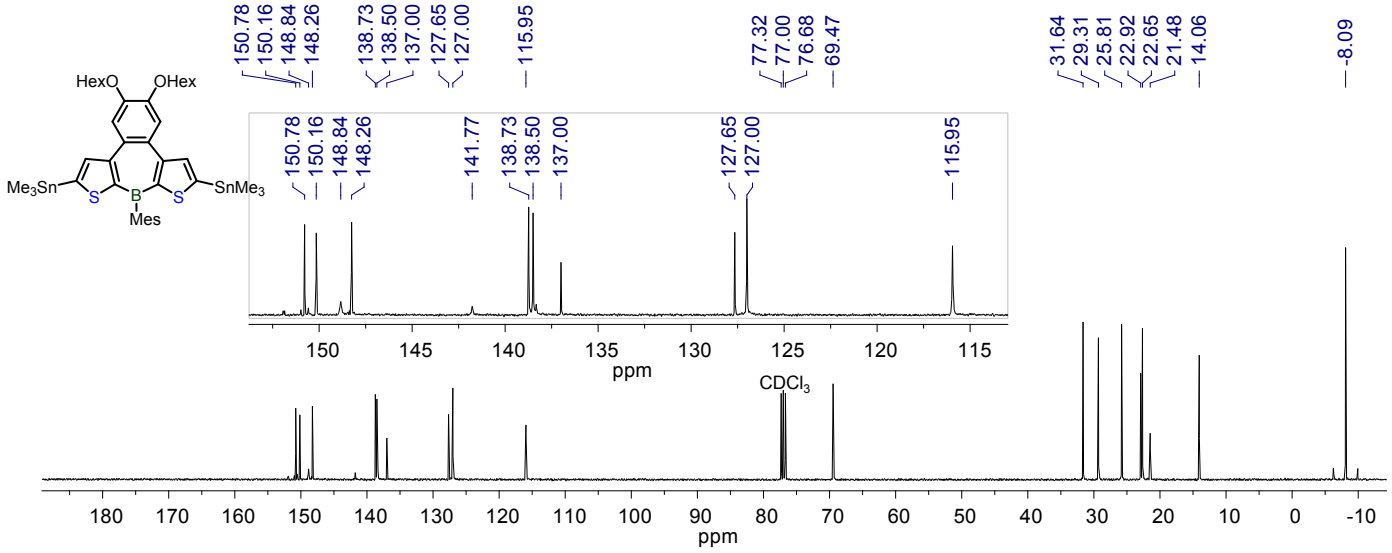


Figure S22. ^{13}C NMR spectrum of **4** in $CDCl_3$ at room temperature (100 MHz).

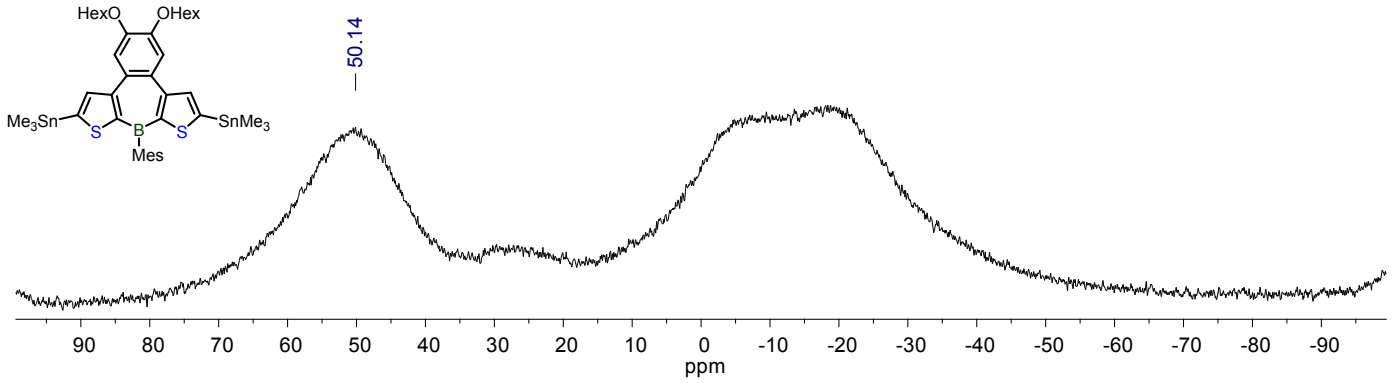


Figure S23. ^{11}B NMR spectrum of **4** in $CDCl_3$ at room temperature (128 MHz).

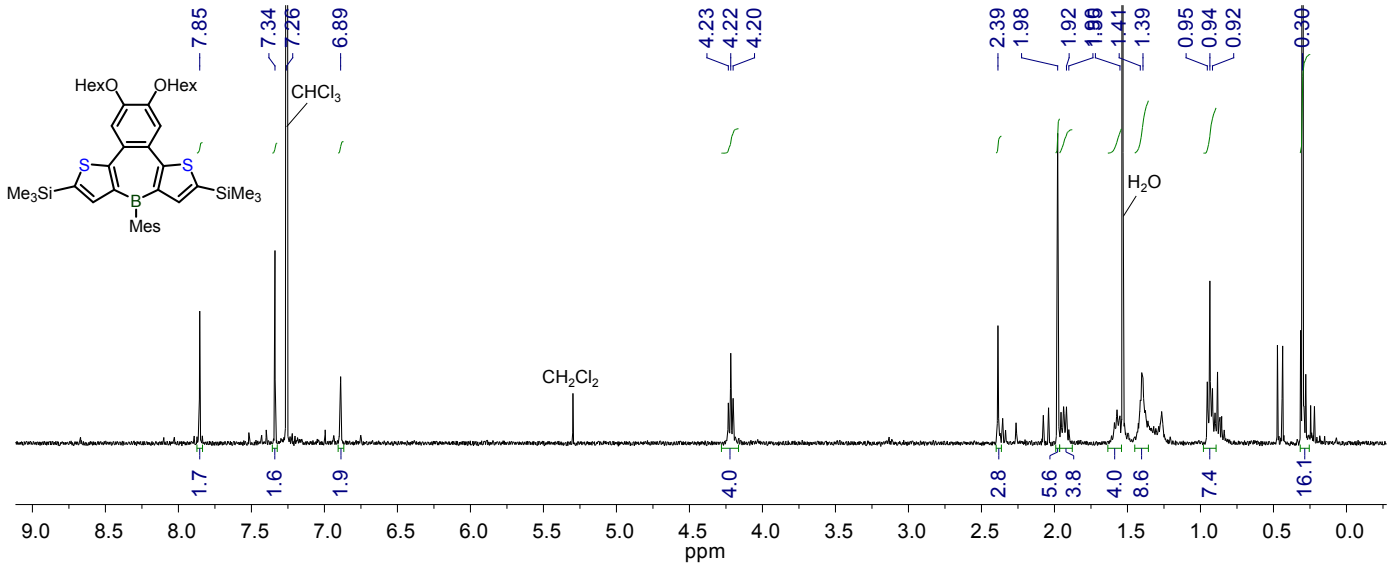


Figure S24. ^{1}H NMR spectrum of **6** in $CDCl_3$ at room temperature (400 MHz).

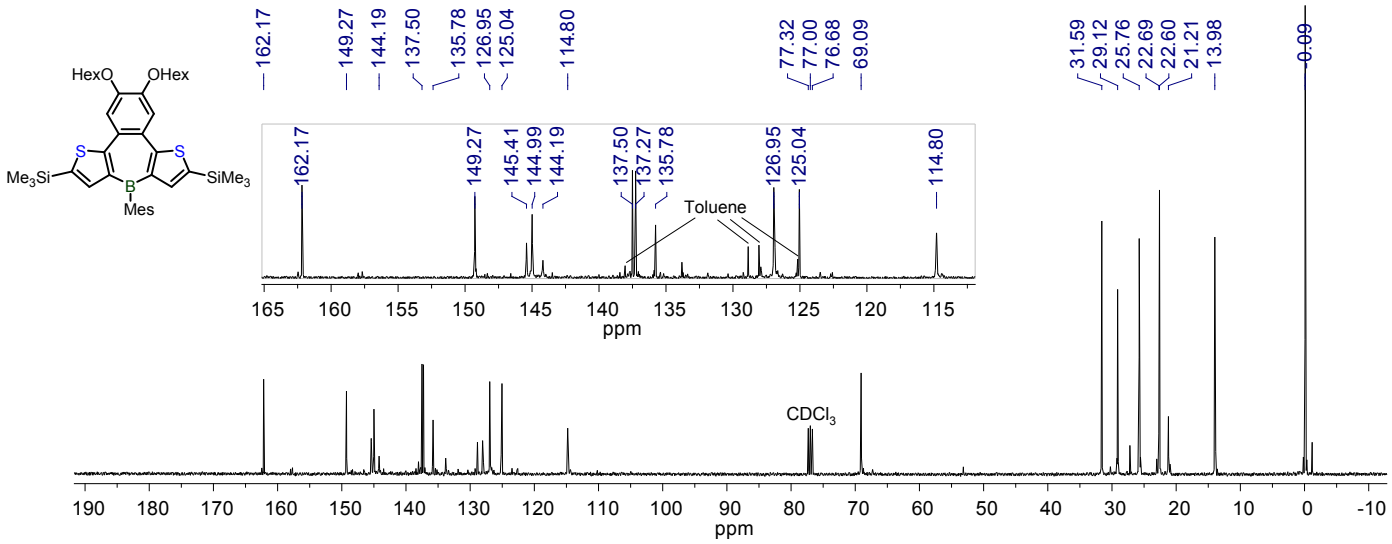


Figure S25. ^{13}C NMR spectrum of **6** in $CDCl_3$ at room temperature (100 MHz).

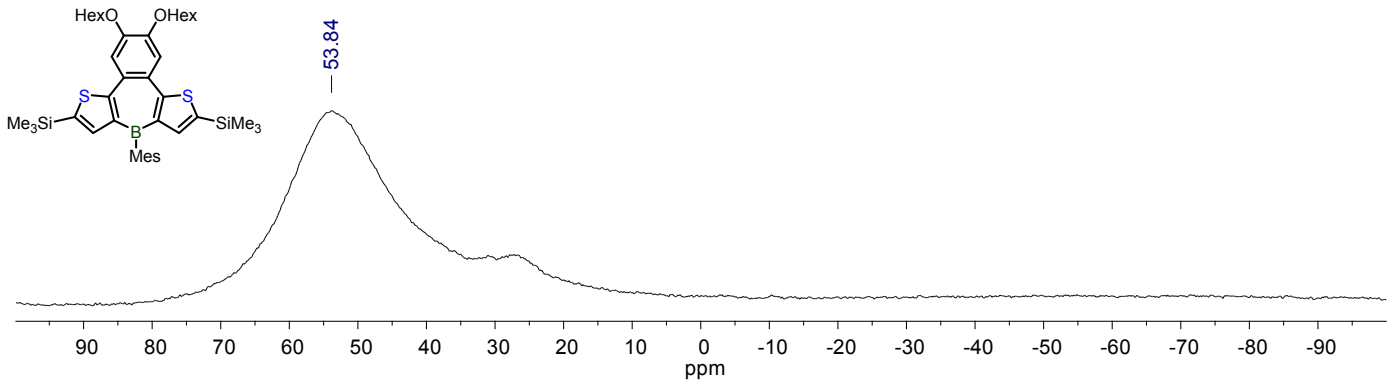


Figure S26. ^{11}B NMR spectrum of **6** in $CDCl_3$ at room temperature (160 MHz).

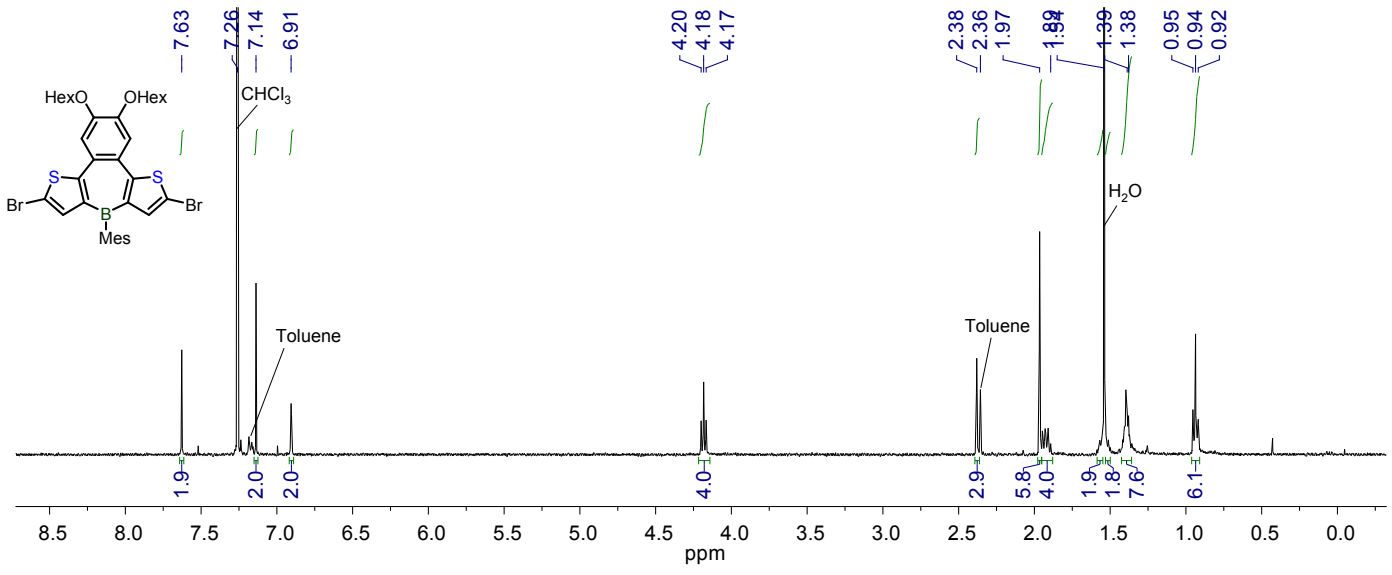


Figure S27. ^{1}H NMR spectrum of **7** in $CDCl_3$ at room temperature (400 MHz).

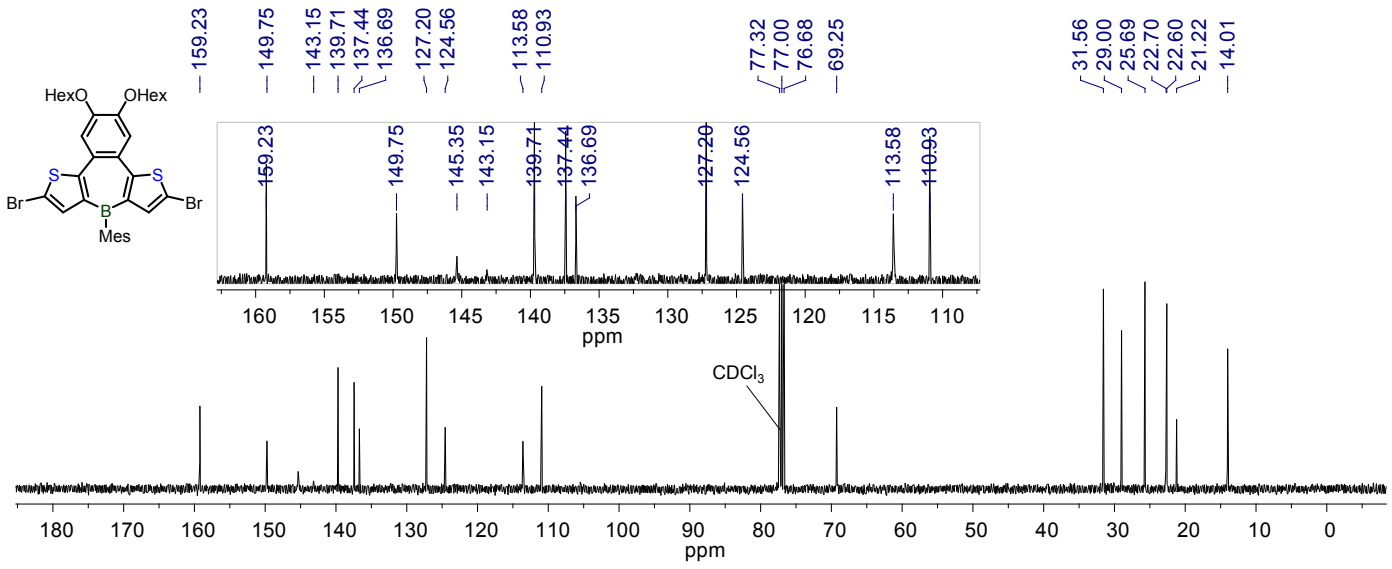


Figure S28. ^{13}C NMR spectrum of **7** in $CDCl_3$ at room temperature (100 MHz).

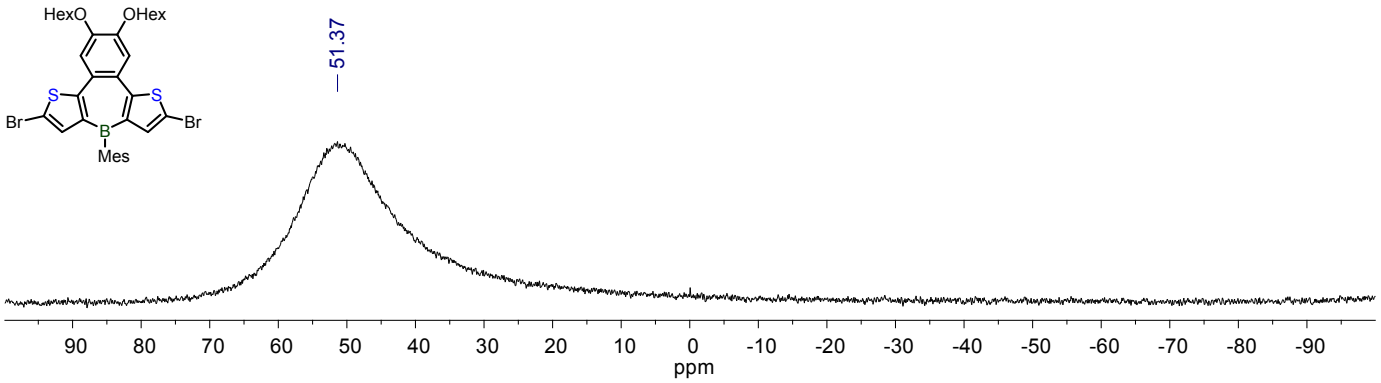


Figure S29. ^{11}B NMR spectrum of **7** in $CDCl_3$ at room temperature (160 MHz).

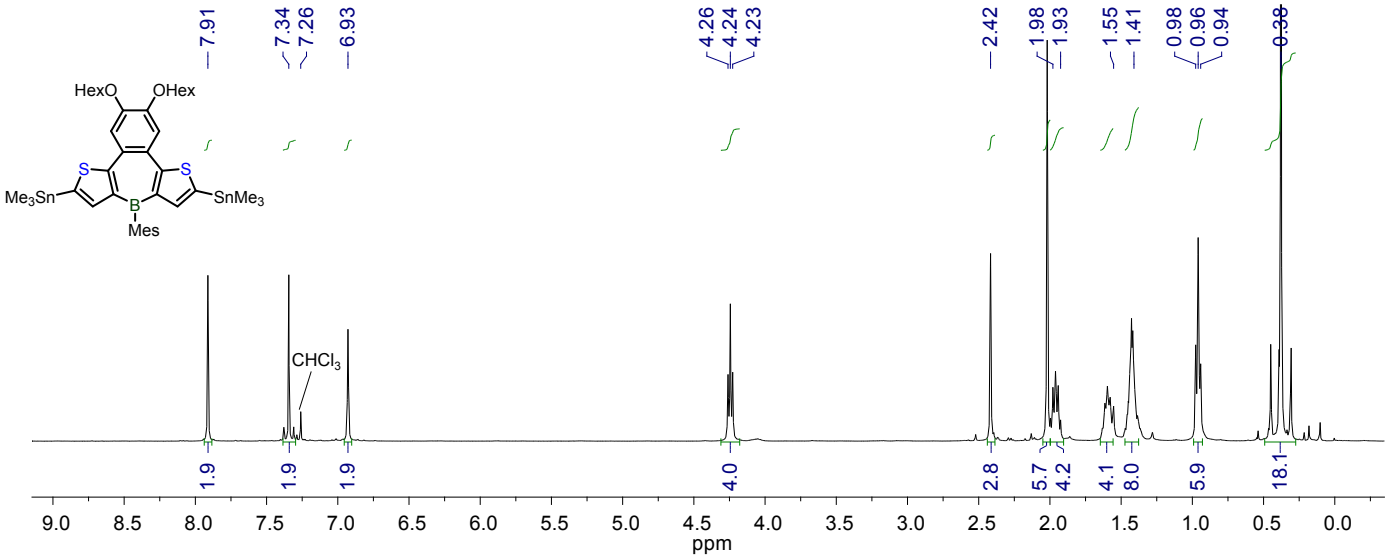


Figure S30. ^{1}H NMR spectrum of **8** in $CDCl_3$ at room temperature (400 MHz).

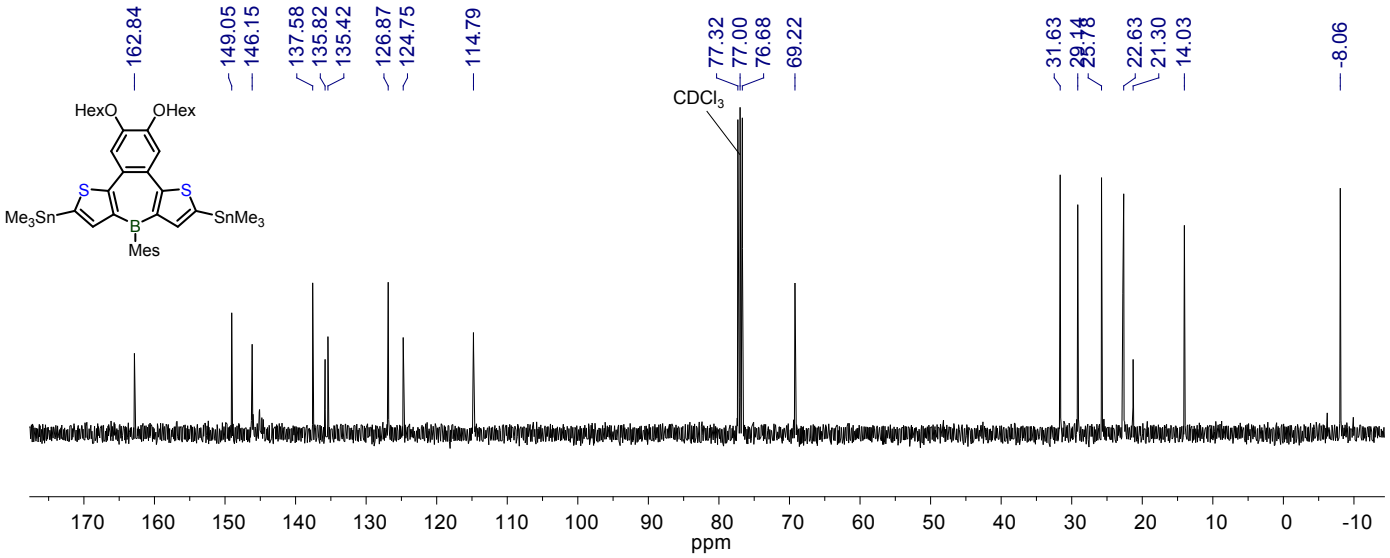


Figure S31. ^{13}C NMR spectrum of **8** in $CDCl_3$ at room temperature (100 MHz).

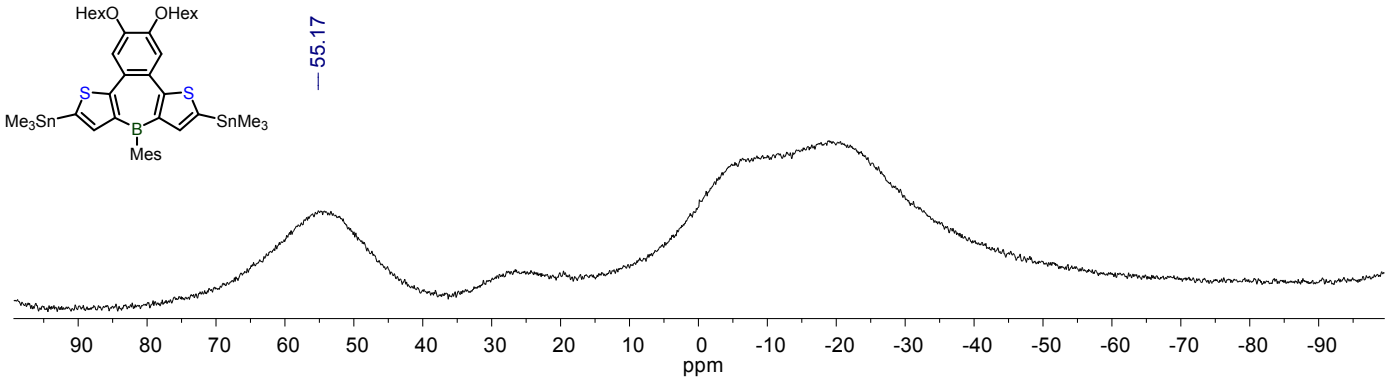


Figure S32. ^{11}B NMR spectrum of **8** in $CDCl_3$ at room temperature (128 MHz).

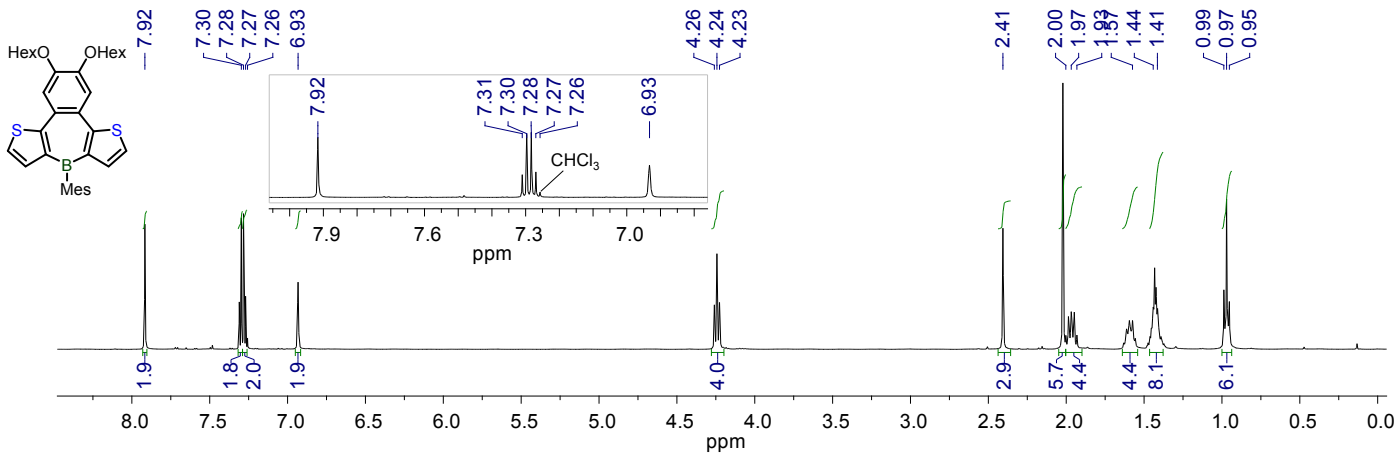


Figure S33. ^{1}H NMR spectrum of **8'** in $CDCl_3$ at room temperature (400 MHz).

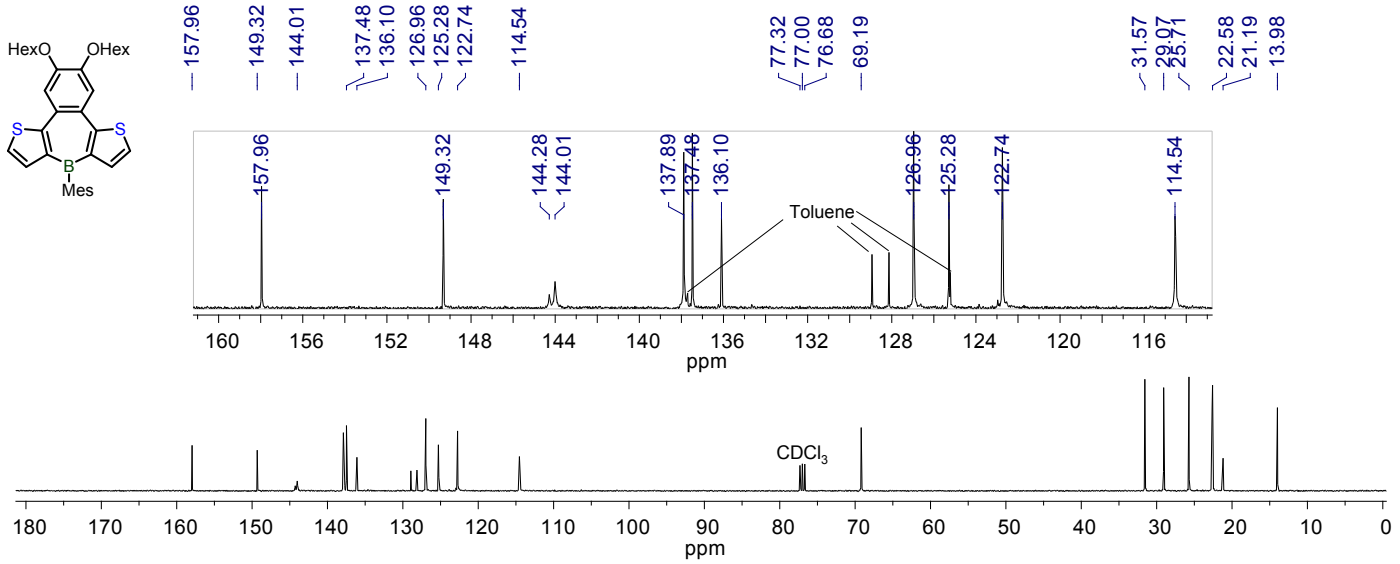


Figure S34. ^{13}C NMR spectrum of **8'** in $CDCl_3$ at room temperature (100 MHz).

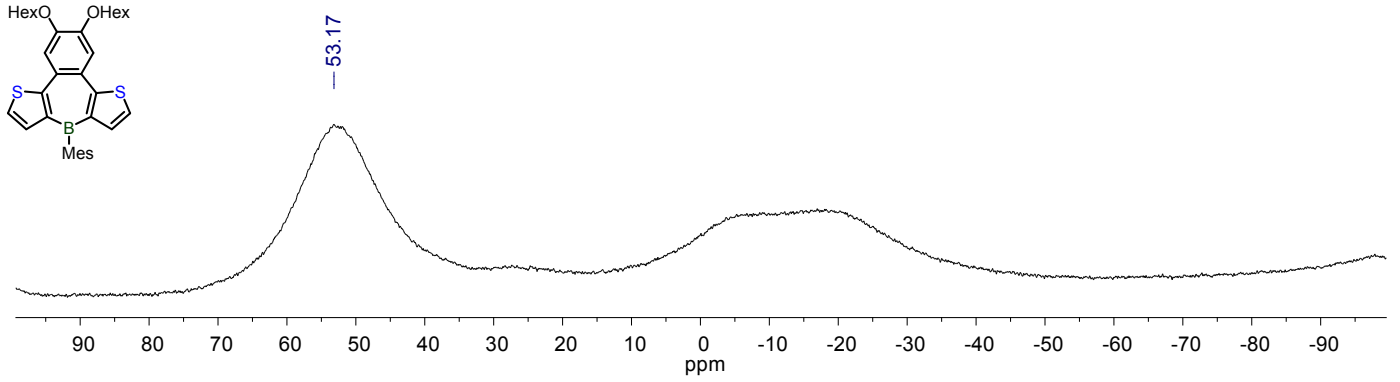


Figure S35. ^{11}B NMR spectrum of **8'** in $CDCl_3$ at room temperature (128 MHz).

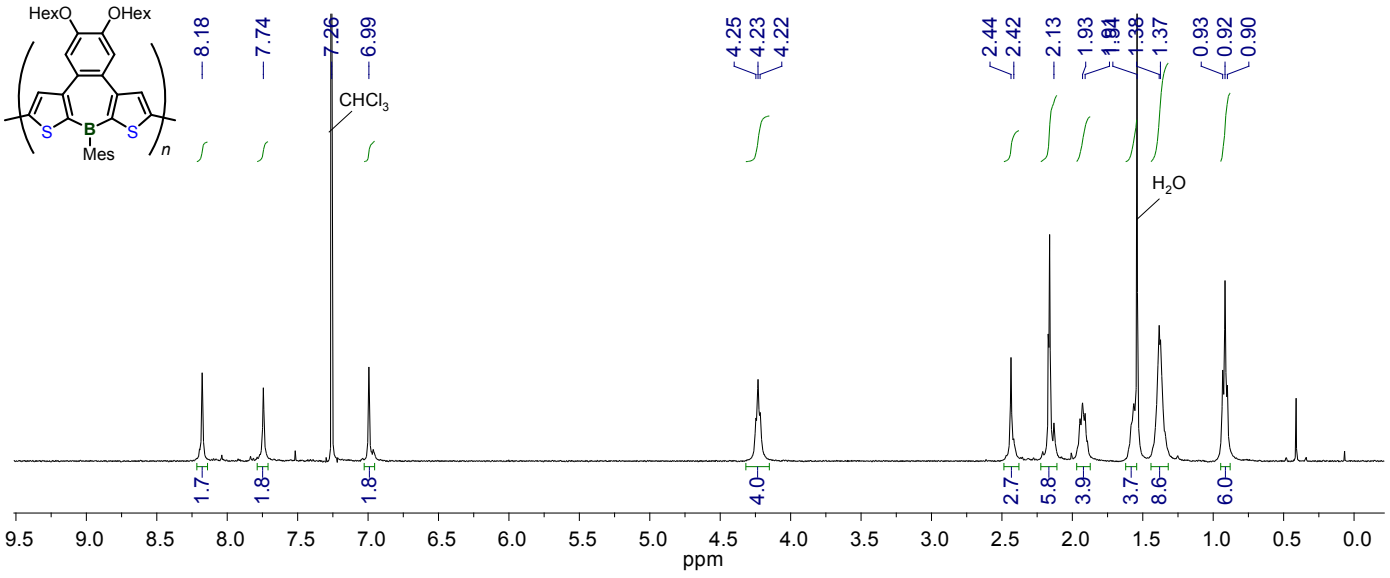


Figure S36. ^{1}H NMR spectrum of **P1** in $CDCl_3$ at room temperature (400 MHz).

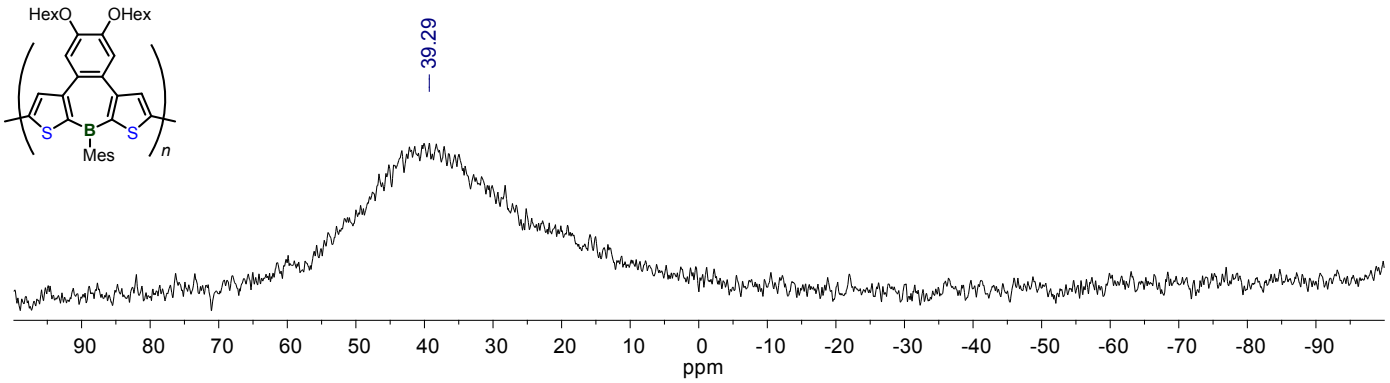


Figure S37. ^{11}B NMR spectrum of **P1** in $CDCl_3$ at room temperature (160 MHz).

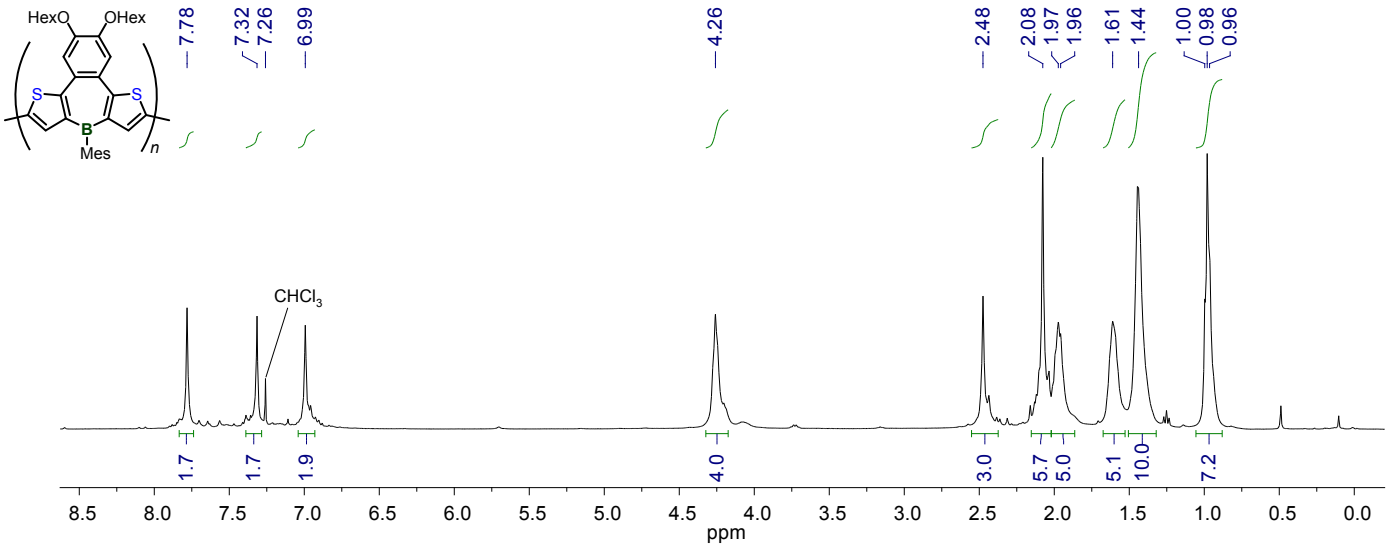


Figure S38. ^{1}H NMR spectrum of **P2** in $CDCl_3$ at room temperature (400 MHz).

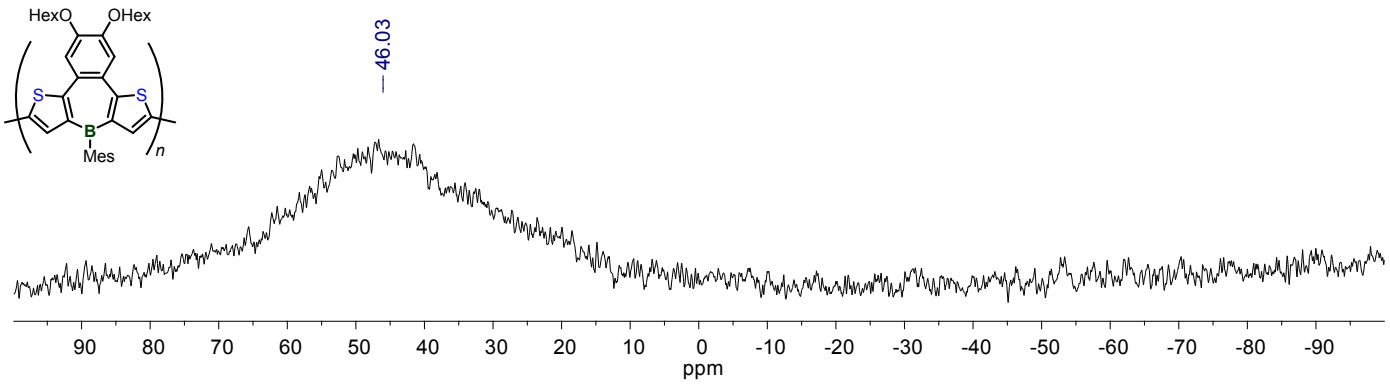


Figure S39. ^{11}B NMR spectrum of **P2** in $CDCl_3$ at room temperature (160 MHz).

Cartesian coordinates for optimized structures

Table S2. Coordinates for optimized structure of **O1** in the ground state (S_0).

Total Energy: −9686.27159846 Hartree

opt b3lyp/6-31g(d) geom=connectivity

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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2	6	0	1.052137	0.872346	-7.236548
3	6	0	2.202951	1.109431	-8.125365
4	6	0	2.206407	1.105998	-9.547995
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6	6	0	-0.297262	1.089271	-10.153874
7	6	0	3.431248	1.387016	-7.465138
8	6	0	4.620741	1.633644	-8.123097
9	6	0	4.624260	1.630110	-9.541100
10	6	0	3.437926	1.380287	-10.203565
11	1	0	3.426603	1.456306	-6.387488
12	1	0	3.438518	1.444191	-11.281545
13	5	0	-1.046059	1.330180	-8.845643
14	6	0	-2.598847	1.663234	-8.850183
15	6	0	-3.589941	0.654153	-8.851278
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49	1	0	5.207773	2.718750	-5.694906

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96	1	0	-5.187737	-2.153862	-3.138189
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105	6	0	1.238844	0.476576	5.873857
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107	6	0	1.052137	0.872346	7.236548
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109	5	0	-1.046059	1.330180	8.845643
110	6	0	2.202951	1.109431	8.125365
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112	6	0	-2.598847	1.663234	8.850183
113	6	0	2.206407	1.105998	9.547995
114	6	0	3.431248	1.387016	7.465138
115	6	0	1.060060	0.864947	10.441530
116	16	0	-1.269918	0.884746	11.605473
117	6	0	-3.589941	0.654153	8.851278
118	6	0	-3.012903	3.017683	8.849793
119	6	0	3.437926	1.380287	10.203565
120	6	0	4.620741	1.633644	8.123097
121	1	0	3.426603	1.456306	6.387488
122	6	0	1.253894	0.462825	11.801339
123	6	0	-4.944731	1.009643	8.853202
124	6	0	-3.216026	-0.814660	8.846420
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127	6	0	4.624260	1.630110	9.541100
128	1	0	3.438518	1.444191	11.281545
129	8	0	5.808059	1.915191	7.527828
130	1	0	2.212327	0.162856	12.206909
131	6	0	-5.359214	2.342674	8.856052
132	1	0	-5.695605	0.220966	8.851569
133	1	0	-2.628935	-1.080661	7.959312
134	1	0	-2.612417	-1.082132	9.721840
135	1	0	-4.109572	-1.447545	8.854189
136	1	0	-4.671634	4.381992	8.848220
137	1	0	-1.332554	4.081871	9.723355
138	1	0	-1.338896	4.079971	7.961057
139	1	0	-2.469501	5.115731	8.845222
140	8	0	5.814385	1.908566	10.131917
141	6	0	5.859196	1.938166	6.109291
142	6	0	-6.825543	2.707435	8.883247
143	6	0	5.872555	1.924108	11.550467
144	1	0	6.896626	2.160324	5.854163
145	1	0	5.578305	0.967198	5.680685
146	1	0	5.207773	2.718750	5.694906
147	1	0	-7.138032	3.035201	9.883912
148	1	0	-7.048024	3.530046	8.193577
149	1	0	-7.455604	1.855563	8.606540
150	1	0	5.593653	0.950958	11.975301
151	1	0	6.911263	2.144796	11.801556
152	1	0	5.223320	2.702605	11.972055
153	6	0	0.108405	0.423095	12.564054
154	6	0	-0.018936	0.042714	-13.956321
155	16	0	1.363096	-0.395241	-14.920618
156	6	0	-1.166521	-0.014517	-14.714594
157	6	0	0.388296	-0.615452	-16.367763
158	6	0	-0.970712	-0.412028	-16.075831
159	1	0	-2.128699	0.267644	-14.304976
160	5	0	1.135956	-0.846087	-17.680571
161	6	0	-2.115773	-0.670374	-16.966355
162	6	0	0.386724	-0.613810	-18.990791
163	6	0	2.690483	-1.169119	-17.676987
164	6	0	-2.115737	-0.668778	-18.389033
165	6	0	-3.340150	-0.968007	-16.307563
166	6	0	-0.972215	-0.409831	-19.280182
167	16	0	1.358002	-0.384797	-20.441893
168	6	0	3.676646	-0.155267	-17.678636
169	6	0	3.110907	-2.521346	-17.664310
170	6	0	-3.341851	-0.964971	-19.045861
171	6	0	-4.523851	-1.236897	-16.967099
172	1	0	-3.335866	-1.035252	-15.229735
173	6	0	-1.169556	-0.009037	-20.648410

174	6	0	-0.018328	0.046700	-21.379325
175	6	0	5.032935	-0.504069	-17.666708
176	6	0	3.296818	1.311806	-17.703900
177	6	0	4.472875	-2.831702	-17.654530
178	6	0	2.091038	-3.641391	-17.656404
179	6	0	-4.524174	-1.235910	-18.384803
180	1	0	-3.338679	-1.029323	-20.123836
181	8	0	-5.707581	-1.538507	-16.373451
182	1	0	-2.129240	0.271675	-21.064239
183	1	0	0.084412	0.340557	-22.416234
184	6	0	5.453869	-1.835125	-17.658685
185	1	0	5.779823	0.288336	-17.664273
186	1	0	2.829579	1.589380	-18.656803
187	1	0	2.582689	1.562925	-16.911370
188	1	0	4.178097	1.948082	-17.571767
189	1	0	4.776290	-3.877540	-17.640905
190	1	0	1.440366	-3.588582	-16.774305
191	1	0	1.437279	-3.597225	-18.536608
192	1	0	2.577805	-4.622031	-17.652269
193	8	0	-5.709058	-1.537767	-18.977439
194	6	0	-5.759930	-1.561357	-14.955052
195	6	0	6.922301	-2.191670	-17.676300
196	6	0	-5.761695	-1.566517	-20.394713
197	1	0	-5.496890	-0.585254	-14.526705
198	1	0	-6.793507	-1.801874	-14.700798
199	1	0	-5.095074	-2.329759	-14.539212
200	1	0	7.134417	-3.054373	-17.034335
201	1	0	7.257557	-2.454399	-18.688818
202	1	0	7.542021	-1.355656	-17.335025
203	1	0	-6.794787	-1.810131	-20.648265
204	1	0	-5.500869	-0.591361	-20.827282
205	1	0	-5.095101	-2.334988	-20.808023
206	6	0	-0.018936	0.042714	13.956321
207	16	0	1.363096	-0.395241	14.920618
208	6	0	-1.166521	-0.014517	14.714594
209	6	0	0.388296	-0.615452	16.367763
210	6	0	-0.970712	-0.412028	16.075831
211	1	0	-2.128699	0.267644	14.304976
212	5	0	1.135956	-0.846087	17.680571
213	6	0	-2.115773	-0.670374	16.966355
214	6	0	0.386724	-0.613810	18.990791
215	6	0	2.690483	-1.169119	17.676987
216	6	0	-2.115737	-0.668778	18.389033
217	6	0	-3.340150	-0.968007	16.307563
218	6	0	-0.972215	-0.409831	19.280182
219	16	0	1.358002	-0.384797	20.441893
220	6	0	3.676646	-0.155267	17.678636
221	6	0	3.110907	-2.521346	17.664310
222	6	0	-3.341851	-0.964971	19.045861
223	6	0	-4.523851	-1.236897	16.967099
224	1	0	-3.335866	-1.035252	15.229735
225	6	0	-1.169556	-0.009037	20.648410
226	6	0	5.032935	-0.504069	17.666708
227	6	0	3.296818	1.311806	17.703900
228	6	0	4.472875	-2.831702	17.654530
229	6	0	2.091038	-3.641391	17.656404
230	6	0	-4.524174	-1.235910	18.384803
231	1	0	-3.338679	-1.029323	20.123836
232	8	0	-5.707581	-1.538507	16.373451
233	1	0	-2.129240	0.271675	21.064239
234	6	0	5.453869	-1.835125	17.658685
235	1	0	5.779823	0.288336	17.664273

236	1	0	2.582689	1.562925	16.911370
237	1	0	2.829579	1.589380	18.656803
238	1	0	4.178097	1.948082	17.571767
239	1	0	4.776290	-3.877540	17.640905
240	1	0	1.437279	-3.597225	18.536608
241	1	0	1.440366	-3.588582	16.774305
242	1	0	2.577805	-4.622031	17.652269
243	8	0	-5.709058	-1.537767	18.977439
244	6	0	-5.759930	-1.561357	14.955052
245	6	0	6.922301	-2.191670	17.676300
246	6	0	-5.761695	-1.566517	20.394713
247	1	0	-6.793507	-1.801874	14.700798
248	1	0	-5.496890	-0.585254	14.526705
249	1	0	-5.095074	-2.329759	14.539212
250	1	0	7.257557	-2.454399	18.688818
251	1	0	7.134417	-3.054373	17.034335
252	1	0	7.542021	-1.355656	17.335025
253	1	0	-5.500869	-0.591361	20.827282
254	1	0	-6.794787	-1.810131	20.648265
255	1	0	-5.095101	-2.334988	20.808023
256	6	0	-0.018328	0.046700	21.379325
257	1	0	0.084412	0.340557	22.416234

Table S3. Coordinates for optimized structure of **O2** in the ground state (S_0).

Total Energy: −9686.24474719 Hartree

opt b3lyp/6-31g(d) geom=connectivity

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-1.732225	-0.204435	3.275777
2	6	0	0.682647	0.259546	2.553196
3	6	0	-1.451520	0.204129	1.576602
4	6	0	-0.080493	0.395553	1.345538
5	1	0	1.758164	0.399639	2.563450
6	6	0	-2.615757	0.349599	0.715280
7	5	0	0.626107	0.635480	0.000000
8	6	0	-2.615757	0.349599	-0.715280
9	6	0	-3.873975	0.491987	1.369411
10	6	0	-0.080493	0.395553	-1.345538
11	6	0	2.170430	1.009428	0.000000
12	6	0	-1.451520	0.204129	-1.576602
13	6	0	-3.873975	0.491987	-1.369411
14	6	0	-5.080133	0.600780	0.710776
15	1	0	-3.882360	0.550873	2.448978
16	6	0	0.682647	0.259546	-2.553196
17	6	0	3.174732	0.016148	0.000000
18	6	0	2.565633	2.368216	0.000000
19	16	0	-1.732225	-0.204435	-3.275777
20	6	0	-5.080133	0.600780	-0.710776
21	1	0	-3.882360	0.550873	-2.448978
22	8	0	-6.291586	0.742943	1.301895
23	1	0	1.758164	0.399639	-2.563450
24	6	0	4.526027	0.387581	0.000000
25	6	0	2.809267	-1.454777	0.000000
26	6	0	3.921816	2.703996	0.000000
27	6	0	1.523000	3.467190	0.000000
28	8	0	-6.291586	0.742943	-1.301895

29	6	0	-6.348343	0.754686	2.721740
30	6	0	4.922353	1.725983	0.000000
31	1	0	5.286818	-0.391704	0.000000
32	1	0	2.212247	-1.724144	0.880320
33	1	0	2.212247	-1.724144	-0.880320
34	1	0	3.703829	-2.086233	0.000000
35	1	0	4.205245	3.755707	0.000000
36	1	0	0.871785	3.404490	-0.881191
37	1	0	0.871785	3.404490	0.881191
38	1	0	1.987974	4.458397	0.000000
39	6	0	-6.348343	0.754686	-2.721740
40	1	0	-7.404980	0.856066	2.974016
41	1	0	-5.958197	-0.179181	3.146248
42	1	0	-5.790767	1.603291	3.138753
43	6	0	6.383380	2.113682	0.000000
44	1	0	-5.958197	-0.179181	-3.146248
45	1	0	-7.404980	0.856066	-2.974016
46	1	0	-5.790767	1.603291	-3.138753
47	1	0	6.640072	2.715242	-0.881310
48	1	0	6.640072	2.715242	0.881310
49	1	0	7.031185	1.230844	0.000000
50	6	0	-0.031916	-0.067467	-3.676501
51	6	0	-0.031916	-0.067467	3.676501
52	6	0	0.432552	-0.295583	-5.026511
53	16	0	2.134196	-0.170025	-5.425317
54	6	0	-0.283323	-0.614557	-6.151280
55	6	0	1.851948	-0.571309	-7.126033
56	6	0	0.479805	-0.752543	-7.358703
57	1	0	-1.359921	-0.746212	-6.142447
58	6	0	3.015725	-0.722284	-7.986987
59	5	0	-0.227587	-0.983026	-8.705472
60	6	0	3.016630	-0.718066	-9.417552
61	6	0	4.272481	-0.875469	-7.332471
62	6	0	0.481510	-0.743888	-10.049738
63	6	0	-1.774675	-1.345571	-8.707649
64	6	0	1.854052	-0.561579	-10.279201
65	6	0	4.274220	-0.867467	-10.071310
66	6	0	5.478244	-0.990914	-7.990679
67	1	0	4.279767	-0.937608	-6.253072
68	6	0	-0.279752	-0.598611	-11.257531
69	6	0	-2.771787	-0.344493	-8.706535
70	6	0	-2.179966	-2.700950	-8.707347
71	16	0	2.138848	-0.149414	-11.976803
72	6	0	5.479179	-0.986743	-9.412253
73	1	0	4.282913	-0.923237	-11.151040
74	8	0	6.688285	-1.143459	-7.399251
75	1	0	-1.356177	-0.731428	-11.269114
76	6	0	-4.125494	-0.705552	-8.706318
77	6	0	-2.394887	1.123526	-8.702395
78	6	0	-3.539041	-3.026538	-8.706911
79	6	0	-1.145895	-3.807989	-8.704571
80	8	0	6.689903	-1.135736	-10.002972
81	6	0	6.744080	-1.160064	-5.979445
82	6	0	-4.531923	-2.041336	-8.708937
83	1	0	-4.880397	0.079506	-8.703221
84	1	0	-1.796291	1.386002	-7.821068
85	1	0	-1.795212	1.390338	-9.581680
86	1	0	-3.284502	1.761936	-8.701386
87	1	0	-3.830486	-4.075999	-8.704026
88	1	0	-0.492667	-3.750847	-9.584653
89	1	0	-0.495758	-3.749875	-7.822282
90	1	0	-1.618549	-4.795560	-8.704932

91	6	0	6.747673	-1.143589	-11.422894
92	1	0	7.799807	-1.269753	-5.726841
93	1	0	6.360319	-0.224776	-5.552230
94	1	0	6.180220	-2.005981	-5.565418
95	6	0	-5.996064	-2.416254	-8.731035
96	1	0	6.364459	-0.205705	-11.844813
97	1	0	7.803751	-1.251662	-11.674669
98	1	0	6.184463	-1.986991	-11.842838
99	1	0	-6.301266	-2.785534	-9.719369
100	1	0	-6.218584	-3.212426	-8.010691
101	1	0	-6.632730	-1.558037	-8.491177
102	6	0	0.432552	-0.295583	5.026511
103	6	0	-0.283323	-0.614557	6.151280
104	16	0	2.134196	-0.170025	5.425317
105	6	0	0.479805	-0.752543	7.358703
106	1	0	-1.359921	-0.746212	6.142447
107	6	0	1.851948	-0.571309	7.126033
108	5	0	-0.227587	-0.983026	8.705472
109	6	0	3.015725	-0.722284	7.986987
110	6	0	0.481510	-0.743888	10.049738
111	6	0	-1.774675	-1.345571	8.707649
112	6	0	3.016630	-0.718066	9.417552
113	6	0	4.272481	-0.875469	7.332471
114	6	0	-0.279752	-0.598611	11.257531
115	6	0	1.854052	-0.561579	10.279201
116	6	0	-2.771787	-0.344493	8.706535
117	6	0	-2.179966	-2.700950	8.707347
118	6	0	4.274220	-0.867467	10.071310
119	6	0	5.478244	-0.990914	7.990679
120	1	0	4.279767	-0.937608	6.253072
121	1	0	-1.356177	-0.731428	11.269114
122	16	0	2.138848	-0.149414	11.976803
123	6	0	-4.125494	-0.705552	8.706318
124	6	0	-2.394887	1.123526	8.702395
125	6	0	-3.539041	-3.026538	8.706911
126	6	0	-1.145895	-3.807989	8.704571
127	6	0	5.479179	-0.986743	9.412253
128	1	0	4.282913	-0.923237	11.151040
129	8	0	6.688285	-1.143459	7.399251
130	6	0	-4.531923	-2.041336	8.708937
131	1	0	-4.880397	0.079506	8.703221
132	1	0	-1.795212	1.390338	9.581680
133	1	0	-1.796291	1.386002	7.821068
134	1	0	-3.284502	1.761936	8.701386
135	1	0	-3.830486	-4.075999	8.704026
136	1	0	-0.495758	-3.749875	7.822282
137	1	0	-0.492667	-3.750847	9.584653
138	1	0	-1.618549	-4.795560	8.704932
139	8	0	6.689903	-1.135736	10.002972
140	6	0	6.744080	-1.160064	5.979445
141	6	0	-5.996064	-2.416254	8.731035
142	6	0	6.747673	-1.143589	11.422894
143	1	0	6.360319	-0.224776	5.552230
144	1	0	7.799807	-1.269753	5.726841
145	1	0	6.180220	-2.005981	5.565418
146	1	0	-6.218584	-3.212426	8.010691
147	1	0	-6.301266	-2.785534	9.719369
148	1	0	-6.632730	-1.558037	8.491177
149	1	0	7.803751	-1.251662	11.674669
150	1	0	6.364459	-0.205705	11.844813
151	1	0	6.184463	-1.986991	11.842838
152	6	0	0.437939	-0.273094	12.379242

153	6	0	0.437939	-0.273094	-12.379242
154	6	0	-0.023813	-0.036943	13.728896
155	6	0	0.696101	0.273061	14.853729
156	16	0	-1.727335	-0.137014	14.127058
157	6	0	-0.065712	0.422769	16.060553
158	1	0	1.774520	0.389173	14.845472
159	6	0	-1.439557	0.261074	15.827101
160	5	0	0.643649	0.640311	17.409741
161	6	0	-2.601811	0.433631	16.687534
162	6	0	-0.068272	0.394271	18.750341
163	6	0	2.193149	0.991553	17.414638
164	6	0	-2.603271	0.421521	18.116398
165	6	0	-3.853591	0.621296	16.032413
166	6	0	0.694374	0.211842	19.962060
167	6	0	-1.441708	0.228778	18.977352
168	6	0	3.184262	-0.016005	17.413534
169	6	0	2.606983	2.343847	17.418151
170	6	0	-3.854973	0.601471	18.771193
171	6	0	-5.056107	0.764664	16.691273
172	1	0	-3.858131	0.688886	14.953288
173	1	0	1.772399	0.323348	19.983846
174	16	0	-1.729720	-0.210309	20.667978
175	6	0	4.539870	0.336190	17.418846
176	6	0	2.798110	-1.481633	17.402841
177	6	0	3.968474	2.660859	17.423127
178	6	0	1.580222	3.457774	17.412276
179	6	0	-5.056812	0.755148	18.112255
180	1	0	-3.860804	0.652267	19.851256
181	8	0	-6.262252	0.950855	16.100370
182	6	0	4.954878	1.669725	17.427353
183	1	0	5.289783	-0.453600	17.416366
184	1	0	2.195313	-1.748192	18.280062
185	1	0	2.199161	-1.736863	16.519593
186	1	0	3.683757	-2.125478	17.400822
187	1	0	4.266712	3.708402	17.422683
188	1	0	0.938302	3.409465	16.523363
189	1	0	0.917720	3.399657	18.285374
190	1	0	2.059359	4.442204	17.423119
191	8	0	-6.263575	0.934150	18.704128
192	6	0	-6.316800	0.974881	14.680794
193	6	0	6.421533	2.033232	17.463687
194	6	0	-6.320363	0.941994	20.123455
195	1	0	-5.956689	0.031998	14.249591
196	1	0	-7.369251	1.112459	14.428031
197	1	0	-5.731396	1.807869	14.270375
198	1	0	6.635349	2.905826	16.835764
199	1	0	6.747624	2.283238	18.482463
200	1	0	7.048507	1.205125	17.116092
201	1	0	-7.372901	1.078818	20.376294
202	1	0	-5.963037	-0.006687	20.544357
203	1	0	-5.733810	1.768926	20.544442
204	6	0	-0.023813	-0.036943	-13.728896
205	16	0	-1.727335	-0.137014	-14.127058
206	6	0	0.696101	0.273061	-14.853729
207	6	0	-1.439557	0.261074	-15.827101
208	6	0	-0.065712	0.422769	-16.060553
209	1	0	1.774520	0.389173	-14.845472
210	6	0	-2.601811	0.433631	-16.687534
211	5	0	0.643649	0.640311	-17.409741
212	6	0	-2.603271	0.421521	-18.116398
213	6	0	-3.853591	0.621296	-16.032413
214	6	0	-0.068272	0.394271	-18.750341

215	6	0	2.193149	0.991553	-17.414638
216	6	0	-1.441708	0.228778	-18.977352
217	6	0	-3.854973	0.601471	-18.771193
218	6	0	-5.056107	0.764664	-16.691273
219	1	0	-3.858131	0.688886	-14.953288
220	6	0	0.694374	0.211842	-19.962060
221	6	0	3.184262	-0.016005	-17.413534
222	6	0	2.606983	2.343847	-17.418151
223	16	0	-1.729720	-0.210309	-20.667978
224	6	0	-5.056812	0.755148	-18.112255
225	1	0	-3.860804	0.652267	-19.851256
226	8	0	-6.262252	0.950855	-16.100370
227	1	0	1.772399	0.323348	-19.983846
228	6	0	4.539870	0.336190	-17.418846
229	6	0	2.798110	-1.481633	-17.402841
230	6	0	3.968474	2.660859	-17.423127
231	6	0	1.580222	3.457774	-17.412276
232	8	0	-6.263575	0.934150	-18.704128
233	6	0	-6.316800	0.974881	-14.680794
234	6	0	4.954878	1.669725	-17.427353
235	1	0	5.289783	-0.453600	-17.416366
236	1	0	2.199161	-1.736863	-16.519593
237	1	0	2.195313	-1.748192	-18.280062
238	1	0	3.683757	-2.125478	-17.400822
239	1	0	4.266712	3.708402	-17.422683
240	1	0	0.917720	3.399657	-18.285374
241	1	0	0.938302	3.409465	-16.523363
242	1	0	2.059359	4.442204	-17.423119
243	6	0	-6.320363	0.941994	-20.123455
244	1	0	-7.369251	1.112459	-14.428031
245	1	0	-5.956689	0.031998	-14.249591
246	1	0	-5.731396	1.807869	-14.270375
247	6	0	6.421533	2.033232	-17.463687
248	1	0	-5.963037	-0.006687	-20.544357
249	1	0	-7.372901	1.078818	-20.376294
250	1	0	-5.733810	1.768926	-20.544442
251	1	0	6.747624	2.283238	-18.482463
252	1	0	6.635349	2.905826	-16.835764
253	1	0	7.048507	1.205125	-17.116092
254	6	0	-0.043022	-0.122940	-21.052535
255	1	0	0.293608	-0.330836	-22.059835
256	6	0	-0.043022	-0.122940	21.052535
257	1	0	0.293608	-0.330836	22.059835

Table S4. Coordinates for optimized structure of **O1'** in the ground state (S_0).

Total Energy: −7582.38609200 Hartree

opt b3lyp/6-31g(d) geom=connectivity

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.268549	-0.650932	0.010508
2	6	0	1.271211	0.741164	0.013063
3	6	0	-0.000127	1.549421	-0.000197
4	6	0	-1.271435	0.741146	-0.015454
5	6	0	-1.268754	-0.650962	-0.016276
6	5	0	-0.000075	-1.516628	-0.003946
7	6	0	-2.570030	1.304158	-0.028645

8	6	0	-3.582306	0.359187	-0.039763
9	16	0	-2.909599	-1.256132	-0.035633
10	16	0	2.909397	-1.256147	0.028340
11	6	0	3.582095	0.359171	0.036522
12	6	0	2.569800	1.304148	0.027666
13	6	0	0.000451	-3.092579	-0.005871
14	6	0	0.010820	-3.811201	-1.223183
15	6	0	0.007640	-5.209364	-1.206384
16	6	0	-0.002736	-5.931087	-0.009448
17	6	0	-0.017118	-5.212429	1.189047
18	6	0	-0.014248	-3.814113	1.209432
19	1	0	0.009588	2.222759	-0.870900
20	1	0	-0.009870	2.220608	0.872165
21	1	0	-2.763841	2.372674	-0.026512
22	1	0	2.763588	2.372671	0.028343
23	1	0	0.011965	-5.748466	-2.152485
24	1	0	-0.032211	-5.753899	2.133654
25	6	0	-0.030960	-3.085361	2.537532
26	1	0	-0.043613	-3.788552	3.376474
27	1	0	0.850656	-2.442708	2.656413
28	1	0	-0.912543	-2.438789	2.632826
29	6	0	0.020951	-3.078969	-2.549428
30	1	0	0.029539	-3.779948	-3.390270
31	1	0	-0.860753	-2.435439	-2.662605
32	1	0	0.902532	-2.432701	-2.646989
33	6	0	0.026803	-7.442019	-0.011485
34	1	0	-0.478167	-7.852270	-0.892920
35	1	0	1.057717	-7.821468	-0.023383
36	1	0	-0.459071	-7.854113	0.879617
37	6	0	-5.011144	0.582864	-0.053496
38	6	0	-6.023755	-0.360747	-0.009917
39	16	0	-5.683384	2.196449	-0.133217
40	6	0	-7.322287	0.201956	-0.038605
41	1	0	-5.830362	-1.427947	0.044734
42	6	0	-7.324506	1.592425	-0.104951
43	6	0	-8.593997	-0.604911	-0.000509
44	5	0	-8.593234	2.457337	-0.148762
45	6	0	-9.865105	0.202775	-0.041135
46	1	0	-8.593355	-1.318891	-0.838257
47	1	0	-8.595140	-1.233903	0.902813
48	6	0	-9.861968	1.593213	-0.108751
49	6	0	-8.592728	4.031498	-0.225774
50	6	0	-11.163951	-0.359417	-0.016047
51	16	0	-11.503082	2.197788	-0.139850
52	6	0	-8.586911	4.691175	-1.476048
53	6	0	-8.593082	4.810280	0.953732
54	6	0	-12.176085	0.584402	-0.063626
55	1	0	-11.357942	-1.426742	0.033515
56	6	0	-8.582778	6.088539	-1.526020
57	6	0	-8.580866	3.896458	-2.765840
58	6	0	-8.588903	6.206054	0.866645
59	6	0	-8.593623	4.145755	2.315209
60	6	0	-8.587222	6.866626	-0.364886
61	1	0	-8.574438	6.581820	-2.496787
62	1	0	-8.578051	4.556486	-3.639243
63	1	0	-7.698460	3.247910	-2.836895
64	1	0	-9.461733	3.246570	-2.843603
65	1	0	-8.585516	6.792020	1.784442
66	1	0	-8.593005	4.888181	3.119748
67	1	0	-9.476045	3.507960	2.452687
68	1	0	-7.712705	3.505962	2.453065
69	6	0	-8.615414	8.375749	-0.439584

70	1	0	-8.096400	8.743335	-1.331639
71	1	0	-9.645663	8.754417	-0.485743
72	1	0	-8.143081	8.829901	0.438258
73	6	0	5.010918	0.582886	0.050922
74	6	0	6.023600	-0.360678	0.007909
75	16	0	5.683065	2.196504	0.130823
76	6	0	7.322096	0.202073	0.037252
77	1	0	5.830284	-1.427899	-0.046598
78	6	0	7.324224	1.592542	0.103552
79	6	0	8.593862	-0.604744	-0.000083
80	5	0	8.592890	2.457513	0.148024
81	6	0	9.864917	0.202996	0.041233
82	1	0	8.592779	-1.318689	0.837694
83	1	0	8.595548	-1.233765	-0.903385
84	6	0	9.861682	1.593436	0.108768
85	6	0	8.592277	4.031675	0.224953
86	6	0	11.163800	-0.359141	0.016910
87	16	0	11.502750	2.198081	0.140793
88	6	0	8.585729	4.691420	1.475188
89	6	0	8.593266	4.810393	-0.954596
90	6	0	12.175868	0.584723	0.065012
91	1	0	11.357867	-1.426459	-0.032534
92	6	0	8.581511	6.088787	1.525082
93	6	0	8.579002	3.896774	2.765020
94	6	0	8.588984	6.206171	-0.867586
95	6	0	8.594585	4.145795	-2.316037
96	6	0	8.586581	6.866811	0.363907
97	1	0	8.572604	6.582121	2.495817
98	1	0	8.575600	4.556849	3.638385
99	1	0	7.696625	3.248133	2.835588
100	1	0	9.459895	3.246986	2.843341
101	1	0	8.586091	6.792088	-1.785416
102	1	0	8.594483	4.888179	-3.120615
103	1	0	9.477055	3.507948	-2.452957
104	1	0	7.713714	3.506043	-2.454385
105	6	0	8.614668	8.375939	0.438539
106	1	0	8.095111	8.743554	1.330266
107	1	0	9.644875	8.754649	0.485288
108	1	0	8.142838	8.830023	-0.439608
109	6	0	-13.605345	0.361074	-0.055739
110	6	0	-14.617087	1.303008	-0.132478
111	16	0	-14.278518	-1.249807	0.060711
112	6	0	-15.916447	0.741051	-0.099066
113	1	0	-14.423095	2.368535	-0.212493
114	6	0	-15.919156	-0.646510	0.004165
115	6	0	-17.188020	1.545993	-0.168010
116	5	0	-17.190344	-1.509164	0.060303
117	6	0	-18.459577	0.740358	-0.115463
118	1	0	-17.192497	2.282519	0.650306
119	1	0	-17.181281	2.151279	-1.087662
120	6	0	-18.459273	-0.646280	-0.011896
121	6	0	-17.188053	-3.080778	0.177447
122	6	0	-19.766538	1.303843	-0.165429
123	16	0	-20.105075	-1.245023	0.022778
124	6	0	-17.192540	-3.708481	1.443969
125	6	0	-17.176179	-3.889130	-0.981822
126	6	0	-20.751770	0.351871	-0.100269
127	1	0	-19.967878	2.367680	-0.246061
128	6	0	-17.186386	-5.104103	1.529428
129	6	0	-17.200518	-2.881155	2.713079
130	6	0	-17.170338	-5.282212	-0.859383
131	6	0	-17.166309	-3.259166	-2.359593

132	1	0	-21.822369	0.511141	-0.118586
133	6	0	-17.178909	-5.911383	0.388438
134	1	0	-17.186513	-5.572585	2.512442
135	1	0	-17.203778	-3.518704	3.603032
136	1	0	-16.320700	-2.228141	2.775588
137	1	0	-18.084030	-2.232412	2.765908
138	1	0	-17.157902	-5.891216	-1.761985
139	1	0	-17.157272	-4.021637	-3.145121
140	1	0	-18.048922	-2.627137	-2.520261
141	1	0	-16.285574	-2.620971	-2.506079
142	6	0	-17.205904	-7.418159	0.501100
143	1	0	-16.694941	-7.762275	1.407077
144	1	0	-18.236103	-7.796929	0.547080
145	1	0	-16.724711	-7.893737	-0.360453
146	6	0	13.605141	0.361453	0.057937
147	6	0	14.616807	1.303478	0.134571
148	16	0	14.278440	-1.249472	-0.057194
149	6	0	15.916207	0.741558	0.102108
150	1	0	14.422733	2.369050	0.213794
151	6	0	15.919025	-0.646065	-0.000278
152	6	0	17.187713	1.546597	0.171138
153	5	0	17.190277	-1.508699	-0.055310
154	6	0	18.459329	0.740983	0.119683
155	1	0	17.192539	2.282611	-0.647636
156	1	0	17.180522	2.152458	1.090407
157	6	0	18.459133	-0.645719	0.016963
158	6	0	17.188103	-3.080381	-0.171536
159	6	0	19.766242	1.304555	0.169915
160	16	0	20.104977	-1.244411	-0.016576
161	6	0	17.193194	-3.708815	-1.437693
162	6	0	17.175735	-3.888063	0.988194
163	6	0	20.751545	0.352586	0.105798
164	1	0	19.967498	2.368450	0.249992
165	6	0	17.187142	-5.104487	-1.522348
166	6	0	17.201712	-2.882222	-2.707278
167	6	0	17.170013	-5.281216	0.866558
168	6	0	17.165214	-3.257301	2.365596
169	1	0	21.822128	0.511913	0.124520
170	6	0	17.179183	-5.911107	-0.380896
171	1	0	17.187744	-5.573538	-2.505091
172	1	0	17.205420	-3.520284	-3.596861
173	1	0	16.321887	-2.229293	-2.770569
174	1	0	18.085212	-2.233460	-2.760072
175	1	0	17.157198	-5.889699	1.769506
176	1	0	17.155842	-4.019317	3.151562
177	1	0	18.047733	-2.625151	2.526301
178	1	0	16.284392	-2.619048	2.511307
179	6	0	17.206311	-7.417947	-0.492673
180	1	0	16.695863	-7.762611	-1.398733
181	1	0	18.236553	-7.796694	-0.537866
182	1	0	16.724668	-7.893052	0.368890

Table S5. Coordinates for optimized structure of **O2'** in the ground state (S_0).

Total Energy: −7582.32466967 Hartree

opt b3lyp/6-31g(d) geom=connectivity

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

1	6	0	-0.000186	-1.997459	-0.004765
2	5	0	0.000115	1.055312	0.004014
3	6	0	0.000004	2.631685	0.009287
4	6	0	-0.029285	3.356111	-1.203349
5	6	0	-0.024830	4.754560	-1.180853
6	6	0	0.004589	5.471124	0.018853
7	6	0	0.037302	4.746358	1.213635
8	6	0	0.034376	3.347873	1.226770
9	1	0	-0.005502	-2.664025	-0.880256
10	1	0	0.004996	-2.668535	0.867280
11	1	0	-0.043325	5.297695	-2.124561
12	1	0	0.067117	5.283030	2.160759
13	6	0	0.070503	2.609555	2.549283
14	1	0	0.098254	3.305220	3.394160
15	1	0	-0.810635	1.967484	2.677205
16	1	0	0.951527	1.959296	2.625338
17	6	0	-0.058938	2.626871	-2.531055
18	1	0	-0.083123	3.328305	-3.371259
19	1	0	0.822604	1.985495	-2.659621
20	1	0	-0.939768	1.977346	-2.615324
21	6	0	-0.024181	6.982175	0.024975
22	1	0	0.440657	7.396135	-0.876503
23	1	0	-1.054120	7.362701	0.062160
24	1	0	0.502068	7.390177	0.894921
25	6	0	-1.306140	0.222598	0.010064
26	6	0	-1.247963	-1.160361	0.005710
27	6	0	-2.664226	0.688837	0.028445
28	16	0	-2.828519	-1.886593	0.013215
29	6	0	-3.611523	-0.303502	0.036666
30	1	0	-2.917010	1.744328	0.048269
31	6	0	1.306198	0.222386	-0.007303
32	6	0	1.247742	-1.160548	-0.010862
33	6	0	2.664384	0.688446	-0.023191
34	16	0	2.828148	-1.887069	-0.022900
35	6	0	3.611498	-0.304020	-0.037231
36	1	0	2.917344	1.744002	-0.036736
37	6	0	5.057761	-0.203636	-0.057163
38	6	0	6.000236	-1.170187	-0.301629
39	16	0	5.847954	1.341433	0.271665
40	6	0	7.359928	-0.712142	-0.241449
41	1	0	5.742273	-2.198337	-0.535593
42	6	0	7.424190	0.638030	0.056615
43	5	0	8.661900	-1.520717	-0.467656
44	6	0	8.674816	1.459459	0.193746
45	6	0	8.655272	-3.059908	-0.808308
46	6	0	9.970821	-0.703270	-0.333347
47	1	0	8.646243	2.301642	-0.513896
48	1	0	8.709018	1.923178	1.191053
49	6	0	9.918278	0.646678	-0.031735
50	6	0	8.605168	-3.500701	-2.149738
51	6	0	8.694361	-4.025733	0.222138
52	6	0	11.326618	-1.155081	-0.474850
53	16	0	11.500690	1.361729	0.068548
54	6	0	8.596330	-4.869998	-2.434268
55	6	0	8.556390	-2.497880	-3.284385
56	6	0	8.684226	-5.387376	-0.097165
57	6	0	8.743080	-3.595450	1.674012
58	6	0	12.277553	-0.183887	-0.288615
59	1	0	11.575825	-2.187743	-0.698096
60	6	0	8.638957	-5.832337	-1.421413
61	1	0	8.553812	-5.192884	-3.473446

62	1	0	8.524104	-2.997786	-4.257832
63	1	0	7.672570	-1.850682	-3.214128
64	1	0	9.434288	-1.838955	-3.278609
65	1	0	8.711085	-6.118814	0.709197
66	1	0	8.767836	-4.459497	2.345840
67	1	0	9.631248	-2.985758	1.884642
68	1	0	7.869383	-2.988859	1.945333
69	6	0	8.661634	-7.307580	-1.748938
70	1	0	8.128089	-7.519904	-2.681911
71	1	0	9.689789	-7.674107	-1.873508
72	1	0	8.201040	-7.902632	-0.952761
73	6	0	-5.057791	-0.202958	0.056881
74	6	0	-6.000311	-1.169220	0.302245
75	16	0	-5.847864	1.341912	-0.273126
76	6	0	-7.359968	-0.711059	0.241944
77	1	0	-5.742348	-2.197147	0.537180
78	6	0	-7.424151	0.638887	-0.057163
79	5	0	-8.661985	-1.519305	0.469138
80	6	0	-8.674723	1.460356	-0.194593
81	6	0	-8.655452	-3.058161	0.811281
82	6	0	-9.970860	-0.701889	0.334166
83	1	0	-8.646056	2.302777	0.512771
84	1	0	-8.708935	1.923730	-1.192054
85	6	0	-9.918243	0.647777	0.031306
86	6	0	-8.605288	-3.497641	2.153140
87	6	0	-8.694710	-4.024990	-0.218215
88	6	0	-11.326690	-1.153552	0.475854
89	16	0	-11.500626	1.362756	-0.069934
90	6	0	-8.596558	-4.866655	2.439015
91	6	0	-8.556318	-2.493707	3.286795
92	6	0	-8.684677	-5.386322	0.102427
93	6	0	-8.743531	-3.596133	-1.670507
94	6	0	-12.277572	-0.182524	0.288524
95	1	0	-11.575968	-2.186018	0.699922
96	6	0	-8.639352	-5.829986	1.427107
97	1	0	-8.553986	-5.188523	3.478507
98	1	0	-8.524050	-2.992655	4.260733
99	1	0	-7.672410	-1.846702	3.215856
100	1	0	-9.434126	-1.834667	3.280412
101	1	0	-8.711664	-6.118549	-0.703213
102	1	0	-8.768239	-4.460839	-2.341488
103	1	0	-9.631767	-2.986732	-1.881694
104	1	0	-7.869903	-2.989727	-1.942465
105	6	0	-8.662139	-7.304901	1.756094
106	1	0	-8.128176	-7.516407	2.689014
107	1	0	-9.690301	-7.671111	1.881536
108	1	0	-8.202046	-7.900818	0.960277
109	6	0	13.723019	-0.278427	-0.351197
110	6	0	14.678238	0.615529	0.061927
111	16	0	14.493518	-1.707981	-1.045703
112	6	0	16.032614	0.189899	-0.153705
113	1	0	14.433675	1.564968	0.527959
114	6	0	16.080138	-1.060487	-0.745130
115	5	0	17.346446	0.935431	0.192269
116	6	0	17.321307	-1.824319	-1.110823
117	6	0	17.357004	2.360073	0.867967
118	6	0	18.645381	0.177589	-0.174676
119	1	0	17.319537	-2.800311	-0.602925
120	1	0	17.310925	-2.058965	-2.185712
121	6	0	18.576766	-1.072911	-0.765311
122	6	0	17.360457	2.489869	2.274887
123	6	0	17.357836	3.532029	0.079002

124	6	0	20.013010	0.593655	0.012720
125	16	0	20.154847	-1.731572	-1.087736
126	6	0	17.366327	3.760847	2.858503
127	6	0	17.353284	1.258680	3.157855
128	6	0	17.363687	4.787903	0.694669
129	6	0	17.347101	3.437614	-1.433112
130	1	0	20.282507	1.544395	0.460618
131	6	0	17.371575	4.925499	2.085568
132	1	0	17.365348	3.843073	3.944432
133	1	0	17.362277	1.528344	4.218894
134	1	0	16.464671	0.639182	2.980317
135	1	0	18.227252	0.621821	2.969484
136	1	0	17.360510	5.681195	0.071772
137	1	0	17.353544	4.430137	-1.895145
138	1	0	18.220829	2.890149	-1.809594
139	1	0	16.458258	2.907151	-1.798536
140	6	0	17.410585	6.290317	2.733608
141	1	0	16.908858	6.286736	3.707518
142	1	0	18.443588	6.623707	2.903151
143	1	0	16.926127	7.046512	2.106244
144	6	0	-13.723060	-0.276995	0.350803
145	6	0	-14.678176	0.615653	-0.065365
146	16	0	-14.493716	-1.704587	1.049156
147	6	0	-16.032606	0.190510	0.150898
148	1	0	-14.433487	1.563711	-0.534135
149	6	0	-16.080266	-1.058156	0.745941
150	5	0	-17.346363	0.934803	-0.198026
151	6	0	-17.321521	-1.821046	1.113307
152	6	0	-17.356751	2.357268	-0.878294
153	6	0	-18.645383	0.177892	0.170530
154	1	0	-17.319365	-2.798587	0.608406
155	1	0	-17.311654	-2.052391	2.188917
156	6	0	-18.576904	-1.070855	0.764881
157	6	0	-17.358639	2.482518	-2.285631
158	6	0	-17.359013	3.531765	-0.093122
159	6	0	-20.012973	0.593168	-0.018896
160	16	0	-20.155059	-1.728814	1.088359
161	6	0	-17.364404	3.751601	-2.873359
162	6	0	-17.350052	1.248489	-3.164614
163	6	0	-17.364699	4.785640	-0.712853
164	6	0	-17.349856	3.442249	1.419303
165	1	0	-20.282373	1.542523	-0.469779
166	6	0	-17.371047	4.918739	-2.104197
167	1	0	-17.362238	3.830318	-3.959546
168	1	0	-17.357637	1.514727	-4.226528
169	1	0	-16.461593	0.629705	-2.983856
170	1	0	-18.224186	0.612107	-2.975391
171	1	0	-17.362637	5.680943	-0.092845
172	1	0	-17.357948	4.436254	1.878115
173	1	0	-18.223354	2.894985	1.796598
174	1	0	-16.460794	2.914013	1.787423
175	6	0	-17.409919	6.281436	-2.756696
176	1	0	-16.906896	6.274975	-3.729923
177	1	0	-18.442873	6.613719	-2.928694
178	1	0	-16.926699	7.039916	-2.131138
179	6	0	-20.928178	-0.313909	0.419149
180	1	0	-22.008267	-0.254127	0.397449
181	6	0	20.928116	-0.314586	-0.423117
182	1	0	22.008207	-0.254572	-0.402191
