Supporting Information for

Construction of Thiophene-Based Double Helices with Through-space Conjugation for Luminescene Enhancement

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1. Experimental Section

Materials and General Methods

Ether and tetrahydrofuran (THF) for use on vacuum line were freshly distilled from sodium/benzophenone prior to use. n-BuLi (hexane) was obtained from Energy Chemical, and their concentrations were determined by titration with N-pivaloyl-o-toluidine. Column chromatography was carried out on silica gel (300−400 mesh). All starting materials and reagents were commercially available.

The ^{1}H NMR (500 MHz, 400 MHz) and ^{13}C NMR (125 MHz, 100 MHz) spectra were recorded on Bruker spectrometer. Chemical shifts in ^{1}H NMR spectra were recorded in delta (δ) units, parts per million (ppm) relative to residual $CDCl_3$ (δ = 7.26 ppm). Chemical shifts in ^{13}C NMR spectra were recorded in delta (δ) units, parts per million (ppm) relative to $CDCl_3$ (δ = 77.00 ppm) as solvent. HRMS analysis was carried out on a mass spectrometer equipped with an AP-MALDI ion source (positive mode) and an ESI-TOF mass analyzer. Melting point determination was taken on a Melt-Temp apparatus and was uncorrected. X-ray diffraction (XRD) patterns were recorded on a Bruker D8-advance diffractometer. Ultraviolet-visible (UV-vis) absorption spectra were recorded on PE Lambda 950 equipment. The photoluminescence spectra were collected on a JY HORIBA FluoroLog-3 fluorescence spectrophotometer with 450 W Xe lamp. Fluorescence quantum yields (Φ_F) were measured on a JY HORIBA FluoroLog-3 equipment using quinine sulfate (Φ_F = 0.55, 1.0×10^{-5} M in 5.0×10^{-1} H_2SO_4) as the reference.

Starting materials **1** and **4** are commercially available. Compounds **2**[S1], **5**[S2], **6**[S2], **7**[S3], **8**[S4, S5], and **9**[S6] are known compounds, and prepared according to the literature methods.

Synthesis of 2

Compound 3-bromothiophene (compound **1**) (1 mL, 10.6 mmol, 1.0 eq.), 2-bromobenzeneboronic acid (2.3 g, 11.2 mmol, 1.1 eq.), anhydrous K_2CO_3 (4.5 g, 32.0 mmol, 3.0 eq.), and $Pd(PPh_3)_4$ (950 mg, 0.9 mmol, 0.1 eq.) were added to a 250 mL Schlenk flask. The mixture was dried under vacuum for 30 min, then THF(120 mL) and anhydrous water(30 mL) were added under argon. The reaction was heated at 85 °C with stirring overnight, monitored

by TLC, cooled to room temperature and concentrated. The residue was dissolved in CH_2Cl_2 (40 mL), washed with saturated aqueous NaCl solution (30 mL), and the aqueous layer was re-extracted with CH_2Cl_2. The combined organic phases were dried over Na_2SO_4, filtered and concentrated to give 3.9 g of crude product. Purification by silica-gel column chromatography (300–400 mesh, petroleum ether) afforded compound **2** (1.9 g, 79 %).

Synthesis of 3

Compound **2** (0.2 g, 0.86 mmol, 1.0 eq.) was added in a 100 mL round-bottom flask and cooled to 0 °C (ice-water bath). Anhydrous DMF (4 mL) was added slowly via syringe. N-Bromosuccinimide (176 mg, 0.99 mmol, 1.2 eq.) was dissolved in DMF and added drop-wise to the stirred solution. The mixture was kept at 0 °C overnight, and the reaction was monitored by TLC. When complete, the mixture was quenched with saturated aqueous $Na_2S_2O_3$ at 0 °C, allowed to warm to room temperature, and stirred for 10 min. The product was extracted with EtOAc, washed with saturated aqueous NaCl solution, dried over Na_2SO_4, filtered, and concentrated to give 322 mg of crude material. Purification by silica-gel column chromatography (300–400 mesh, petroleum ether) afforded compound **3** (151 mg, 55 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, J = 8.4 Hz, 1H), 7.39-7.36 (m, 1H), 7.34 (d, J = 2.0 Hz, 1H), 7.31 (d, J = 5.6 Hz, 1H), 7.27-7.23 (m, 1H), 6.98 (d, J = 5.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.3, 136.4, 133.1, 131.9, 129.7, 129.5, 127.3, 125.5, 123.7, 111.4. HRMS (EI) *m/z* $[M]^+$ calcd for $[C_{10}H_6Br_2S]$ 315.8551; found 315.8548.

Synthesis of 5

Compound **4** (0.1 g, 0.32 mmol, 1.0 eq.) was placed in a 100 mL Schlenk flask and dried under vacuum for 0.5 h. After back-filling with argon, anhydrous THF (20 mL) was added. The flask was transferred to to a −78 °C cryostat, and the stirred solution was equilibrated for 10 min. *n*-Butyllithium (0.7 mL, 2.4 M, 1.1 eq.) was added drop-wise via syringe under a positive argon flow. The reature mixture was kept at −78 °C for 2 h, after which a freshly prepared, anhydrous $CuCl_2$ (51.6 mL, 0.38 M, 1.2 eq.) was added. The cooling bath was removed, and the mixture was allowed to warm slowly to room temperature and stirred overnight. The mixture was re-cooled to −78 °C and quenched with a few drops of MeOH. Volatiles were removed in vacuo, and the residue was dissolved in CH_2Cl_2 (40 mL). The solution was transferred to a 250 mL separatory funnel and washed with saturated aqueous NaCl (30 mL).

The combined organic phases were dried over Na_2SO_4, filtered, and concentrated to give 317 mg of crude product. Purification by flash column chromatography on silica gel (300–400 mesh, petroleum ether) afforded **5** (24.3 mg, 57 %).

Synthesis of 6

Compound **5** (150 mg 0.56 mmol, 1.0 eq.) was placed in a 100 mL Schlenk flask and dried under vacuum for 0.5 h. After back-filling with argon, anhydrous THF (20 mL) was added. The flask was cooled to –78 °C, and the stirred solution was equilibrated for 10 min. *n*-Butyllithium (0.54 mL, 1.95 M, 2.1 eq) was added drop-wise via syringe under a positive argon flow, and the resulting mixture was stirred at –78 °C for 2 h. Dried 1,2-dibromo-1,1,2,2-tetrachloroethane (733.5 mg, 1.34 mmol, 1.2 eq) was then added in one portion. The cooling bath was removed, and the reaction was allowed to warm slowly to room temperature and stirred overnight. The mixture was re-cooled to –78 °C and quenched with a few drops of MeOH. Volatiles were removed in vacuo, and the residue was dissolved in CH_2Cl_2 (40 mL). The solution was transferred to a separatory funnel and washed with saturated aqueous NaCl (30 mL). The combined organic phases were dried over Na_2SO_4, filtered, and concentrated to give 267 mg of crude product. Purification by flash column chromatography on silica gel (300–400 mesh, petroleum ether) afforded **6** (216.2 mg, 91 %).

Synthesis of 7

Compound **4** (100 mg, 0.47 mmol, 1.0 eq.), pinacolborane (179.7 mg, 0.71 mmol, 1.5 eq.), KOAc (139 mg, 1.42 mmol, 3.0 eq.) and $Pd(dppf)Cl_2$ (30.8 mg, 0.047 mmol, 0.10 eq.) were added in a 100 mL Schlenk flask and dired under high vacuum for 30 min. After back-filled with argon, 1,4-dioxane (30 mL) was added. The flask was immersed in a 100 °C oil bath and stirred for 36 h (TLC monitoring showed complete consumption of starting material). After cooling to room tempurate, the mixture was concentrated in vacuo. The residue was taken up in CH_2Cl_2 (20 mL) and transferred to a 125 mL separatory funnel. The aqueous layer was extracted with CH_2Cl_2 (3 × 15 mL); the combined organics were washed with saturated aqueous (3 × 15 mL), dried over $MgSO_4$, filtered, and evaporated to give 175 mg of crude product. Flash column chromatography on silica gel (300–400 mesh, petroleum ether) afforded **7** (74.9 mg, 61 %).

Synthesis of 8

Compound **7** (100 mg, 0.32 mmol, 1.0 eq), 3-Bromo-5-(trimethylsilyl)thiophene (225.8 mg, 0.96 mmol, 3.0 eq), anhydrous K_2CO_3 (220 mg, 1.60 mmol, 5.0 eq) and $Pd(PPh_3)_4$ (38 mg, 0.032 mmol, 0.10 eq) were placed in a 100 mL Schlenk flask. The flask was evacuated and dried under high vacuum for 30 min, back-filled with argon, and toluene solvent (20 mL) and oxygen-free H_2O (4 mL) were added. After sealing with a screw cap, the vessel was immersed in a 110 °C oil bath and stirred vigorously for 48 h (TLC monitoring showed complete conversion). After cooling to room tempurate, the mixture was concentrated in vacuo. The residue was taken up in CH_2Cl_2 and transferred to a 125 mL separatory funnel. Dilute the mixture with CH_2Cl_2 (40 mL) and saturated aqueous NaCl (30 mL), and separate the phases. Extract the aqueous layer and combine the organic portions, dry over anhydrous Na_2SO_4, filter, and concentrated to give 175 mg of crude product. Flash column chromatography on silica gel (300–400 mesh, petroleum ether) afforded **8** (67.1 mg, 55 %).

Synthesis of 9

A 50 mL Schlenk flask was evacuated and dried for 30 min, then back-filled with argon. Under a positive argon flow, anhydrous Et_2O (10 mL) was added. Diisopropylamine (4.61 mL, 32 mmol, 1.2 eq) was added in a separate 100 mL Schlenk flask under argon and cooled to 0 °C, and *n*-Butyllithium (10.9 mL, 2.5 M in hexanes, 27.3 mmol, 1.0 eq) was added drop-wise and the resulting LDA solution was stirred at 0 °C for 30 min. Meanwhile, compound **8** (5 mL, 44 mmol) was added into a 500 mL Schlenk flask, evacuated for 30 min, and back-filled with argon. Anhydrous Et_2O (150 mL) was added, and the solution was cooled to –78 °C. The pre-formed LDA was transferred drop-wise to the –78 °C solution of **8**. The mixture was kept at –78 °C for 2 h, then $C_2Br_2Cl_4$ (1.09 g, 3.34 mmol, 2.1 eq) was added in one portion. After 5–10 min the cryostat was switched off, and the reaction was allowed to warm to room temperature and stirred for 12 h (TLC monitoring showed complete consumption of starting material). The mixture was re-cooled to –78 °C and carefully quenched with saturated aqueous $NaHCO_3$ (10 mL). The volatiles were removed in vacuo, and the residue was dissolved in CH_2Cl_2. The solution was transferred to a 125 mL separatory funnel. Addtional CH_2Cl_2(40 mL) was added, and the organic phase was washed with saturated aqueous NaCl (30 mL). The combined organic phases were dried over Na_2SO_4, filtered, and concentrated to afford 405 mg of crude product.

Flash column chromatography on silica gel (300–400 mesh, petroleum ether) gave **9** (187.3 mg, 75 %).

Synthesis of BPDH

Compound **4TCOTh** (100 mg, 0.16 mmol) was placed in a 100 mL Schlenk flask, evacuated for 30 min (three argon back-fill cycles), and cooled to −78 °C. Anhydrous, degassed Et_2O (10 mL) was added under Ar, and the mixture was stirred for 20 min to give a clear solution. *n*-BuLi (0.17 mL, 2.5 M, 2.1 eq.) was added drop-wise; the cooling bath was removed, and the solution was allowed to warm slowly to room temperature and subsequently heated at 60 °C for 2 h. After cooling to room temperature, the flask was re-cooled to −78 °C and anhydrous $ZnCl_2$ was added in one portion under Ar. The mixture was warmed to room temperature and stirred for 1 h to furnish the Negishi reagent. In a separate 50 mL Schlenk flask, 2,2'-dibromo-1,1'-biphenyl (74 mg, 0.24 mmol, 1.5 eq.) was subjected to the same evacuation/Ar cycle (30 min, three cycles. Anhydrous, degassed Et_2O (20 mL) was added, and the resulting solution together with $Pd(PPh_3)_4$ (23 mg, 0.02 mmol, 0.1 eq) were transferred into a glove-box and poured into the Negishi reagent. The combined mixture was sealed and stirred at 100 °C for 5 d. After cooling to room temperature, the mixture was re-cooled to −78 °C, stirred for 10 min, and quenched with MeOH (1 mL). The volatiles were removed in vacuo; the residue was taken up in CH_2Cl_2 and transferred to a 100 mL separatory funnel. The aqueous layer was extracted with CH_2Cl_2 (2 × 40 mL), and the combined organic phases were washed with saturated aqueous NaCl (30 mL), dried over Na_2SO_4, filtered, and evaporated to give a brownish-red crude product (197.6 mg). Purification by flash column chromatography (silica gel 300–400 mesh, petroleum ether) afforded **BPDH** as a white powder (32.1 mg, 26 %). Mp: 105–107 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.33-7.27 (m, 8H), 7.11 (d, J = 12 Hz, 2H), –0.05 (s, 18H), -0.29 (s, 18H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 145.72, 145.58, 143.71, 142.56, 140.19, 139.66, 138.13, 137.90, 134.59, 131.70, 131.31, 127.82, 126.91, 125.61, 0.26, 0.11. HRMS (AP-MALDI POSITIVE) *m/z* $[M]^+$ calcd for $[C_{40}H_{46}S_4Si_4]$ 766.1559; found 766.1547.

Synthesis of TPDH

Compund 4**TCOTh** (100 mg, 0.16 mmol) was placed in a 100 Ml Schlenk flask, evacuated for 0.5 h (three argon back-fill cyclyes), and cooled to −78 °C. Anhydrous, degassed Et_2O (10

mL) was added under Ar, and the mixture was stirred for 20 min to give a clear solution. *n*-BuLi (0.17 mL, 2.5 M, 2.1 eq.) was added drop-wise; the cooling bath was removed, and the solution was allowed to warm slowly to room temperature and subsequently heated at 60 °C for 2 h. After cooling to room temperature, the flask was re-cooled to −78 °C and anhydrous $ZnCl_2$ was added in one portion under Ar. The mixture was warmed to room temperature and stirred for 1 h to furnish the Negishi reagent. In a separate 50 mL Schlenk flask, compound **3** (56.7 mg, 0.18 mmol, 1.1 eq.) was subjected to the same evacuation/Ar cycle (30 min, three cycles. Anhydrous, degassed Et_2O (20 mL) was added, and the resulting solution together with $Pd(PPh_3)_4$ (23 mg, 0.02 mmol, 0.1 eq) were transferred into a glove-box and poured into the Negishi reagent. The combined mixture was sealed and stirred at 100 °C for 5 d. After cooling to room temperature, the mixture was re-cooled to −78 °C, stirred for 10 min, and quenched with MeOH (1 mL). The volatiles were removed in vacuo; the residue was taken up in CH_2Cl_2 and transferred to a 100 mL separatory funnel. The aqueous layer was extracted with CH_2Cl_2 (40 mL), and the combined organic phases were washed with saturated aqueous NaCl (30 mL), dried over Na_2SO_4, filtered, and evaporated to give a brownish-red crude product (241.1 mg). Purification by flash column chromatography (silica gel 300–400 mesh, petroleum ether) afforded **TPDH** as a pale yellow powder (34.7 mg, 28 %). Mp: 260-262 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.35-7.30 (m, 5H), 7.28-7.27 (m, 2H), 7.19 (d, J = 8.0 Hz, 1H), 6.95 (d, J = 4 Hz, 1H), –0.03 (s, 9H), –0.08 (s, 9H), –0.17 (s, 9H), –0.23 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 146.00, 145.78, 145.69, 145.47, 144.13, 140.99, 140.47, 140.29, 140.21, 139.92, 139.52, 139.20, 138.93, 137.89, 137.23, 134.65, 132.53, 132.37, 131.53, 131.14, 127.86, 127.11, 125.91, 125.66, 125.23, 0.22, 0.19, 0.15, 0.09. HRMS (ESI-TOF) *m/z* $[M]^+$ calcd for $[C_{38}H_{45}S_5Si_4]$ 773.1202; found 773.1190.

Synthesis of TBTDH

Compound **4TCOTh** (100 mg, 0.16 mmol) was placed in a 100 mL Schlenk flask, evacuated for 30 min (three Ar back-fill cycles) and cooled to −78 °C. Anhydrous, degassed Et_2O (10 mL) was added under Ar and the mixture was stirred for 20 min to complete dissolution. *n*-BuLi (0.17 mL, 2.5 M, 2.1 eq.) was added drop-wise; the cooling bath was then removed and the solution was allowed to warm to room temperature and subsequently heated at 60 °C for 2 h. After cooling to room temperature, the flask was re-cooled to −78 °C and

anhydrous $ZnCl_2$ (weighed in a glove-box) was introduced in one portion under Ar. The mixture was warmed to room temperature and stirred for 1 h to furnish the Negishi reagent. In parallel, compound **9** (79.5 mg, 0.18 mmol, 1.1 eq) was placed in a 50 mL Schlenk flask, evacuated for 30 min (three Ar cycles) and dissolved in anhydrous, degassed Et_2O (20 mL) under Ar. This solution together with $Pd(PPh_3)_4$ (23 mg, 0.02 mmol, 0.1 eq) was transferred into a glove-box and added to the Negishi reagent. The combined mixture was sealed, removed from the glove-box and stirred at 100 °C for 5 d. After cooling to room temperature, the mixture was re-cooled to −78 °C, stirred for 10 min and quenched with MeOH (1 mL). The volatiles were removed in vacuo; the residue was taken up in CH_2Cl_2 (40 mL) and transferred to a 100 mL separatory funnel. The aqueous layer was extracted with CH_2Cl_2 (3 × 40 mL), and the combined organic phases were washed with saturated aqueous NaCl (30 mL), dried over Na_2SO_4, filtered, and evaporated to give a yellow solid (211.1 mg). Purification by flash column chromatography (silica gel 300–400 mesh, petroleum ether) afforded **TBTDH** as a pale-yellow powder (29.8 mg, 21 %). Mp:178–180 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.80-7.78 (m, 1H), 7.61-7.59 (m, 1H), 7.35-7.33 (m, 4H), 7.17 (s, 1H), 0.32 (s, 9H), –0.05 (s, 9H), –0.08 (s, 9H), –0.14 (s, 9H), –0.15 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 146.26, 146.03, 145.19, 141.97, 141.73, 140.68, 140.66, 140.32, 140.21, 140.11, 139.61, 139.53, 139.02, 138.97, 136.66, 135.84, 135.45, 133.77, 130.96, 125.43, 125.25, 124.54, 124.41, 123.84, 122.05, 0.24, 0.14, 0.07, 0.01, –0.21. HRMS (ESI-TOF) *m/z* $[M]^+$ calcd for $[C_{43}H_{53}S_6Si_5]$ 901.1318; found 901.1308.

Synthesis of BBTDH

Compound **4TCOTh** (100 mg, 0.16 mmol, 1.0 eq.) was placed in a 100 mL Schlenk flask, evacuated for 30 min (three Ar back-fill cycles) and cooled to −78 °C. Anhydrous, degassed Et_2O (10 mL) was added under Ar and the mixture was stirred for 20 min to complete dissolution. *n*-BuLi (0.17 mL, 2.5 M, 2.1 eq.) was added drop-wise; the cooling bath was then removed and the solution was allowed to warm to room temperature and subsequently heated at 60 °C for 2 h. After cooling to room temperature, the flask was re-cooled to −78 °C and anhydrous $ZnCl_2$ (weighed in a glove-box) was introduced in one portion under Ar. The mixture was warmed to room temperature and stirred for 1 h to furnish the Negishi reagent. In parallel, compound **6** (76.7 mg, 0.18 mmol, 1.1 eq) was placed in a 50 mL Schlenk flask,

evacuated for 30 min (three Ar cycles) and dissolved in anhydrous, degassed Et_2O (20 mL) under Ar. This solution together with $Pd(PPh_3)_4$ (23 mg, 0.02 mmol, 0.1 eq.) was transferred into a glove-box and added to the Negishi reagent. The combined mixture was sealed, removed from the glove-box and stirred at 100 °C for 5 d. After cooling to room temperature, the mixture was re-cooled to −78 °C, stirred for 10 min and quenched with MeOH (1 mL). The volatiles were removed in vacuo; the residue was taken up in CH_2Cl_2 (40 mL) and transferred to a 100 mL separatory funnel. The aqueous layer was extracted with CH_2Cl_2 (3 × 40 mL), and the combined organic phases were washed with saturated aqueous NaCl (30 mL), dried over Na_2SO_4, filtered, and evaporated to give a yellow solid (188.1 mg). Purification by flash column chromatography (silica gel 300–400 mesh, petroleum ether) afforded **BBTDH** as a pale-yellow powder (19.1 mg, 18 %). Mp:152-154 ℃. ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 7.83 (d, J = 10 Hz, 2H), 7.36 (s, 2H), 7.32 (t, J = 10 Hz, 2H), 7.19 (d, J = 5 Hz, 4H), –0.07 (s, 18H), –0.19 (s, 18H). ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 146.16, 145.00, 141.73, 140.56, 140.29, 140.22, 139.75, 139.07, 135.79, 135.29, 129.61, 125.40, 124.75, 124.52, 124.00, 122.02, 0.14, 0.08. HRMS (AP-MALDI POSITIVE) *m/z* $[M]^+$ calcd for $[C_{44}H_{46}S_6Si_4]$ 878.1001; found 878.0986.

2. NMR and HRMS Spectra

NMR and HRMS Spectra of 3

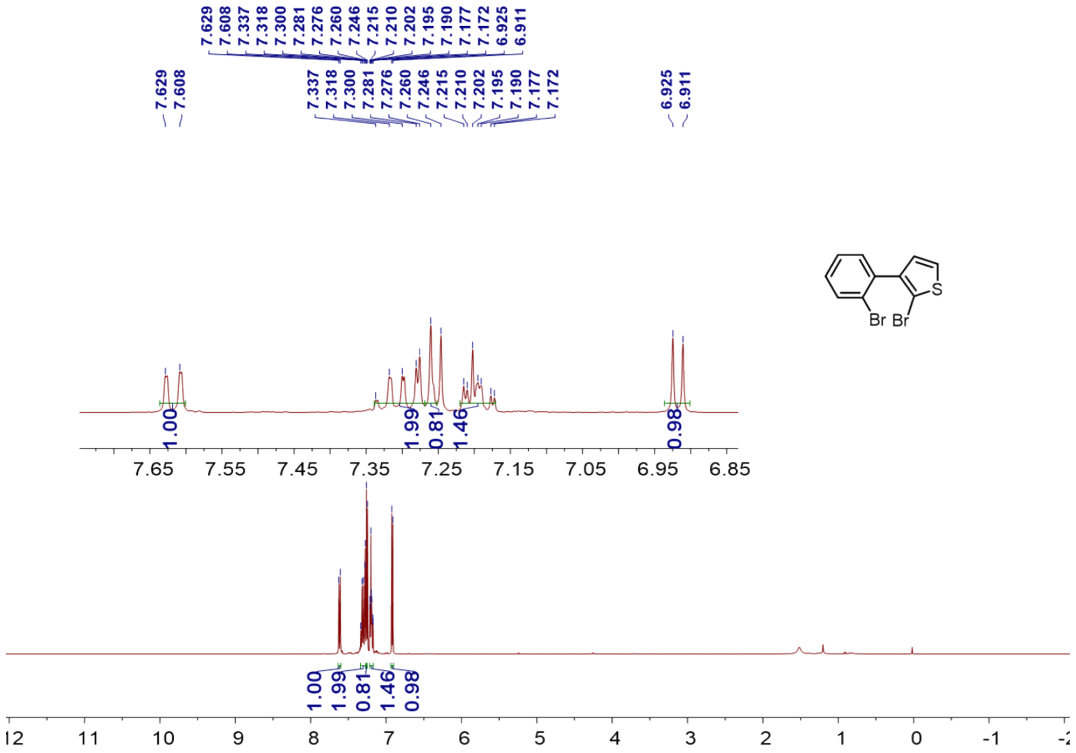


Figure S1. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3**.

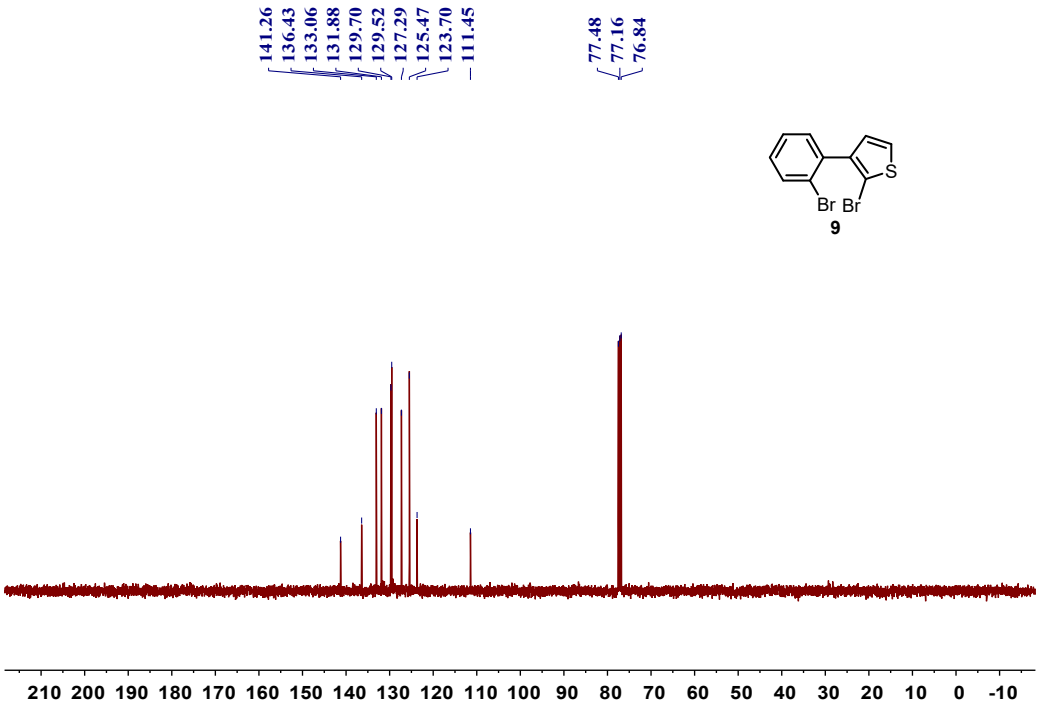


Figure S2. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3**.

National Center for Organic Mass Spectrometry in Shanghai
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution EI-MS Report
Low Resolution EI-MS Report

Instrument:	Waters Premier GC-TOF MS		
Operation Mode:	**EI** Positive Ion Mode	Electron Energy: 70eV	
Card Serial Number:	GCT-P-EI-T24-01-OS-006		
Sample Serial Number:	HNU-ML-1		
Operator:	Liguangping	Date:	2023/12/21

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
315.8548	315.8551	-1.10	7.0	$C_{10}H_6Br_2S$
	315.8552	-1.28	0.0	$C_4H_5O_3Br_2F_3$
	315.8541	2.33	4.0	$C_7H_4O_2Br_2F_2$
	315.8563	-4.72	3.0	$C_7H_7OBr_2FS$
	315.8563	-4.90	-4.0	$CH_6O_4Br_2F_4$

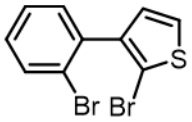


Figure S3. HRMS-EI spectrum of **3**.

NMR and HRMS Spectra of BPDH

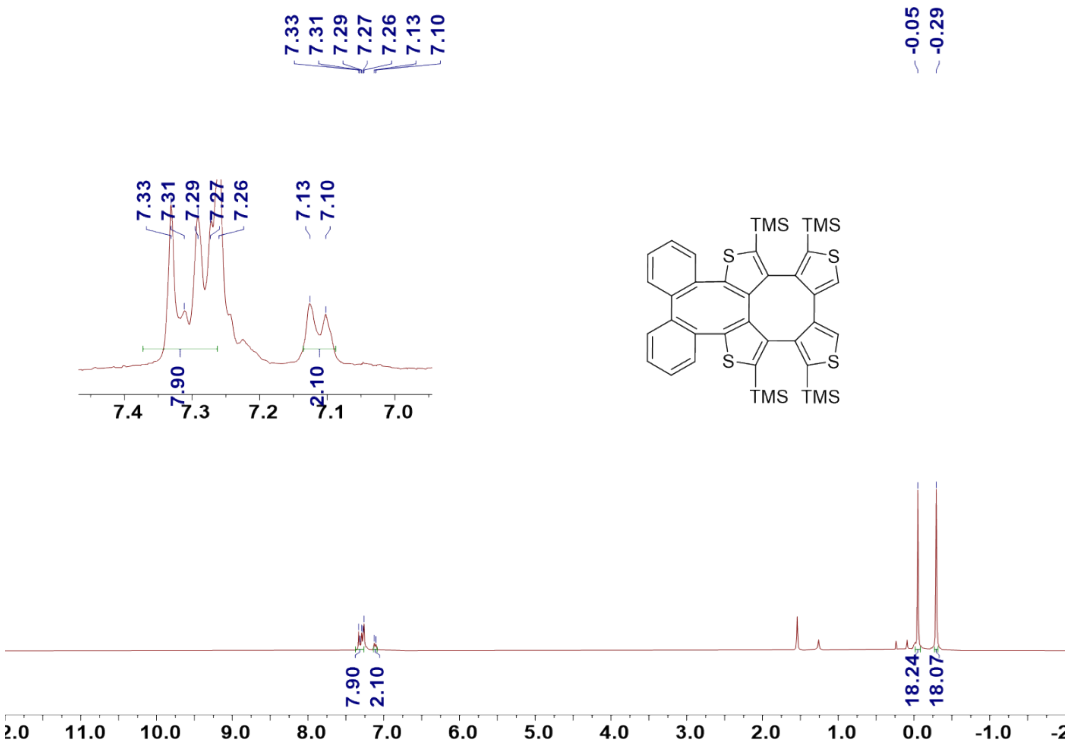


Figure S4. ^{1}H NMR (400 MHz, $CDCl_3$) spectra of **BPDH**.

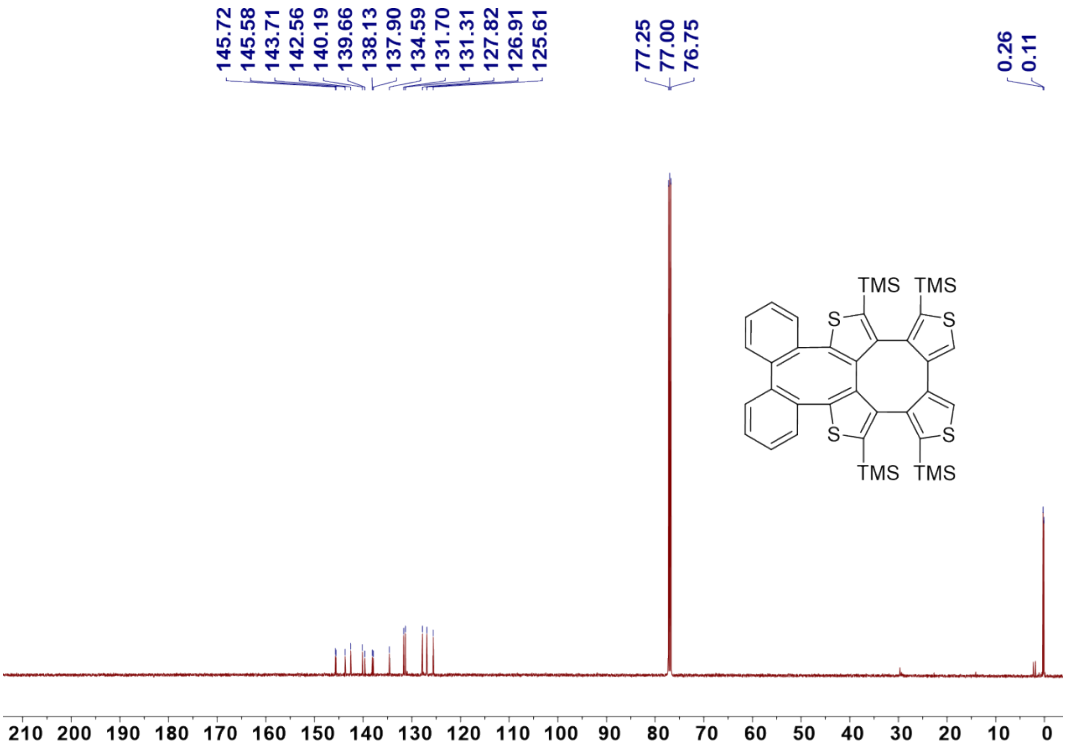


Figure S5. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **BPDH**.

National Center for Organic Mass Spectrometry in Shanghai
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution AP-MALDI- MS REPORT

Instrument: Thermo Scientific Q Exactive HF Orbitrap-FTMS

Card Serial Number: E-W2024031827

Sample Serial Number: PLY-1

Operator: Wang Haoyang Date: 2024/03/18

Operation Mode: AP-MALDI Positive Ion Mode

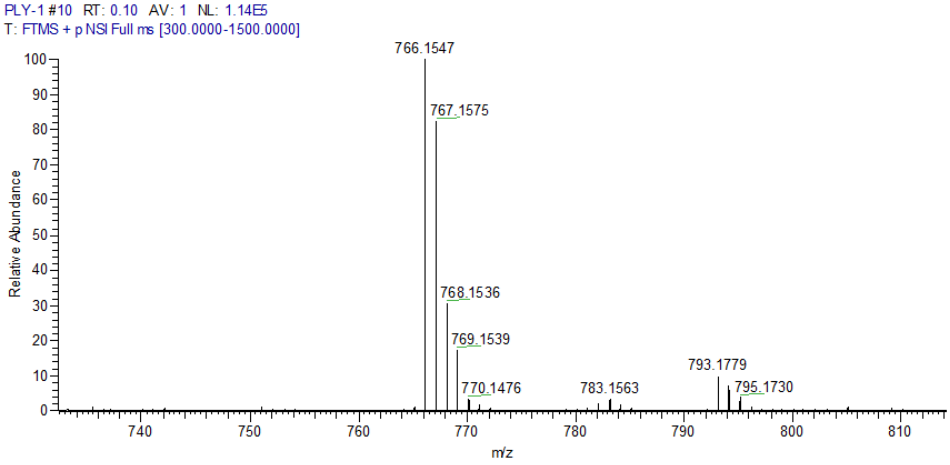


Figure S6. HRMS data of **BPDH**.

NMR and HRMS Spectra of TPDH

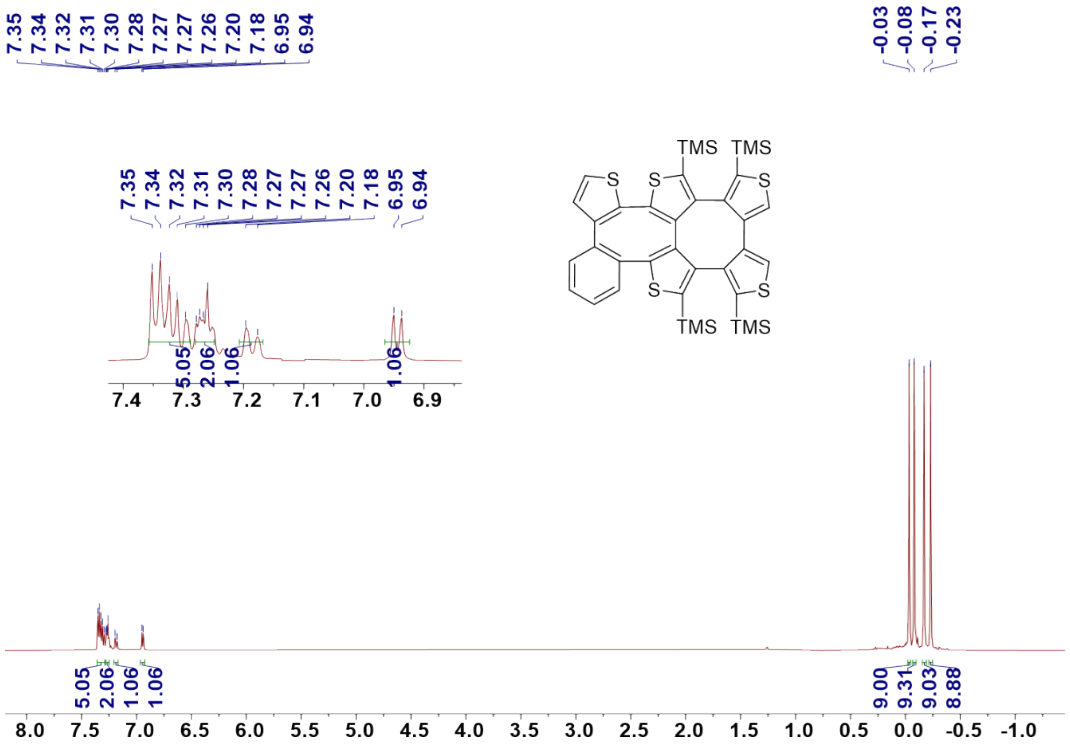


Figure S7. ^{1}H NMR (400 MHz, $CDCl_3$) spectra of **TPDH**.

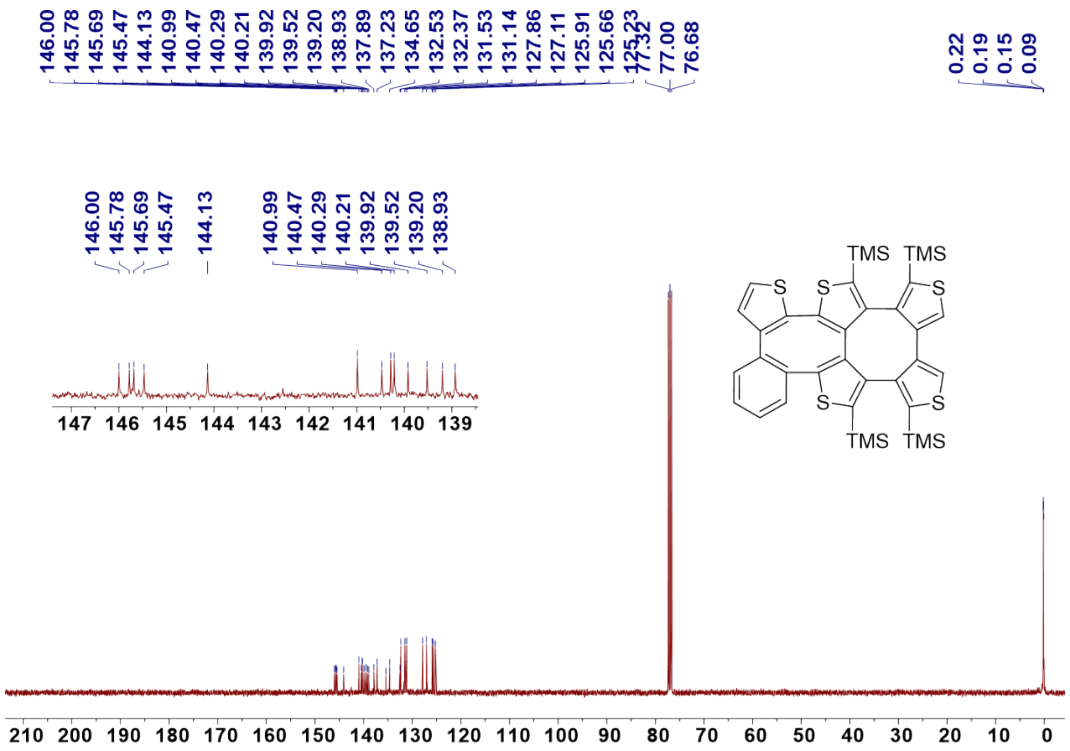


Figure S8. ^{13}C NMR (100 MHz, $CDCl_3$) spectra of **TPDH**.

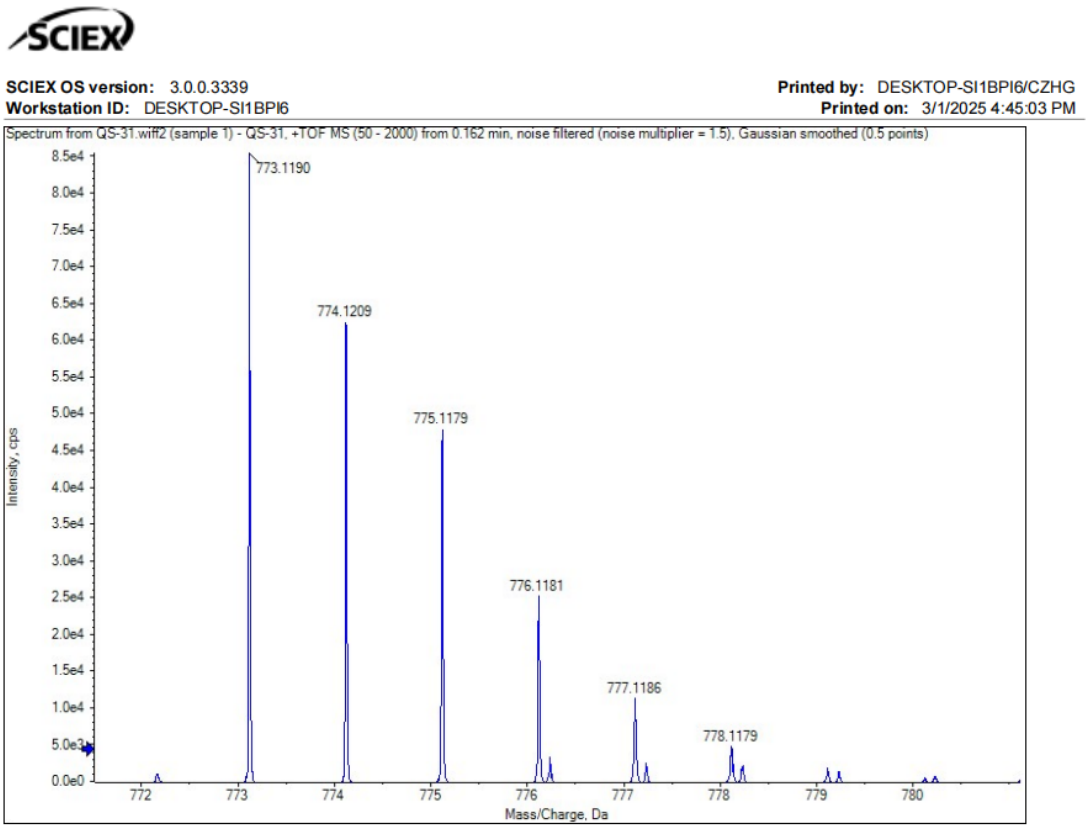


Figure S9. HRMS data of **TPDH**.

NMR and HRMS Spectra of TBTDH

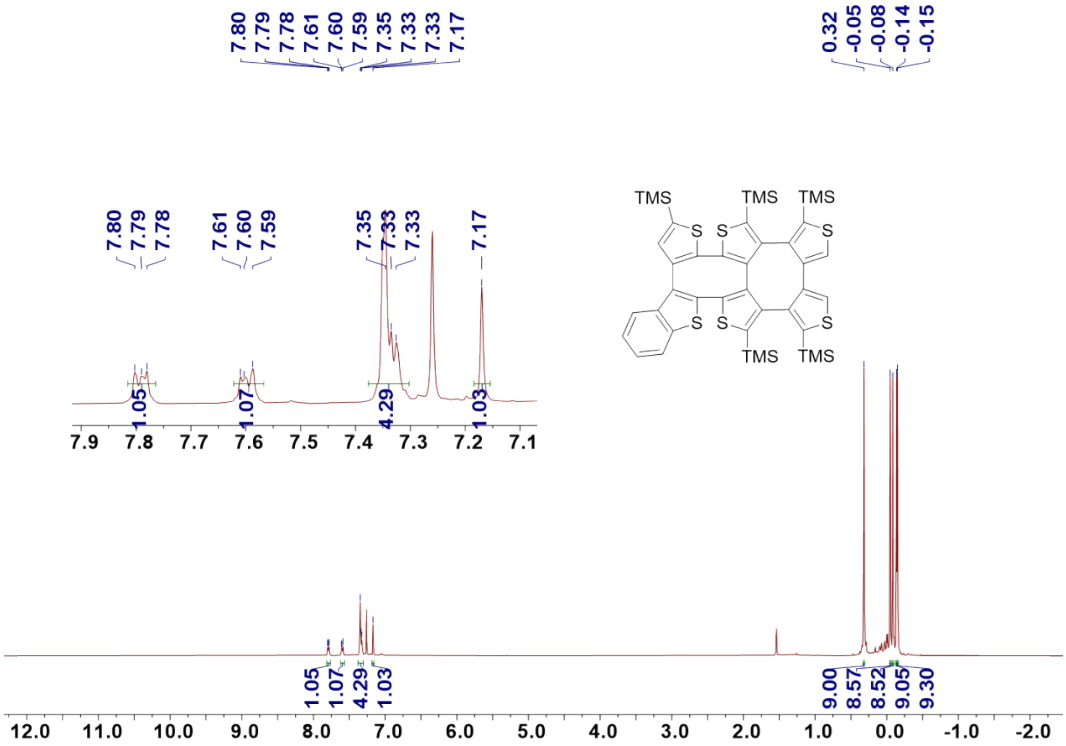


Figure S10. ^{1}H NMR (400 MHz, $CDCl_3$) spectra of **TBTDH**.

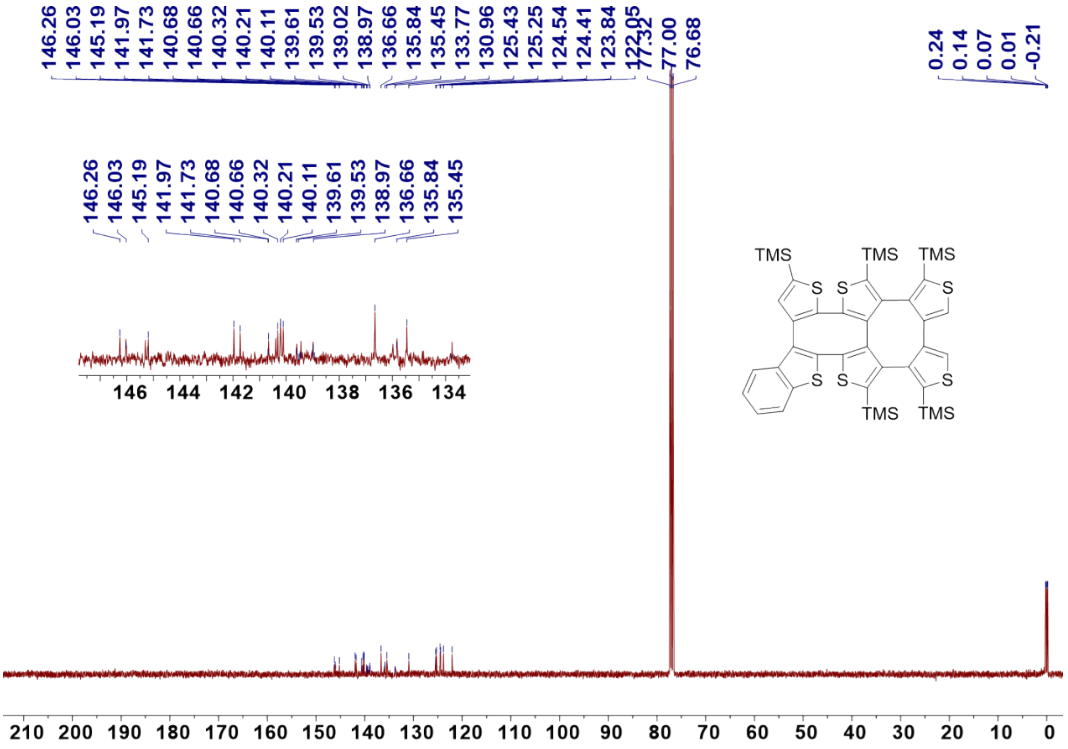


Figure S11. ^{13}C NMR (100 MHz, $CDCl_3$) spectra of **TBTDH**.

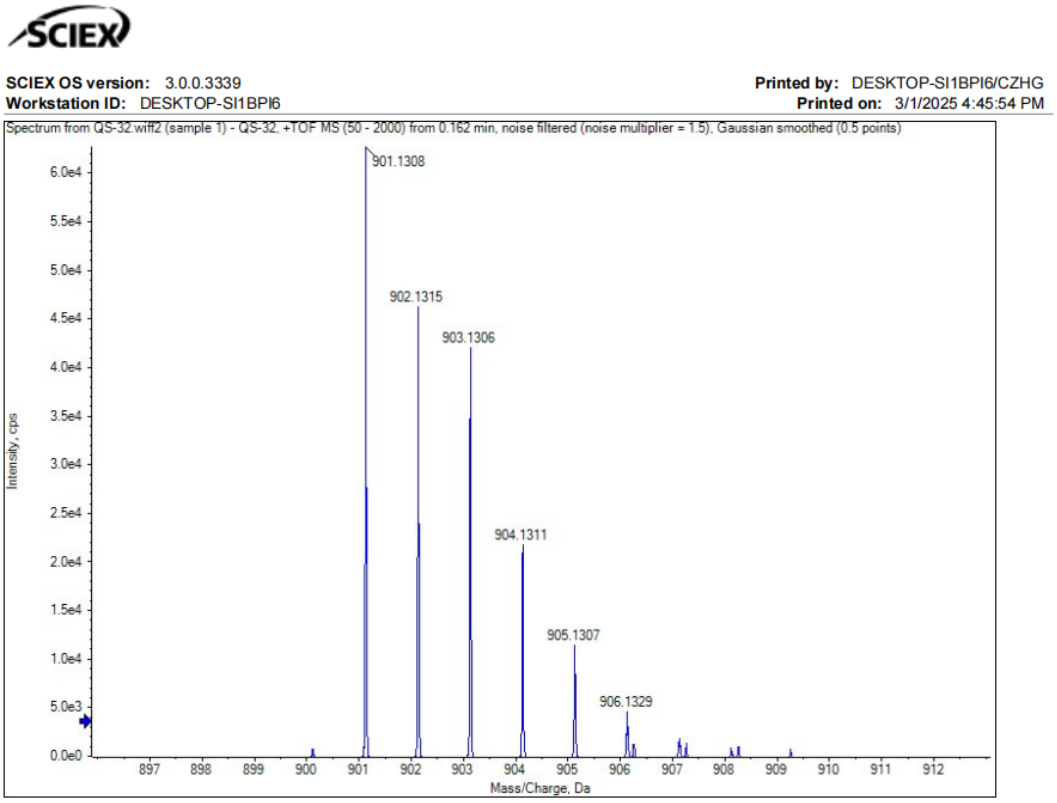


Figure S12. HRMS data of **TBTDH**.

NMR and HRMS Spectra of BBTDH

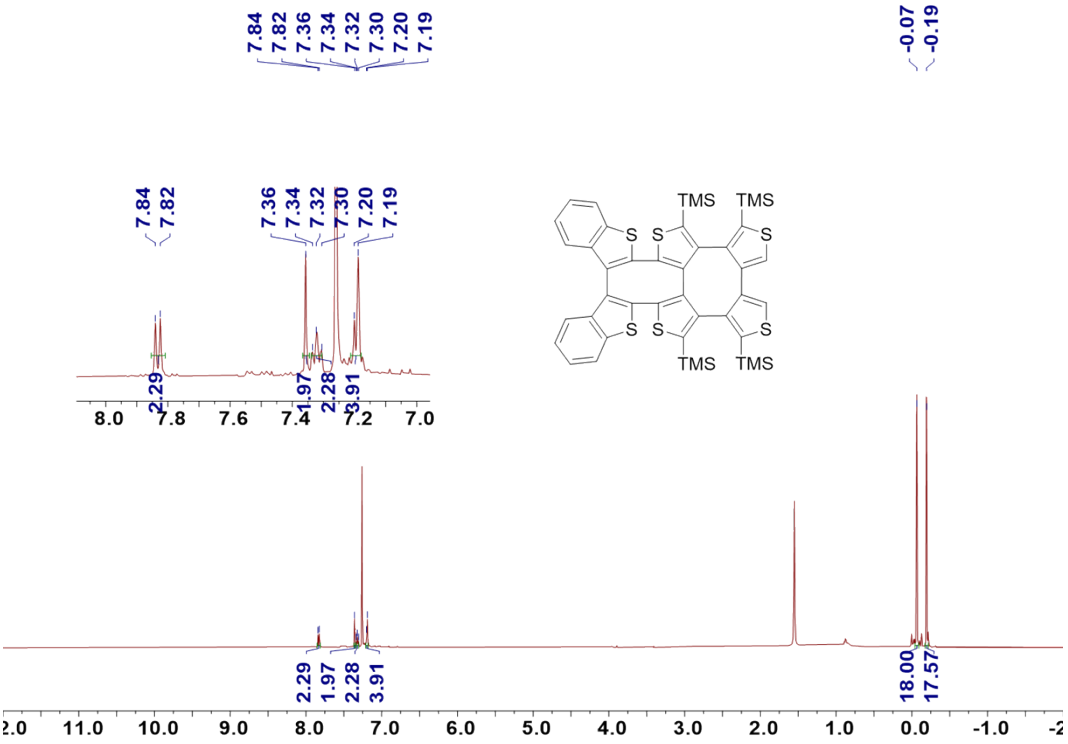


Figure S13. ^{1}H NMR (500 MHz, $CDCl_3$) spectra of **BBTDH**.

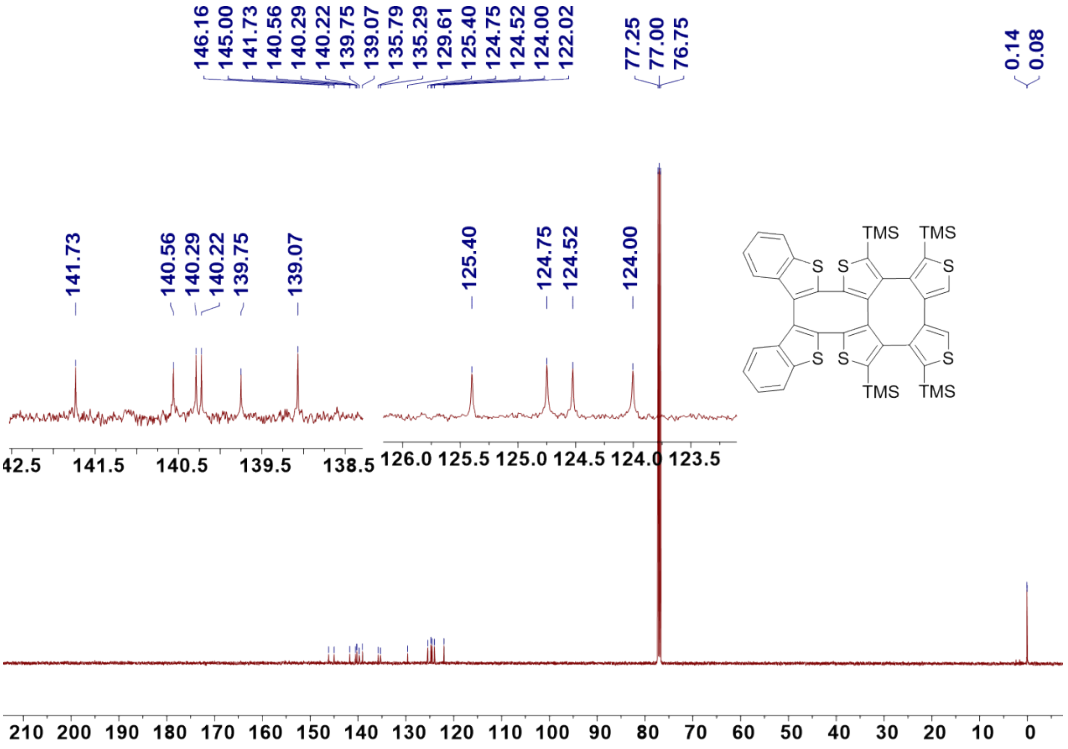


Figure S14. ^{13}C NMR (125 MHz, $CDCl_3$) spectra of **BBTDH**.

National Center for Organic Mass Spectrometry in Shanghai
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution AP-MALDI- MS REPORT

Instrument: Thermo Scientific Q Exactive HF Orbitrap-FTMS

Card Serial Number: E-W2024031825

Sample Serial Number: PLY-2

Operator: Wang Haoyang Date: 2024/03/18

Operation Mode: AP-MALDI Positive Ion Mode

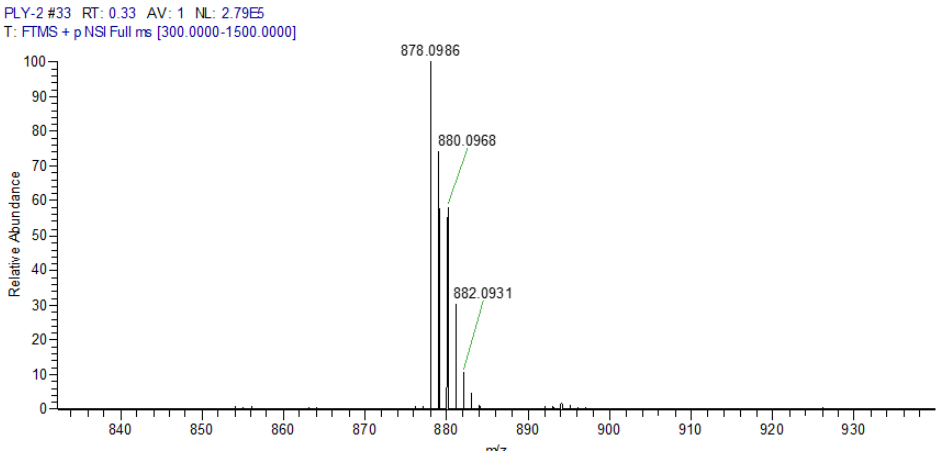


Figure S15. HRMS data of **BBTDH**.

3. Chiral Resolution of Racemic BPDH and Circular Dichroism Analysis

To support the proposed double-helical structures, the racemic mixture of **BPDH** was chirally resolved by preparative high-performance liquid chromatography (HPLC), and the CD spectra were subsequently measured. As shown in Figure S16, the enantiomerically pure **BPDH** exhibit obvious Cotton effects in the range of 230 to 340 nm. The CD spectra of the two enantiomers display perfect mirror-image profiles, confirming their enantiomeric nature. The absorption dissymmetry factor at 289 nm were determined to be -9.33×10-2 and 9.27×10-2 for the two enantiomers, respectively. To determine the absolute configuration, the CD spectra of (*M*)-**BPDH** and (*P*)-**BPDH** were calculated using TD-DFT (Figure S17). The calculated CD spectrum of (*P*)-**BPDH** shows good agreement with the experimental spectrum of (-)-**BPDH**, while that of (*M*)-**BPDH** is consistent with (+)-**BPDH**.

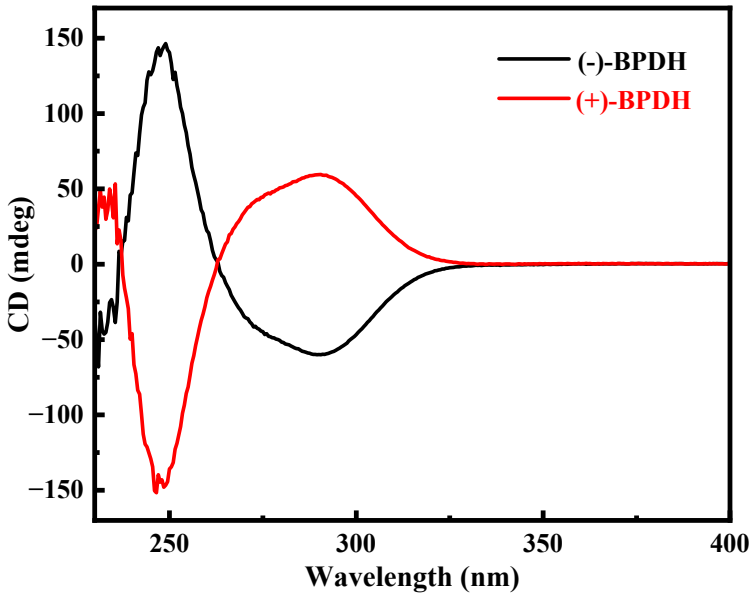


Figure S16. CD spectra of enantiomers of **BPDH** in DCM (1×10^{-5} M)

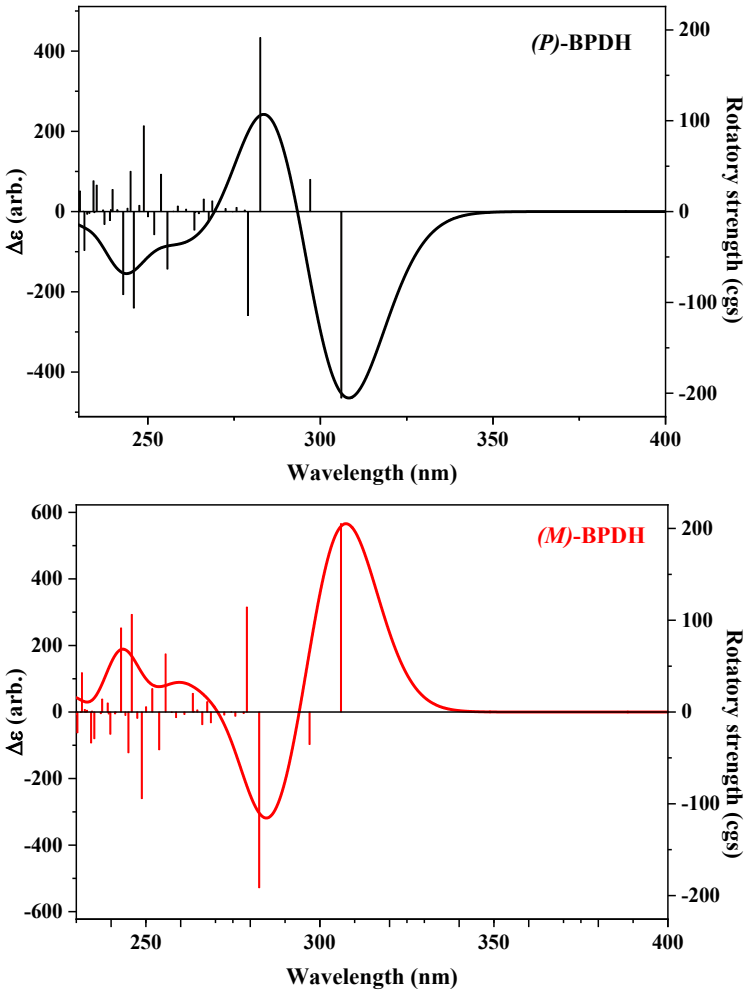


Figure S17. TD-DFT simulated CD spectra of **BPDH** enantiomers at B3LYP/6-311G(d) level

4. Optimized Dihedral Angles of the Four Double-helix Compounds

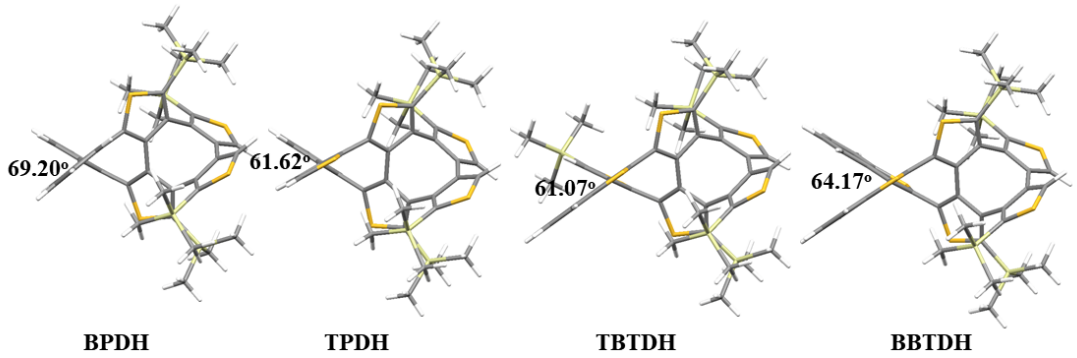


Figure S18. Optimized dihedral angles of the four double-helix compounds.

5. X-ray Crystallographic Data

Table S1. Crystal data and structure refinement for **BPDH**.

Empirical formula	$C_{40}H_{46}S_4Si_4$
Formula weight	767.37
Temperature/K	150.0
Crystal system	trigonal
Space group	*R*-3
a/Å	48.046(2)
b/Å	48.046(2)
c/Å	9.8834(9)
α/°	90
β/°	90
γ/°	120
Volume/Å^3	19758(3)
Z	18
D_{calc}g/cm^3	1.161
μ/mm^{-1}	0.351
F(000)	7308.0
Crystal size/mm^3	0.16 × 0.08 × 0.08
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.236 to 56.566
Index ranges	-59 ≤ h ≤ 64, -64 ≤ k ≤ 61, -12 ≤ l ≤ 13
Reflections collected	73823
Independent reflections	10870 [R_{int} = 0.1208, R_{sigma} = 0.0784]
Data/restraints/parameters	10870/0/445
Goodness-of-fit on F^2	1.009
Final R indexes [I>=2σ (I)]	R_1 = 0.0516, wR_2 = 0.0954
Final R indexes [all data]	R_1 = 0.1097, wR_2 = 0.1174
Largest diff. peak/hole / e Å^{-3}	0.27/-0.26

6. Photophysical Parameters of double-helical compounds and 4TCOTh

Table S2 Photophysical properties of double-helical compounds and **4TCOTh**

Comp.	$\lambda_{abs}{}^{a}$ (nm)	$\lambda_{FL}{}^{a}$ (nm)	$\lambda_{PL}{}^{b}$ (nm)	$\Phi_{FL}{}^{a,c}$ (%)	$\tau_{FL}{}^{a}$ (ns)	$k_r{}^{a}$	$k_{nr}{}^{a}$
4TCOTh	258	355	369	0.11	1.13	0.97	8.8
BPDH	276	395	400, 520	0.37	1.49	2.5	6.7
TPDH	290	450	410	0.23	1.21	1.9	8.2
TBTDH	310	430	400	0.08	1.19	0.67	8.4
BBTDH	310	415	402	0.09	1.13	0.80	8.8

[a] In DCM solution (1×10^{-5} M), k_r ($\times 10^6$ s^{-1}), k_{nr} ($\times 10^8$ s^{-1}). [b] In 2-MTHF solution (1×10^{-5} M) at 77 K. [c] Relative fluorescence quantum yield using quinine sulfate (Φ_{FL} = 0.55, 1×10^{-5} M in 0.5 M H_2SO_4) as a standard.

7. Concentration-Dependent and Film State Photophysical Properites

We have performed concentration-dependent absorption and photoluminescence measurements on the four target compounds to distinguish the contributions of through-space conjugation (TSC) and through-bond conjugation (TBC) to the emission. As shown in the Figure S19 and S20, with increasing concentration from 1×10^{-5} M to 5×10^{-4} M, the absorption intensity increased while the peak positions remained largely unchanged. The emission intensity decreased with increasing concentration, accompanied by a slight red shift in the emission peaks and no clear emergence of a new emission band. This concentration-quenching behavior indicates that emission at high concentrations is dominated by through-bond conjugation (TBC), whereas the contribution from intramolecular through-space conjugation (ITSC) is negligible under the conditions examined.

We have further measured the solid-state optical properties, including photoluminescence and fluorescence lifetimes, in the film state. As shown in Figures S21 and S22, the emission peaks range from 393 to 424 nm, and the lifetimes range from 1.18 to 1.51 ns. These values are close to those observed in solution (Fig. 5a) at room temperature, indicating that the emission originates primarily from local excited states. This is likely because the effective electron cloud overlap required for intramolecular spatial conjugation is not achieved in the film state.

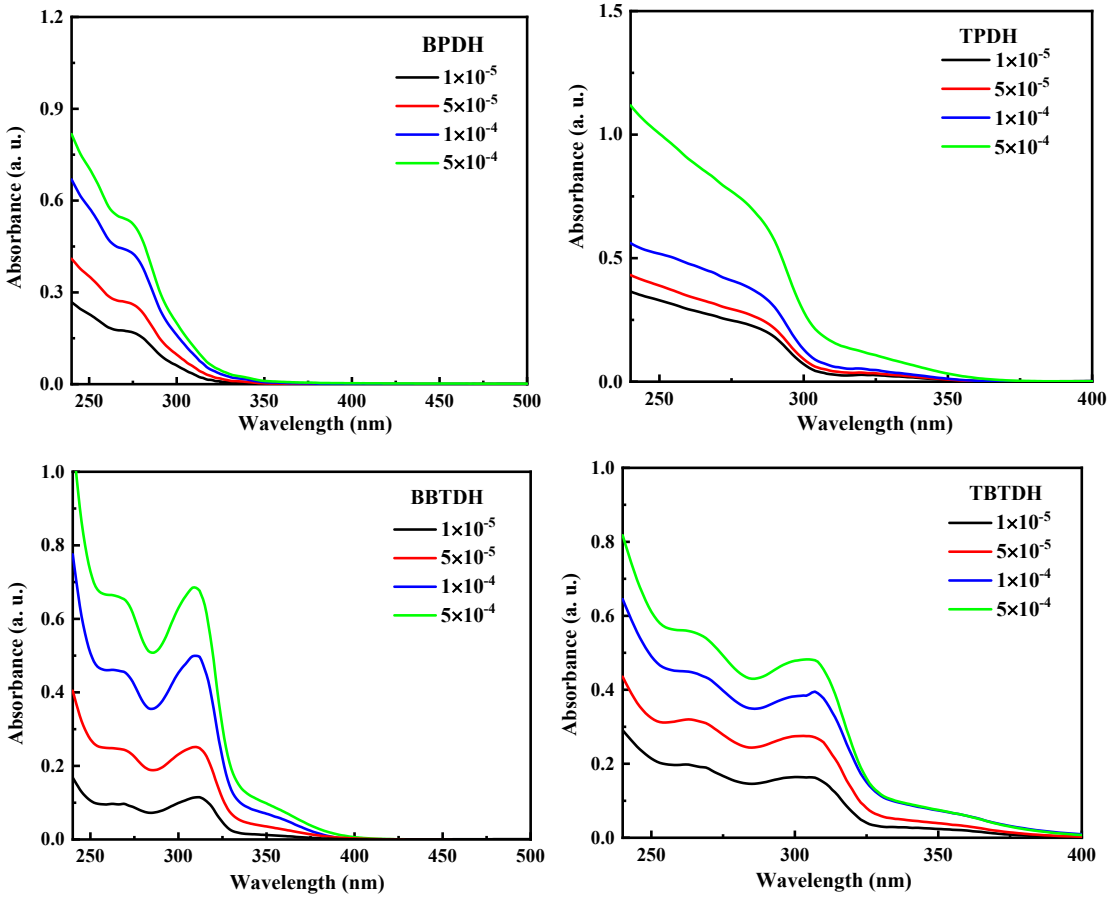
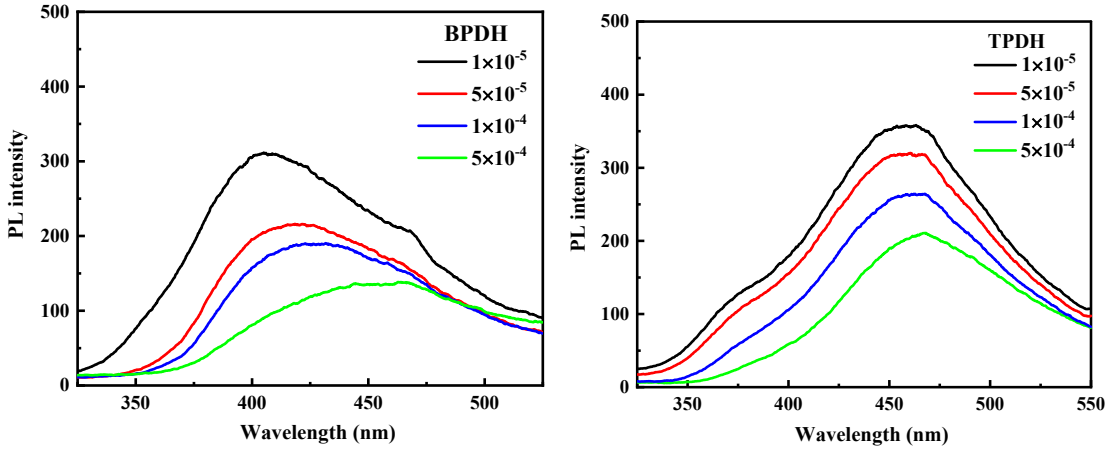


Figure S19. Concentration-dependent UV-Vis Asoption spectra in DCM solution at room temerature.



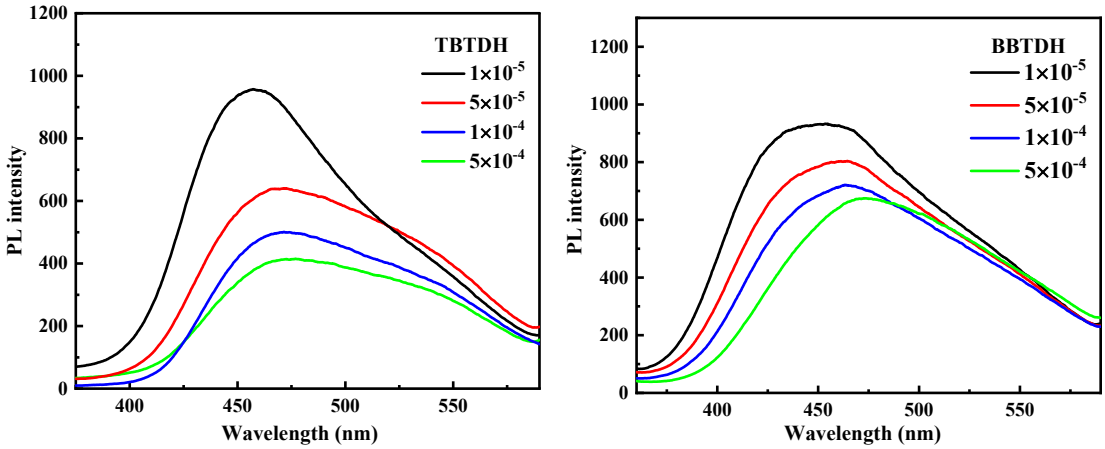


Figure S20. Concentration-dependent fluorescence spectra measured in DCM at room-temperature. λ_{ex}: **BPDH**, 280 nm; **TPDH**, 290 nm; **TBTDH**, 320 nm **BBTDH**, 320 nm.

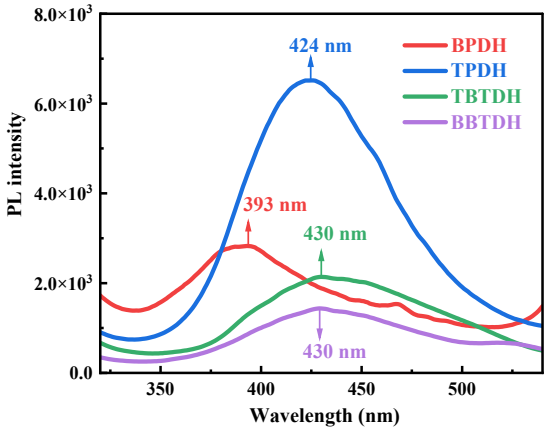
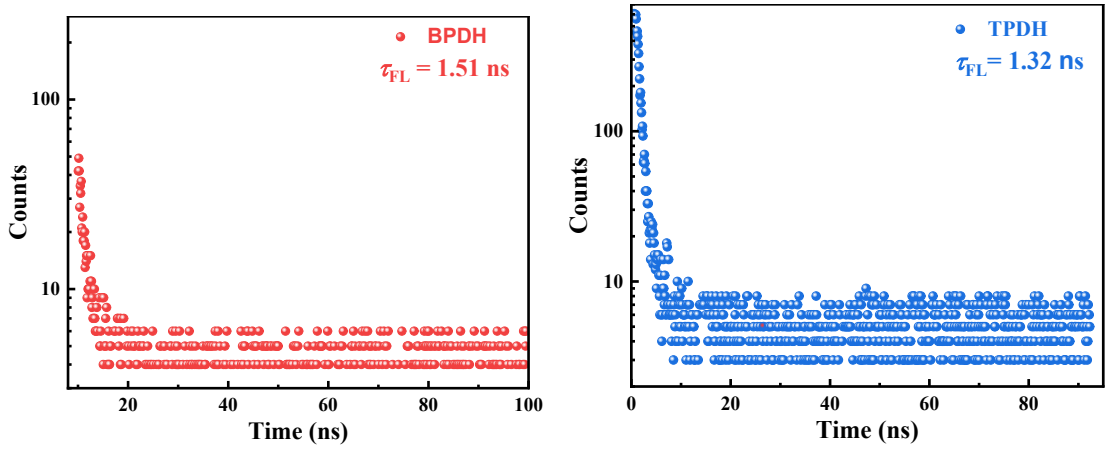


Figure S21. Fluorescence spectra of film states deposited from DCM, measured at room temperature. λ_{ex}: **BPDH**, 280 nm; **TPDH**, 290 nm; **TBTDH**, 320 nm; **BBTDH**, 320 nm.



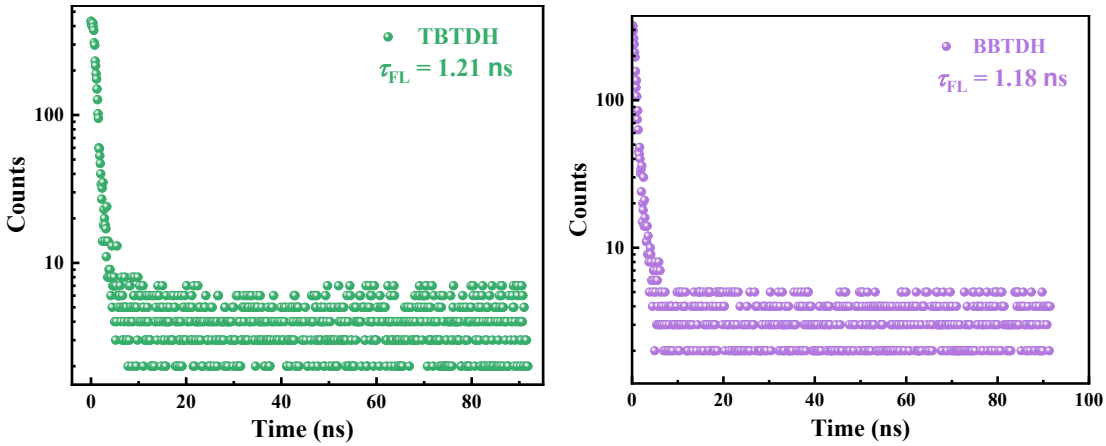


Figure S22. Fluorescence decay curves of films deposited from DCM, measured at room temperature.

8. Computational Methods and Coordinates of all Optimized Molecules

All quantum chemical calculations were carried out using the Gaussian 16 program package. The ground state (S_0) geometry was fully optimized using density functional theory (DFT) at the B3LYP/6-311G(d) level. Vibrational frequency analysis was performed at the same theoretical level to verify that the optimized structure corresponds to a local minimum on the potential energy surface, as evidenced by the absence of imaginary frequencies. Subsequently, absorption and circular dichroism spectra were simulated based on the optimized S_0 geometry using time-dependent DFT (TD-DFT) at the same level. The optimized cartesian coordinates for the S_0 state are provided below:

(1).BPDH

	S_0						
	X	Y	Z		X	Y	Z
Si	3.442667	-1.56278	2.592036	C	-0.416169	3.685645	0.676962
Si	3.967406	-0.320023	-1.69071	C	-3.831563	1.223281	0.765725
Si	-3.931234	-0.391033	1.7169	H	-4.04531	1.104697	-0.296334
Si	-3.500473	-1.409188	-2.638297	H	-2.847924	1.68702	0.85665
C	3.561556	-3.151996	1.60018	H	-4.565213	1.920541	1.183371
H	3.997585	-2.999204	0.612659	C	-3.663241	-0.044586	3.549258
H	2.580082	-3.609889	1.457215	H	-4.391854	0.683907	3.918273

H	4.190067	-3.865572	2.142784	**H**	-2.66457	0.363451	3.72431
C	5.120368	-0.71605	2.713145	**H**	-3.763141	-0.950812	4.153133
H	5.509521	-0.435586	1.731618	**C**	-5.611275	-1.212726	1.489872
H	5.854175	-1.376049	3.18594	**H**	-5.787616	-1.507859	0.452757
H	5.05896	0.195288	3.315196	**H**	-6.418774	-0.535854	1.785606
C	2.823202	-1.954956	4.327042	**H**	-5.693701	-2.113629	2.105244
H	3.497867	-2.651964	4.833715	**C**	-5.196844	-0.59454	-2.567218
H	1.830741	-2.413299	4.292125	**H**	-5.533709	-0.431978	-1.541274
H	2.750689	-1.055706	4.94522	**H**	-5.944256	-1.218422	-3.067158
C	2.202309	-0.36697	1.830995	**H**	-5.18795	0.377364	-3.06913
C	1.445125	-0.445435	0.682871	**C**	-3.526464	-3.086535	-1.795654
C	0.498513	0.627113	0.54144	**H**	-3.90092	-3.035212	-0.772701
C	0.573093	1.554162	1.547714	**H**	-2.529054	-3.530616	-1.758032
C	1.572718	-1.4935	-0.357366	**H**	-4.174803	-3.762991	-2.361857
C	0.609269	-2.560918	-0.487422	**C**	-3.002674	-1.619583	-4.442726
C	0.944173	-3.443774	-1.474682	**H**	-3.704043	-2.277916	-4.964633
H	0.402927	-4.324888	-1.786272	**H**	-2.004692	-2.059066	-4.525547
C	2.592184	-1.545645	-1.281988	**H**	-2.988878	-0.664199	-4.975016
C	5.631546	-1.151338	-1.39164	**S**	1.777975	1.086569	2.718044
H	6.453517	-0.478177	-1.654312	**S**	2.398644	-2.970332	-2.286333
H	5.736794	-2.054739	-1.999606	**S**	-2.390567	-3.090122	2.119014
H	5.762341	-1.442086	-0.346558	**S**	-1.791777	1.216519	-2.677746
C	3.80374	0.081897	-3.523905	**C**	-0.290466	2.731384	1.706781
H	4.565475	0.805052	-3.831423	**C**	-1.32418	4.738034	0.845687
H	2.824334	0.516435	-3.740283	**C**	-1.042532	2.881662	2.879956
H	3.918887	-0.807832	-4.149232	**C**	-2.086247	4.861796	2.003318
C	3.825843	1.264859	-0.696778	**H**	-1.425374	5.470908	0.052731
H	4.573744	1.9753	-1.063888	**C**	-1.935569	3.934914	3.031876
H	4.000332	1.111761	0.368244	**H**	-0.93754	2.14262	3.665944

H	2.84579	1.731076	-0.809117	**H**	-2.787897	5.682689	2.102971
C	-0.615145	-2.58387	0.331139	**H**	-2.518614	4.023007	3.941894
C	-0.944753	-3.520547	1.269218	**C**	0.443073	3.704378	-0.548699
H	-0.403171	-4.419107	1.525529	**C**	1.365415	4.750018	-0.676816
C	-2.587091	-1.609184	1.199806	**C**	1.060172	2.976052	-2.780693
C	-1.576161	-1.507913	0.269877	**C**	2.129667	4.907288	-1.828949
C	-1.454968	-0.40722	-0.715339	**H**	1.476594	5.450342	0.143733
C	-2.222544	-0.270296	-1.851351	**C**	1.967637	4.022085	-2.89196
C	-0.499675	0.651586	-0.533654	**H**	0.94641	2.267679	-3.593413
C	-0.573344	1.621274	-1.498791	**H**	2.842661	5.721598	-1.897155
C	0.304749	2.792767	-1.614438	**H**	2.553296	4.136437	-3.797372

(2).TPDH

	S0						
	X	**Y**	**Z**		**X**	**Y**	**Z**
Si	3.492383	-1.469764	2.607849	**C**	0.186651	2.774244	-1.584259
Si	3.921892	-0.301905	-1.709048	**C**	-0.393703	3.75959	0.692522
Si	-3.917767	-0.398817	1.760139	**C**	-3.809478	1.199464	0.782451
Si	-3.448568	-1.565123	-2.592117	**H**	-3.997107	1.06099	-0.28246
C	3.629711	-3.075577	1.645892	**H**	-2.831678	1.672819	0.888949
H	4.055425	-2.934379	0.652156	**H**	-4.558512	1.897839	1.169917
H	2.655361	-3.553146	1.519863	**C**	-3.670731	-0.017745	3.588417
H	4.274928	-3.767387	2.197013	**H**	-4.410023	0.710265	3.936608
C	5.155742	-0.591013	2.694536	**H**	-2.677774	0.403542	3.765838
H	5.531053	-0.324372	1.703738	**H**	-3.768059	-0.913252	4.208452
H	5.905614	-1.227779	3.173959	**C**	-5.592927	-1.227335	1.526052
H	5.083681	0.331577	3.277966	**H**	-5.757686	-1.532554	0.490011
C	2.898438	-1.838651	4.356839	**H**	-6.405036	-0.549696	1.806949
H	3.59024	-2.514229	4.869386	**H**	-5.678966	-2.12246	2.149228

H	1.913605	-2.314202	4.341874	**C**	-5.154364	-0.768721	-2.562538
H	2.817316	-0.928819	4.958227	**H**	-5.494367	-0.566898	-1.5444
C	2.223981	-0.307808	1.839666	**H**	-5.894067	-1.420876	-3.037066
C	1.446341	-0.423208	0.708761	**H**	-5.154658	0.181608	-3.104111
C	0.485314	0.636547	0.557247	**C**	-3.460682	-3.210076	-1.688516
C	0.568263	1.590659	1.536419	**H**	-3.844493	-3.12444	-0.671267
C	1.575991	-1.493775	-0.308501	**H**	-2.458782	-3.640782	-1.626225
C	0.63271	-2.582927	-0.39926	**H**	-4.096565	-3.914872	-2.233861
C	0.973477	-3.484751	-1.367107	**C**	-2.922006	-1.827738	-4.38077
H	0.446216	-4.383959	-1.649553	**H**	-3.602905	-2.517814	-4.888499
C	2.584932	-1.549844	-1.244438	**H**	-1.914517	-2.24967	-4.434467
C	5.61268	-1.081253	-1.420171	**H**	-2.919461	-0.891366	-4.945956
H	6.411202	-0.39239	-1.712796	**S**	1.800482	1.162329	2.696336
H	5.732491	-1.995422	-2.009062	**S**	2.407799	-3.003509	-2.209282
H	5.769447	-1.343657	-0.371143	**S**	-2.347596	-3.070946	2.238006
C	3.7115	0.046511	-3.547943	**S**	-1.799627	1.095457	-2.691574
H	4.451279	0.776347	-3.891375	**C**	-0.274649	2.784594	1.704824
H	2.719293	0.456038	-3.75433	**C**	-1.229763	4.861813	0.916072
H	3.832384	-0.857942	-4.15073	**C**	-0.981595	2.952963	2.904193
C	3.756987	1.302685	-0.7498	**C**	-1.937591	5.008407	2.103942
H	4.456202	2.034237	-1.167794	**H**	-1.323928	5.609941	0.136606
H	3.986156	1.184216	0.309413	**C**	-1.810009	4.049441	3.106245
H	2.753583	1.724383	-0.824929	**H**	-0.887669	2.196873	3.675157
C	-0.585643	-2.6005	0.427741	**H**	-2.584339	5.867364	2.245143
C	-0.901564	-3.512626	1.394163	**H**	-2.356601	4.150341	4.037283
H	-0.349996	-4.397907	1.67429	**C**	0.355633	3.717314	-0.590962
C	-2.562709	-1.619265	1.277437	**C**	1.245369	4.766008	-0.992635
C	-1.557108	-1.536322	0.340129	**C**	1.733216	4.609945	-2.256852
C	-1.446975	-0.462891	-0.676606	**H**	1.502856	5.598917	-0.350842

C	-2.200918	-0.376702	-1.827255	**H**	2.416042	5.249691	-2.795507
C	-0.514827	0.617366	-0.516098	**S**	1.124932	3.171872	-3.005731
C	-0.600391	1.559269	-1.510045				

(3).TBTDH

	S_0						
	X	**Y**	**Z**		**X**	**Y**	**Z**
Si	1.235635	-3.493707	-3.257534	**H**	3.483459	4.460955	-2.474457
Si	-1.273554	-3.975496	0.484527	**H**	2.856047	2.846144	-2.819106
Si	3.48109	3.055672	-0.418335	**H**	4.597637	3.102753	-2.662171
Si	3.018552	1.265377	3.724237	**C**	4.852105	3.974255	0.489394
C	2.22301	-4.615557	-2.122701	**H**	4.832543	3.777617	1.564043
H	1.611434	-5.060551	-1.337253	**H**	4.755	5.055054	0.347575
H	3.04031	-4.077909	-1.636895	**H**	5.838144	3.679002	0.118851
H	2.658827	-5.426756	-2.714796	**C**	3.076044	3.089561	4.186038
C	-0.246553	-4.401203	-3.981092	**H**	3.294913	3.720281	3.321095
H	-0.942077	-4.729734	-3.205323	**H**	3.848269	3.276028	4.938641
H	0.074901	-5.287166	-4.537257	**H**	2.120756	3.422284	4.602379
H	-0.802581	-3.760625	-4.671739	**C**	4.683519	0.68331	3.083293
C	2.337562	-2.884315	-4.657276	**H**	5.050325	1.292733	2.256911
H	2.73635	-3.724965	-5.23331	**H**	4.64242	-0.351064	2.734812
H	3.184307	-2.312953	-4.266504	**H**	5.415816	0.736017	3.895461
H	1.792809	-2.236897	-5.35025	**C**	2.538405	0.251764	5.236696
C	0.622159	-1.960107	-2.347116	**H**	3.285694	0.356435	6.029295
C	0.723905	-1.583635	-1.025643	**H**	2.461468	-0.809946	4.985564
C	0.236684	-0.2579	-0.762214	**H**	1.57441	0.565332	5.646984
C	-0.300126	0.348402	-1.870241	**S**	-0.147513	-0.685528	-3.270603
C	1.245887	-2.437958	0.067556	**S**	1.535256	-4.244608	1.863935
C	2.570347	-2.25406	0.610869	**S**	5.120939	0.425537	-0.938668

C	2.867434	-3.176247	1.573639	**S**	-0.005201	1.309593	2.914493
H	3.777943	-3.265196	2.147611	**C**	-0.934223	1.652406	-1.914117
C	0.532927	-3.455913	0.660446	**C**	-2.323573	3.464746	-1.400869
C	-1.33588	-5.737827	-0.17781	**C**	-1.575354	4.014634	-2.46794
H	-2.370854	-6.082536	-0.265946	**C**	-2.634669	1.28863	-0.083403
H	-0.812812	-6.428772	0.489819	**C**	-4.039684	1.017282	-0.121714
H	-0.873322	-5.820959	-1.164189	**C**	-4.514697	0.284593	0.93868
C	-2.017629	-3.940831	2.213937	**H**	-4.672263	1.354323	-0.933871
H	-3.075689	-4.219302	2.183844	**S**	-3.20372	-0.081885	2.031209
H	-1.950303	-2.939225	2.645894	**S**	-0.405292	2.863195	-3.085152
H	-1.510031	-4.633457	2.891184	**C**	-3.291596	4.263724	-0.770093
C	-2.238388	-2.812546	-0.628761	**C**	-1.780105	5.322652	-2.909617
H	-3.297201	-3.087461	-0.585967	**C**	-3.497216	5.562209	-1.208266
H	-1.917954	-2.863555	-1.669735	**H**	-3.865223	3.860676	0.056852
H	-2.155425	-1.773464	-0.306881	**C**	-2.746846	6.089179	-2.272743
C	3.398491	-1.11024	0.192292	**H**	-1.197727	5.731188	-3.727629
C	4.581333	-1.157976	-0.489278	**H**	-4.242576	6.181877	-0.722102
H	5.144119	-2.032904	-0.779404	**H**	-2.920882	7.108113	-2.600464
C	3.735886	1.199337	-0.192144	**Si**	-6.253734	-0.369861	1.220455
C	2.935443	0.242498	0.390063	**C**	-6.873366	0.230006	2.891481
C	1.698412	0.540524	1.150419	**H**	-6.907568	1.322208	2.932357
C	1.657014	1.009608	2.445376	**H**	-6.225391	-0.112447	3.703567
C	0.402223	0.372748	0.554382	**H**	-7.881338	-0.144985	3.093083
C	-0.624244	0.771967	1.372839	**C**	-6.182761	-2.250149	1.197589
C	-2.035049	0.751587	1.037961	**H**	-7.172358	-2.685432	1.366184
C	-1.943213	2.10193	-1.102809	**H**	-5.514455	-2.631638	1.97508
C	1.793224	3.612629	0.185532	**H**	-5.81328	-2.616488	0.235831
H	1.682548	3.526749	1.266905	**C**	-7.332588	0.278934	-0.173866
H	0.98506	3.042875	-0.275829	**H**	-7.356291	1.372021	-0.189867

H	1.653042	4.663872	-0.08651	**H**	-8.361745	-0.072339	-0.05484
C	3.621676	3.395623	-2.265126	**H**	-6.978103	-0.064093	-1.14971

(4).BBTDH

	S_0						
	X	**Y**	**Z**		**X**	**Y**	**Z**
Si	-2.22843	-3.00505	3.109056	**H**	0.93663	2.862471	0.424866
Si	-0.93342	-4.15423	-1.07822	**H**	1.191602	4.605934	0.479884
Si	-1.12692	4.091784	1.113678	**C**	-0.77627	4.142115	2.963003
Si	-2.28879	2.974406	-3.12097	**H**	-0.06654	4.940556	3.200992
C	-3.79471	-3.34381	2.133277	**H**	-0.34003	3.198685	3.300809
H	-3.6112	-3.93692	1.237048	**H**	-1.6846	4.319599	3.545543
H	-4.28245	-2.41814	1.819786	**C**	-1.94677	5.706276	0.596087
H	-4.4958	-3.8953	2.768049	**H**	-2.22938	5.702465	-0.45926
C	-1.32856	-4.60525	3.525003	**H**	-1.27366	6.5539	0.757512
H	-1.0043	-5.13548	2.626302	**H**	-2.85476	5.889367	1.178268
H	-1.97592	-5.27896	4.094612	**C**	-1.47215	4.648629	-3.39288
H	-0.43866	-4.41076	4.130801	**H**	-1.22971	5.1431	-2.44951
C	-2.66344	-2.09912	4.701202	**H**	-2.13217	5.314211	-3.95761
H	-3.35041	-2.69294	5.311946	**H**	-0.54194	4.546031	-3.95912
H	-3.14729	-1.14237	4.485064	**C**	-3.91784	3.159956	-2.20884
H	-1.77625	-1.89238	5.306341	**H**	-3.81424	3.71441	-1.27558
C	-1.04655	-1.88445	2.157085	**H**	-4.35669	2.189345	-1.96731
C	-1.13341	-1.324	0.901359	**H**	-4.62451	3.699042	-2.84795
C	-0.06965	-0.40535	0.603091	**C**	-2.58744	2.151135	-4.7874
C	0.864104	-0.32042	1.606458	**H**	-3.28103	2.742528	-5.393
C	-2.18396	-1.63361	-0.09762	**H**	-3.01881	1.154289	-4.66014
C	-3.28449	-0.73491	-0.35022	**H**	-1.66127	2.04117	-5.35849
C	-4.16371	-1.23815	-1.26654	**S**	0.40514	-1.32237	2.960634

H	-5.06439	-0.77681	-1.64379	**S**	-3.6457	-2.77853	-1.86574
C	-2.20715	-2.77765	-0.86342	**S**	-3.80396	2.605998	1.805078
C	-1.68407	-5.77858	-0.49034	**S**	0.386846	1.359787	-2.96524
H	-0.98444	-6.60602	-0.64392	**C**	2.072102	0.481291	1.581159
H	-2.59974	-6.01285	-1.04111	**C**	4.056222	1.477873	0.838643
H	-1.93714	-5.75168	0.572208	**C**	3.87132	2.162326	2.062281
C	-0.57544	-4.27026	-2.92316	**C**	3.033012	-0.39756	-0.57948
H	0.162445	-5.0529	-3.12522	**C**	3.945063	-2.03187	-2.04537
H	-0.17129	-3.32725	-3.30015	**S**	2.482782	-1.534	-2.87606
H	-1.4746	-4.50447	-3.49992	**S**	2.416441	1.624327	2.880706
C	0.660759	-3.78851	-0.15706	**C**	5.160116	1.810406	0.036035
H	1.404958	-4.54362	-0.43024	**C**	4.760904	3.14781	2.493323
H	0.53636	-3.81513	0.925984	**C**	6.04325	2.789331	0.461609
H	1.071546	-2.81248	-0.41906	**H**	5.311295	1.301457	-0.90882
C	-3.32182	0.595923	0.278678	**C**	5.846783	3.45344	1.68421
C	-4.24172	1.051353	1.179877	**H**	4.606122	3.664125	3.433866
H	-5.12888	0.546858	1.533175	**H**	6.895585	3.049188	-0.15629
C	-2.34429	2.676476	0.836293	**H**	6.548875	4.217235	1.999713
C	-2.25562	1.543708	0.058555	**C**	4.101947	-1.34139	-0.8212
C	-1.17503	1.289432	-0.92434	**C**	4.863864	-2.9939	-2.46789
C	-1.09253	1.864174	-2.17423	**C**	5.207499	-1.64397	-0.00911
C	-0.08048	0.409749	-0.61947	**C**	5.950627	-3.27016	-1.64947
C	0.866097	0.365236	-1.6132	**H**	4.73043	-3.51498	-3.40907
C	2.097964	-0.39919	-1.58063	**C**	6.119452	-2.5999	-0.42609
C	3.015161	0.505879	0.587509	**H**	5.337372	-1.13019	0.936299
C	0.482772	3.825289	0.185339	**H**	6.675067	-4.01566	-1.95815
H	0.360098	3.87274	-0.89703	**H**	6.973118	-2.8368	0.199161

(5).COTh-4TMS

	S_0						
	X	**Y**	**Z**		**X**	**Y**	**Z**
Si	3.765872	2.163914	0.538184	**C**	-0.772622	1.462221	2.533962
Si	3.765634	-2.16406	-0.538076	**H**	-0.197823	1.668911	3.424617
Si	-3.766061	2.163958	-0.53807	**C**	-2.432328	1.543244	0.640236
Si	-3.765427	-2.164122	0.538158	**C**	-1.526643	0.509463	0.539148
C	3.734026	1.236069	2.169744	**C**	-1.526549	-0.5092	-0.539376
H	4.030253	0.191861	2.069136	**C**	-2.43212	-1.543035	-0.640404
H	2.738005	1.251554	2.618282	**C**	-0.556986	-0.480485	-1.608563
H	4.424745	1.719519	2.868168	**C**	-0.772355	-1.461905	-2.534138
C	5.446527	2.014558	-0.298548	**C**	-3.734474	1.235729	-2.169429
H	5.688734	0.982204	-0.559792	**H**	-4.031188	0.191696	-2.068451
H	6.240085	2.386957	0.356628	**H**	-2.738373	1.250558	-2.617817
H	5.476594	2.602055	-1.220897	**H**	-4.424864	1.719216	-2.868143
C	3.404625	3.985172	0.855029	**C**	-3.404777	3.985141	-0.855214
H	4.142139	4.413897	1.540632	**H**	-4.142676	4.413908	-1.540378
H	2.414979	4.115735	1.301801	**H**	-2.415408	4.115541	-1.302657
H	3.431112	4.571268	-0.067929	**H**	-3.430581	4.571321	0.067707
C	2.43233	1.543172	-0.640312	**C**	-5.446636	2.014867	0.298859
C	1.526589	0.509464	-0.539277	**H**	-5.688857	0.982625	0.560532
C	0.557031	0.480939	-1.608474	**H**	-6.240142	2.386949	-0.356569
C	0.772502	1.462396	-2.533989	**H**	-5.476797	2.602794	1.220927
C	1.526534	-0.509242	0.539221	**C**	-5.446262	-2.01499	-0.298279
C	0.556902	-0.480568	1.608354	**H**	-5.689678	-0.982518	-0.557894
C	0.772305	-1.461982	2.533971	**H**	-6.239352	-2.389309	0.356382
H	0.19747	-1.668591	3.424623	**H**	-5.475742	-2.601136	-1.22151
C	2.43218	-1.543046	0.64039	**C**	-3.733299	-1.236544	2.169851
C	5.446594	-2.014379	0.297959	**H**	-4.028724	-0.192101	2.069321
H	6.239869	-2.385986	-0.358022	**H**	-2.737341	-1.252807	2.618519

H	5.477572	-2.602473	1.219891	**H**	-4.42446	-1.71957	2.868125
H	5.688517	-0.982082	0.559673	**C**	-3.404065	-3.985435	0.854551
C	3.404435	-3.985421	-0.854296	**H**	-4.141049	-4.414152	1.540723
H	4.141855	-4.414311	-1.539896	**H**	-2.414052	-4.11618	1.300454
H	2.414721	-4.116164	-1.30087	**H**	-3.431414	-4.571406	-0.068464
H	3.431106	-4.571254	0.068823	**S**	2.12046	2.458252	-2.103296
C	3.733227	-1.236429	-2.169759	**S**	2.120114	-2.457932	2.103391
H	4.42405	-1.719493	-2.868334	**S**	-2.120398	2.458153	2.103223
H	4.028969	-0.192081	-2.069109	**S**	-2.120018	-2.458137	-2.103355
H	2.737129	-1.252344	-2.618114	**H**	0.197776	1.66908	-3.4247
C	-0.557079	0.480851	1.608329	**H**	-0.197608	-1.668488	-3.424861

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