Supporting Information

C-H-activated Csp^2-Csp^3 diastereoselective gridization enables ultraviolet-emitting stereo-molecular nanohydrocarbons with mulitple H···H interactions

Wei et al.

Supplementary Methods

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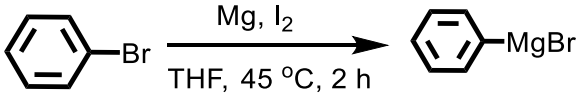
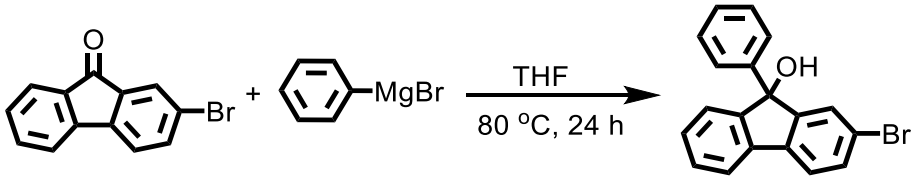
General Information

The progress of all reactions was monitored by thin-layer chromatography to ensure the reactions had reached completion. Gas chromatographic analyses were performed on Varian GC 2000 gas chromatography instrument with a FID detector and biphenyl was added as internal standard. Some products were purified via column chromatography over silica gel (200-300 mesh) (from Nanjing Wanqing Chemical Instruments Company) and a little of them were purified by recrystallization. All solvents were dried and distilled before use according to the standard methods. ^{1}H NMR and ^{13}C NMR spectra were recorded at 20 ºC on a Varian 400 MHz and 100 MHz, respectively. Chemical shifts are exhibited as δ in units of parts per million (ppm) relative to internal standard (^{1}H NMR: TMS = 0.00 ppm) or relative residual peaks (^{1}H NMR: 7.26 for $CDCl_3$; ^{13}C NMR: 77.0 triplet for $CDCl_3$). Multiplicities in briefly were shown as: s (singlet); d (doublet); t (triplet); dd (doublet of doublets); m (multiplet). Cycle preparation liquid chromatography (CPLC) were recorded on LaboACE LC-5060. High performance liquid chromatography (HPLC) were recorded on Agilent technologies. The Matrix-Assisted Laser Desorption/Ionization Time of Flight Mass Spectrometry (MALDI-ToF-MS, Bruker, reflective mode) and High Resolution Mass Spectroscopy HRMS (Bruker solanX 70 FT-MS) were used as the determination of molecular weight. UV absorption spectra were recorded on LAMBDA 35 spectrophotometer. Fluorescence emission spectra were recorded on RF-6000 Plus spectrophotometer. Single crystals were analyzed by single crystal X-ray diffraction. Photoluminescence quantum yields were recorded on Hamamatsu C9920-02G. Unless otherwise noted, materials were obtained from commercial suppliers and used without further purification.

Experimental Details and Characterization Data

Typical procedure for the preparation of 2-bromo-9-phenyl-9*H*-fluoren-9-ol from 2-bromo-9*H*-fluoren-9-one

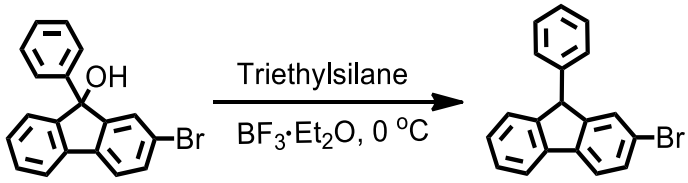




Put bromobenzene (0.236 mg, 1.5 mmol, 1.5 equiv), magnesium (0.036 mg, 1.5 mmol, 1.5 equiv), iodine (one pill) in tetrahydrofuran (2 ml) in a reaction flask. Then the reaction mixture was stirred at 50 ºC for 2 h. After that, dissolve 2-bromo-9*H*-fluoren-9-on (0.259 mg, 1 mmol) in tetrahydrofuran (8 ml) and transfer the reaction mixture to it. After reacting at 80 ºC for 24 h, the reaction was quenched with water and extracted with methylene chloride. The organic layers were then combined, dried (Na_2SO_4) and concentrated under reduced pressure. The residue was purified by flash column

chromatography on silica gel to obtain the pure product. The products 2-bromo-9-phenyl-9*H*-fluoren-9-ol were obtained in 89% yield. (White powders, 0.3 g, 0.89 mmol). The NMR spectral data match the previously published data.[1]

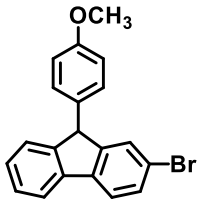
Typical procedure for the preparation of 2-bromo-9-phenyl-9-*H*-fluorene (**1a**) from 2-bromo-9-phenyl-9*H*-fluoren-9-ol



1a

Put 2-bromo-9-phenyl-9*H*-fluoren-9-ol (0.036 g, 1 mmol), triethylsilane (0.128 g, 1.1 mmol, 1.1 equiv), $BF_3{\cdot}Et_2O$ (0.426 g, 3 mmol, 3 equiv) in methylene chloride in a reaction flask. Then the reaction mixture was stirred at 0 °C for a while. Upon completion, the reaction was quenched with water and extracted with methylene chloride. The organic layers were then combined, dried (Na_2SO_4) and concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel to obtain the pure product. The product **1a** was obtained in 95% yield. (White powders, 0.304 g, 0.95 mmol). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.80 - 7.78 (d, *J* = 7.2 Hz, 1H), 7.68 - 7.66(d, *J* = 8.0 Hz, 1H), 7.54 - 7.52 (d, *J* = 7.6 Hz, 1H), 7.47 (s, 1H), 7.43-7.40 (t, *J* = 6.0 Hz, 1H), 7.32 - 7.30 (m, 5H), 7.11 - 7.09 (d, *J* = 6.8 Hz, 2H), 5.04 (s,1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.9, 147.6, 140.7, 140.0, 130.6, 128.9, 128.6, 128.4, 127.8, 127.6, 127.2, 125.5, 121.3, 121.1, 120.0, 54.4; m/z $(M)^+$ calcd for $C_{19}H_{13}Br$: 320.020, found: 320.000.

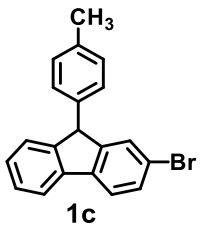
2-Bromo-9-(4-methoxyphenyl)-9H-fluorene (**1b**):



1b

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 - 7.76 (d, *J* = 7.8 Hz, 1H), 7.66 - 7.64 (d, *J* = 8.4 Hz, 1H), 7.51 - 7.49 (dd, *J* = 8.4 Hz, 1H), 7.44 (s, 1H), 7.41 - 7.37 (t, *J* = 6.8 Hz, 1H), 7.31 - 7.27 (m, 2H), 7.01 - 6.99 (d, *J* = 8.8 Hz, 2H), 6.84-6.82 (d, *J* = 8.4 Hz, 2H), 4.98 (s, 1H), 3.79 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.7, 150.3, 147.9, 139.9, 132.6. 130.4, 129.3, 128.5, 127.7, 125.4, 121.2, 121.0, 119.9, 114.3, 55.3, 53.6.

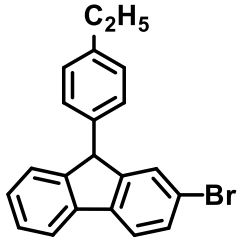
2-Bromo-9-(p-tolyl)-9H-fluorene (**1c**):



1c

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.79 - 7.77 (d, *J* = 7.6 Hz, 1H), 7.67 - 7.65 (d, *J* = 8 Hz, 1H), 7.52 - 7.50 (dd, *J* = 8 Hz, 1H), 7.46 (s, 1H), 7.42 - 7.38 (t, *J* = 6.8 Hz, 1H), 7.33 - 7.27 (m, 2H), 7.13 - 7.11 (d, *J* = 8 Hz, 2H), 6.99-6.97 (d, *J* = 8 Hz, 2H), 5.01 (s, 1H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.1, 147.8, 140.0, 137.6. 136.8, 130.5, 129.6, 128.6, 128.2, 127.8, 127.5, 127.3, 125.4, 121.2, 121.1, 119.9, 54.0, 21.2.

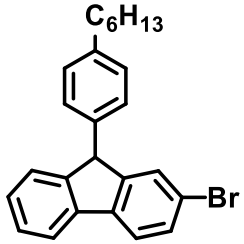
2-Bromo-9-(4-ethylphenyl)-9H-fluorene (**1d**):



1d

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.77 - 7.76 (d, *J* = 7.6 Hz, 1H), 7.65 - 7.63 (d, *J* = 8 Hz, 1H), 7.51 - 7.49 (d, *J* = 8 Hz, 1H), 7.46 (s, 1H), 7.40 - 7.37 (t, *J* = 8.4 Hz, 1H), 7.32 - 7.24 (m, 2H), 7.14 - 7.12 (d, *J* = 8 Hz, 2H), 7.00-6.98 (d, *J* = 8 Hz, 2H), 5.01 (s, 1H), 2.67-2.61 (m, 2H), 1.26-1.22 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 148.2, 145.9, 141.2, 138.1, 135.9, 126.7, 126.3, 125.8, 125.6, 123.5, 119.3, 119.2, 118.0, 52.2, 26.6, 13.6.

2-Bromo-9-(4-hexylphenyl)-9H-fluorene (**1e**):

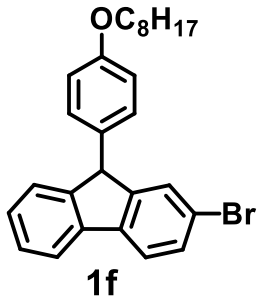


1e

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72- 7.70 (d, *J* = 7.6 Hz, 1H), 7.60 - 7.58 (d, *J* = 8 Hz,

1H), 7.46 - 7.44 (d, *J* = 9.2 Hz, 1H), 7.41 (s, 1H), 7.35 - 7.32 (t, *J* = 7.2 Hz, 1H), 7.23 - 7.19 (m, 2H), 7.07 - 7.05 (d, *J* = 8 Hz, 2H), 6.94-6.92 (d, *J* = 8 Hz, 2H), 4.96 (s, 1H), 2.56-2.52 (t, *J* = 7.6 Hz,2H), 1.60-1.52 (m, 2H), 1.28 (s, 6H),0.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 148.2, 145.9, 140.0, 138.1, 135.8, 128.6, 127.0, 126.7, 126.3, 125.8, 125.6, 123.6, 119.3, 119.2, 118.0, 52.2, 33.8, 29.9, 29.5, 27.3, 20.8, 12.3.

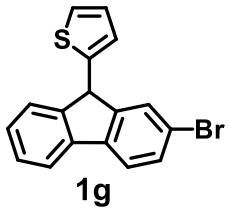
2-Bromo-9-(4-(octyloxy)phenyl)-9H-fluorene (**1f**):



1f

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.75- 7.73 (d, *J* = 7.2 Hz, 1H), 7.63 - 7.61 (d, *J* = 8 Hz, 1H), 7.48 - 7.46 (d, *J* = 8 Hz, 1H), 7.42 (s, 1H), 7.38 - 7.36 (t, *J* = 7.2 Hz, 1H), 7.29 - 7.23 (m, 2H), 6.97 – 6.95 (d, *J* = 8.4 Hz, 2H), 6.81-6.79 (d, *J* = 8.4 Hz, 2H), 4.95 (s, 1H), 3.92-3.89 (t, *J* = 12.8 Hz,2H), 1.79-1.72 (m, 2H), 1.52-1.28 (m, 10H),0.88 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.4, 150.3, 148.0, 139.9, 132.3, 130.4, 129.3, 128.6, 127.7, 127.5, 125.4, 121.2, 121.1, 119.9, 114.8, 68.0, 53.7, 31.9, 29.4, 29.3, 26.1, 22.7, 14.2.

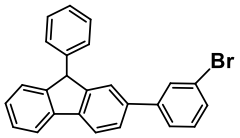
2-(2-Bromo-9H-fluoren-9-yl)thiophene (**1g**):



1g

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.44- 7.42 (d, *J* = 7.6 Hz, 1H), 7.32 - 7.30 (d, *J* = 8 Hz, 1H), 7.27 (s, 1H), 7.21 - 7.18 (d, *J* = 9.6 Hz, 1H), 7.15 - 7.13 (d, *J* = 9.6 Hz, 1H), 7.10 – 7.07 (m, 1H), 7.02-6.98 (m, 1H), 6.83-6.85 (m, 1H), 6.66-6.65 (m,2H), 5.00 (s, 1H), ^{13}C NMR (100 MHz, $CDCl_3$): δ 146.4, 144.2, 140.6, 137.2, 128.5, 126.2, 125.6, 125.5, 124.6, 123.2, 123.0, 122.2, 119.0, 118.8, 117.7, 46.6.

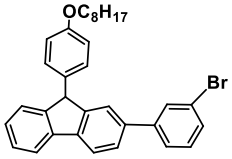
2-(3-Bromophenyl)-9-phenyl-9H-fluorene (**1h**)



1h

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85 - 7.80 (m, 2H), 7.70 (s, 1H), 7.58 - 7.56 (dd, *J* = 8 Hz, 1H), 7.53 - 7.51 (m, 2H), 7.48 - 7.43 (m, 2H), 738 - 7.26 (m, 6H), 7.18 - 7.16 (d, *J* = 8.4 Hz, 2H), 5.14 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 148.7, 148.3, 143.4, 141.3, 140.9, 138.9, 130.2, 130.1, 128.8, 128.4, 127.6, 127.5, 127.0, 126.6, 125.8, 122.9, 54.5.

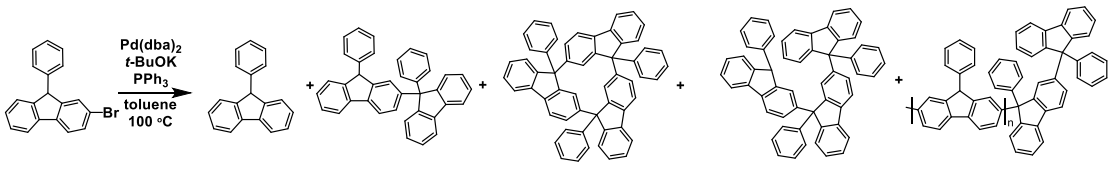
2-(3-bromophenyl)-9-(4-(octyloxy)phenyl)-9H-fluorene (**1i**)



1i

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.88 - 7.84 (t, *J* = 7.8 Hz, 2H), 7.78 (s, 1H), 7.62 - 7.60 (d, *J* = 8 Hz, 1H), 7.54 - 7.42 (m, 4H), 7.39 - 7.28 (m, 3H), 7.09 - 7.07 (d, *J* = 8 Hz, 2H), 6.88 - 6.86 (d, *J* = 8 Hz, 2H), 5.08 (s, 1H), 3.97 - 3.94 (t, *J* = 6.6 Hz, 2H), 1.84 - 1.77 (m, 2H), 1.51 - 1.47 (t, *J* = 7.4 Hz, 2H), 1.41 - 1.34 (m, 8H), 0.97 - 0.94 (t, *J* = 6.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.3, 149.1, 148.7, 143.5, 140.9, 140.4, 138.8, 133.2, 133.0, 130.3, 130.1, 129.4, 127.6, 127.4, 126.5, 125.8, 125.4, 124.0, 122.9, 120.3, 120.1, 114.8, 68.0, 53.9, 31.9, 29.5, 29.4, 26.2, 22.8, 14.3.

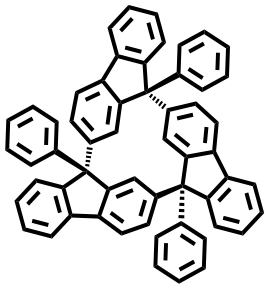
Typical procedure for the preparation of windmill gridarene of phenyl-fluorene from 2-bromo-9-phenyl-9*H*-fluorene



To a solution of 2-bromo-9-phenyl-9*H*-fluorene (**1a**) (0.32 g, 1 mmol), $Pd(dba)_2$ (0.040 g, 0.07 mmol, 0.07 equiv), PPh_3 (0.037 g, 0.14 mmol, 0.14 equiv) in dry toluene (25 ml) in a Schlenk tube, KO^{t}Bu (0.135 g, 1.2 mmol, 1.2 equiv) was added under argon atmosphere in a glove box. Then the reaction mixture was stirred at 100 °C for 56 h.

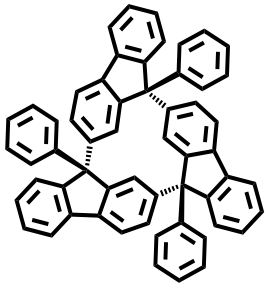
Upon completion, the reaction was quenched with water and extracted with methylene chloride. The organic layers were then combined, dried (Na_2SO_4) and concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel to obtain the pure product. The products **TWGs** were obtained in 32% yield (White powders, 0.077 g, 0.107 mmol). The product **2a** was obtained in 17% yield (White powders, 0.041 g, 0.17 mmol). The product **3a** was obtained in 10% yield (White powders, 0.024 g, 0.05 mmol). The product **4a** was obtained in 7% yield (White powders, 0.017 g, 0.023 mmol). The product **LPs1** was obtained in 33% yield.

***cis-trans*-TWG1**



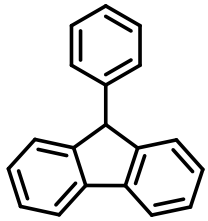
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.75 - 7.73 (d, *J* = 7.6 Hz, 2H), 7.66 - 7.64 (d, *J* = 7.2 Hz, 1H), 7.56 - 7.54 (d, *J* = 8.0 Hz, 4H), 7.49 - 7.46 (m, 3H), 7.41 - 7.35 (m, 5H), 7.31 - 7.27(m, 8H), 7.23 - 7.16 (m, 5H), 7.02- 6.95 (m, 3H), 6.69 - 6.65 (m, 4H), 6.01 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.4, 152.8, 151.5, 150.7, 149.9 (d, *J* = 6.2 Hz), 147.1, 146.4, 146.3, 145.2, 144.2, 141.6, 140.5, 140.4, 139.4, 138.1, 137.6, 130.6, 130.2, 129.6, 128.9, 128.8, 128.5, 128.2, 128.1, 128.0, 127.9,127.8, 127.7 (overlapping), 127.6, 127.4, 127.3, 127.0, 126.9, 126.8, 126.4 (d, *J* = 3.6 Hz), 126.2, 123.8, 120.7, 120.5, 120.4, 119.8, 119.4, 119.3, 67.4, 65.4, 65.3; HRMS (MOLDI-TOF): m/z calcd for $[M+Na]^+$ $C_{57}H_{36}Na^+$: 720.3, found: 720.5.

***cis-cis*-TWG1**



^{1}H NMR (400 MHz, $CDCl_3$): δ8.19 (s, 3H), 7.60 - 7.58 (d, *J* = 8.4 Hz, 3H), 7.39 - 7.37 (d, *J* = 7.6 Hz, 6H), 7.34 - 7.28 (m, 13H), 7.24 - 7.22 (m, 5H), 7.15 - 7.12 (d, *J* = 7.6 Hz, 6H), 6.60 - 6.57 (d, *J* = 9.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ153.9, 149.4, 146.1, 144.2, 139.6, 138.2, 129.9, 128.7, 128.5, 127.6, 127.2, 127.0, 126.7, 124.5, 120.5, 118.0, 66.8; MALDI-TOF-MS: m/z calcd for [M+] $C_{57}H_{36}$: 720.3; Found: 720.1.

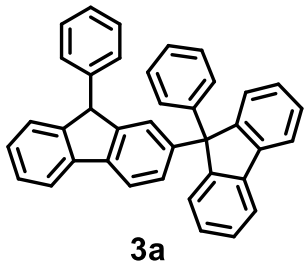
9-Phenyl-fluorene (**2a)**:



2a

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.80 - 7.78 (d, *J* = 7.6 Hz, 2H), 7.39 - 7.35 (t, *J* = 7.2 Hz, 2H), 7.32- 7.30 (d, *J* = 7.2 Hz, 2H), 7.27 - 7.26 (m, 2H), 7.24 - 7.21 (m, 3H), 7.09 - 7.07 (d, *J* = 8.0 Hz, 2H), 5.00 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 147.9, 141.6, 141.0, 128.7, 128.4, 127.4, 126.9, 125.4, 119.9, 54.5; m/z $(M)^+$ calcd for $C_{19}H_{14}$: 242.110; found, 242.000.[2]

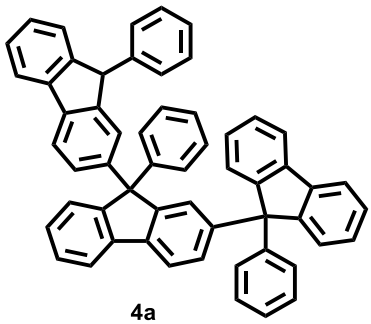
9-9'-Diphenyl-9*H*,9'*H*-2,9'-bifluorene (**3a)**:



3a

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81 - 7.79 (d, *J* = 7.6 Hz, 2H), 7.76 - 7.74 (d, *J* = 7.6 Hz, 1H), 7.64 - 7.62 (d, *J* = 8.0 Hz, 1H), 7.44 - 7.42 (d, *J* = 7.6 Hz, 1H), 7.40 - 7.33 (m, 6H), 7.30 - 7.25 (m, 6H), 7.20 - 7.16 (m, 6H), 7.09 - 7.07 (dd, *J* = 8.0 Hz, 2.0 Hz, 2H), 5.05 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.3 (d, J = 7.9 Hz), 148.0, 147.7, 146.3, 145.2, 141.6, 140.5, 140.2 (d, *J* = 5.3 Hz), 140.0, 128.6, 128.3, 128.1, 127.8, 127.5, 127.3, 127.2, 127.1, 126.8, 126.7,126.2, 125.9, 125.2, 120.3, 119.9, 119.5, 65.8, 54.3; m/z $(M)^+$ calcd for $C_{38}H_{26}$: 482.203, found: 482.321.

9,9',9''-Triphenyl-9*H*,9'*H*,9''*H*-2,9':2',9''-terfluorene (**Trimerized product, 4a)**:

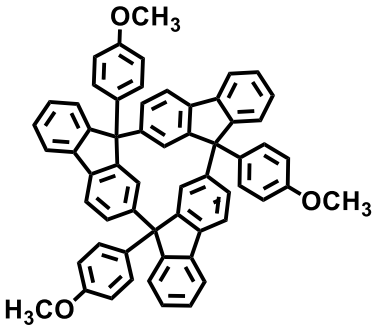


4a

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 (3H), 7.70- 7.65 (m, 1H), 7.63- 7.57 (m, 1H), 7.53 - 7.52 (d, J = 6.4Hz, 2H), 7.36- 7.24 (m, 13H), 7.21 - 7.16 (m, 8H), 7.12 - 7.11 (4H), 7.06 - 7.05 (d, J = 6.8 Hz, 3H), 7.02 - 6.96 (m, 2H); 4.98 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.3, 151.2, 151.1, 148.1, 147.9, 147.7, 147.4, 146.1, 145.9, 145.5, 145.3, 145.2, 141.6, 141.2, 140.4, 140.2, 140.1, 139.9, 139.8, 138.7, 138.6, 128.7,128.6, 128.2,128.1, 128.0, 127.8, 127.7, 127.5, 127.4, 127.3, 127.2,126.9, 126.8, 126.7, 126.6,

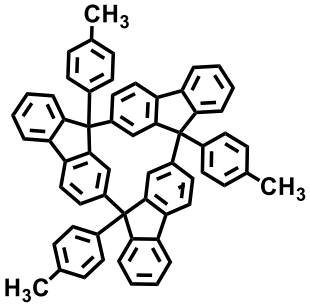
126.5, 126.2,126.1, 125.7, 125.3, 125.2, 125.1, 120.2, 119.8 (d, *J* = 3.1 Hz), 119.5, 119.4,65.8, 65.7, 54.3; MALDI-TOF-MS: m/z calcd for [M+] $C_{57}H_{38}$: 722.30; Found: 721.95.

TWG2



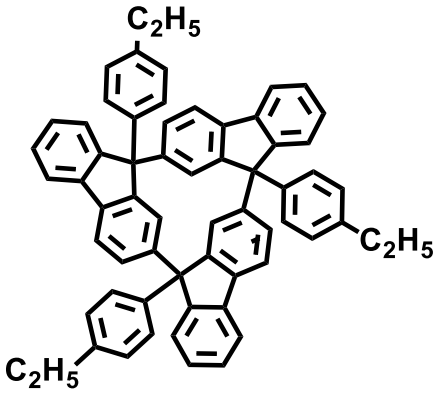
^{1}H NMR (400 MHz, $CDCl_3$): δ7.78 - 7.75 (m, 2H), 7.68 - 7.66 (d, *J* = 7.6 Hz, 1H), 7.60 - 7.56 (m, 4H), 7.50 - 7.48 (d, *J* = 7.6 Hz, 1H), 7.46 - 7.40 (m, 4H), 7.38 - 7.30 (m, 6H), 7.28 - 7.22 (m, 4H), 6.88 – 6.85 (d, *J* = 8.8 Hz, 2H), 6.75 – 6.73 (d, *J* = 8.8 Hz, 2H), 6.96 – 6.63 (m, 4H), 6.55 – 6.53 (d, *J* = 8.8 Hz, 2H), 6.01 (s, 1H), 3.83 (s, 3H), 3.75 (s, 3H), 3.65 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ158.5, 158.1, 157.7, 153.3, 152.7, 151.0, 150.2, 147.3, 146.6, 140.5, 140.3, 140.2, 139.3, 138.0, 137.4, 137.2, 136.2, 130.5, 130.1, 130.0, 129.5, 129.3, 128.8, 128.7, 127.7, 127.6, 127.3, 126.9, 126.3, 126.2, 120.6, 120.5, 120.4, 119.7, 119.3, 113.9, 113.5, 113.3, 31.6, 22.7, 14.6. MALDI-TOF-MS: m/z calcd for [M+] $C_{60}H_{42}O_3$: 810.00; Found: 810.30.

TWG3



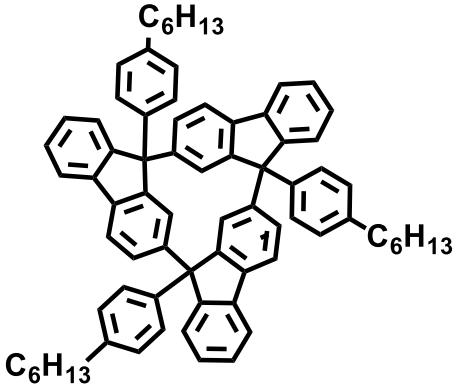
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.17 (s, 3H), 7.74 - 7.72 (d, *J* = 7.6 Hz, 2H), 7.65 - 7.63 (d, *J* = 8.4 Hz, 1H), 7.60 - 7.58 (d, *J* = 6.8 Hz, 1H), 7.56 - 7.52 (m, 3H), 7.46 - 7.44 (d, *J* = 7.2 Hz, 1H), 7.39 - 7.37 (d, *J* = 8.0 Hz, 3H), 7.35 - 7.33 (d, *J* = 7.6 Hz, 3H), 7.31 - 7.28 (m, 5H), 7.23 - 7.18 (m, 4H), 7.11 - 7.09 (d, *J* = 8.0 Hz, 3H), 7.00 - 6.98 (d, *J* = 8.0 Hz, 2H), 6.79 - 6.77 (d, *J* = 7.6 Hz, 2H), 6.67 - 6.63 (m, 1H), 6.58 - 6.56 (d, *J* = 8.0 Hz, 1H), 6.00 (s, 1H), 2.28 – 2.35 (m, 9H);^{13}C NMR (100 MHz, $CDCl_3$): δ157.6, 154.1, 153.1, 151.7, 150.9, 150.2, 150.1, 147.0, 146.6, 146.3, 142.2, 141.2, 140.5, 140.4,140.2,139.6, 139.4, 138.5, 138.1, 137.5, 136.5, 136.3, 136.0,130.6, 130.2,129.9, 129.6, 129.4, 129.2, 128.8, 128.7, 128.4, 128.1, 127.8, 127.7, 127.6, 127.5, 127.2, 127.0, 126.6, 126.3, 126.2, 123.7, 120.6, 120.5, 120.3, 120.1, 119.7, 119.2, 117.9, 29.7, 21.0. MALDI-TOF-MS: m/z calcd for [M+] $C_{60}H_{42}$: 762.32; Found: 762.13.

TWG4



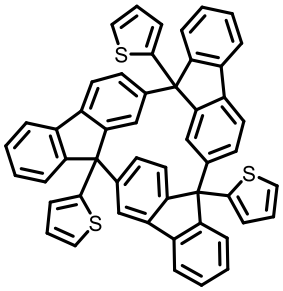
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.21 (s, 3H), 7.73 - 7.71 (d, *J* = 7.2 Hz, 2H), 7.64 - 7.62 (d, *J* = 6.8 Hz, 1H), 7.58 - 7.52 (m, 4H), 7.46 - 7.44 (m, *J* = 8.0 Hz, 1H), 7.40 - 7.34 (m, 6H), 7.31 - 7.28 (m, 4H), 7.21 - 7.19 (m, 4H), 7.11 - 7.09 (d, *J* = 7.2 Hz, 2H), 7.00 – 6.988 (d, *J* = 7.6 Hz, 2H), 6.80 – 6.78 (d, *J* = 7.6 Hz, 2H), 6.67 (s, 1H), 6.00 (s, 1H), 3.65 - 3.59 (m, 8H), 2.66 -2.54 (m, 5H), 2.47 -2.41 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ157.5, 153.1, 151.7, 150.9, 150.2, 147.2, 146.6, 146.4, 142.8, 142.5, 142.4, 142.2, 141.3, 140.5, 10.4, 140.3, 139.4, 138.7, 138.1, 137.5, 130.7, 130.2, 129.6, 128.9, 128.8, 128.1, 127.9, 127.7, 127.6, 127.5, 127.4, 127.2, 127.0, 126.4, 126.3, 123.7, 120.6, 120.5, 120.3, 119.7, 119.2, 119.2, 28.4, 28.1, 15.5, 15.3, 15.2. MALDI-TOF-MS: m/z calcd for [M+] $C_{63}H_{48}$: 804.38; Found: 804.02.

TWG5



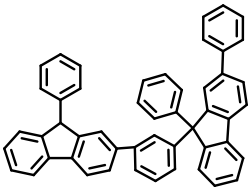
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.74 - 7.72 (m, 2H), 7.65 - 7.63 (d, *J* = 7.2 Hz, 1H), 7.54 (s, 4H), 7.47 - 7.45 (d, *J* = 7.2 Hz, 1H), 7.41 - 7.34 (m, 6H), 7.30 - 7.28 (m, 4H), 7.22 - 7.18 (m, 4H), 7.08 - 7.06 (d, *J* = 8.0 Hz, 2H), 6.98 - 6.96 (d, *J* = 7.6 Hz, 2H), 6.78 - 6.76 (d, *J* = 8.0 Hz, 2H), 6.68 (s, 1H), 6.64 - 6.56 (m, 2H), 6.00 (s, 1H), 2.60 -2.50 (m, 4H), 2.40 -2.37 (m, 2H), 1.62 -1.55 (m, 7H), 1.32 - (m, 26H); ^{13}C NMR (100 MHz, $CDCl_3$): δ156.5, 149.1, 145.5, 140.3, 139.9, 139.3, 129.7, 129.2, 128.6, 127.8, 127.4, 127.0, 126.9, 126.8, 126.6, 126.5, 126.4, 126.2, 126.1, 126.0, 125.4, 125.3, 122.6, 119.5, 119.4, 119.3, 118.6, 118.2, 118.1, 66.1, 64.1, 64.0 ,34.5, 34.3, 30.7, 30.6, 30.3, 30.2, 30.1, 28.7, 28.1, 28.0, 21.6, 21.5, 13.1, 13.0. MALDI-TOF-MS: m/z calcd for [M+] $C_{75}H_{72}$: 972.16; Found: 972.55.

TWG7



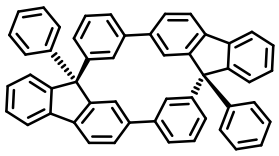
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.51 (s, 1H) 7.74 -7.71 (m, 2H), 7.65 – 7.59 (m, 4H), 7.54 -7.52 (d, *J* = 8.0 Hz, 1H), 7.48 (m,1H), 7.42 - 7.39 (m, 3H), 7.35 - 7.30 (m, 4H), 7.25 - 7.23 (m, 3H), 7.15 -7.11 (d, *J* = 9.2 Hz, 2H), 7.09 - 7.06 (m, 1H), 7.00 - 6.98 (m, 1H), 6.93 -6.91 (d, *J* = 8.0 Hz, 1H), 6.87-6.85 (d, *J* = 7.2 Hz 1H), 6.67 (s, 1H), 6.60-6.56 (m, 2H), 6.45 (s, 1H), 6.00 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ156.1, 151.3, 150.3, 149.0, 147.8, 146.5, 145.9, 145.2, 144.8, 144.1, 138.9, 138.8, 138.7, 138.5, 136.1, 129.3, 128.7, 128.5, 127.6, 127.3, 127.1, 127.0, 126.8, 126.6, 126.5, 126.4, 126.3, 126.1, 125.7, 125.4, 125.2, 125.1, 124.7, 124.1, 124.0, 123.9, 123.3, 123.1, 122.2, 119.7, 119.6, 119.4, 118.7, 118.5. MALDI-TOF-MS: m/z calcd for [M+] $C_{51}H_{30}S_3$: 738.16; Found: 738.46.

3h



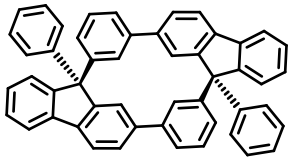
^{1}H NMR (400 MHz, $CDCl_3$): δ ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.11 -8.09 (d, *J* = 7.2, 2H), 7.89 - 7.87 (d, *J* = 8.0, 1H), 7.85 -7.81 (t, *J* = 7.2, 3H), 7.69 -7.68 (d, *J* = 9.6, 1H), 7.58 - 7.56 (d, *J* = 8.8, 4H), 7.50 (s, 1H), 7.48 -7.46 (d, *J* = 7.6, 2H), 7.44 - 7.42 (m, 1H), 7.41 - 7.37 (m, 2H), 7.34 (s, 1H), 7.32 -7.31 (m, 2H), 7.29 - 7.21 (m, 6H), 7.27 - 7.19 (m, 5H), 7.14 -7.13 (d, *J* = 6.4, 2H), 4.68 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ147.6, 147.2, 139.6, 139.4, 128.1, 127.7, 127.4, 126.4, 125.9, 125.7, 125.2, 124.4, 123.2, 119.2, 119.0, 53.5, 30.9, 30.4, 29.3, 28.7, 21.7, 13.1. (MALDI-TOF): m/z calcd for $[M+Na]^+$ $C_{57}H_{36}Na^+$: 634.6, found: 634.3.

***meso*-DWG1**



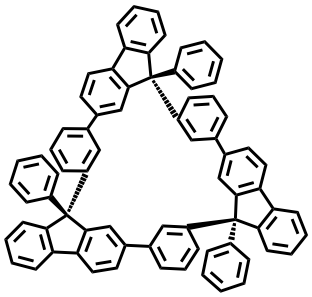
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.82 - 7.76 (m, 4H), 7.78 (s, 2H), 7.65 -7.54 (d, *J* = 7.2, 2H), 7.56 -7.54 (d, *J* = 7.6, 2H), 7.48 - 7.41 (m, 4H), 7.39 - 7.34 (m, 6H),7.25 (s,*2*H),7.16 - 7.12 (m, 6H), 7.06 - 7.04(m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ151.0, 145.7, 139.1, 134.1, 129.4, 128.3, 127.9, 127.7, 126.7, 126.6, 126.2, 125.8, 123.5, 120.4, 119.9. (MALDI-TOF): m/z calcd for $[M+Na]^+$ $C_{57}H_{36}Na^+$: 632.0, found: 632.2.

***rac*-DWG1**



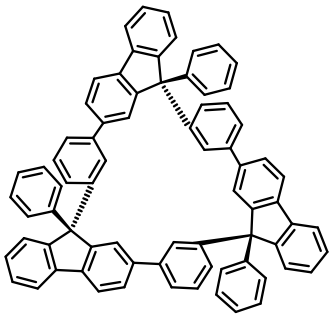
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81 - 7.74 (m, 7H),7.71 -7,69 (d, *J* = 6.8, 4H), 7.53 - 7.45 (m, 4H), 7.44 - 7.32 (m, 7H), 7.19 - 7.17 (d, *J* = 4.8, 6H),7.02 -7.00 (d, *J* = 8, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ150.8, 149.9, 146.4, 142.4, 142.1, 140.7, 139.0, 128.9, 128.6, 128.3, 127.9, 127.8, 127.0, 1266.6, 126.1, 123.7, 120.2, 119.9. (MALDI-TOF): m/z calcd for $[M+Na]^+$ $C_{57}H_{36}Na^+$: 632.1, found: 632.2.

***cis-trans*-TWG8**



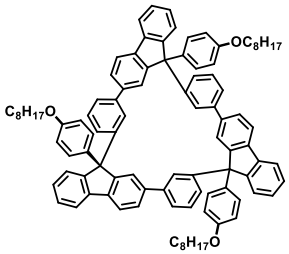
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81 - 7.74 (m, 5H),7.70 -7,69 (d, *J* = 7.6, 1H), 7.62 - 7.60 (d, *J* = 6.0, 2H), 7.47 - 7.41 (m, 2H), 7.38 - 7.33 (m, 9H),7.31 -7.27 (m, 8H), 7.23 - 7.20 (m, 8H),7.18 -7.14 (m, 9H), 7.02 - 7.00 (d, *J* = 8.8, 1H),6.89 – 6.86 (d, *J* = 9.6,1H), 6.65 - 6.63 (d, *J* = 8.8, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ155.3, 152.2, 151.8, 151.4, 147.1, 146.9, 146.2, 145.2, 144.1, 142.2, 141.8, 141.6, 141.4, 140.0, 139.9, 139.3, 133.4, 128.4, 128.3, 128.1, 127.8, 127.0, 126.8, 126.5, 124.8, 120.3. (MALDI-TOF): m/z calcd for $[M+Na]^+$ $C_{57}H_{36}Na^+$: 948.0, found: 948.4.

***cis-cis*-TWG8**



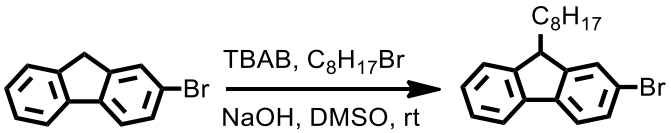
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.75 - 7.73 (d, *J* = 7.6, 3H), 7.71 -7,69 (d, *J* = 8, 2H), 7.46 -7.44 (d, *J* = 7.2, 3H), 7.39 - 7.37 (d, *J* = 6.4, 3H), 7.36 - 7.34 (t, *J* = 7.6, 6H),7.31 -7.30 (t, *J* = 6.8, 10H), 7.27 - 7.25 (d, *J* = 8.4, 4H),7.22 -7.20 (d, *J* = 6.8, 5H), 7.12 (s, 3H), 7.09 - 7.05 (m, 4H), 7.02 (s, 2H), 6.92 - 6.90 (d, *J* = 8.0, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ151.6, 146.4, 145.0, 142.5, 141.8, 139.9, 139.1, 128.3, 128.1, 127.7, 127.5, 127.4, 126.7, 126.1, 126.0, 125.8, 125.4, 120.2, 120.1. (MALDI-TOF): m/z calcd for $[M+Na]^+$ $C_{57}H_{36}Na^+$: 948.1, found: 948.4.

TWG9



^{1}H NMR (400 MHz, $CDCl_3$): δ 7.82 - 7.80 (d, *J* = 8 Hz, 2H), 7.77 - 7.65 (m, 16H), 7.45 - 7.28 (m, 29H), 7.25 - 7.03 (m, 39H), 6.97 (S, 1H), 6.92 (s, 1H), 6.85- 6.80 (m, 8H), 6.70- 6.65 (m, 8H), 6.64 - 6.62 (d, *J* = 8 Hz, 2H), 3.99 - 3.79 (m, 15H), 1.83-1.76 (m, 15H), 1.52-1.43 (m, 15H), 1.38-1.26 (m, 61H), 0.91-0.83 (m, 22H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.2, 158.0, 157.9, 157.7, 152.8, 152.6, 152.1, 151.9, 151.8, 147.4, 147.2, 146.4, 142.2, 141.8, 141.7, 141.6, 141.4, 139.9, 139.8, 139.8, 139.8, 139.6, 139.2, 139.2, 139.0, 138.9, 136.7, 135.9, 135.4, 129.3, 129.2, 128.5, 128.4, 128.1, 128.1, 127.8, 127.7, 127.6, 127.4, 127.3, 127.1, 126.8, 126.7, 126.4, 126.0, 125.9, 125.5, 125.4, 125.2, 124.7, 124.6, 120.2, 120.1, 120.0, 114.2, 114.1, 114.1, 68.0, 67.9, 65.0, 64.9, 64.4, 31.9, 31.9, 31.8, 31.8, 29.7, 29.5, 29.5, 29.5, 29.4, 29.4, 29.4, 29.3, 29.3, 26.2, 26.2, 26.1, 22.7, 22.7, 22.7, 14.1. MALDI-TOF-MS (m/z): calcd. For $C_{99}H_{96}O_3$: 1333.739 [M+]; Found: 1334.104.

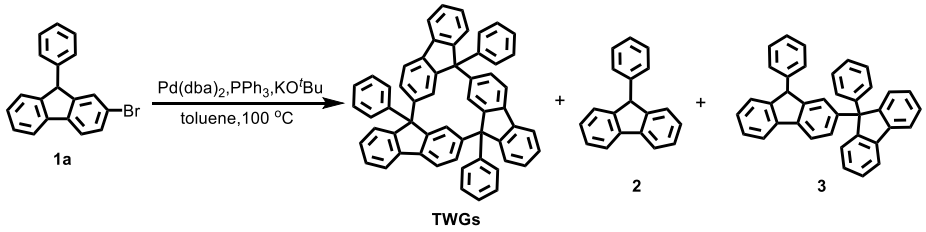
Procedure for the preparation of 2-bromo-9-octyl-9*H*-fluorene from 2-bromo-9*H*-fluorene.



In a dried reaction flask (150 mL), add 2-Bromo-9*H*-fluorene (0.244 g, 1 mmol) and tetrabutylammonium bromide (TBAB) (0.005 g, 0.016 mmol), evacuate and fill with nitrogen three times. Then inject 1-bromooctane (0.173 g, 0.9 mmol, 0.9 equiv) and DMSO (20 ml) into the reaction flask with a syringe and stir well, finally add sodium hydroxide solution (0.036 g, 0.9 mmol, 0.9 equiv) slowly. The mixture was stirred at room temperature for 5 hours. Upon completion, the reaction was quenched with water and extracted with methylene chloride. The organic layers were then combined, dried (Na_2SO_4) and concentrated under reduced pressure.[3] The residue was purified by flash column chromatography on silica gel to obtain the pure product. The product 2-bromo-9-octyl-9-H-fluorene was obtained in 50% yield. (White liquid, 0.178 g, 0.5 mmol). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78-7.71 (d, *J* = 6.8 Hz, 1H), 7.69-7.65 (s, 1H), 7.65-7.60 (d, *J* = 8.0 Hz, 1H), 7.56-7.48 (t, *J* = 8.0 Hz, 2H), 7.43-7.32 (m, 2H), 4.02-3.95 (t, *J* = 5.6 Hz, 1H), 2.09-1.92 (m, 2H), 1.36-1.13 (m, 12H), 0.96-0.84 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.8, 147.3, 140.2, 130.0, 127.6, 127.2, 127.1, 124.4, 121.1, 119.9, 47.6, 32.9, 31.9, 29.9,29.3, 25.6, 22.7, 14.1; m/z $(M)^+$ calcd for $C_{21}H_{25}Br$: 356.114; found, 356.000.

Section 1. Characteristics of C-H gridization

Supplementary Table 1 | Optimization studies for Pd-PPh$_3$-controlled reaction of 2-bromo-9-aryl-9*H*-fluorenes[a].

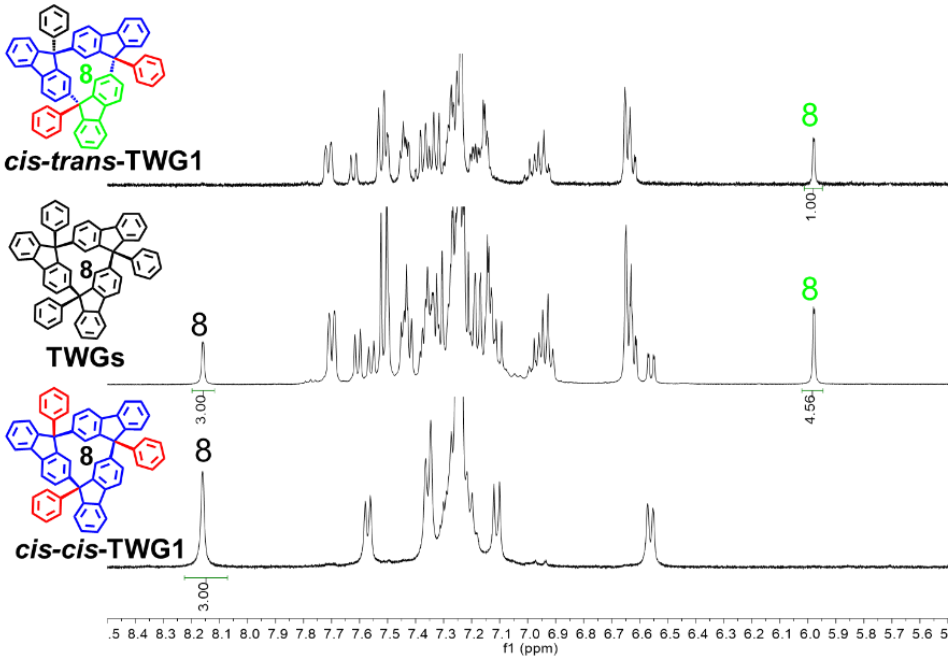


Entry	**1**	Ligand	Base	Conc. (mM)	Yield[b] (%)	*Dr*[e] *cis-trans/cis-cis*
1	**1a**	PPh_3	KO^{t}Bu	0.4	51[c] 49[d]	-
2	**1a**	PPh_3	KO^{t}Bu	10	10	-
3	**1a**	PPh_3	KO^{t}Bu	20	22	-
4	**1a**	PPh_3	KO^{t}Bu	60	20	-
5	**1a**	PPh_3	KO^{t}Bu	80	0	-
6	**1a**	PPh_3	KO^{t}Bu	100	0	-
7	**1a**	PPh_3	KO^{t}Bu	30	32	77:23
8	**1a**	PPh_3	KO^{t}Bu	40	35	80:20
9	**1a**	PPh_3	KO^{t}Bu	50	30	74:26
10	**1a**	Dppf	KO^{t}Bu	40	0	-
11	**1a**	PCy_3	KO^{t}Bu	40	0	-
12	**1a**	P^{t}Bu$_3$	KO^{t}Bu	40	0	-
13	**1b**[f]	PPh_3	KO^{t}Bu	40	0	-
14	**1a**	PPh_3	$KN(SiMe_3)_2$	40	33	76:24
15	**1a**	PPh3	KOH	40	0	-

[a] Conditions: **1** (0.1 mmol), $Pd(dba)_2$ (0.07 equiv), ligand (0.14 equiv), base (1.2 equiv), dry toluene, 100 °C, 56 h. [b] Yield of **TWGs** (mixed diastereoisomers). [c] Yield of debromination product **2**. [d] Yield of dimerization product **3**. [e] *Dr* ratio determined by ^{1}H NMR. [f] **1b** is 2-bromo-9-octyl-9*H*-fluorene.

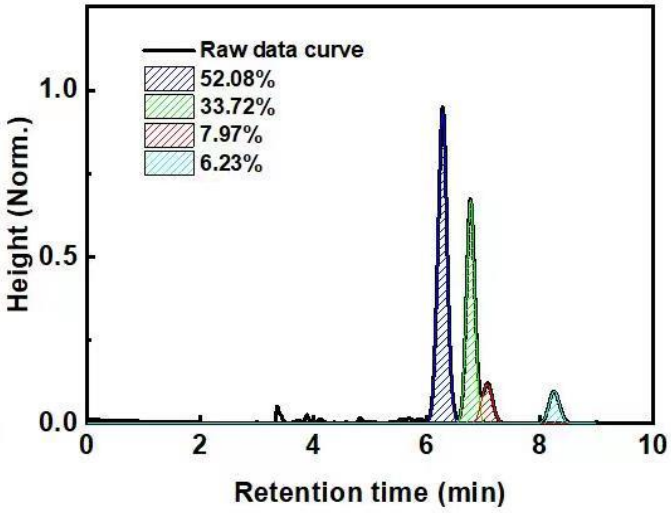
The stereoselectivity of TWGs was confirmed by the following two methods: First, TWGs was formed with 82:18 *cis-trans*-TWG1/*cis-cis*-TWG1 selectivity, determined

by ^{1}H NMR (Supplementary Fig.3). According to ^{1}H NMR spectrums of *cis-trans*-TWG1 and *cis-cis*-TWG1 in supplementary Figure 2. In the ^{1}H NMR spectrums of *cis-trans*-TWG1, a singlet peak at 6.00 ppm correspond to one hydrogen and belong to proton 8. Furthermore, in the ^{1}H NMR spectrums of *cis-cis*-TWG1, proton 8 resonated as a single at 8.19 ppm integrating for three hydrogens. Compared to ^{1}H NMR spectrums of *cis-trans*-TWG1, TWGs, and *cis-cis*-TWG1 in Supplementary Fig.3, the single peaks at 6.00 ppm and 8.19 ppm in ^{1}H NMR spectrums of TWGs are characteristic peaks at proton 8 of *cis-trans*-TWG1 and *cis-cis*-TWG1, respectively. In ^{1}H NMR spectrum of TWGs, when the integral of single at 8.19 ppm is 3 hydrogens, the integral of single at 6.00 ppm is 4.56 hydrogens, so the ratio of *cis-trans*-TWG1 and *cis-cis*-TWG1 existing in TWGs calculated from ^{1}H NMR of TWGs is 4.56/1:3/3=4.56:1. Then, *cis-trans*-TWG1 selectivity was calculated as 4.56/ (1+4.56) =0.82 and *cis-cis*-TWG1 selectivity was calculated as 1/ (1+4.56) =0.18. Hence, TWGs was formed with 82:18 *cis-trans*-TWG1/*cis-cis*-TWG1 selectivity.



Supplementary Fig. 1 | ^{1}H NMR spectra of *cis-trans*-TWG1, TWGs and *cis-cis*-TWG1.

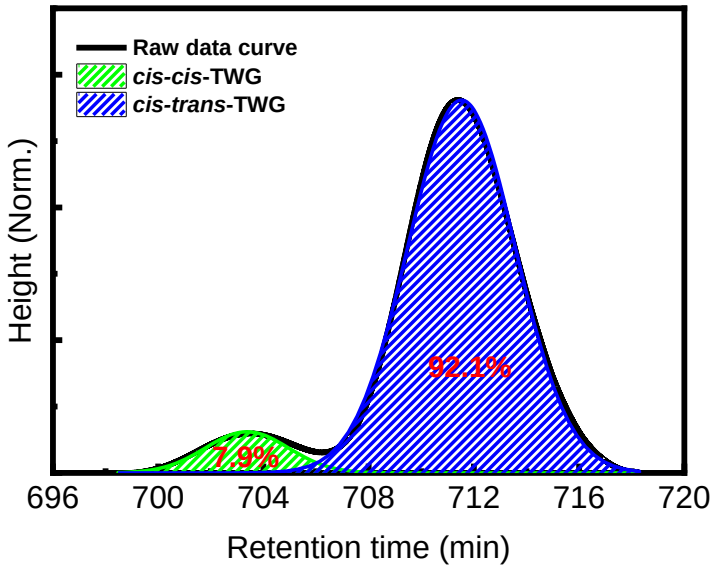
Second, TWGs was formed with 87:13 *cis-trans*-TWG1/*cis-cis*-TWG1 selectivity, determined by chiral HPLC. In the chiral HPLC spectrum of TWGs, it is clearly that TWGs was composed of (52.269+34.532): (6.347+6.652) = 87: 13 *cis-trans*-TWG1/*cis-cis*-TWG1 selectivity. The selectivity is almost identical to that obtained by ^{1}H NMR. In addition, two enantiomers of *cis-trans*-TWG1 have some enantioselectivity (52.269% and 34.532%, respectively), while the content of two enantiomers of *cis-cis*-TWG1 is basically the same (6.347% and 6.852%, respectively).



Supplementary Fig. 2 | Chiral HPLC chromatogram of TWGs.

Supplementary Table 2 | Separation method of TWGs in HPLC.

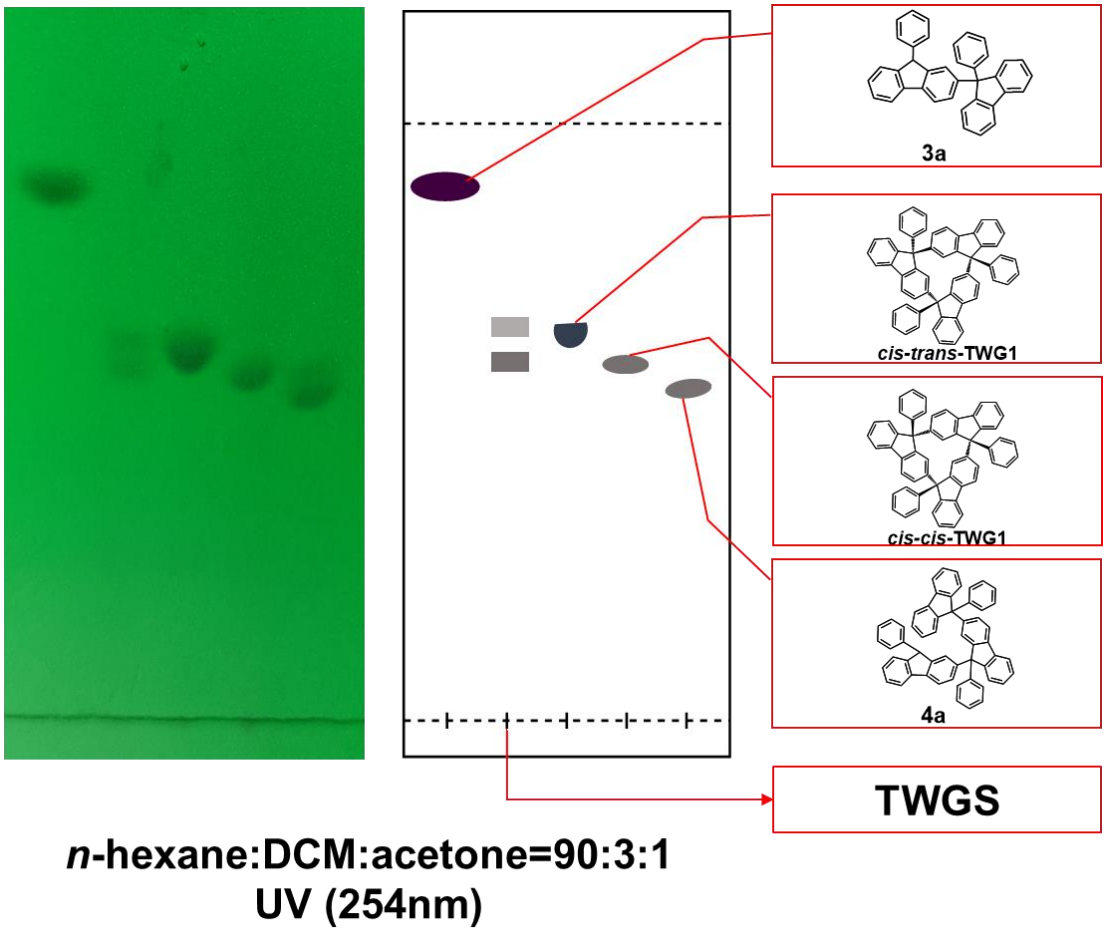
Column	CHIRALPAK IG IG00CE-UC054
Column size	0.46 cm I.D. × 25 cm L
Injection	2 ul
Mobile phase	dichloromethane / methanol =20/80(V/V)
Flow rate	1.0 ml/min
Wave length	UV 254 nm
Temperature	room temperature
Sample name	mixture
Solution	1 mg/ml in dichloromethane



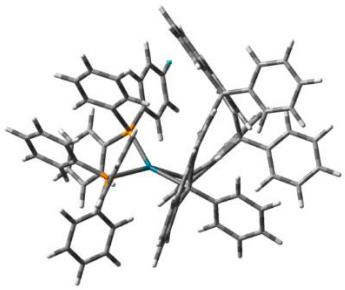
Supplementary Fig. 3 | The CPLC spectrum of TWGs, the peak area ratio of *cis-*

***cis*-TWG1 to *cis-trans*-TWG1 is 7.9% : 92.1%.** The mother liquor of recrystallization was processed by cycle preparation liquid chromatography (CPLC) using dichloromethane as the mobile phase. In the CPLC, *cis-cis*-TWG1 (shaded in green) and *cis-trans*-TWG1 (shaded in blue) were successfully separated and prepared when the retention time reaches 700 min.

Section 2. Theoretical calculation datas of TWG-TS1 and TWG-TS2



Supplementary Fig. 4 | The thin layer chromatography (TLC) of TWGs.
First, TWGs was purified by column chromatography. [Silica gel, eluent is petroleum: DCM=8:1]. Second, *cis-trans*-TWG1 was prepared by Recrystallizing TWGs with dichloromethane, and then repeatedly wash the recrystallized sample with n-hexane (5-8 times).



TWG-TS1

Energy： -4393.01061931

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C	0.59197100	-2.26677000	3.31124200
C	0.11131700	-2.61242200	4.57802700
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C	1.06180900	-4.11842600	-0.10076400
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C	1.34443300	2.22919500	1.63811200
C	1.92115100	2.61035900	0.41905500
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C	3.25085600	4.80777900	0.84506800
C	4.15333600	5.71355300	0.28253900
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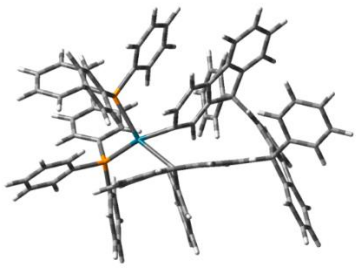

TWG-TS2

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Structure：

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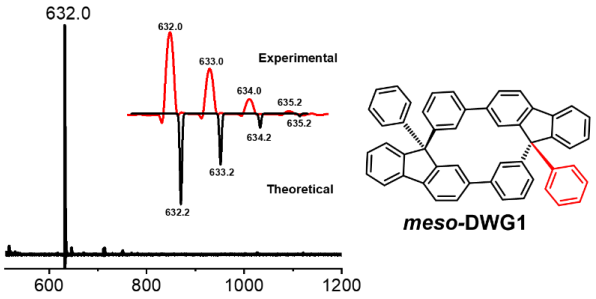
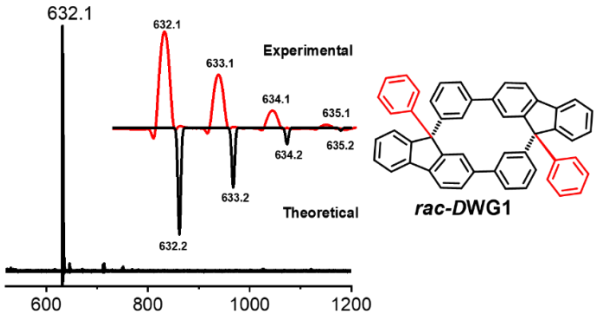
C	5.52006200	-4.32742500	1.66491600
C	6.27892300	-4.39305400	2.83437400
C	5.90591300	-3.61744300	3.93227700

C	4.78495500	-2.78788300	3.86373700
H	1.55978700	-4.26612600	2.73218300
H	-0.19871000	-5.18172900	1.27083900
H	1.47311100	-0.60324200	0.53737600
H	-1.90110100	-5.76205100	-0.62927300
H	-3.29024400	-5.94124200	-2.68310800
H	-3.26665800	-4.11523300	-4.36420900
H	-1.83612200	-2.13246100	-4.04778300
H	2.21628900	-3.43518300	-1.44528500
H	3.83197500	-4.19935800	-3.12779700
H	3.65967600	-3.42238600	-5.48944800
H	1.84743300	-1.82349400	-6.11239900
H	0.26582600	-1.01846900	-4.41462900
H	-0.92544700	1.30107100	-3.28485400
H	0.57699200	3.16859800	-3.75906700
H	2.22492400	-0.62470600	-1.09536100
H	2.51469000	5.08311700	-3.66088000
H	4.49217800	6.51347200	-3.19533100
H	6.33971700	5.67363500	-1.77104800
H	6.24812700	3.38442100	-0.81498000
H	3.97864500	0.13827600	-3.65990700
H	5.76218100	-1.15626900	-4.75200900
H	7.96912700	-1.45561000	-3.63297800
H	8.34510200	-0.44706700	-1.38510400
H	6.54950200	0.83579100	-0.28611800
H	-6.65647200	-1.05199100	-1.16493700
H	-7.78920700	-0.95437800	-3.35219100
H	-6.49712600	-0.41930300	-5.40986900
H	-4.04959500	0.00205400	-5.25314400
H	-2.90762500	-0.14009100	-3.04878600
H	-5.28067100	1.83194400	-0.70254600
H	-6.94899300	3.04417900	0.62077100
H	-7.72018300	2.13573600	2.81257900
H	-6.75552900	-0.00128200	3.65403900
H	-5.07394800	-1.20977900	2.34064300
H	-2.45834400	-2.02157100	1.81737700
H	-2.74404800	-4.19421200	2.94884100
H	-4.41166700	-5.83956600	2.09764400
H	-5.76406300	-5.28514900	0.08382400
H	-5.49041100	-3.11420400	-1.03853400
H	0.52898100	3.81613300	-0.81655600
H	2.14328900	5.58194300	-0.23740200
H	2.46865000	6.25163700	2.14292600
H	1.17573100	5.09468900	3.92859400
H	-0.43933000	3.32926700	3.34985600
H	-0.69400600	0.19177400	2.53582500
H	-1.43277000	-0.44345700	4.79918800

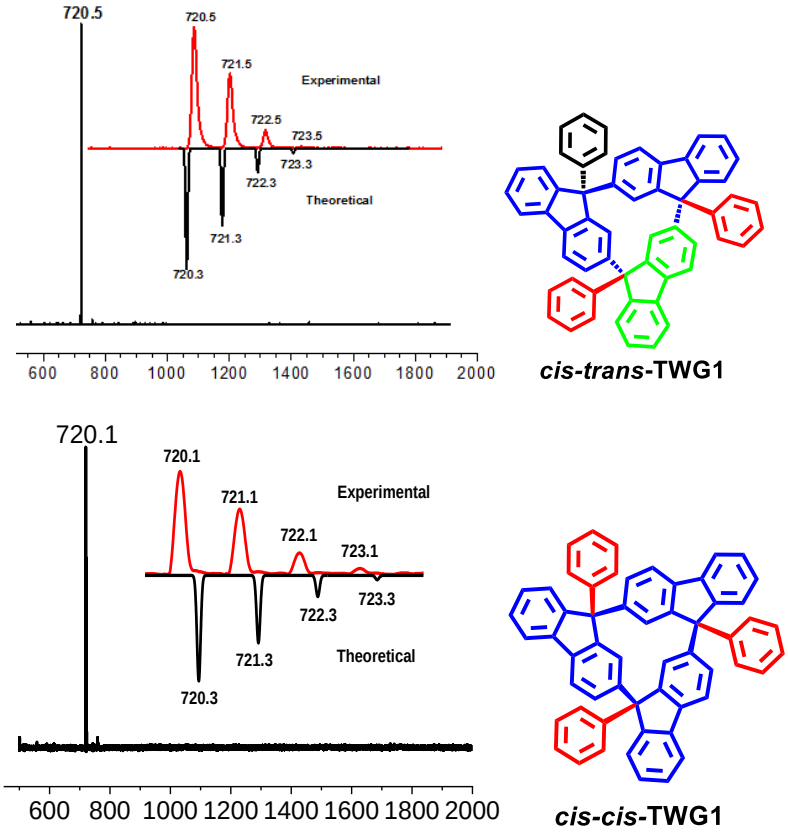
H	-3.33269900	0.75911800	5.87915500
H	-4.46807200	2.60651000	4.65939600
H	-3.71325800	3.26310400	2.41171600
H	-2.86330000	2.19771100	-1.82255300
H	-4.31198300	3.81750800	-3.01867000
H	-4.81884700	6.02730400	-1.98766200
H	-3.84165100	6.60525400	0.22619500
H	-2.36412600	5.00934300	1.38672800
H	4.03301300	-0.92768500	0.04360300
H	3.89678600	3.28110600	0.91648700
H	3.21408400	2.79656400	3.22751500
H	2.21142900	1.81146600	5.43042000
H	1.14931200	0.45982500	7.22458900
H	0.80972200	-1.97827600	6.92086100
H	1.52848500	-3.09598100	4.82743100
H	3.81638300	-3.46827400	0.68344700
H	5.79794400	-4.92263600	0.79885200
H	7.14989700	-5.04080000	2.88888000
H	6.48704300	-3.65535000	4.85028700
H	4.51391200	-2.19011100	4.72738000

Section 3. Structural characterization of DWGs and TWGs.

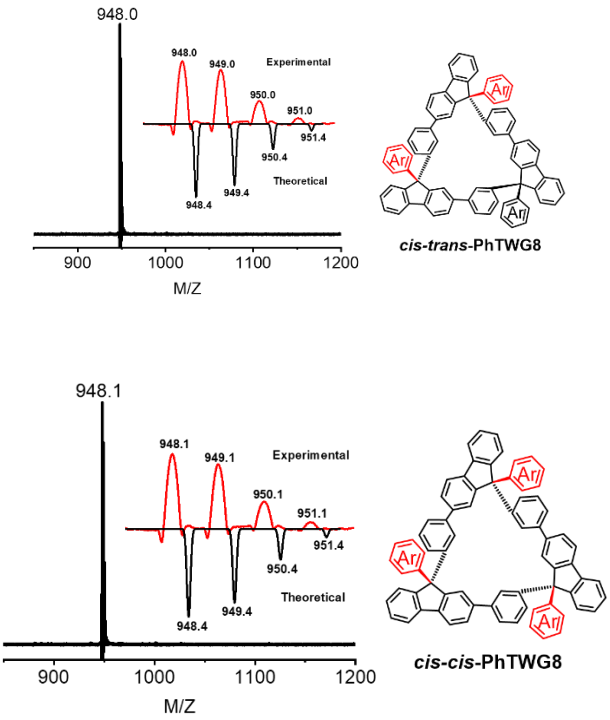




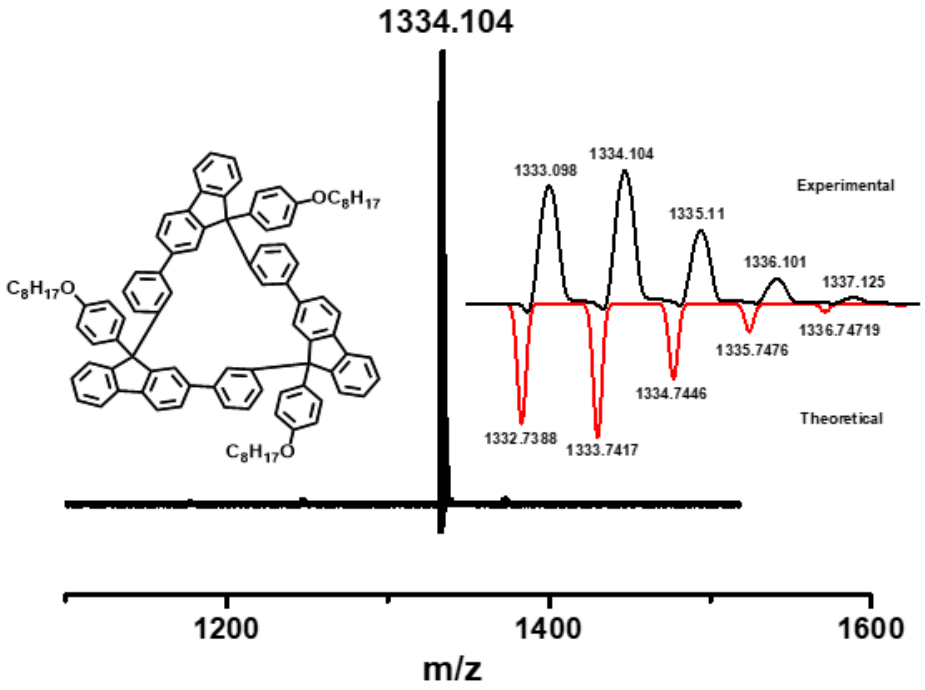
Supplementary Fig. 5 | MALDI-TOF spectra of *meso*-DWG1 and *rac*-DWG1;



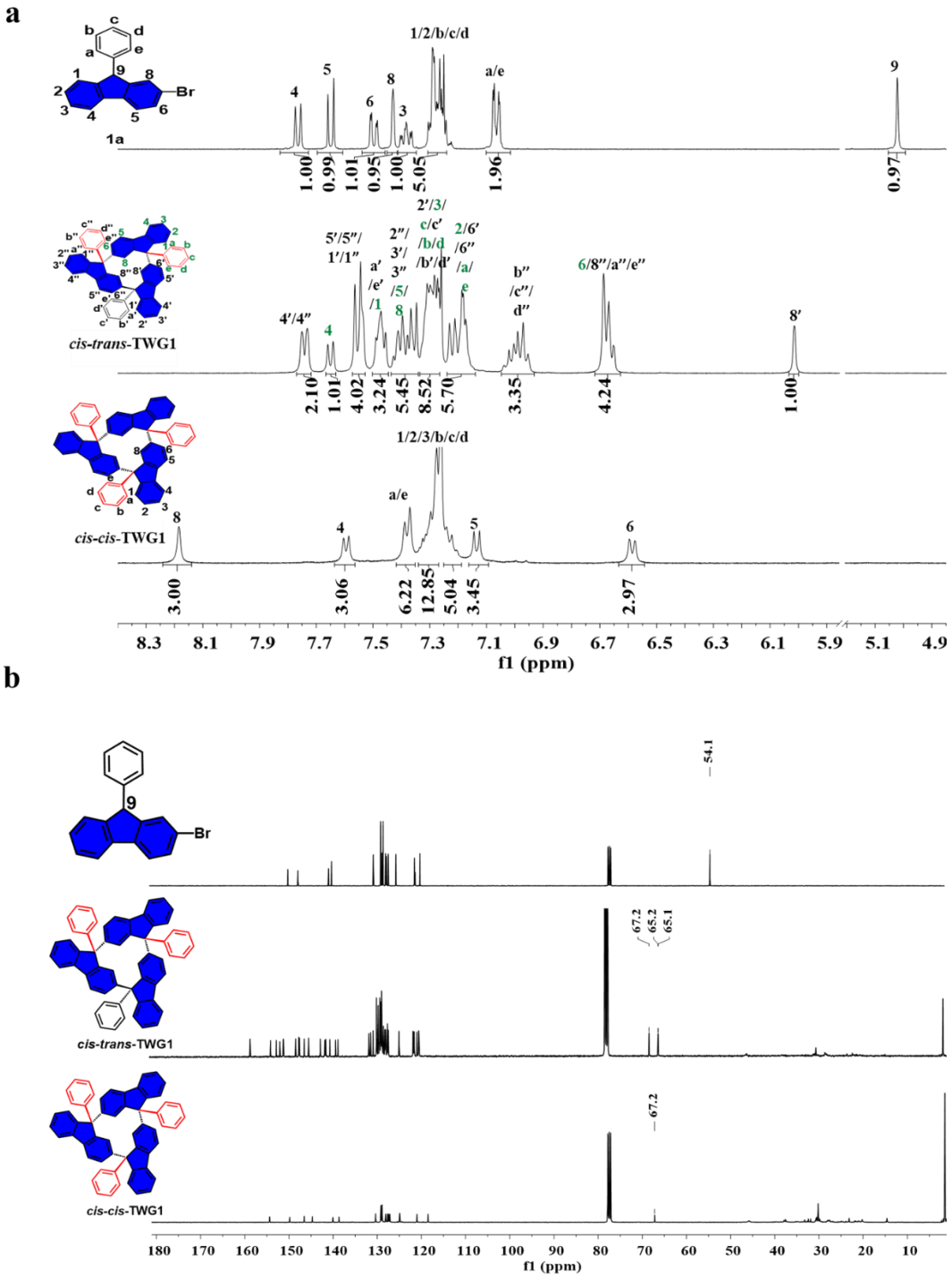
Supplementary Fig. 6 | MALDI-TOF spectra of *cis-trans*-TWG1 and *cis-cis*-TWG1.



Supplementary Fig. 7 | MALDI-TOF spectra of *cis-trans*-TWG8 and *cis-cis*-TWG8.



Supplementary Fig. 8 | MALDI-TOF spectra of TWGS9.

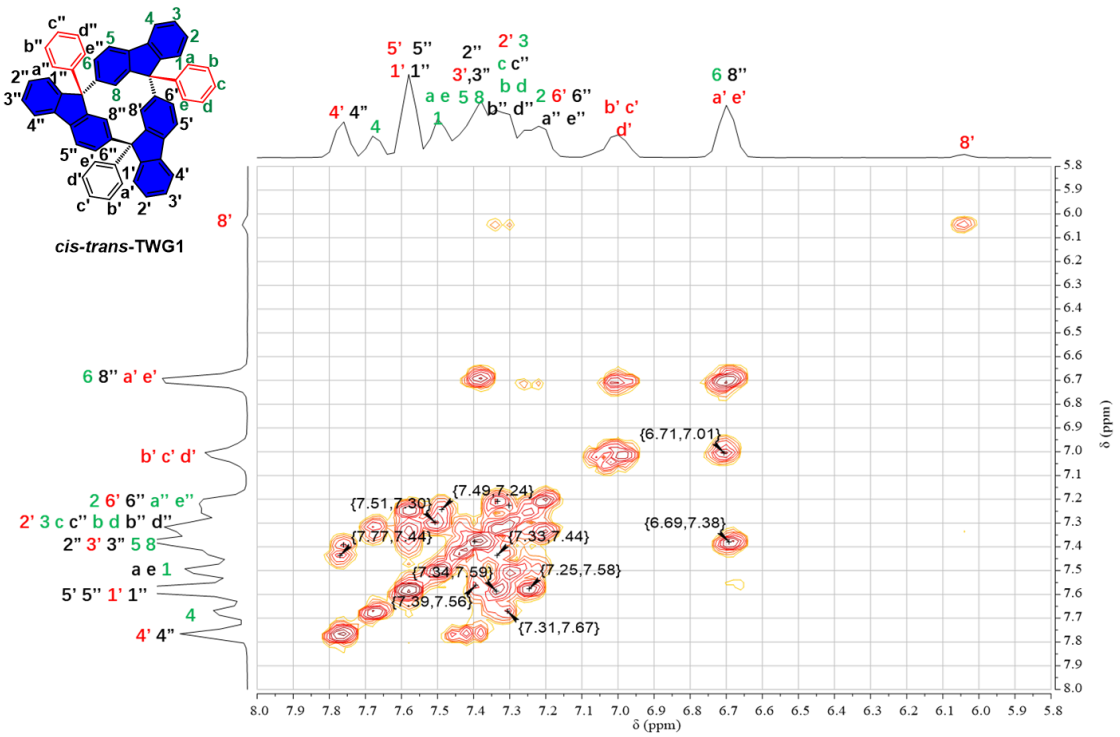


Supplementary Fig. 9 | (a) ^{1}H NMR spectra of 1a, *cis-trans*-TWG1 and *cis-cis*-TWG1; (b) ^{13}C NMR spectra of 1a, *cis-trans*-TWG1 and *cis-cis*-TWG1

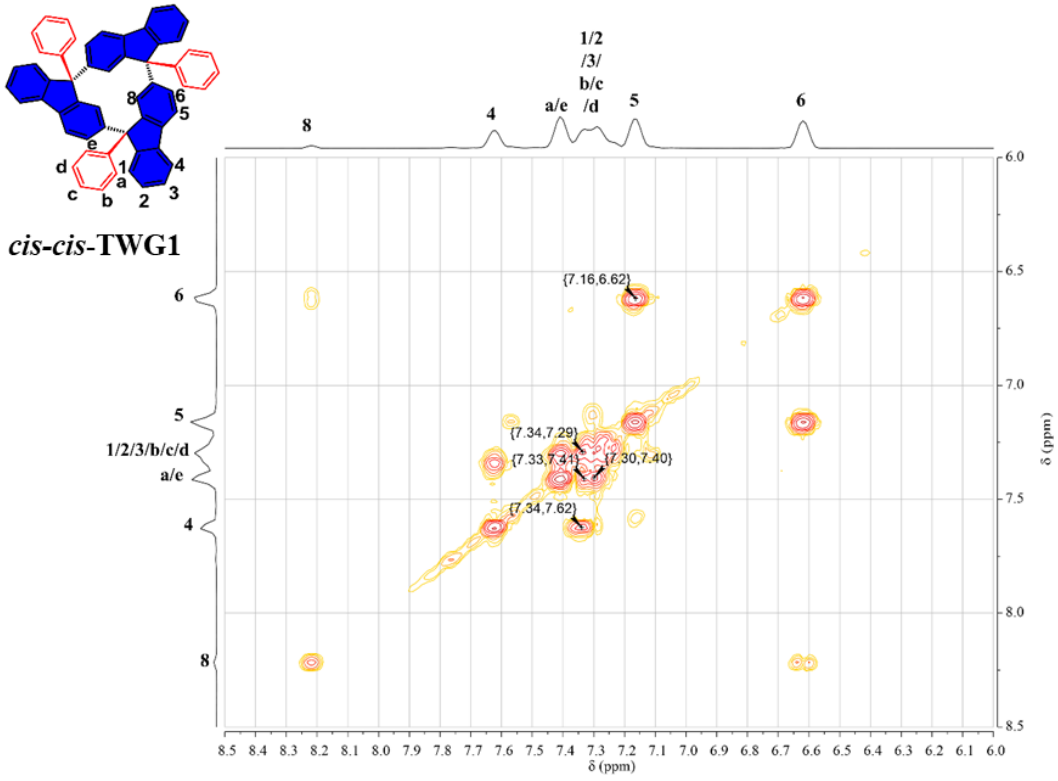
^{1}H NMR spectrum of *cis-trans*-TWG1 shows a complex resonances because it is an asymmetrical structure. In detail, in the ^{1}H NMR spectrum of **1a**, a doublet at 7.78-7.76 ppm corresponds to one hydrogen and is assigned to proton 4 of fluorene. Therefore, in the ^{1}H NMR spectrum of *cis-trans*-TWG1, protons 4' and 4'' of fluorenes resonated as a doublet at 7.75-7.7 ppm integrating for two hydrogens. Then, based on the cross peaks at (7.77 ppm, 7.44 ppm) and (7.76 ppm, 7.39 ppm) in ^{1}H-^{1}H COSY spectrum of *cis-*

trans-TWG1, we infer that protons 3' and 3" are located at 7.42-7.34 ppm. Based on the cross peaks at (7.33 ppm, 7.44 ppm) and (7.40 ppm, 7.38 ppm), protons 2' and 2" are located at 7.32-7.28 ppm and 7.42-7.34 ppm, respectively. The cross peaks at (7.34 ppm, 7.59 ppm) and (7.39 ppm, 7.56 ppm) show the protons 1', 1" are located at 7.56 -7.52 ppm. Next, proton 4 resonated as a doublet at 7.66-7.64 ppm integrating for one hydrogen owing to the deshielding reduction from fluorene's bending mode. Therefore, according to the cross peak at (7.31 ppm, 7.67 ppm), the proton 3 is located at 7.32-7.28 ppm. Further, we confirmed the proton 2 is located at 7.23-7.17 ppm based on the cross peak at (7.30 ppm, 7.23 ppm). The cross peak at (7.49 ppm, 7.24 ppm) shows the proton 1 at 7.48 -7.45 ppm. Moreover, the protons 5' and 5" can be assigned to the area of 7.56 -7.7.52 ppm. Thus, the proton 6' and 6" are located at 7.23-7.17 ppm based on the cross peak at (7.25 ppm, 7.58 ppm). However, because the shielding effect of proton 6 by adjacent fluorene, the proton 6 can be assigned to the area of 6.68 -6.64 ppm. According to the cross peak at (6.69 ppm, 7.38 ppm), the proton 5 is located at 7.42-7.34 ppm. For phenyl connected at 9-position of fluorene, we assign the protons a' and e' to the 6.68 -6.64 ppm region because the protons a' and e' are shielded by fluorene. According to the cross peak at (6.71 ppm, 7.01 ppm), multiplet at 7.03-6.95 ppm integrating to three hydrogens can be assigned to protons b", c" and d". On the contrary, we assign the protons a and e to the 7.48 -7.45 ppm region because the protons a and e are deshielded by fluorene. Therefore, the proton b', c' and d' are located at 7.32-7.28 ppm based on the cross peak at (7.51 ppm, 7.30 ppm). Moreover, we infer that protons a" and e" are located at 7.23-7.17 ppm. According to the cross peak at 7.33-7.21 ppm, we assign the protons b, c and d to the 7.32-7.28 ppm region. In addition, in the ^{1}H NMR spectrum of **1a**, a singlet at 7.43 ppm corresponds to one hydrogen and is assigned to proton 8 of fluorene. Therefore, in the ^{1}H NMR spectrum of *cis-trans*-TWG1, we attribute proton 8 to 7.42-7.34 ppm region. Then, we assign the proton 8" to the 6.68-6.64 ppm region because the proton 8" is shielded by adjacent fluorene. Significant, chemical shift of proton 8' shifts to highfield (singlet peak at 6.00 ppm) due to strong shielding of adjacent fluorene.

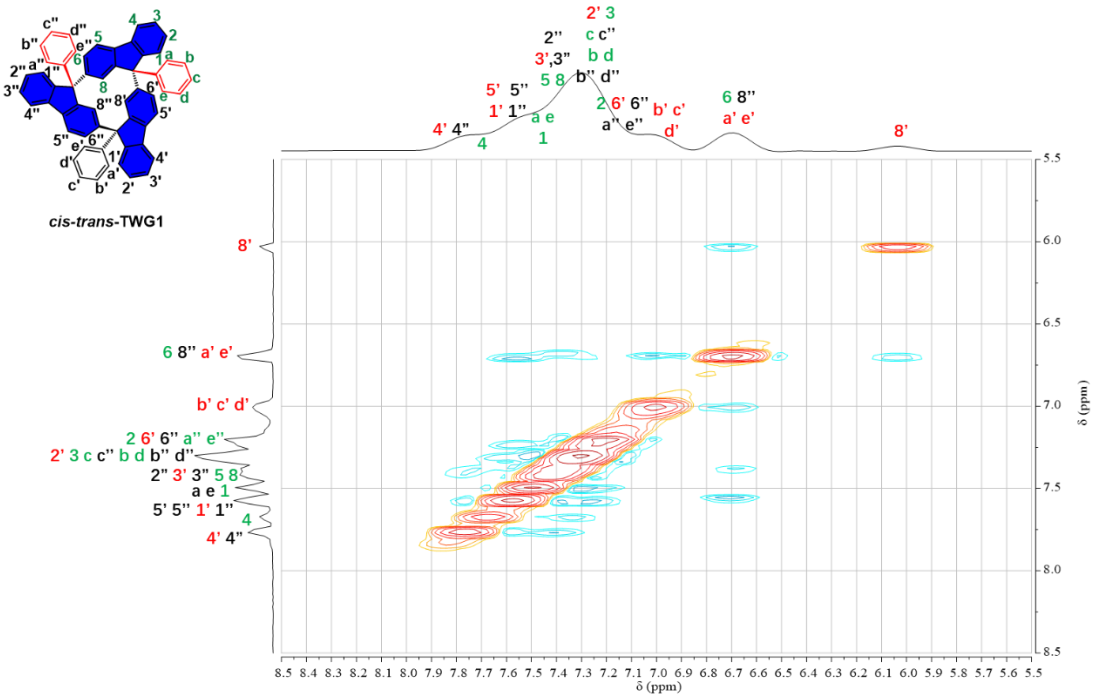
^{1}H NMR spectrum of *cis-cis*-TWG1 (C_3 symmetry) shows one set of resonance for phenyl fluorene units because it is a symmetrical structure. In detail, the doublet (three hydrogens) at 7.60-7.59 ppm is assigned to proton 4 due to the strong deshielding of adjacent phenyl. Further, proton 3 are assigned to the region at 7.34-7.20 ppm based on the cross peak at (7.34 ppm, 7.62 ppm) in in ^{1}H-^{1}H COSY spectrum of *cis-cis*-TWG1. Moreover, the doublet (six hydrogens) at 7.39-7.37 ppm is assigned to protons a and e due to the deshielding of fluorene and adjacent fluorene. Therefore, according to the cross peak at (7.33 ppm, 7.41 ppm) and (7.30 ppm, 7.40 ppm), the protons b and d are assigned to the area at 7.34-7.20 ppm. However, the doublet (three hydrogens) at 6.60 -6.57 ppm can be assigned to proton 6 because of the shielding of adjacent fluorene. Then, we assign the proton 5 to the 7.14-7.12 ppm region according to the cross peak at (7.16 ppm, 6.62 ppm). Especially, due to the double deshielding of two adjacent fluorene and two phenyl linked at 9-position, the chemical shift value of proton 8 dramatically moves to 8.19 ppm. Finally, the protons 1, 2 and c can be assigned to the region at 7.34-7.20 ppm.



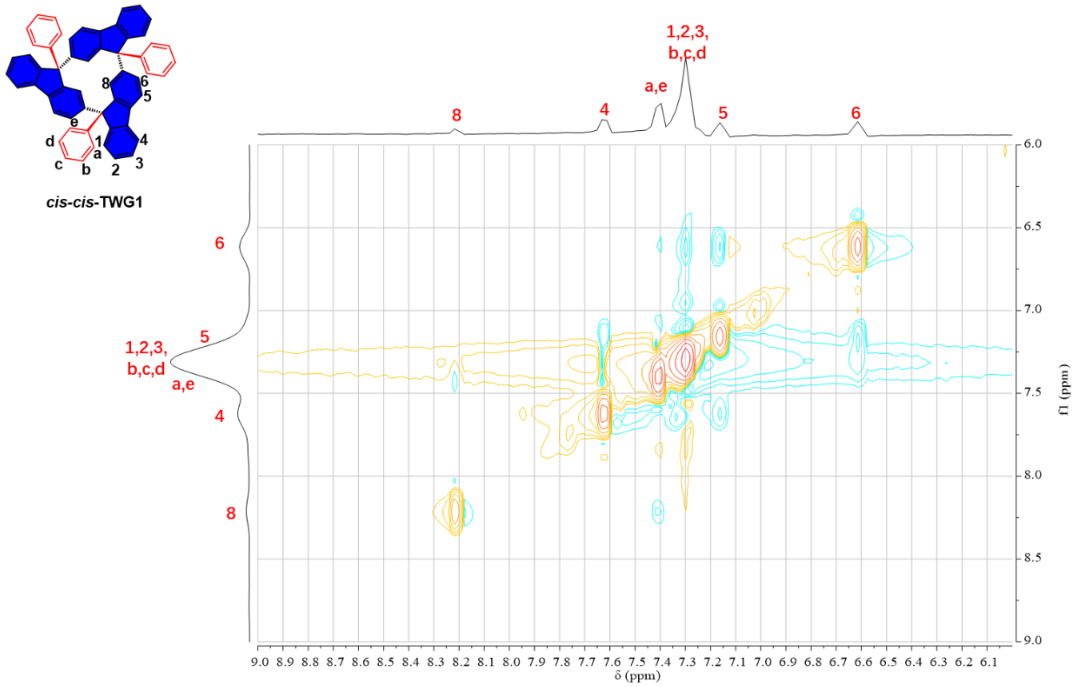
Supplementary Fig. 10 | ^{1}H-^{1}H COSY spectrum of *cis-trans*-TWG1.



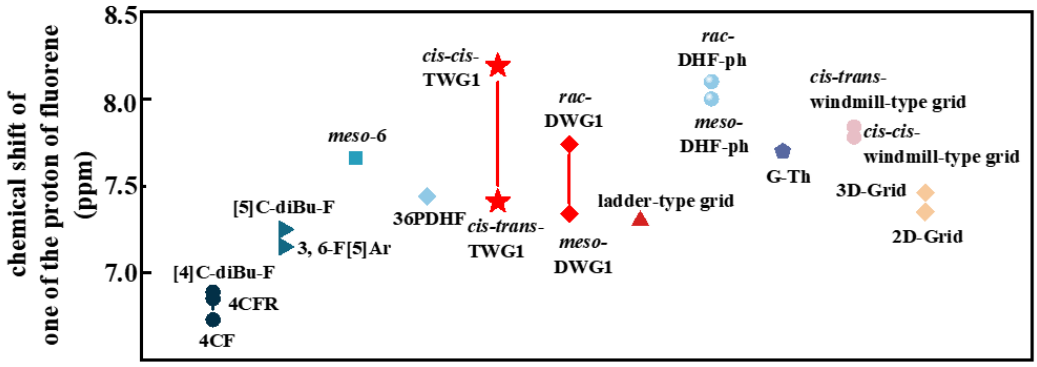
Supplementary Fig. 11 | ^{1}H-^{1}H COSY spectrum of *cis-cis*-TWG1.



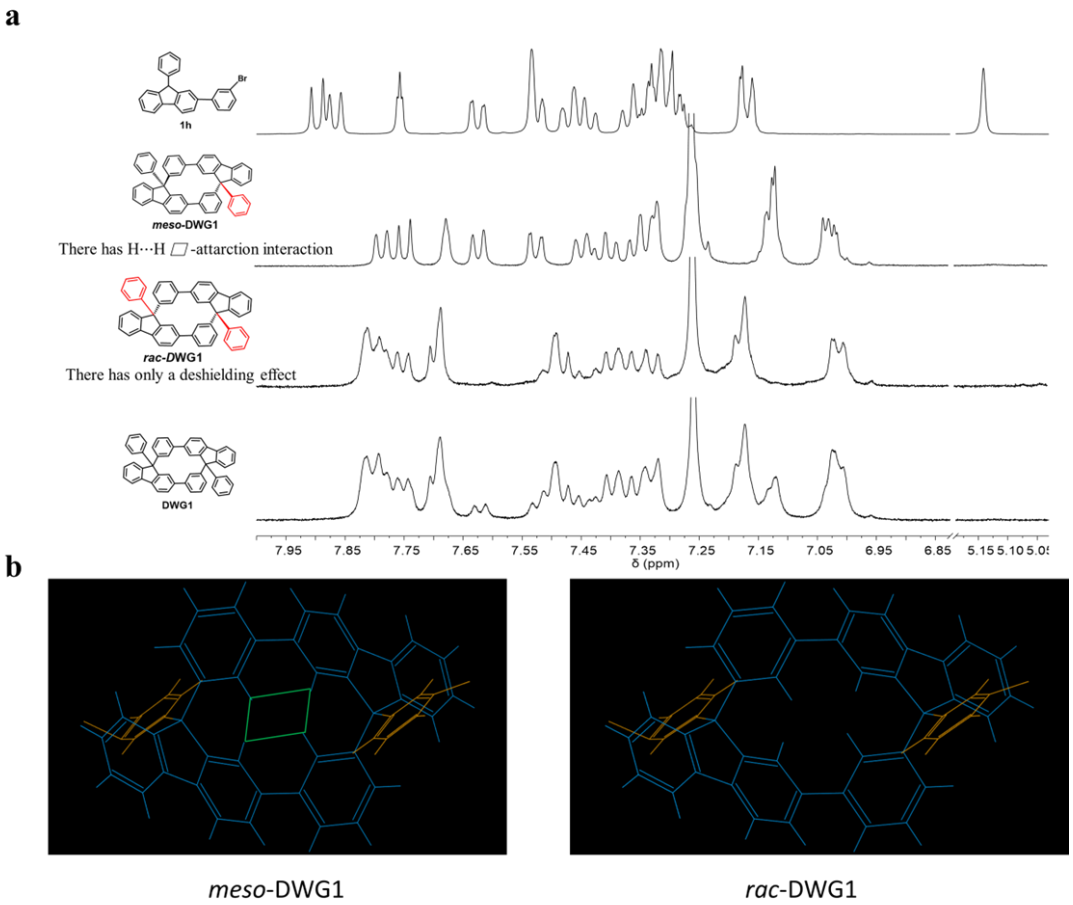
Supplementary Fig. 12 | ^{1}H-^{1}H NOESY spectrum of *cis-trans*-TWG1.



Supplementary Fig. 13 | ^{1}H-^{1}H NOESY spectrum of *cis-cis*-TWG1.



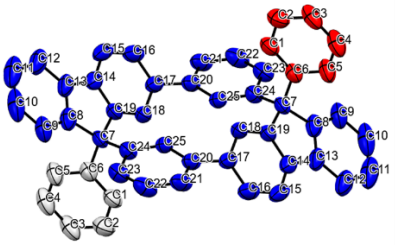
Supplementary Fig. 14 | Chemical shift of one of the proton of fluorene. [4]Cyclofluorenequare (4CF)[36]; [4]C-diBu-F[35]; [5]C-diBu-F[35] [2]spirobifluorenylenes (*meso*-6)[37]; tetrofluorene (36PDHF)[38]; 3D Grid;[39] 2D Grid;[39] windmill-type nanogrids[16]; ladder-type nanogrids[15]; fluorenes-based DHGs (DHGs-F)[17].

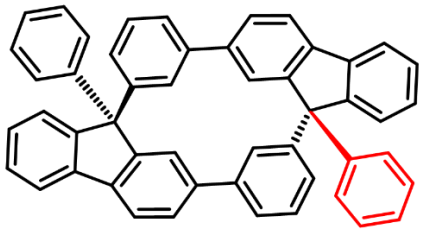


Supplementary Fig. 15 | (a) :^{1}H NMR spectra of 1h, *meso*-DWG1, *rac*-DWG1; (b) H···H ▱-attraction interaction (green) of *meso*-DWG1 and *rac*-DWG1. H···H ▱-attraction interaction: we define a triangle formed by four stacking interactions as H···H ▱-attraction interaction. The structure of *meso*-DWG1 has only an H···H ▱-attraction interaction, while the structure of *rac*-DWG1 has only a deshielding effect.

Section 4. The crystal data of single crystal of *meso*-DWG1 and *rac*-DWG1 and *cis-trans*-TWG1 and *cis-cis*-TWG1 and co-crystal of *cis-cis*-TWG1 and *cis-trans*-TWG1.

Supplementary Table 3 | The displacement ellipsoids are drawn at the 50% probability level. Single crystals suitable for X-ray analysis were obtained by slow evaporation of dichloromethane mixed with isopropanol solvent.



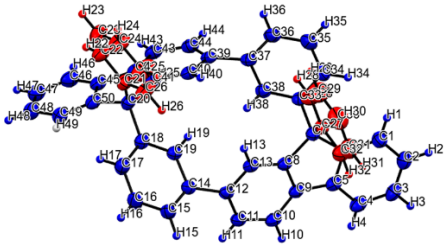


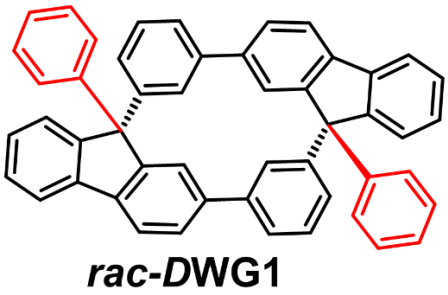
***meso*-DWG1**

Moiety formula	$C_{50}H_{32}$
CCDC	2248637
Bond precision	C-C = 0.0124 Å
Wavelength	1.34139
Cell	a=17.542(5) b=27.270(8) c=6.5789(19) alpha=90 beta=90 gamma=90
Temperature	193K
Volume	3147.2(16)
Space group	Pccn
Hall group	-P 2ab 2ac
$D_{x,g\ cm-3}$	1.335
Z	4
M_u (mm-1)	0.365
F000	1328.0
h,k,l_{max}	21,32,7
Nref	2898
Tmin,Tmax	0.957,0.964
Correction method= # Reported T Limits	Tmin=0.465 Tmax=0.751
AbsCorr	MULTI-SCAN
Data completeness	0.994
Theta(max)	54.202
R(reflections)	0.1517(1937)

wR2(reflections)	0.3489(2882)
S	1.107
Npar	226

Supplementary Table 4 | The displacement ellipsoids are drawn at the 50% probability level. Single crystals suitable for X-ray analysis were obtained by slow evaporation of dichloromethane mixed with isopropanol solvent.

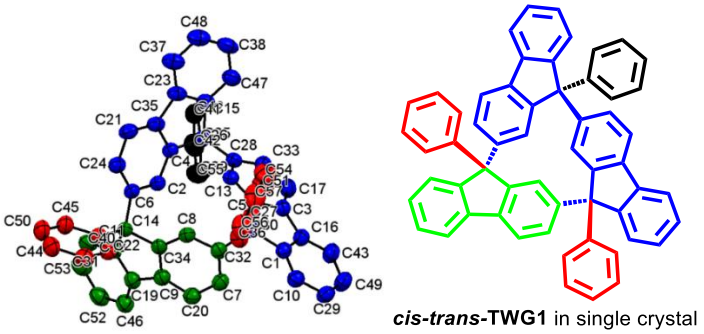




Moiety formula	$C_{50}H_{32}$
CCDC	2248641
Bond precision	C-C = 0.052Å
Wavelength	1.54178
Cell	a=11.3411(2) b=12.2038(3) c=15.3609(3) alpha=108.401(1) beta=98.498(1) gamma=108.4621(1)
Temperature	193K
Volume	1839.58(7)
Space group	P-1
Hall group	-P -
$D_{x,g\ cm-3}$	1.296
Z	2
M_u (mm-1)	1.858
F000	748.0
h,k,l_{max}	13,14,18
Nref	6764
Tmin,Tmax	0.748,0.800
Correction method= # Reported T Limits	Tmin=0.377 Tmax=0.0.467
AbsCorr	MULTI-SCAN
Data completeness	0.994
Theta(max)	68.402

R(reflections)	0.0281(5077)
wR2(reflections)	0.2445(6722)
S	1.079
Npar	478

Supplementary Table 5 | The displacement ellipsoids are drawn at the 50% probability level. Single crystals suitable for X-ray analysis were obtained by slow evaporation of dichloromethane mixed with isopropanol solvent.

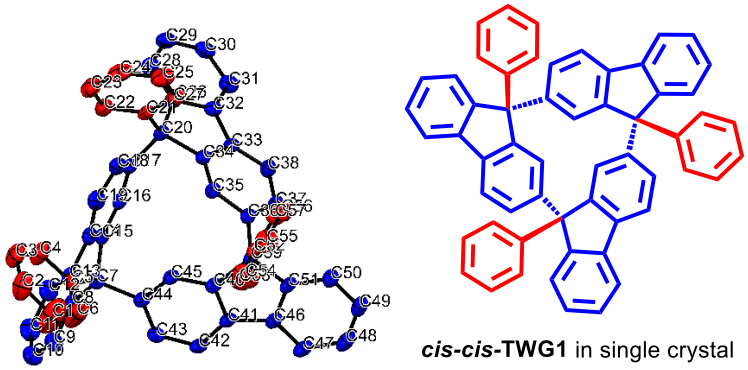


***cis-trans*-TWG1** in single crystal

Moiety formula	$C_{57}H_{36}$
CCDC	2052303
Bond precision	C-C = 0.0037 Å
Wavelength	1.34138
Cell	a=26.3387(7) b=20.6806(7) c=17.3390(5) alpha=90 beta=110.254(2) gamma=90
Temperature	193K
Volume	8860.6(5)
Space group	C12/c1
Hall group	-C2yc
$D_{x,g\ cm-3}$	1.081
Z	8
M_u (mm-1)	0.299
F000	3024.0
h,k,l_{max}	31,24,20
Nref	8125
Tmin,Tmax	0.200,0.301
Correction method= # Reported T Limits	Tmin=0.200 Tmax=0.301
AbsCorr	MULTI-SCAN
Data completeness	0.994

Theta(max)	54.079
R(reflections)	0.0634(5887)
wR2(reflections)	0.1846(8125)
S	1.035
Npar	514

Supplementary Table 6 | The displacement ellipsoids are drawn at the 50% probability level. Single crystals suitable for X-ray analysis were obtained by slow evaporation of dichloromethane mixed with *n*-hexane solvent.

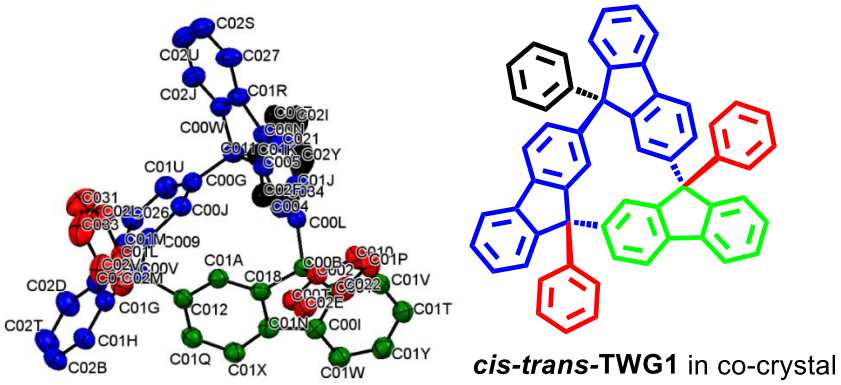


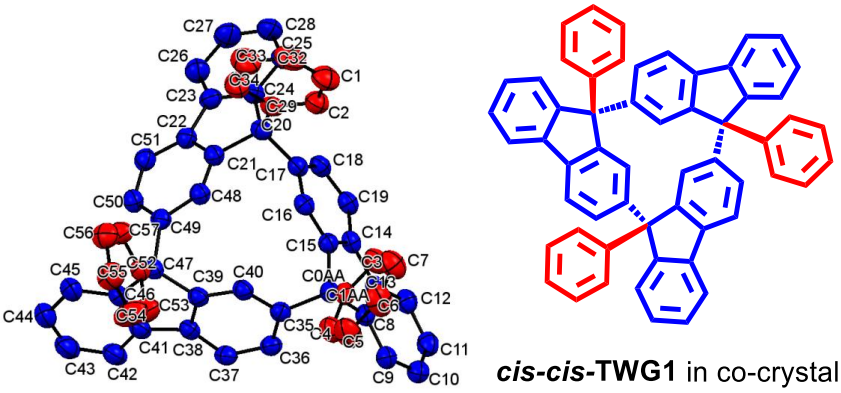
***cis-cis*-TWG1** in single crystal

Moiety formula	$C_{57}H_{36}$
CCDC	2124396
Bond precision	C-C = 0.0048 Å
Wavelength	0.71073
Cell	a=14.3732(7) b=11.6437(5) c=27.9984(15) alpha=90 beta=103.558(2) gamma=90
Temperature	191K
Volume	4555.2(4)
Space group	P121/n1
Hall group	-P2yn
$D_{x,g\ cm-3}$	1.238
Z	4
M_u (mm-1)	0.183
F000	1780.0
h,k,l_{max}	18, 15, 36
Nref	10472
Tmin,Tmax	0.667, 0.746
Correction method= # Reported T Limits	Tmin= 0.667 Tmax=0.746
AbsCorr	MULTI-SCAN

Data completeness	0.998
Theta(max)	27.529
R(reflections)	0.0817 (6763)
wR2(reflections)	0.2367 (10472)
S	1.060
Npar	570

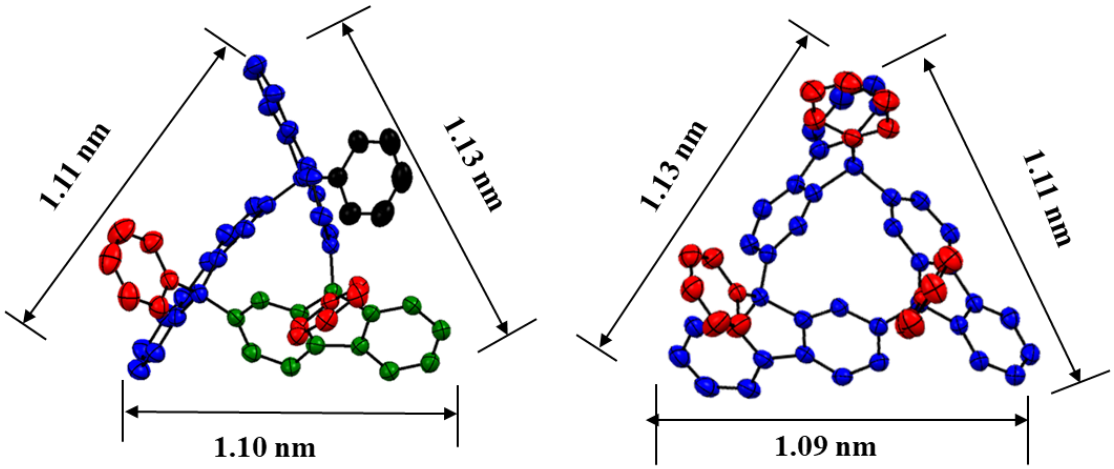
Supplementary Table 7 | The displacement ellipsoids are drawn at the 50% probability level. Single crystals suitable for X-ray analysis were obtained by slow evaporation of tetrahydrofuran mixed with water solvent.





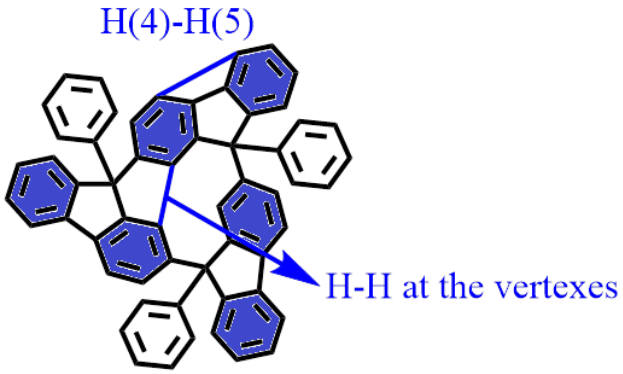
Moiety formula	$C_{114}H_{72}$
CCDC	2052304
Bond precision	C-C = 0.0031 Å
Wavelength	1.34138
Cell	a=26.9960(11) b=20.4249(9) c=17.8631(7) alpha=90 beta=93.411(2) gamma=90
Temperature	193K
Volume	9832.1(7)
Space group	P121/c1
Hall group	-P 2ybc

$D_{x,g\ cm-3}$	0.974
Z	8
M_u (mm-1)	0.269
F000	3024.0
h,k,l_{max}	32,24,21
Nref	18003
Tmin,Tmax	0.213,0.301
Correction method= # Reported T Limits	Tmin=0.213 Tmax=0.301
AbsCorr	NONE
Data completeness	0.996
Theta(max)	53.994
R(reflections)	0.0522(11040)
wR2(reflections)	0.1500(18003)
S	0.958
Npar	1027

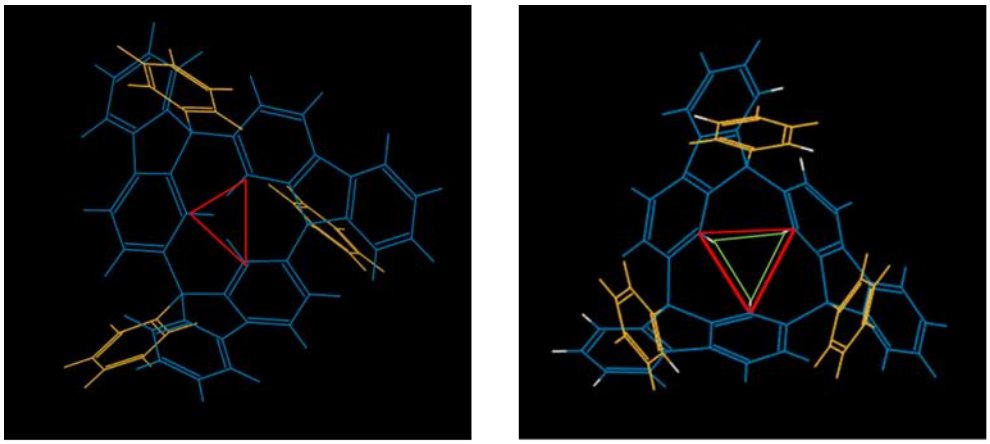


Supplementary Fig. 16 | co-crystallography of *cis-cis*-TWG1 and *cis-trans*-TWG1. (The red and black lines represent phenyl at the same side or the other side, respectively. The green lines exhibit the bent skeleton and blue lines exhibits the stretched skeleton.).

Supplementary Table 8 | Relevant H-H distances of the X-Ray structures of *cis-trans*-TWG1 and *cis-cis*-TWG1.



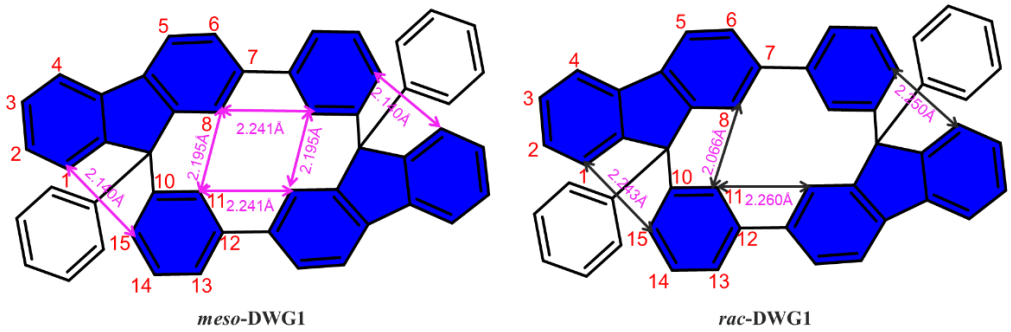
	H(4)-H(5)	H-H at the vertexes
***cis-trans*-TWG1**	2.69 Å, 2.70 Å,	3.10 Å, 2.18 Å,
(single crystal)	2.71 Å	3.55 Å
***cis-trans*-TWG1**	2.72 Å,2.70 Å,	3.30 Å, 2.33 Å
(co-crystal)	2.67 Å	3.60 Å
***cis-cis*-TWG1**	2.72 Å， 2.75 Å	2.19 Å,2.19 Å,
(single crystal)	2.70 Å	2.31 Å
***cis-cis*-TWG1**	2.67 Å, 2.70 Å,	2.15 Å, 2.19 Å,
(co-crystal)	2.74 Å	2.34 Å



cis-trans-TWG1 *cis-cis*-TWG1

Supplementary Fig. 17 | H···H *Δ*-attraction interaction (green) and π···π *Δ*-repulsion interaction (red) of TWGs. Delta (*Δ*)-stacking motif: we define a triangle formed by three stacking interactions as delta-stacked motif, as shown in the figure. A symmetric H···H delta (*Δ*)-attraction interaction can be extracted with mutually three H···H interactions among the adjacent hydrogen at the 8-position of fluorenes. π···π *Δ*-repulsion interaction can be extracted with mutually three π···π stacking interactions on the vertexes between adjacent fluorenes.

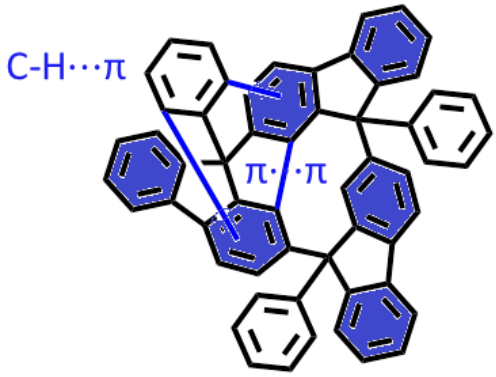
Supplementary Table 9 | Relevant H-H distances of the X-Ray structures of *meso*-DWG1 and *rac*-DWG1.



meso-DWG1 *rac*-DWG1

	H(1)-H(15)	H(8)-H(11)
***meso*-DWG1**	2.140 Å,2.140 Å	2.195 Å,2.195 Å,
(single crystal)		2.241 Å,2.241 Å
***rac*-DWG1**	2.243 Å,2.250 Å	2.066 Å,2.260 Å
(single crystal)		

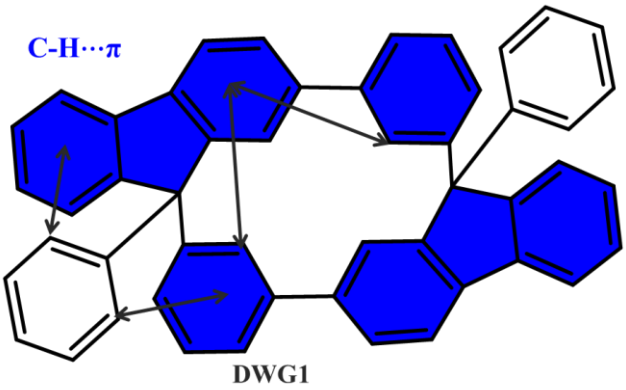
Supplementary Table 10 | Relevant C-H···π and π···π distances of the X-Ray structures of *cis-trans*-TWG1 and *cis-cis*-TWG1.



	C-H···π	π···π
***cis-trans*-TWG1**	3.18 Å, 3.59 Å,	3.04 Å, 3.08 Å,
(single crystal)	3.38 Å, 3.37 Å,	3.18 Å
	4.83 Å, 4.06 Å	
***cis-trans*-TWG1**	3.33 Å, 3.66 Å	3.05 Å, 3.05 Å,
(co-crystal)	3.31 Å, 4.74 Å	3.24 Å
	3.98 Å, 3.17 Å	

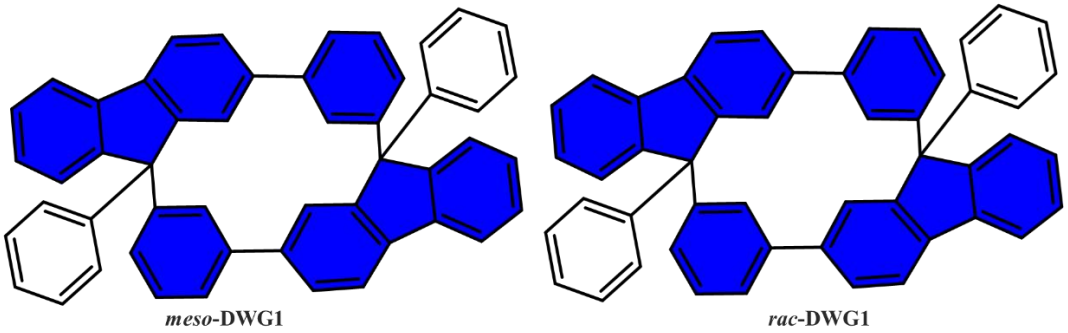
***cis-cis*-TWG1**	3.44 Å, 3.44 Å,	3.06 Å, 3.06 Å,
(single crystal)	3.44 Å, 3.47 Å	3.05 Å
	3.47 Å, 3.37 Å	
***cis-cis*-TWG1**	3.39 Å, 3.47 Å,	3.04 Å, 3.05 Å,
(co-crystal)	3.49 Å, 3.37 Å,	3.08 Å
	3.45 Å, 3.50 Å	

Supplementary Table 11 | Relevant C-H···π distances of the X-Ray structures of *meso*-DWG1 *and rac*-DWG1.

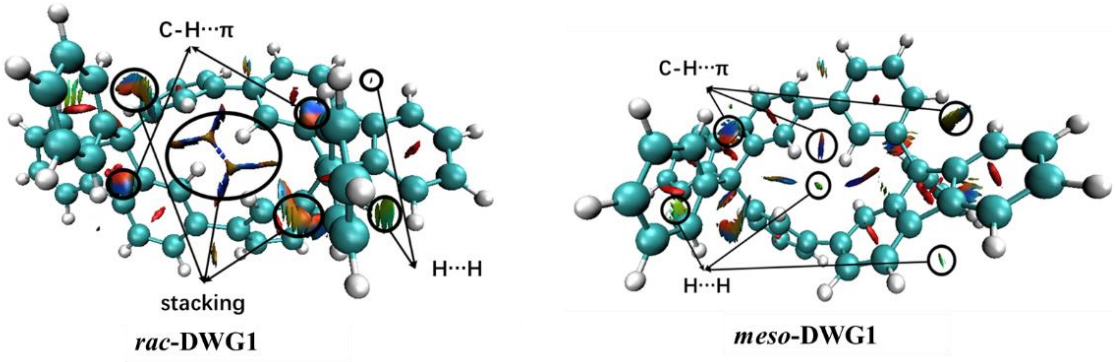


	C-H···π
***meso*-DWG1**	2.57 Å，2.51 Å，2.78 Å, 2.55 Å 2.80 Å，2.77 Å，
(single crystal)	2.90 Å，2.50 Å，2.24 Å，2.56 Å，2.76 Å
***rac*- DWG1**	2.57 Å, 2.51 Å, 2.78 Å,2.64 Å,2.56 Å, 2.62 Å, 2.78 Å,
(single crystal)	2.89 Å, 2.45 Å, 2.38 Å, 2.69 Å, 2.51 Å, 2.23 Å, 2.28
	Å, 2.72 Å,2.88 Å，2.74 Å

Supplementary Table 12 | Relevant π···π distances of the X-Ray structures of *meso*-DWG1 *and rac*-DWG1.

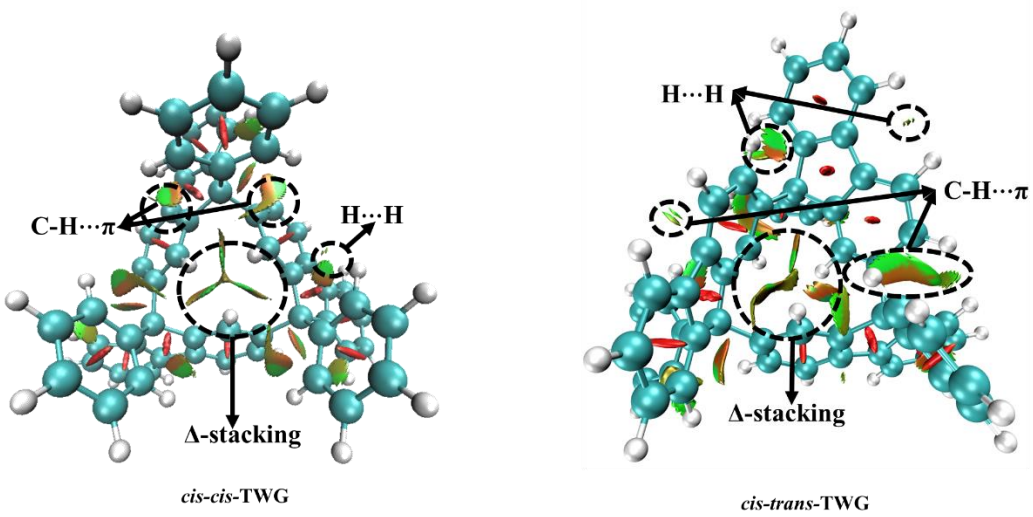


	π···π
***meso*-DWG1 (single crystal)**	3.326 Å， 3.028 Å,3.326 Å,3.028 Å
***rac*- DWG1 (single crystal)**	3.27 Å,.33 Å,3.39 Å,3.03 Å,3.06 Å 3.27 Å,3.33 Å,3.39 Å 3.40 Å,3.39 Å



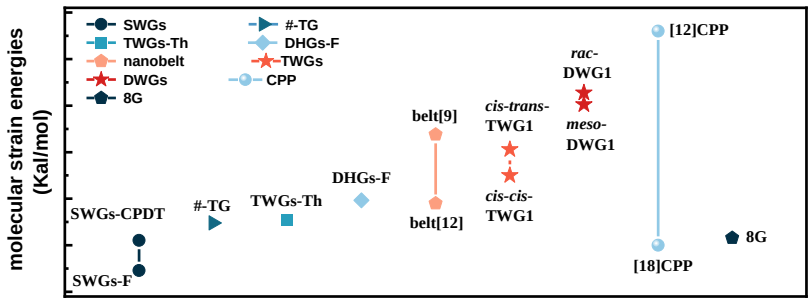
Supplementary Fig. 18 | The non-covalent interactions (NCI) isosurfaces for the *rac*-DWG1 and *meso*-DWG1.

The interactions include H-bonds (strong interactions) in blue, van der Waals interactions in green and steric repulsions in red. in the fluorenes and H···H interactions between benzene ring and fluorene. In the scatter plot of *rac*-DWG1, the spikes corresponding to all two H···H interactions were around ±0.005 a.u., while those of *meso*-DWG1 were around ±0.006 a.u.. Similarly, the C-H···π interactions were divided into two types: C-H···π interactions between fluorene and benzene ring and C-H···π interactions between two benzene rings. In the scatter plot of *rac*-DWG1, the corresponding spikes were mainly located around ±0.012 a.u., while for *meso*-DWG1, the spikes were mainly located around ±0.011a.u. Moreover, stacking motif include H ···H interaction and C-H···π interaction.The scatter plots of rac-DWG1 show that the spike positions corresponding to stacking motifs were around ±0.011 a.u..



Supplementary Fig. 19 | The non-covalent interactions (NCI) isosurfaces for the *cis-trans*-TWG1 and *cis-cis*-TWG1.

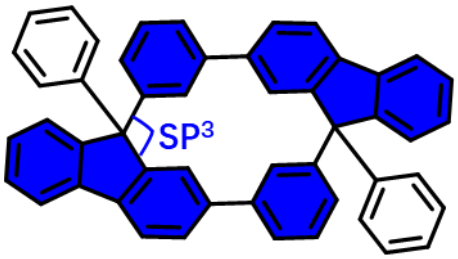
The interactions include H-bonds (strong interactions) in blue, van der Waals interactions in green and steric repulsions in red. in the fluorenes and H···H interactions between fluorene and fluorene. In the scatter plot of *cis-cis*-TWG1, the spikes corresponding to all three H···H interactions were around ±0.04 a.u., while those of *cis-trans*-TWG1 were around ±0.05 a.u.. Similarly, the C-H···π interactions were divided into two types: C-H···π interactions between fluorene and benzene ring and C-H···π interactions between two fluorenes. In the scatter plot of *cis-cis*-TWG1, the corresponding spikes were mainly located around ±0.012 a.u., while for *cis-tans*-TWG, the spikes were mainly located around ±0.017a.u. Moreover, *Δ*-stacking motif include H···H *Δ*-attraction interaction and π···π *Δ*-repulsion interaction. The scatter plots of *cis-cis*-TWG1 and *cis-tans*-TWG show that the spike positions corresponding to *Δ*-stacked motifs were around ±0.01 a.u..



Supplementary Fig. 20 | Summary of MSE for other nanogrids nanorbelt and CPPs.

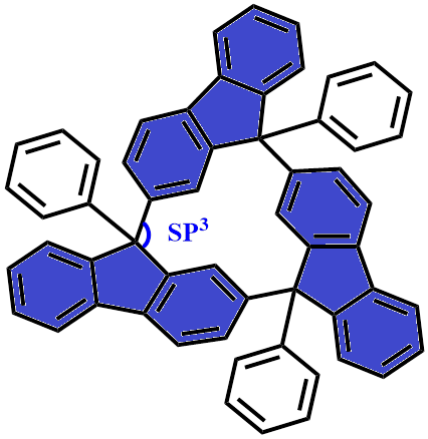
Supplementary Table 13 | Angle strain of DWGs1 is defined as relevant angles of SP^3 including the measurements of X-Ray structures of *meso*-DWG1and *rac*-

DWG1.



	SP^3	Average angle strain
***meso*-DWG1 (single crystal)**	113.04°	3.54°
***rac*-DWG1 (single crystal)**	110.29° 112.22°	1.76°

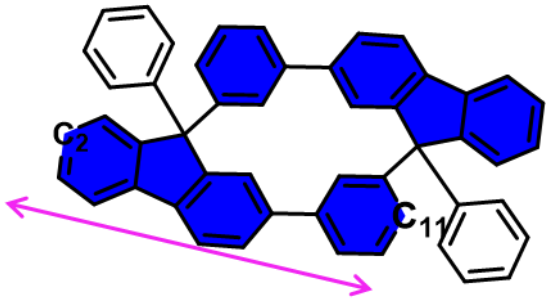
Supplementary Table 14 | Angle strain of TWGs is defined as relevant angles of SP^3 including the measurements of X-Ray structures of *cis-trans*-TWG1 and *cis-cis*-TWG1.



	SP^3	**Average angle strain**
***cis-trans*-TWG1 (single crystal)**	106.05°, 108.46°, 109.56°	1.44°
***cis-trans*-TWG1 (co-crystal)**	105.28°, 107.21°, 108.82°	2.36°
***cis-cis*-TWG1 (single crystal)**	106.75°, 106.22°, 104.13°	3.77°
***cis-cis*-TWG1 (co-crystal)**	104.71°, 105.96°, 107.01°	3.57°

Definition of bending strain: The bending strain is the absolute value of difference in C2-C11 distance between DWG1 and normal *m*-BrPhF measured by single crystal XRD. The out-of-plane distorsion is the distance between the carbon atoms C2 and C11 localized on the same *m*-BrPhF unit.

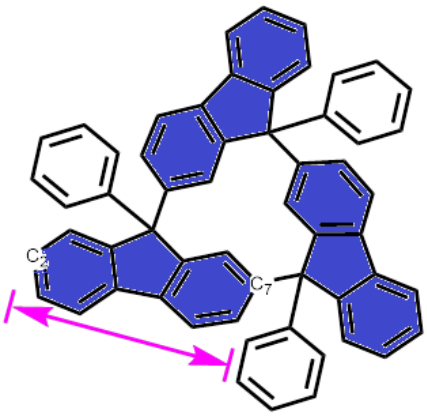
Supplementary Table 15 | Relevant C2-C11 distances of the X-Ray structures of DWG1



	C2-C11	average	Bending strain
***meso*-DWG1 (single crystal)**	10.914 Å 10.914 Å	10.914 Å	0.16 Å
***rac*-DWG1 (single crystal)**	10.946 Å, 10.942 Å	10.944 Å	0.19 Å

Definition of bending strain: The bending strain is the absolute value of difference in C2-C7 distance between TWGs and normal fluorene measured by single crystal XRD. The out-of-plane distorsion is the distance between the carbon atoms C2 and C7 localized on the same fluorene unit.

Supplementary Table 16 | Relevant C2-C7 distances of the X-Ray structures of *cis-trans*-TWG1 and *cis-cis*-TWG1.

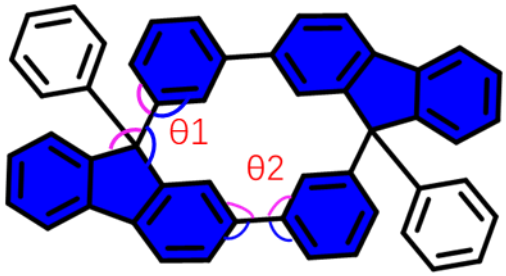


	C2-C7	average	Bending strain
***cis-trans*-TWG1 (single crystal)**	6.89 Å, 6.87 Å, 6.76 Å	6.84 Å	0.01 Å

***cis-trans*-TWG1 (co-crystal)**	6.88 Å, 6.84 Å, 6.89 Å	6.87 Å	0.02 Å
***cis-cis*-TWG1 (single crystal)**	6.90 Å, 6.91 Å, 6.93 Å	6.91 Å	0.06 Å
***cis-cis*-TWG1 (co-crystal)**	6.90 Å, 6.90 Å, 6.91 Å	6.90 Å	0.05 Å

Definition of a torsion angle: The external torsion angle (θ1 and θ2) is the dihedral angle between fluorene and two adjacent backbone phenyl.

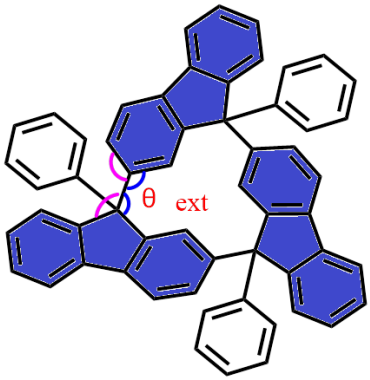
Supplementary Table 17 | Relevant external torsion angles of the X-Ray structures of DWG1.



	θ1	Average (°)	θ2	Average (°)
***meso*-DWG1 (single crystal)**	57.77°,17.39°, 57.77°,17.39°,	37.58	33.74°,36.49°, 36.49°,33.74°,	35.115
***rac*-DWG1 (single crystal)**	40.23,31.28, 64.94，5.01	35.37	60.65°,49.07°, 34.33°,39.68°,	35.15

Definition of a torsion angle: The external torsion angle (θ_{ext}) is the dihedral angle between two fluorene building units. Two angles are measured for each C7-C9 link.

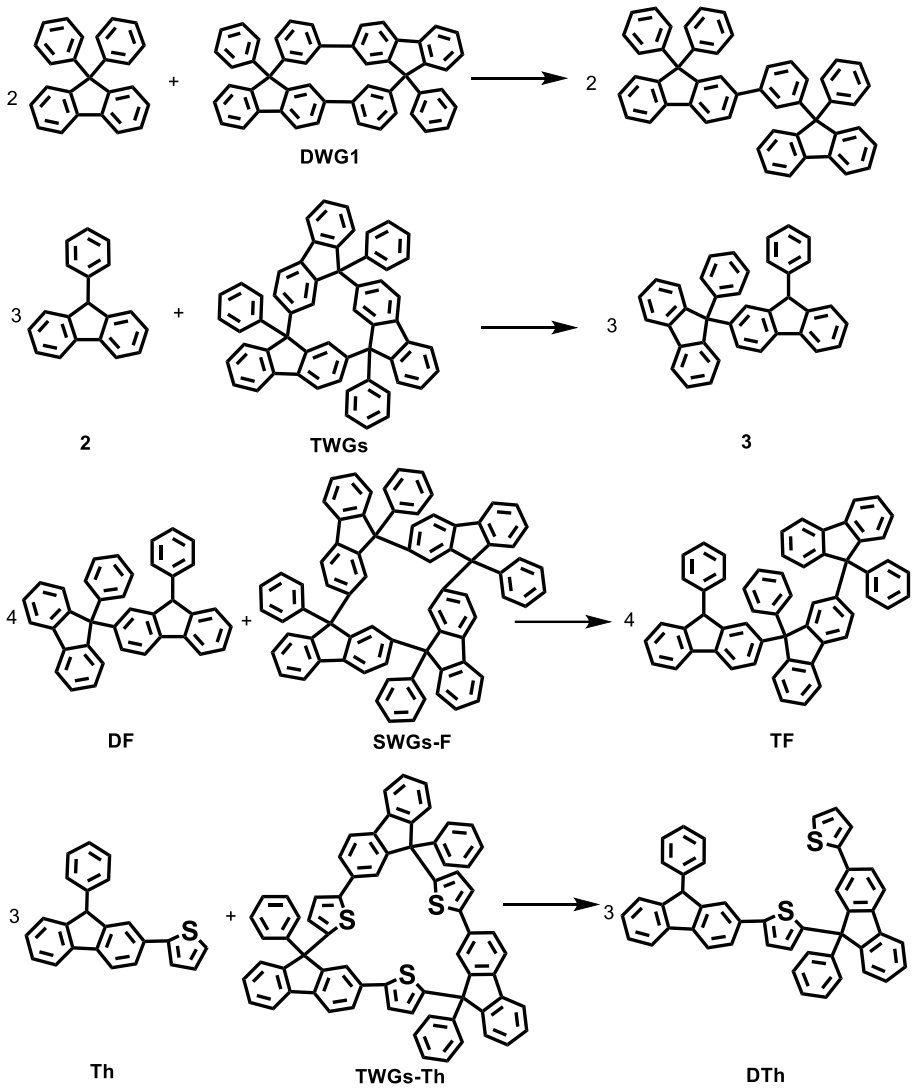
Supplementary Table 18 | Relevant external torsion angles of the X-Ray structures of *cis-trans*-TWG1 and *cis-cis*-TWG1.



	θ_{ext}	average

***cis-trans*-TWG1 (single crystal)**	49.57° 67.11° 21.75° 127.52° 9.52° 95.38°	61.82°
***cis-trans*-TWG1 (co-crystal)**	17.49° 51.57° 70.22° 91.89° 132.47° 13.28°	62.82°
***cis-cis*-TWG1 (single crystal)**	65.42° 3.87° 57.54° 6.98° 64.24° 0.72°	33.13°
***cis-cis*-TWG1 (co-crystal)**	55.49° 63.77° 65.05° 8.67° 1.59° 0.92°	32.58

Section 5. The Calculation of strain energies of DWGs, TWGs, SWGs-F and TWGs-Th



Supplementary Fig. 21 | Calculation formula of strain energies of DWGs, TWGs, SWGs-F and TWGs-Th.

Energy (**Ph**) = -963.8190078 a.u., Energy (***rac*-DWG1**) = -1925.238837 a.u., Energy (***meso*-DWG1**) = -1925.240847 a.u., Energy (**DPh**) = -1926.455465 a.u.,

Molecular strain energies (MSE, ***rac*-DWG1**) = 2*(energy of **Ph**)+(energy of ***rac*-DWG1**)-2*(energy of **DPh**) = 2*(-963.8190078)+(-1925.238837)-2*(-1926.455465） = 0.0340772 a.u.

MSE (*rac*-DWG1) =0.0340772*627.51 = 21.38378377 kcal/mol

MSE (***meso*-DWG1**) = 2*(energy of **Ph**)+(energy of ***meso*-DWG1**)-2*(energy of **DPh**) = 2*(-963.8190078)+(-1925.240847)-2*(-1926.455465） = 0.03206701 a.u.

MSE (*meso*-DWG1) = 0.03206701*627.51 = 20.12236945 kcal/mol

Energy (**2**) = -732.4727164 a.u., Energy (***cis-cis*-TWG1**) = -2193.7729125 a.u., Energy (***cis-trans*-TWG1**) = -2193.7684481 a.u., Energy (**3**) = -1463.7369963 a.u.

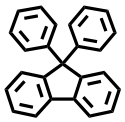
Molecular strain energies (MSE, ***cis-cis*-TWG1**) = 3*(energy of **2**)+(energy of ***cis-cis*-TWG1**)-3*(energy of **3**） = 3*(-732.4727164)+(-2193.7729125)-3*(-1463.7369963）

=0.019927 a.u.
MSE (***cis-cis*-TWG1**) =0.019927*627.51 = 12.49854 kcal/mol
MSE (***cis-trans*-TWG1**) = 3*(energy of **2**)+(energy of ***cis-trans*-TWG1**)-3*(energy of **3**) = 3*(-732.4727164)+(-2193.7684481)-3*(-1463.7369963) =0.024392 a.u.
MSE (*cis-trans*-TWG1) = 0.024392*627.51 = 15.29866 kcal/mol

Energy (**DF**) = -1463.7369963 a.u., Energy (**SWGs-F**) = -2925.0446609 a.u., Energy (**TF**) = -2194.9990723. a.u.
MSE (**SWGs-F**) = 4*(energy of **DF**)+(energy of **SWGs-F**)-4*(energy of **TF**) = =4*(-1463.7369963)+(-2925.0446609)-4*(-2194.9990723) = 0.0036431 a.u.
MSE (**SWGs-F**) = 0.0036431*627.51 = 2.284988751 kcal/mol

Energy (**Th**) = -1284.28601943 a.u., Energy (**SWGs-Th**) = -3849.22100722 a.u., Energy (**DTh**) = -2567.36377595 a.u.
MSE (**SWGs-Th**) = 3*(energy of **Th**)+(energy of **SWGs-Th**)-3*(energy of **DTh**) = 3*(-1284.28601943)+(-3849.22100722)-3*(-2567.36377595) = 0.01226234 a.u.
MSE (*cis-trans*-TWG1) = 0.01226234*627.51 = 7.691062273 kcal/mol

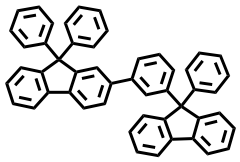
Theoretical calculation datas:



Energy: -963.8190078 a.u
Structure:

C	-1.77157	0.06061	1.14207
C	-1.11819	-0.28831	2.26211
C	-1.76202	-0.92262	3.25632
C	-3.06758	-1.21864	3.14443
C	-3.71525	-0.86858	2.024
C	-3.07599	-0.23147	1.02876
C	-4.99901	-1.05416	1.68188
C	-5.21371	-0.54017	0.4593
C	-3.9728	0.07952	-0.15397
C	-5.9922	-1.63979	2.36602
C	-7.21253	-1.70317	1.80797
C	-7.43241	-1.18731	0.58699
C	-6.4341	-0.60217	-0.09433
C	-4.03353	1.59036	-0.31374
C	-3.13902	2.23222	-1.08962
C	-3.15302	3.56758	-1.22131
C	-4.06001	4.29719	-0.55608
C	-4.93882	3.68002	0.24677
C	-4.91548	2.34368	0.37066
C	-2.62251	-2.49851	-2.51829
C	-3.12894	-2.09473	-3.69227
C	-3.90767	-1.00409	-3.73152
C	-4.16306	-0.32129	-2.60489
C	-3.63836	-0.69173	-1.421
C	-2.88501	-1.80781	-1.39769

H	-1.24	0.57523	0.32678
H	-0.04524	-0.05416	2.36488
H	-1.21351	-1.20453	4.17091
H	-3.58185	-1.74078	3.96648
H	-5.82721	-2.06447	3.36865
H	-8.04144	-2.18024	2.35762
H	-8.43993	-1.24225	0.14149
H	-6.61901	-0.17524	-1.09209
H	-2.36939	1.66222	-1.63567
H	-2.4136	4.06706	-1.8696
H	-4.07267	5.39523	-0.65586
H	-5.67544	4.27457	0.81306
H	-5.64113	1.87847	1.05665
H	-1.99684	-3.40591	-2.47414
H	-2.91999	-2.66296	-4.61382
H	-4.3444	-0.67418	-4.68908
H	-4.821	0.56109	-2.66741
H	-2.46641	-2.1858	-0.45141



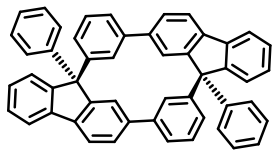
Energy: -1926.455465 a.u.

Structure:

C	5.02698	0.5402	3.06982
C	5.6518	0.27584	4.22884
C	4.99598	-0.32562	5.23573
C	3.70479	-0.67043	5.09955
C	3.08691	-0.40373	3.94042
C	3.73862	0.19407	2.92882
C	1.82213	-0.64425	3.5674
C	1.62837	-0.21055	2.31646
C	2.86935	0.41252	1.70446
C	0.80796	-1.21574	4.22338
C	-0.37969	-1.34674	3.60632
C	-0.62628	-0.93336	2.33974
C	0.43334	-0.35589	1.72612
C	3.46234	-0.37614	0.54711
C	4.39555	0.17896	-0.24982
C	4.95118	-0.50327	-1.26301
C	4.59366	-1.77529	-1.49018
C	3.68936	-2.35661	-0.68894
C	3.14081	-1.66447	0.32184
C	-1.8354	-1.08729	1.72887
C	-2.90417	-1.65521	2.33031
C	-4.08126	-1.82878	1.70993
C	-4.24995	-1.42198	0.44659
C	-3.24235	-0.8112	-0.19612
C	-2.06941	-0.69409	0.45586
C	-2.25024	1.90822	-1.69249
C	-1.26372	2.67217	-2.1884

C	-0.39863	2.16967	-3.08518
C	-0.50737	0.89638	-3.49911
C	-1.49487	0.13803	-3.00198
C	-2.36458	0.63782	-2.10799
C	-1.79913	-1.14487	-3.24946
C	-2.86856	-1.49933	-2.51756
C	-3.39626	-0.37555	-1.6473
C	-1.20505	-2.02471	-4.06814
C	-1.70017	-3.2711	-4.14672
C	-2.77064	-3.62853	-3.41739
C	-3.36118	-2.74439	-2.59719
C	-4.77184	0.13994	-2.03721
C	-5.31013	-0.11185	-3.2457
C	-6.51218	0.37511	-3.59155
C	-7.19754	1.14692	-2.73576
C	-6.6644	1.43584	-1.54002
C	-5.46194	0.94331	-1.20507
C	2.37999	4.11102	2.07208
C	1.93113	4.45889	0.85757
C	1.77593	3.51384	-0.08046
C	2.07801	2.23609	0.19657
C	2.56337	1.87119	1.39928
C	2.68229	2.83042	2.33713
H	5.56619	1.039	2.24984
H	6.71081	0.55728	4.35531
H	5.52121	-0.53572	6.18272
H	3.17617	-1.1607	5.93212
H	0.94076	-1.5805	5.25492
H	-1.1404	-1.83405	4.23315
H	0.4138	0.03312	0.7013
H	4.72105	1.21856	-0.08043
H	5.70682	-0.02107	-1.90569
H	5.04969	-2.34229	-2.31862
H	3.40315	-3.40851	-0.8576
H	2.41644	-2.1869	0.96662
H	-2.88808	-2.03258	3.36271
H	-4.9185	-2.31938	2.23607
H	-5.21774	-1.5974	-0.04998
H	-1.27458	-0.2475	-0.14999
H	-2.94841	2.31969	-0.94751
H	-1.15998	3.71711	-1.85104
H	0.4108	2.8063	-3.48049
H	0.21261	0.49614	-4.23002
H	-0.32704	-1.74595	-4.67168
H	-1.22393	-4.00735	-4.81598
H	-3.16761	-4.65488	-3.49196
H	-4.23907	-3.03695	-2.00028
H	-4.77151	-0.72411	-3.98632
H	-6.9347	0.14898	-4.58508
H	-8.18278	1.55305	-3.01876
H	-7.21161	2.0851	-0.83611
H	-5.04295	1.21295	-0.2216
H	2.4923	4.87899	2.85591
H	1.6778	5.50906	0.63681

H	1.39198	3.78837	-1.07685
H	1.91856	1.48248	-0.59234
H	3.02915	2.5842	3.35336

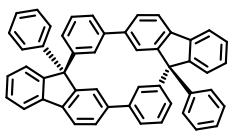


Energy: -1925.238837 a.u.

Structure:

C	3.9386	-2.2487	3.5991
C	5.1877	-1.9947	4.0216
C	5.7332	-0.7794	3.845
C	5.0357	0.2024	3.2496
C	3.7868	-0.0541	2.836
C	3.24	-1.2724	3.0005
C	2.9021	0.7614	2.244
C	1.7615	0.0884	2.0575
C	1.8368	-1.3943	2.4374
C	2.9803	2.0415	1.8567
C	1.9455	2.6074	1.2044
C	0.7795	1.963	0.9687
C	0.7166	0.7275	1.5131
C	0.8591	-1.8276	3.5097
C	0.3856	-0.959	4.4226
C	-0.4595	-1.3545	5.3873
C	-0.8332	-2.6398	5.4683
C	-0.3459	-3.5246	4.5862
C	0.4982	-3.1192	3.625
C	-0.2027	2.4014	0.1282
C	-0.0744	3.4797	-0.6726
C	-0.9402	3.7245	-1.671
C	-1.9398	2.8733	-1.947
C	-2.154	1.8148	-1.1495
C	-1.3362	1.6967	-0.0863
C	-4.8507	1.7192	-3.0829
C	-5.3613	1.721	-4.3249
C	-4.9179	0.8483	-5.2455
C	-3.9624	-0.0441	-4.9364
C	-3.4612	-0.0466	-3.6933
C	-3.8937	0.8325	-2.771
C	-2.53	-0.8459	-3.1528
C	-2.3818	-0.5167	-1.865
C	-3.1885	0.7126	-1.4333
C	-1.799	-1.8457	-3.6634
C	-0.8617	-2.4453	-2.9027
C	-0.6549	-2.1331	-1.6027
C	-1.5235	-1.2204	-1.1135
C	-4.1822	0.4628	-0.3181
C	-4.6173	1.4783	0.4509
C	-5.5178	1.2791	1.4258
C	-6.0172	0.0528	1.6374
C	-5.6184	-0.9646	0.86
C	-4.7175	-0.755	-0.1125

C	0.4145	-2.5414	-0.859
C	1.4689	-3.21	-1.3706
C	2.6127	-3.3586	-0.6807
C	2.7719	-2.7986	0.5279
C	1.7393	-2.1719	1.114
C	0.5789	-2.1725	0.4311
H	3.4953	-3.2481	3.7332
H	5.7714	-2.792	4.5117
H	6.7611	-0.5851	4.1948
H	5.4897	1.1971	3.1171
H	3.9122	2.6111	2.0047
H	2.1284	3.6285	0.8359
H	-0.1725	0.1066	1.4517
H	0.6872	0.1006	4.3957
H	-0.8413	-0.6242	6.1206
H	-1.5231	-2.9693	6.2628
H	-0.6336	-4.5871	4.6569
H	0.8971	-3.8709	2.9244
H	0.7844	4.1651	-0.6134
H	-0.7709	4.5871	-2.339
H	-2.5566	3.0527	-2.8403
H	-1.6324	0.8921	0.5886
H	-5.2055	2.4422	-2.3314
H	-6.146	2.4487	-4.592
H	-5.3443	0.8624	-6.2628
H	-3.612	-0.7602	-5.6965
H	-1.9101	-2.131	-4.7222
H	-0.2402	-3.1876	-3.4267
H	-1.5157	-0.9047	-0.0742
H	-4.2367	2.4999	0.2875
H	-5.8541	2.1251	2.0485
H	-6.7611	-0.1146	2.4339
H	-6.0388	-1.9724	1.0158
H	-4.4254	-1.6086	-0.7454
H	1.4867	-3.5918	-2.4024
H	3.472	-3.865	-1.1541
H	3.7601	-2.8494	1.0092
H	-0.2509	-1.7577	1.0056



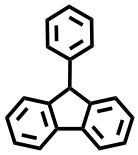
Energy: -1925.240847 a.u.

Structure:

C	5.2138	-1.5954	-1.6887
C	6.3356	-1.0158	-2.1464
C	6.2756	0.1314	-2.8417
C	5.0898	0.7105	-3.0889
C	3.9754	0.1259	-2.6261
C	4.0245	-1.0158	-1.9166
C	2.7028	0.5333	-2.7339

C	1.8992	-0.3293	-2.0985
C	2.6476	-1.5363	-1.5349
C	2.1894	1.6208	-3.3211
C	0.8877	1.9082	-3.1451
C	0.0718	1.1311	-2.3968
C	0.5872	-0.0553	-2.0035
C	2.2087	-2.7333	-2.3777
C	1.1274	-3.457	-2.0268
C	0.7028	-4.4953	-2.7632
C	1.3482	-4.8263	-3.8905
C	2.4093	-4.1025	-4.2744
C	2.8242	-3.066	-3.5292
C	-1.1063	1.6212	-1.921
C	-1.745	2.6919	-2.433
C	-2.7266	3.3102	-1.759
C	-3.0375	2.9257	-0.5134
C	-2.4548	1.8479	0.0394
C	-1.5788	1.1766	-0.7342
C	-5.2129	1.5845	1.6696
C	-6.3342	0.9991	2.121
C	-6.2723	-0.1476	2.8169
C	-5.0851	-0.7209	3.0707
C	-3.971	-0.1309	2.6139
C	-4.0221	1.0107	1.9045
C	-2.6972	-0.533	2.7267
C	-1.8947	0.3329	2.0942
C	-2.6458	1.5383	1.5308
C	-2.1818	-1.6189	3.3149
C	-0.8789	-1.9021	3.1419
C	-0.064	-1.1227	2.395
C	-0.5819	0.0625	2.0008
C	-2.2165	2.7343	2.3798
C	-2.8415	3.0629	3.5273
C	-2.4351	4.099	4.2779
C	-1.3732	4.8265	3.9035
C	-0.7186	4.4998	2.7804
C	-1.1347	3.4619	2.0385
C	1.1152	-1.6108	1.9203
C	1.7569	-2.6785	2.4349
C	2.7388	-3.2968	1.7612
C	3.0467	-2.9154	0.514
C	2.4614	-1.8403	-0.0414
C	1.5852	-1.1685	0.7317
H	5.2908	-2.5487	-1.1481
H	7.3133	-1.4917	-1.9606
H	7.2031	0.5964	-3.2159
H	5.0527	1.6512	-3.6604
H	2.8398	2.3376	-3.848
H	0.586	2.8975	-3.523
H	-0.0298	-0.8123	-1.4981
H	0.5586	-3.2072	-1.1163
H	-0.1821	-5.0727	-2.4469
H	1.0011	-5.675	-4.5028
H	2.9357	-4.3562	-5.21

H	3.6886	-2.4914	-3.8972
H	-1.4659	3.1364	-3.4013
H	-3.2017	4.2105	-2.1855
H	-3.7326	3.5516	0.0662
H	-1.1092	0.3176	-0.2569
H	-5.2911	2.5372	1.128
H	-7.3133	1.4699	1.9294
H	-7.1996	-0.6175	3.1857
H	-5.0465	-1.6618	3.6417
H	-2.8313	-2.3384	3.8394
H	-0.575	-2.8909	3.5198
H	0.0342	0.8205	1.4958
H	-3.7073	2.4855	3.8878
H	-2.9693	4.3494	5.21
H	-1.0332	5.675	4.5201
H	0.1669	5.0805	2.4718
H	-0.5588	3.2156	1.1315
H	1.4796	-3.1207	3.4048
H	3.2159	-4.1951	2.1896
H	3.7412	-3.5427	-0.0648
H	1.1119	-0.3125	0.2528

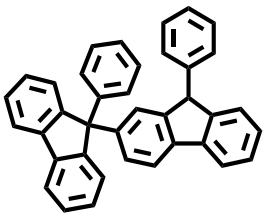


Energy: -732.4727243 a.u.

Structure:

C	3.11100000	-2.21370000	1.64070000
C	2.39290000	-2.79210000	2.61880000
C	1.07090000	-2.98710000	2.47610000
C	0.48090000	-2.59370000	1.33850000
C	1.19920000	-2.01650000	0.36080000
C	2.51750000	-1.82080000	0.50180000
C	-0.80430000	-2.67210000	0.95920000
C	-0.93850000	-2.14700000	-0.27010000
C	0.36370000	-1.63800000	-0.83700000
C	-1.86770000	-3.16650000	1.60890000
C	-3.06850000	-3.12530000	1.00700000
C	-3.20250000	-2.59900000	-0.22260000
C	-2.13550000	-2.10480000	-0.87140000
C	0.35000000	-0.15030000	-1.09830000
C	0.67770000	0.33590000	-2.30910000
C	0.66830000	1.65610000	-2.55030000
C	0.32860000	2.51410000	-1.57680000
C	-0.00040000	2.04360000	-0.36460000
C	0.01130000	0.72200000	-0.13120000
H	4.19510000	-2.05930000	1.77330000
H	2.89380000	-3.10900000	3.54920000
H	0.49520000	-3.46100000	3.28670000
H	3.09700000	-1.34440000	-0.30480000
H	0.66150000	-2.24720000	-1.72020000
H	-1.77340000	-3.59940000	2.61720000
H	-3.95400000	-3.52690000	1.52820000

H	-4.19510000	-2.57130000	-0.70290000
H	-2.23530000	-1.66980000	-1.87850000
H	0.95970000	-0.35320000	-3.12220000
H	0.93990000	2.03700000	-3.54920000
H	0.31990000	3.59940000	-1.77170000
H	-0.28070000	2.74370000	0.44020000
H	-0.26260000	0.35720000	0.87240000

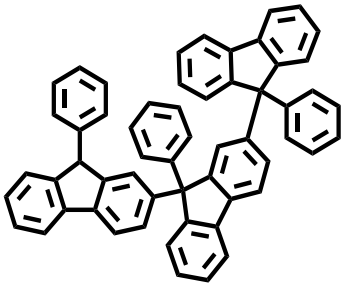


Energy: -1463.7369963 a.u.

Structure:

C	-3.79454500	3.65489200	-1.02176300
C	-3.52567200	2.34205800	-1.41854200
C	-3.30405800	1.33693500	-0.47122000
C	-3.35644300	1.67358300	0.88955700
C	-3.62351500	2.98116100	1.28833200
C	-3.84426100	3.97805000	0.33316600
C	-3.02044500	-0.09309900	-0.91057700
C	-1.71575100	-0.68945100	-0.38843300
C	-1.95845800	-1.92008700	0.24904400
C	-3.40106900	-2.19234700	0.21814100
C	-4.04355400	-1.12397800	-0.43972100
C	-0.42753400	-0.18119300	-0.49764000
C	0.65718900	-0.90385800	0.02575900
C	0.40234700	-2.13353800	0.66086900
C	-0.88950300	-2.64620000	0.77639400
C	-4.14425600	-3.26624400	0.71340400
C	-5.53127600	-3.25842800	0.55002500
C	-6.16775000	-2.19365900	-0.09750000
C	-5.42430600	-1.11808200	-0.59673500
C	3.94447100	-3.35335800	-1.46775000
C	2.95013400	-2.41986500	-1.17656700
C	3.16435500	-1.40403600	-0.23098300
C	4.41021300	-1.35131800	0.40803800
C	5.40652500	-2.28560600	0.11813500
C	5.17942300	-3.29177300	-0.82018500
C	2.08793700	-0.32249300	0.00959600
C	2.28355200	0.79157000	-1.03722600
C	2.57102600	2.02134000	-0.41612200
C	2.56926100	1.82661300	1.03815400
C	2.30015600	0.47269000	1.31250300
C	2.23529100	0.70150700	-2.42409500
C	2.46611300	1.84940900	-3.19015300
C	2.74900000	3.07232800	-2.57243400
C	2.80496900	3.16635700	-1.18078500
C	2.77704800	2.73503500	2.07840700
C	2.71358900	2.27880000	3.39622900

C	2.44211400	0.93378400	3.66928400
C	2.22994800	0.02458500	2.62717900
H	-3.96286200	4.42159900	-1.77368700
H	-3.48613200	2.09694900	-2.47783000
H	-3.18427000	0.90374200	1.63719000
H	-3.65867200	3.22442100	2.34714100
H	-4.05195900	4.99803600	0.64556200
H	-2.99451600	-0.09944600	-2.01068500
H	-0.26146100	0.77652700	-0.98057900
H	1.23284500	-2.70653900	1.06130800
H	-1.05053300	-3.60067500	1.27137100
H	-3.65624100	-4.09489600	1.22041600
H	-6.12247500	-4.08649200	0.93223100
H	-7.24841200	-2.20103500	-0.21208700
H	-5.92183200	-0.28797300	-1.09213400
H	3.75007400	-4.13210800	-2.20091200
H	1.99052600	-2.49168800	-1.67954000
H	4.60689500	-0.57442100	1.13920800
H	6.36272600	-2.22343800	0.63143500
H	5.95368400	-4.02094400	-1.04345400
H	2.02633300	-0.24624200	-2.91204000
H	2.42866100	1.78829800	-4.27449200
H	2.92898200	3.95505900	-3.18027100
H	3.02841900	4.11700100	-0.70332600
H	2.98289800	3.78169100	1.86909300
H	2.87302400	2.97425500	4.21600000
H	2.39168500	0.59169900	4.69951100
H	2.00903000	-1.01585900	2.84785900



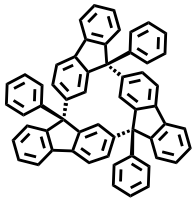
Energy: 194.9990723 a.u.

Structure:

C	2.80631600	-3.74711600	2.98969600
C	3.45954900	-2.60401400	2.52132600
C	3.39957800	-2.24499400	1.17050800
C	2.66090300	-3.05187800	0.29278700
C	2.01303200	-4.19431900	0.75581000
C	2.08542600	-4.54875100	2.10641500
C	4.16210700	-1.03133900	0.65877300
C	5.20001900	-1.35917500	-0.41236400
C	5.01583600	-0.54259800	-1.54521000
C	3.86885200	0.33986200	-1.30052300
C	3.33670400	0.05632800	-0.02870600
C	6.22310800	-2.29919300	-0.37658000
C	7.07378300	-2.41696000	-1.48157500
C	6.89594800	-1.60275100	-2.60584500

C	5.86655500	-0.65990500	-2.64684000
C	3.30263800	1.35072700	-2.07703200
C	2.23578800	2.08531500	-1.56298500
C	1.70725400	1.82978700	-0.28515800
C	2.25794500	0.77861400	0.47038800
C	-0.68659400	3.05887000	3.88104200
C	-0.68608100	2.81381900	2.50630400
C	0.50565000	2.82744800	1.76963000
C	1.69896900	3.10505700	2.45735700
C	1.70065700	3.35056100	3.83001400
C	0.50584600	3.32752800	4.55112800
C	0.50811000	2.66106200	0.23460300
C	0.46846700	4.06755400	-0.40191200
C	-0.66540500	4.21782800	-1.22094200
C	-1.43836500	2.97387200	-1.18242400
C	-0.79897100	2.06103700	-0.32446600
C	1.36850400	5.11738100	-0.25430100
C	1.13291200	6.31790400	-0.93309500
C	0.00610100	6.46595500	-1.74907000
C	-0.90202000	5.41652600	-1.89811700
C	-2.62707300	2.61842500	-1.81869700
C	-3.18431000	1.36632000	-1.56518200
C	-2.57811900	0.45583400	-0.68152400
C	-1.35765300	0.81095800	-0.07988500
C	-6.82679500	0.14612300	0.29913100
C	-5.43520100	0.13736800	0.21439300
C	-4.75462900	-0.89200700	-0.45672300
C	-5.51724800	-1.91526500	-1.03471800
C	-6.91142200	-1.90806200	-0.95093300
C	-7.57400900	-0.87820600	-0.28488700
C	-3.20733800	-0.93464700	-0.45423800
C	-2.63373400	-1.92101300	-1.48793400
C	-2.00984700	-3.01034700	-0.85148600
C	-2.10473400	-2.82483100	0.60105800
C	-2.76701200	-1.61037200	0.85935900
C	-2.66148000	-1.83971100	-2.87572200
C	-2.07466500	-2.86209100	-3.62973300
C	-1.46405700	-3.95073700	-2.99802500
C	-1.42617800	-4.03148200	-1.60462700
C	-1.66052300	-3.62837600	1.65287100
C	-1.87559800	-3.20472700	2.96504300
C	-2.52986200	-1.99564100	3.22206400
C	-2.98344500	-1.19465900	2.16871400
H	2.86751200	-4.01016300	4.04257600
H	4.02827100	-1.98695900	3.21374600
H	2.60325300	-2.78492400	-0.75907900
H	1.45369400	-4.81231100	0.05826000
H	1.58482600	-5.44452200	2.46492500
H	4.67525100	-0.58025200	1.52140300
H	6.35642800	-2.93971800	0.49173600
H	7.87753400	-3.14827600	-1.46732400
H	7.56432700	-1.70662900	-3.45660800
H	5.73192700	-0.03204300	-3.52404000
H	3.69297200	1.58318300	-3.06468600

H	1.81224900	2.88262900	-2.16399800
H	1.86161600	0.54895200	1.45492500
H	-1.62663500	3.03864900	4.42663600
H	-1.62527200	2.61114100	2.00360500
H	2.64032400	3.11609300	1.91674800
H	2.64027100	3.55862200	4.33561600
H	0.50590800	3.51552800	5.62147900
H	2.24299600	5.01539800	0.38136600
H	1.83113600	7.14320700	-0.82243000
H	-0.16469500	7.40525600	-2.26836700
H	-1.77913700	5.53415100	-2.52945100
H	-3.12695800	3.30785000	-2.49445200
H	-4.12183100	1.10071700	-2.04263100
H	-0.86194700	0.11206700	0.58642700
H	-7.32671100	0.95797400	0.82139500
H	-4.87211500	0.94998700	0.66300200
H	-5.02185500	-2.72792700	-1.55482000
H	-7.47769700	-2.71365600	-1.41139800
H	-8.65893300	-0.87129200	-0.22254100
H	-3.12825000	-0.99373900	-3.37258800
H	-2.09161800	-2.80761200	-4.71488800
H	-1.01219800	-4.73756000	-3.59625200
H	-0.95023700	-4.87835600	-1.11683800
H	-1.14847000	-4.56617500	1.45785700
H	-1.52924300	-3.81763900	3.79275800
H	-2.68976200	-1.67536000	4.24803800
H	-3.50207300	-0.26366300	2.37817700



***cis-cis*-TWG1**

Energy: -2193.7729125 a.u.

Structure:

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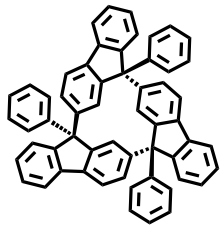
C	-2.89556600	1.79833000	-2.08381200
C	-1.90055200	2.56932100	-1.48516900
C	-1.21295900	2.06857000	-0.36404500
C	-1.56758500	0.84455400	0.17905900
C	-0.27581800	4.16299300	-0.94582000
C	-1.35670100	3.89358700	-1.81012800
C	-1.75709100	4.83782200	-2.75721400
C	-1.07744400	6.05628700	-2.82715000
C	-0.01550100	6.32907300	-1.95909300
C	0.39044400	5.38084700	-1.01176900
C	0.00000000	2.96619900	-0.01972300
C	0.08552100	3.40626500	1.44791700
C	1.32006900	3.70327000	2.04190900
C	1.38944500	4.17204000	3.35525900
C	0.22415200	4.35070900	4.10044700

C	-1.01128500	4.06040400	3.51868300
C	-1.07915600	3.59515200	2.20581100
C	1.23944100	-2.15873800	-0.47477500
C	1.13671700	-2.98845800	-1.60008900
C	-0.10961600	-3.40679900	-2.08381200
C	-1.27482200	-2.93058700	-1.48516900
C	-1.18495400	-2.08473800	-0.36404500
C	0.05238700	-1.77984600	0.17905900
C	-3.46734900	-2.32036200	-0.94582000
C	-2.69359500	-3.12173100	-1.81012800
C	-3.31113100	-3.94059600	-2.75721400
C	-4.70617600	-3.96123800	-2.82715000
C	-5.47338700	-3.17796100	-1.95909300
C	-4.85517200	-2.35228900	-1.01176900
C	-2.56880400	-1.48310000	-0.01972300
C	-2.99267300	-1.62906900	1.44791700
C	-3.86716100	-0.70842200	2.04190900
C	-4.30781500	-0.88272600	3.35525900
C	-3.87990100	-1.98123300	4.10044700
C	-3.01077000	-2.90600000	3.51868300
C	-2.57391500	-2.73215300	2.20581100
C	1.24980100	2.15275600	-0.47477500
C	2.01972200	2.47865500	-1.60008900
C	3.00518300	1.60846900	-2.08381200
C	3.17537300	0.36126500	-1.48516900
C	2.39791300	0.01616800	-0.36404500
C	1.51519800	0.93529200	0.17905900
C	3.74316700	-1.84263100	-0.94582000
C	4.05029600	-0.77185600	-1.81012800
C	5.06822200	-0.89722600	-2.75721400
C	5.78362000	-2.09504900	-2.82715000
C	5.48888800	-3.15111200	-1.95909300
C	4.46472800	-3.02855800	-1.01176900
C	2.56880400	-1.48310000	-0.01972300
C	2.90715100	-1.77719600	1.44791700
C	3.65307100	-0.86299900	2.20581100
C	4.02205500	-1.15440300	3.51868300
C	3.65574800	-2.36947600	4.10044700
C	2.91837000	-3.28931400	3.35525900
C	2.54709100	-2.99484800	2.04190900
H	-3.87695500	-0.10920900	-2.12286600
H	-3.44147200	2.16659200	-2.94884800
H	-1.09499600	0.49897900	1.08894100
H	-2.59120100	4.63576900	-3.42436600
H	-1.38279600	6.80195300	-3.55647100
H	0.49581200	7.28629300	-2.01548200
H	1.20949500	5.60033200	-0.33194700
H	2.23530200	3.55637800	1.47626800
H	2.35865900	4.39237600	3.79543500
H	0.27725300	4.70949800	5.12487200
H	-1.92732400	4.19361000	4.08849200
H	-2.04600400	3.37287800	1.76417800
H	2.03305600	-3.30293700	-2.12286600
H	-0.15558800	-4.06369800	-2.94884800

H	0.11536900	-1.19778400	1.08894100
H	-2.71909300	-4.56193100	-3.42436600
H	-5.19926600	-4.59851400	-3.55647100
H	-6.55802100	-3.21376100	-2.01548200
H	-5.45477700	-1.75271300	-0.33194700
H	-4.19756400	0.15763900	1.47626800
H	-4.98323800	-0.15353000	3.79543500
H	-4.21717100	-2.11464100	5.12487200
H	-2.66811100	-3.76591700	4.08849200
H	-1.89799600	-3.45833000	1.76417800
H	1.84390000	3.41214600	-2.12286600
H	3.59706000	1.89710600	-2.94884800
H	0.97962700	0.69880500	1.08894100
H	5.31029400	-0.07383800	-3.42436600
H	6.58206300	-2.20344000	-3.55647100
H	6.06220900	-4.07253200	-2.01548200
H	4.24528300	-3.84761900	-0.33194700
H	3.94400000	0.08545200	1.76417800
H	4.59543500	-0.42769300	4.08849200
H	3.93991800	-2.59485700	5.12487200
H	2.62458000	-4.23884600	3.79543500
H	1.96226300	-3.71401700	1.47626800



cis-trans-TWG1

Energy: -2193.7684481 a.u.

Structure:

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C	2.23630800	-0.34240700	3.97324500
C	4.84958900	-4.56309000	4.86821600
C	3.04969300	-0.84381900	4.99910900
C	6.87969800	-3.71427500	5.88834100
C	5.77193900	0.92342200	4.50328600
H	5.22839600	1.74040000	4.04052100
C	5.91771700	-0.83352900	6.15399200
H	5.49172000	-1.38331600	6.98745100
C	7.66063300	-0.57560900	4.48943600
C	3.05087000	2.85134900	5.56302400
H	3.67170200	3.16108800	6.39925200
C	8.72741300	-2.45670000	7.20798700
C	3.80574600	-6.26988200	2.11730100
H	3.35599900	-6.99149200	2.79075600
C	3.38232100	-2.18845500	5.04211200
H	4.00667600	-2.55345500	5.84350600
C	7.90599300	-2.54695900	5.90076500
C	2.66278900	-5.46405500	4.69512400

C	2.13808100	1.11459100	4.13034200
C	1.75140900	-1.21687900	2.99475900
H	1.11056300	-0.85656500	2.19382300
C	8.69740300	-1.31870700	8.02388400
H	8.06260100	-0.48191500	7.75630600
C	8.78297500	-1.35932900	3.96330300
C	7.01501700	0.55315800	3.98236400
H	7.42677200	1.09692500	3.13584100
C	5.53323200	-5.40607200	7.03018700
H	5.36682800	-6.02454400	7.90866400
C	8.88213800	-2.55769400	4.70012000
C	3.27270100	-5.97405100	5.85856200
C	6.64048400	-4.54996300	6.98913000
H	7.29238400	-4.50560800	7.85332300
C	3.60168000	-4.49302000	3.95992900
C	3.96592000	-4.93972000	2.52969300
C	3.33254200	0.23525000	7.34683100
C	3.01327200	-3.05392100	4.00288800
C	2.31922700	3.80102600	4.83967400
H	2.38159800	4.85066900	5.11387500
C	3.65800500	0.29694900	5.84766000
C	9.47865800	-1.23626100	9.17983200
H	9.43356800	-0.33794000	9.79021200
C	5.17916400	0.20553900	5.55283800
C	2.15769200	-2.55499600	3.00383900
H	1.84650800	-3.20337400	2.19017800
C	7.12070300	-1.24899600	5.59874400
C	4.60902800	-5.38023600	5.98717400
C	4.13813600	0.90987700	8.27629800
H	5.03738000	1.41630700	7.93670600
C	2.58508400	-6.86178000	6.68878800
H	3.05259900	-7.25650500	7.58732200
C	0.67475200	-6.72246500	5.19785400
H	-0.34059400	-7.01752100	4.94701400
C	4.56284200	-4.03922800	1.63214500
H	4.69604200	-3.00114000	1.91911200
C	9.78286000	-3.54069800	4.30365700
H	9.84315600	-4.49022500	4.82623500
C	4.21754800	-6.68435800	0.84927100
H	4.07714800	-7.72132500	0.55475500
C	4.80371900	-5.77846900	-0.03389600
H	5.12204900	-6.10054400	-1.02182200
C	1.40795300	2.06280700	3.41145500
H	0.76975100	1.76125100	2.58472600
C	10.30797900	-2.29252300	9.54869100
H	10.91503100	-2.22931900	10.44780100
C	9.57166400	-3.51255400	7.59364000
H	9.61824900	-4.41424900	6.99200200
C	9.61553300	-1.12282600	2.86785800
H	9.53915200	-0.19663100	2.30384300
C	1.36194100	-5.82977000	4.36734500
H	0.88177900	-5.43128600	3.47760900
C	1.28334000	-7.23531600	6.34838100
H	0.73746500	-7.92713500	6.98439600

C	1.50472600	3.40855900	3.77289700
H	0.93925900	4.15594700	3.22262300
C	10.34898900	-3.43552700	8.74745400
H	10.98973000	-4.27071300	9.01854100
C	2.18757800	-0.42318900	7.81427500
H	1.55033200	-0.95221600	7.11243100
C	10.53787500	-2.10212500	2.49540200
H	11.19094400	-1.93325400	1.64336300
C	10.61111700	-3.30740100	3.19981300
H	11.31441200	-4.07427000	2.88662500
C	1.85874400	-0.41041000	9.17041000
H	0.96806600	-0.93254300	9.51033400
C	4.97646600	-4.45265200	0.36594100
H	5.43401300	-3.73336500	-0.30847200
C	3.80945600	0.92565800	9.63219500
H	4.45089300	1.45227200	10.33426700
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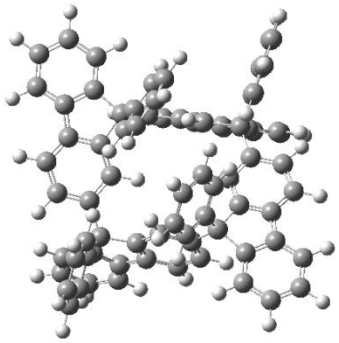
H	2.41306300	0.27077300	11.14228300



SWGs-F

Energy: -2925.0446609 a.u.

Structure:

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C	-1.93378600	-4.10604600	-0.31132800
C	-1.15084000	-2.94209700	-0.27009000
C	-1.70356700	-1.72630800	0.12403100
C	0.26801900	-4.79574000	-0.67168200
C	-1.05864600	-5.25704500	-0.55491700
C	-1.34702300	-6.62171800	-0.60858300
C	-0.29606900	-7.52858000	-0.75973500
C	1.02338100	-7.07434000	-0.84631500
C	1.31143700	-5.70489800	-0.80615800
C	0.30391700	-3.25045400	-0.67421000
C	0.60284100	-2.81325500	-2.13350500
C	-0.37203900	-2.25079700	-2.96528800
C	-0.08453000	-1.92143800	-4.29330800
C	1.18577400	-2.14632300	-4.81790200
C	2.17161200	-2.70158700	-3.99844100
C	1.88091400	-3.03145200	-2.67696300
C	-1.27030200	2.62610800	0.34698300
C	-1.28278100	3.12410400	1.66222500

C	-2.02167900	2.50382100	2.66490200
C	-2.76914600	1.36504200	2.35475700
C	-2.79260000	0.87261700	1.04117400
C	-2.04879400	1.49741200	0.04442400
C	-4.18314700	-0.49373100	2.39738900
C	-3.60878700	0.51304800	3.19794700
C	-3.87123600	0.58160400	4.56787500
C	-4.71952000	-0.36569500	5.14189800
C	-5.29772000	-1.36314200	4.35137900
C	-5.03397200	-1.42994100	2.97852600
C	-3.74374200	-0.33728600	0.92111300
C	-4.92153000	0.07598700	0.00096800
C	-6.04874100	0.73512300	0.51138400
C	-7.06972000	1.17090900	-0.33440100
C	-6.98457800	0.96072500	-1.71093500
C	-5.86480000	0.31214400	-2.23240000
C	-4.84564600	-0.12485200	-1.38538400
C	-1.02338400	7.07433300	-0.84627400
C	0.29606400	7.52857400	-0.75967100
C	1.34701800	6.62171400	-0.60851600
C	1.05864300	5.25703900	-0.55486800
C	-0.26801900	4.79573400	-0.67165100
C	-1.31143800	5.70489000	-0.80613400
C	1.15083900	2.94208700	-0.27007100
C	1.93378300	4.10603800	-0.31128800
C	3.30776100	4.02319700	-0.07711600
C	3.86516500	2.79034800	0.25277600
C	3.07487400	1.63506200	0.41201200
C	1.70356700	1.72629300	0.12403400
C	-0.30391600	3.25044800	-0.67419400
C	-0.60283700	2.81327800	-2.13349900
C	0.37203500	2.25079100	-2.96527200
C	0.08453800	1.92147200	-4.29330500
C	-1.18574400	2.14642900	-4.81792200
C	-2.17157200	2.70172700	-3.99847100
C	-1.88088600	3.03155300	-2.67698100
C	5.29771200	1.36311400	4.35138900
C	4.71950500	0.36566700	5.14190400
C	3.87122100	-0.58162900	4.56787700
C	3.60877700	-0.51307100	3.19794800
C	4.18314300	0.49370800	2.39739300
C	5.03396900	1.42991400	2.97853400
C	2.79259900	-0.87263600	1.04117100
C	2.76913700	-1.36506200	2.35475400
C	2.02166600	-2.50383800	2.66489500
C	1.28276800	-3.12411800	1.66221600
C	1.27029800	-2.62612200	0.34697400
C	2.04879800	-1.49743000	0.04441700
C	3.74374100	0.33726700	0.92111600
C	4.92152900	-0.07599900	0.00096900
C	6.04874200	-0.73513500	0.51138400
C	7.06972300	-1.17091500	-0.33440300
C	6.98458200	-0.96072400	-1.71093600
C	5.86480100	-0.31214400	-2.23239900

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H	-4.93862400	-2.72430200	0.39551400
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H	-1.06852200	-0.85401000	0.22237800
H	-2.37070000	-6.97674300	-0.52020300
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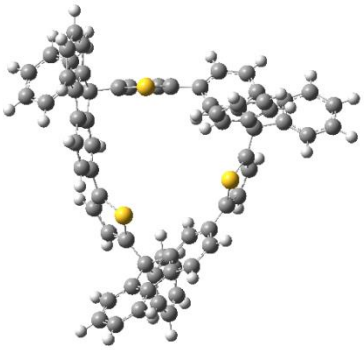
H	1.83541300	-7.78999100	-0.94320900
H	2.34228100	-5.36904800	-0.86685700
H	-1.36879000	-2.06680100	-2.58156700
H	-0.86198000	-1.48115200	-4.91170700
H	1.40883300	-1.89146900	-5.85069700
H	3.17111600	-2.87961000	-4.38671200
H	2.66624400	-3.44918600	-2.05527800
H	-0.68644300	3.99971100	1.90215000
H	-2.00636400	2.90142200	3.67644200
H	-2.06443600	1.10807900	-0.96668300
H	-3.42056600	1.35908200	5.17942800
H	-4.93224900	-0.32728300	6.20695400
H	-5.95989400	-2.09601400	4.80453800
H	-5.49806700	-2.21212400	2.38799200
H	-6.13284300	0.90968300	1.57879500
H	-7.93530600	1.67453900	0.08856100
H	-7.78196600	1.29598000	-2.36890600
H	-5.78186900	0.13926100	-3.30247100
H	-3.98666300	-0.63553400	-1.80898700
H	-1.83541600	7.78998300	-0.94317300
H	0.50397700	8.59457900	-0.79755800
H	2.37069300	6.97673900	-0.52012200
H	-2.34228000	5.36903700	-0.86685500
H	3.94047000	4.90486400	-0.14115800
H	4.93862000	2.72429000	0.39555000
H	1.06852300	0.85399200	0.22236500
H	1.36876900	2.06673900	-2.58153300
H	0.86198000	1.48116200	-4.91169700
H	-1.40879300	1.89160700	-5.85072700
H	-3.17105800	2.87980900	-4.38676100
H	-2.66620600	3.44931900	-2.05530600
H	5.95988500	2.09598300	4.80455100
H	4.93223100	0.32725300	6.20696000
H	3.42054700	-1.35910700	5.17942700
H	5.49806700	2.21209700	2.38800200
H	2.00634500	-2.90144000	3.67643500
H	0.68642600	-3.99972300	1.90213800
H	2.06444600	-1.10809900	-0.96669100
H	6.13284500	-0.90970000	1.57879300
H	7.93531000	-1.67454400	0.08855700
H	7.78197000	-1.29597300	-2.36890900
H	5.78187100	-0.13925600	-3.30246900
H	3.98666100	0.63552700	-1.80898300



TWGs-Th

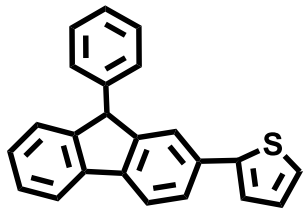
Energy: -3849.22100722 a.u.

Structure:

C	-3.53000800	0.10632600	-1.56889200
C	-3.48342300	-0.73234300	-2.65580300
C	-3.46472600	-2.11537800	-2.31231400
C	-3.52147100	-2.35181900	-0.96109200
S	-3.59454600	-0.83143700	-0.08911200
C	3.34776400	2.33428400	0.54699700
C	4.05819000	2.60987100	1.73104600
C	5.06135400	1.75441700	2.18731000
C	5.35413200	0.59427700	1.46435700
C	4.66367400	0.32517500	0.26948500
C	3.68591600	1.18668500	-0.19617200
C	6.24838300	-0.53367600	1.75197000
C	6.08505200	-1.50825200	0.74763600
C	5.06792800	-1.04636000	-0.31158800
C	7.12587500	-0.75684300	2.81546600
C	7.83242200	-1.96025700	2.86735300
C	7.65914800	-2.93183800	1.87550400
C	6.77856300	-2.71064200	0.81039200
C	2.19106100	3.12497400	0.10119200
C	1.81975400	3.43736000	-1.18510500
C	0.51950100	3.99965000	-1.27986600
C	-0.13025700	4.11103800	-0.07420600
S	0.90999800	3.55422500	1.21827700
C	5.68750600	-0.85351400	-1.71492500
C	7.07425100	-0.75192900	-1.89033300
C	7.62285500	-0.49201200	-3.14783800
C	6.79680000	-0.32401700	-4.25804400
C	5.41360800	-0.41556300	-4.09670500
C	4.86651700	-0.67535900	-2.84047400
C	-3.47868800	1.57639900	-1.55497200
C	-4.21451700	2.32684000	-2.49247500
C	-4.08638900	3.71258500	-2.56386900
C	-3.22011600	4.36617700	-1.68383100
C	-2.51115300	3.63216900	-0.71542100
C	-2.63296600	2.25193900	-0.65313400
C	-2.79570800	5.76874200	-1.61968900
C	-1.81071600	5.89803700	-0.62279900
C	-1.58334400	4.56379200	0.10757300
C	-3.16311700	6.86807200	-2.39969600

C	-2.52898300	8.09273600	-2.18289500
C	-1.53092300	8.21404000	-1.20974000
C	-1.16349300	7.11347300	-0.42729900
C	-2.04852400	4.60651000	1.58731100
C	-2.01615000	3.44257200	2.37524700
C	-2.45916400	3.44864300	3.69699800
C	-2.95943900	4.61948800	4.26716500
C	-3.01133800	5.77838300	3.49613700
C	-2.56326000	5.77117400	2.17307100
C	0.37631500	-3.48604100	0.77736500
C	0.21153200	-3.63909600	2.16794900
C	-1.04977900	-3.81451700	2.73179100
C	-2.17002900	-3.82978800	1.89886000
C	-2.01687400	-3.70254500	0.50634900
C	-0.75921000	-3.53443100	-0.05598300
C	-3.59949500	-3.88613600	2.21719200
C	-4.33517200	-3.75204200	1.02463200
C	-3.38964900	-3.66828900	-0.19696200
C	-4.25200600	-4.00997100	3.44567200
C	-5.64724800	-3.99148100	3.47296500
C	-6.37814100	-3.84676200	2.28915200
C	-5.72469900	-3.72793800	1.05775600
C	1.69828500	-3.17312500	0.20853600
C	2.34038900	-3.68468200	-0.89236800
C	3.57094700	-3.02584900	-1.19104400
C	3.86526000	-1.99012200	-0.33830900
S	2.61993000	-1.84665400	0.88242400
C	-3.63958700	-4.89110900	-1.10940800
C	-4.77002600	-4.93763000	-1.94251800
C	-5.05000600	-6.06353200	-2.71539800
C	-4.20749700	-7.17568800	-2.67128600
C	-3.08608600	-7.14567600	-1.84460300
C	-2.80604400	-6.01615400	-1.07180200
H	-3.41546200	-0.36703400	-3.67528600
H	-3.39409100	-2.90865200	-3.04680200
H	3.81221700	3.50161200	2.30132600
H	5.58630600	1.98179800	3.11151300
H	3.11630200	0.94916900	-1.08840000
H	7.25568200	-0.01059900	3.59508400
H	8.51813100	-2.14631900	3.68969100
H	8.20918800	-3.86712800	1.93406600
H	6.63739600	-3.47010400	0.04586600
H	2.46123100	3.25485600	-2.04126400
H	0.06115800	4.29196600	-2.21874300
H	7.73578300	-0.87537800	-1.04019500
H	8.70233100	-0.42204700	-3.25445900
H	4.75387300	-0.28613900	-4.95089800
H	3.78920800	-0.75196800	-2.73817300
H	-4.88629600	1.80930000	-3.17111600
H	-4.64544200	4.27104100	-3.31036900
H	-2.03125900	1.66793400	0.03500600
H	-3.92214000	6.77253300	-3.17189600
H	-2.80395000	8.95558700	-2.78362700
H	-1.03295400	9.16859900	-1.06296100

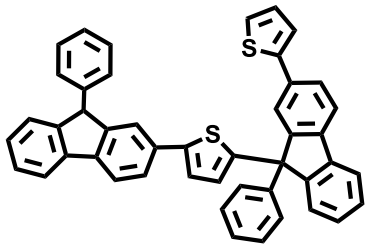
H	-0.37952600	7.20804700	0.31931700
H	-1.64171200	2.51370700	1.96253500
H	-2.41661700	2.53072300	4.27711600
H	-3.40432300	6.69945100	3.91893700
H	-2.62590200	6.68588900	1.59666200
H	1.08877200	-3.61108800	2.80810100
H	-1.15475700	-3.91385000	3.80897800
H	-0.64646700	-3.37629900	-1.12477800
H	-3.68543800	-4.11477300	4.36739200
H	-6.16948300	-4.08570600	4.42128300
H	-7.46393400	-3.82606800	2.32439200
H	-6.30334400	-3.61755900	0.14581800
H	1.94464900	-4.51088900	-1.47439400
H	4.20365800	-3.29706000	-2.02863600
H	-5.43282400	-4.08038600	-1.99888900
H	-5.92999700	-6.06936900	-3.35350300
H	-2.42015300	-8.00335700	-1.79565400
H	-1.93012400	-6.01644500	-0.43294800
H	7.22417300	-0.12486500	-5.23714100
H	-3.30748400	4.62555400	5.29658800
H	-4.42387100	-8.05336200	-3.27440000



Energy: -1284.28601943 a.u.
Structure:

C	-3.96654200	-0.90016800	-0.66624500
C	-4.68341600	-2.03981400	-0.28400100
C	-4.02162500	-3.14919100	0.25443800
C	-2.63562300	-3.13888600	0.42398700
C	-1.91864100	-2.00094900	0.04598500
C	-2.58670900	-0.88697600	-0.50234100
C	-0.48454500	-1.69858400	0.11292200
C	-0.27210600	-0.39914300	-0.39024000
C	-1.58955100	0.21132500	-0.86187600
C	0.59989800	-2.45304600	0.56505500
C	1.87748400	-1.89966400	0.52346100
C	2.10253800	-0.59927900	0.02769200
C	0.99989500	0.14693400	-0.43912100
C	3.44784000	-0.01382000	-0.00330000
C	-1.90554200	1.58577500	-0.28869800
C	-2.08607100	2.68517900	-1.13474900
C	-2.37510800	3.95014400	-0.61530700
C	-2.48724100	4.12959200	0.76240700
C	-2.30891600	3.03736800	1.61700300
C	-2.02121100	1.77791700	1.09615900
C	3.80583400	1.31494800	0.05105600

C	5.21238800	1.53417400	-0.00683000
C	5.92709300	0.37236400	-0.10610800
S	4.88540500	-1.01369300	-0.13822600
H	-2.71204200	5.11151400	1.17020500
H	-4.48376200	-0.03693200	-1.07766400
H	-5.76312000	-2.06276000	-0.40485000
H	-4.59250000	-4.02678000	0.54616400
H	-2.12810300	-4.00263600	0.84602700
H	-1.55642000	0.31131800	-1.95719900
H	0.45741400	-3.45646600	0.95778700
H	2.71725500	-2.47535400	0.90283200
H	1.15564900	1.14148700	-0.84750000
H	-2.00030000	2.55146100	-2.21110900
H	-2.51215000	4.79151700	-1.28968200
H	-2.39480800	3.16839300	2.69261600
H	-1.88478800	0.93281500	1.76593800
H	3.07974000	2.11309700	0.16119000
H	5.67102200	2.51644100	0.03347900
H	6.99969100	0.24477100	-0.16471700



Energy: -2567.36377595 a.u.

Structure:

C	-8.05337900	1.72168900	0.30304200
C	-8.60171200	2.76463600	-0.45242400
C	-7.79436800	3.52572300	-1.30544900
C	-6.42904700	3.25725900	-1.42214900
C	-5.88025200	2.21454000	-0.67115700
C	-6.69452200	1.45342100	0.19288400
C	-4.50867500	1.70170000	-0.59163900
C	-4.47863200	0.62672400	0.31965300
C	-5.86298700	0.40228300	0.92330000
C	-3.33306700	2.09078400	-1.23618300
C	-2.15137400	1.40455500	-0.96927800
C	-2.10610900	0.32338400	-0.06387600
C	-3.30383100	-0.05660800	0.58121500
C	-0.85717400	-0.39661900	0.20951400
C	-6.38877700	-1.02304700	0.82211200
C	-6.71853600	-1.74337500	1.97515800
C	-7.20061900	-3.05251400	1.88962200
C	-7.35839300	-3.65785700	0.64401400
C	-7.03214200	-2.94680200	-0.51484600
C	-6.55203000	-1.64223100	-0.42613300
C	-0.64411100	-1.46818300	1.04931400
C	0.70670300	-1.90681000	1.09530000
C	1.55225600	-1.17592300	0.29738000

S	0.66245800	0.07791300	-0.53387100
C	2.59393500	-3.65949100	-1.37785700
C	2.79149900	-4.33797200	-2.58568200
C	3.49629900	-3.73506100	-3.63374300
C	4.01254000	-2.44581000	-3.49319900
C	3.81806500	-1.76929800	-2.28627300
C	3.11605100	-2.38025600	-1.23047700
C	4.22016500	-0.42540200	-1.86592500
C	3.75575100	-0.19572200	-0.55816400
C	3.02103100	-1.43960500	-0.01290000
C	4.93403400	0.57361700	-2.53151200
C	5.17429500	1.78374400	-1.88943300
C	4.71540200	2.03082400	-0.57756200
C	4.00013700	1.00902500	0.08123800
C	4.98520200	3.31878600	0.07276800
C	3.77767700	-1.97011500	1.22743300
C	3.53642900	-1.42067500	2.49666300
C	4.27345000	-1.82929300	3.60794600
C	5.27010700	-2.79719300	3.47484200
C	5.52123300	-3.34801300	2.21888700
C	4.78403300	-2.93746600	1.10637900
C	5.67393400	4.40917700	-0.41548900
C	5.74704200	5.50235900	0.49286100
C	5.11344200	5.24961600	1.67800800
S	4.41520700	3.66489800	1.69970700
H	-7.73257100	-4.67574000	0.57350100
H	5.84290300	-3.11839400	4.34069400
H	-8.68389400	1.12732400	0.95969400
H	-9.66328600	2.98436700	-0.37698100
H	-8.23517700	4.33246000	-1.88518900
H	-5.80793200	3.85034100	-2.08861400
H	-5.82593100	0.66325100	1.99166200
H	-3.32910900	2.91723700	-1.94213200
H	-1.24294600	1.71344700	-1.47889900
H	-3.30894200	-0.88857000	1.27879100
H	-6.59817900	-1.27609700	2.95035100
H	-7.45162000	-3.59519300	2.79737600
H	-7.15212800	-3.41134600	-1.49016200
H	-6.30000600	-1.09456700	-1.33054700
H	-1.43097200	-1.93501900	1.63110900
H	1.04519200	-2.73393000	1.70933300
H	2.03495300	-4.12568800	-0.57123600
H	2.38948300	-5.33952400	-2.71202600
H	3.63822200	-4.27327800	-4.56711500
H	4.55180100	-1.97728800	-4.31243100
H	5.30169200	0.41632800	-3.54219000
H	5.72894200	2.55340300	-2.41607700
H	3.64319600	1.16381300	1.09517500
H	2.75633100	-0.67640700	2.62025800
H	4.06470700	-1.38954800	4.57979300
H	6.29394300	-4.10286900	2.09800900
H	4.99699300	-3.37609500	0.13755100
H	6.12200200	4.43473200	-1.40220900
H	6.25109000	6.43681100	0.27062000

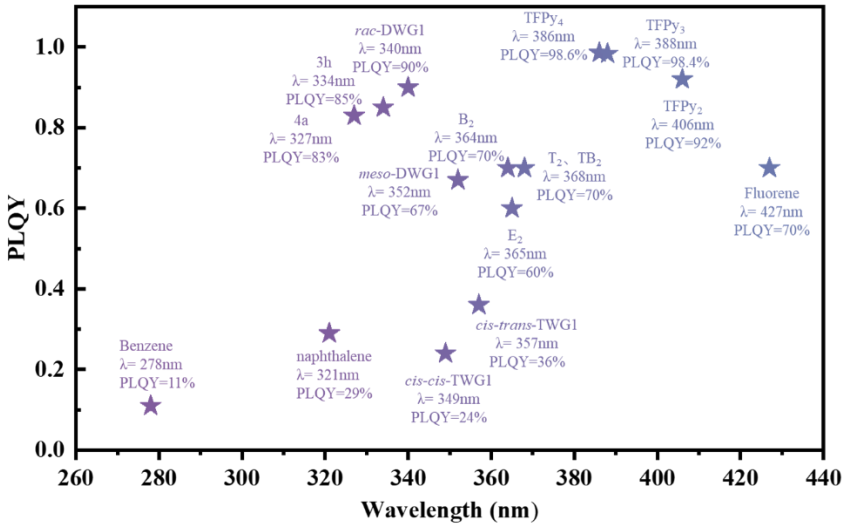
H	5.01276500	5.89603700	2.53941700

Section 6. Strain and aggregate effects of DWGs and TWGs.

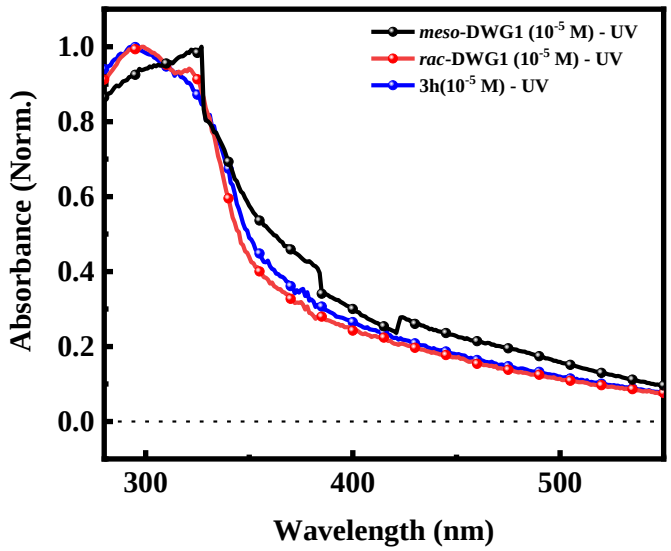
Supplementary Table 19 | Summary of physical for all substrates and products.

λ: First absorption peak in solution (1*10^{-5}M in THF). $\lambda_{max,sol,}$ PL: PL peaks in solutions (1*10^{-5}M in THF). $\lambda_{max,crystal,}$ PL: PL peaks in film (5 mg/ml in THF). QY_{sol}: quantum yield in solution (1*10^{-5}M in THF). QY_{film}: quantum yield in film (5 mg/ml in THF).

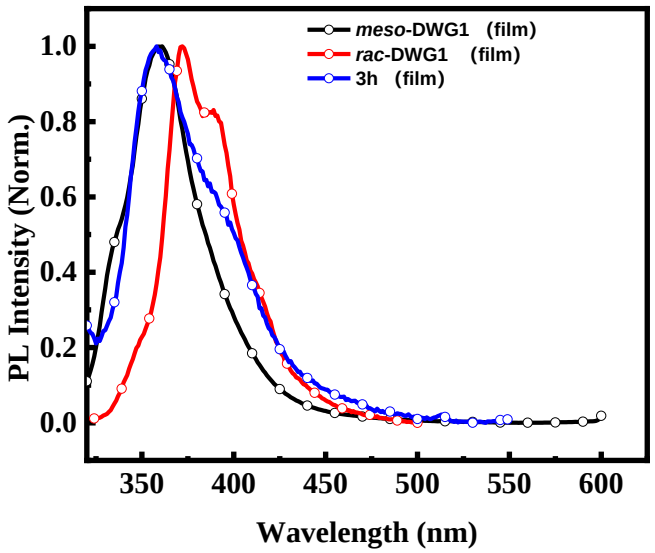
sample	λ	$\lambda_{max,sol,}$ PL	$\lambda_{max,film,}$ PL	$\lambda_{max,crystal,}$ PL	QY_{sol}	QY_{film}	$QY_{crystal}$	CIE_{film}	$CIE_{crystal}$
3h	317	334	358		85	6			
rac-DGW1	315	340	370	370	90	15	28	(0.163, 0.014)	(0.163, 0.014)
meso-DGW1	320	352	360	375	67	20	25	(0.170, 0.047)	(0.155, 0.093)
4a	313	327	334		83	11	-		
cis-cis-TWG1	323	349	392	361	24	25	8	(0.157, 0.022)	(0.161, 0.027)
cis-trans-TWG1	320	357	371	375	36	17	13	(0.163, 0.032)	(0.161, 0.044)



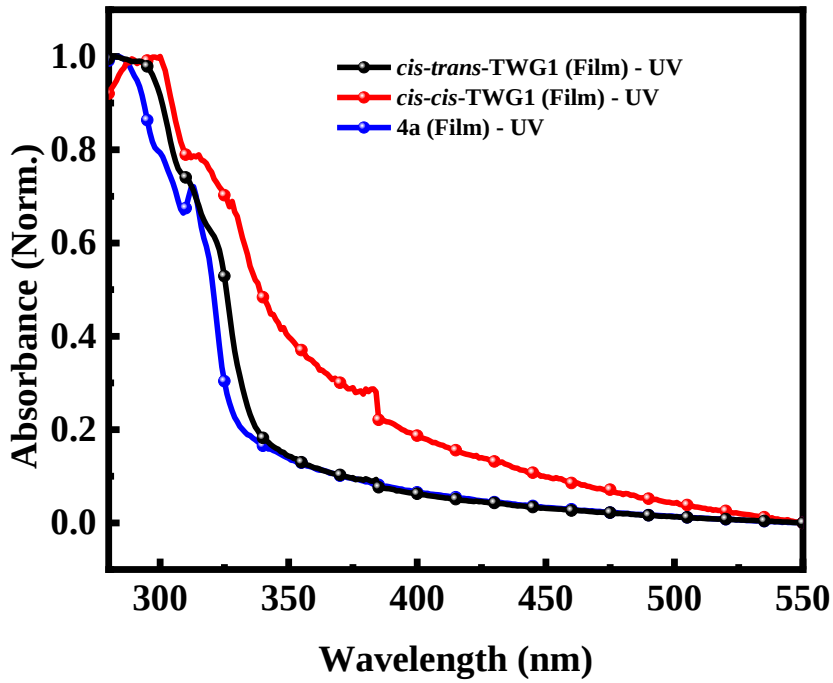
Supplementary Fig. 22 | Summary of physical for all substrates, products and other ultraviolet luminescent material. (Benzene, naphthalene and fluorene[1]; B_2, T_2, TB_2 and E_2[2]; $TFPy_2$, $TFPy_3$ and $TFPy_4$[3].)



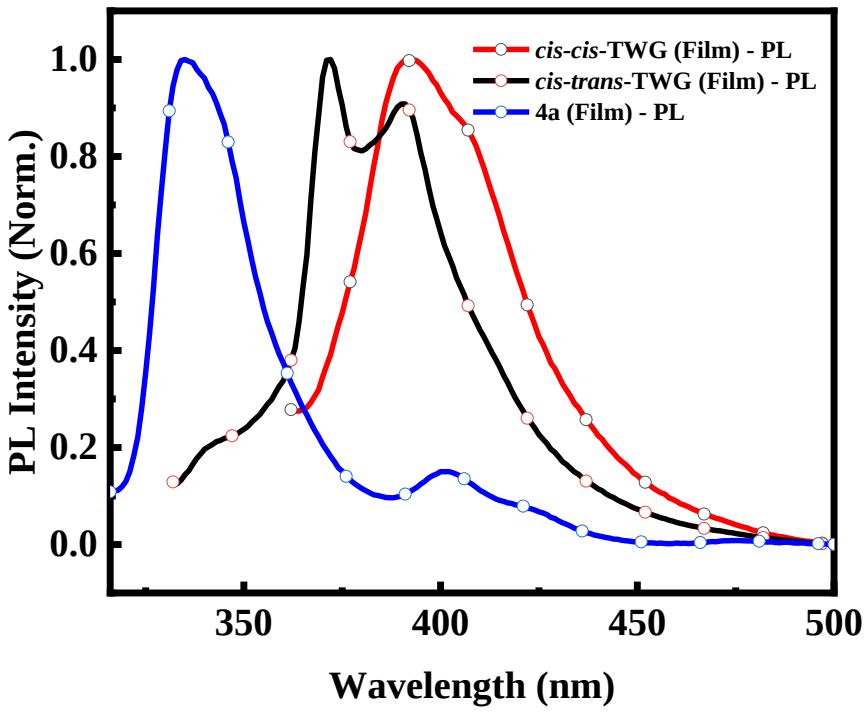
Supplementary Fig. 23 ｜UV-vis absorbance spectra of *meso*-DWG1, *rac*-DWG1 and 3h in film.



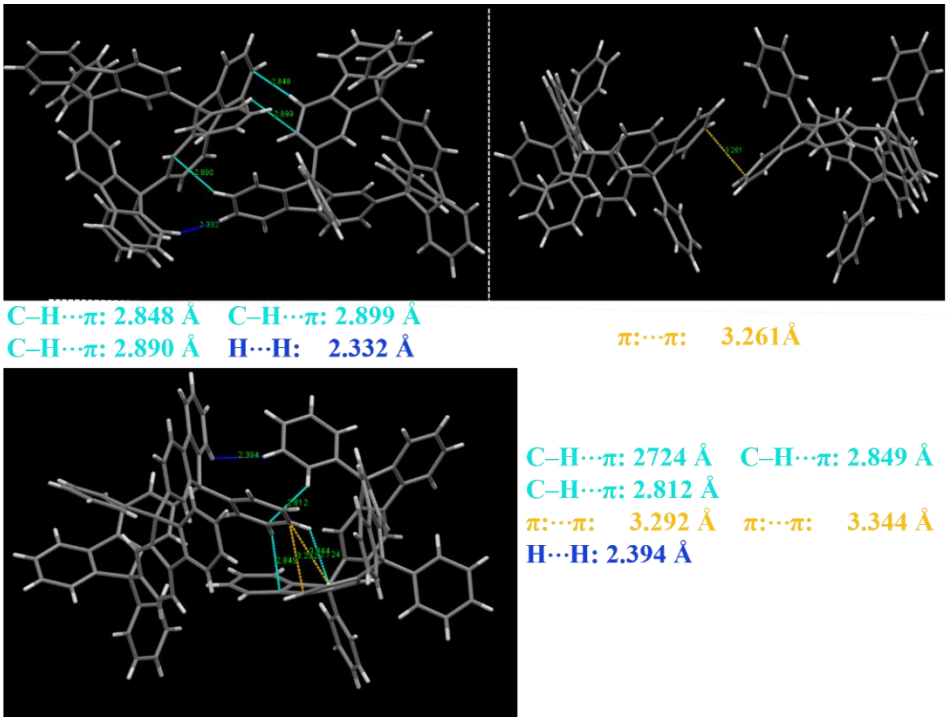
Supplementary Fig. 24 ｜PL spectra of *meso*-DWG1, *rac*-DWG1 and 3h in film.



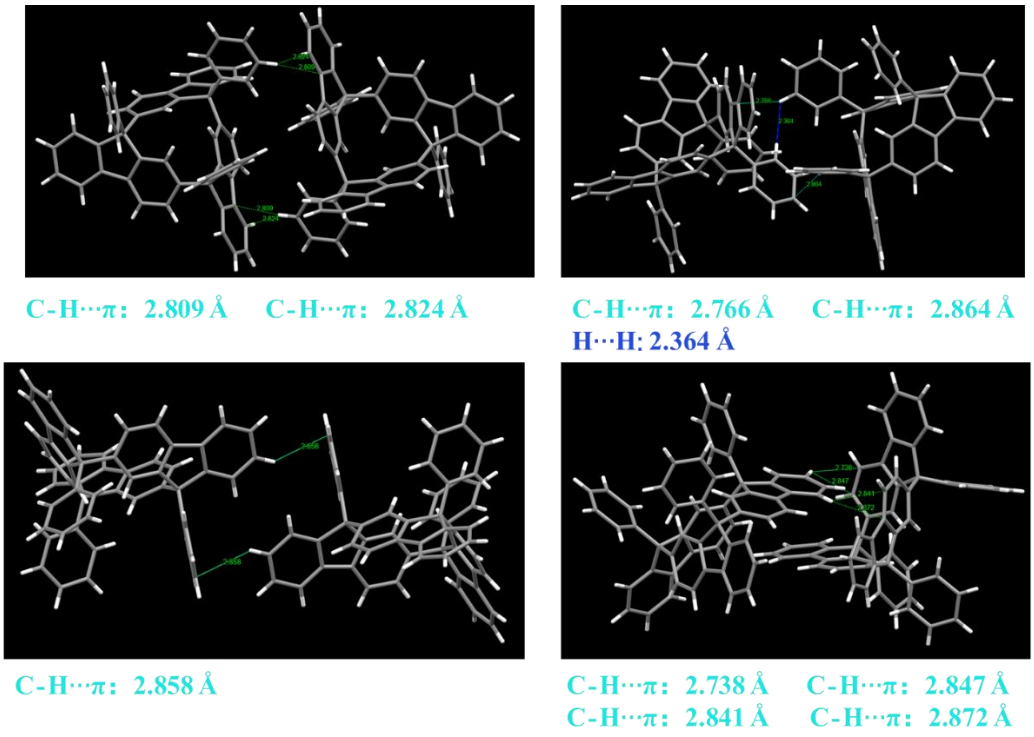
Supplementary Fig. 25 | UV-vis absorbance spectra of *cis-trans*-TWG1, *cis-cis*-TWG1 and 4a in film.



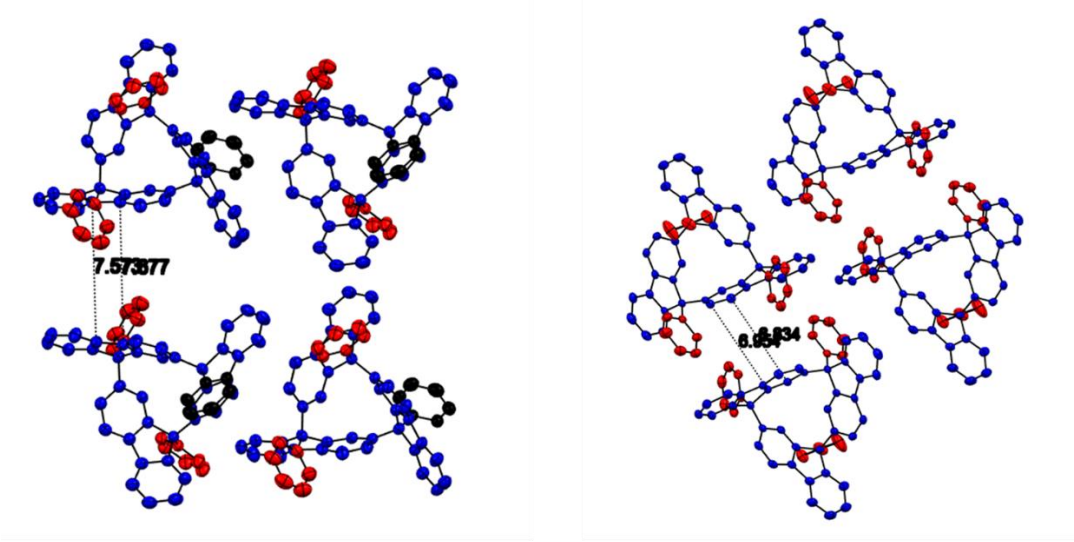
Supplementary Fig. 26 | PL spectra of *cis-trans*-TWG1, *cis-cis*-TWG1 and 4a in film.



Supplementary Fig. 27 | The intermolecular interactions for *cis-trans*-TWG1. In the intermolecular interactions of *cis-trans*-TWG1, interactions include C–H···π interactions (2.724 Å, 2.812 Å, 2.848 Å, 2.849 Å, 2.890 Å and 2.899 Å), π···π interactions (3.261 Å, 3.292 Å and 3.344 Å) and H···H (2.332 Å and 2.394 Å) interactions in repeating units of respective octamers. C–H···π interactions mainly exist between phenyl and fluorene (2.899 Å, 2.724 Å, 2.849 Å, 2.812 Å) and the vertexes between adjacent fluorenes (2.848 Å, 2.890 Å). Then, π···π stacking at the vertexes between adjacent fluorenes (3.261 Å) and between fluorene and phenyl (292 Å, 3.344 Å). One H···H interaction exists between H(1) and H(3) of a fluorene unit (2.332 Å) and another H···H interaction exists between fluorene and phenyl with the distance of 2.394 Å.

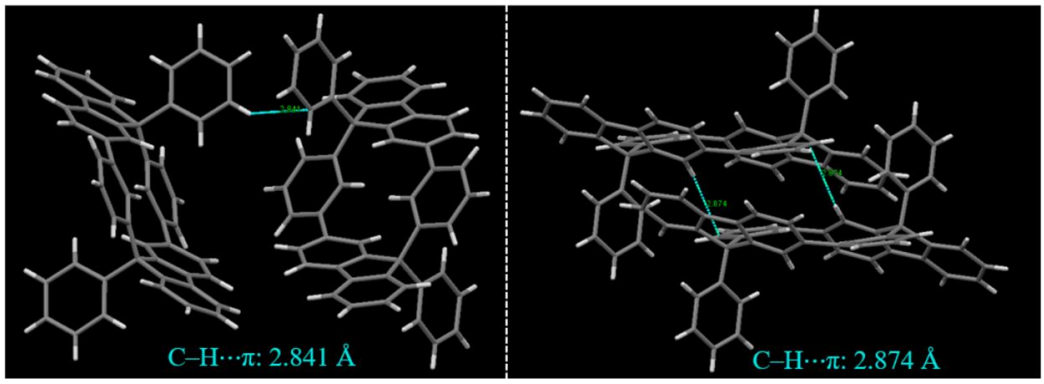


Supplementary Fig. 28 | The intermolecular interactions for *cis-cis*-TWG1. The intermolecular interactions for cis-cis-TWG1. In the intermolecular interactions of cis-cis-TWG1, interactions include C–H···π interactions (2.809 Å, 2.824 Å, 2.766 Å, 2.864 Å, 2.858 Å, 2.738 Å, 2.847 Å, 2.841 Å, 2.872 Å) and H···H interaction (2.364 Å). C–H ···π interactions mainly exist between phenyl and fluorene (2.808Å, 2.824 Å, 2.766 Å, 2.864 Å, 2.858 Å) and the vertexes between adjacent fluorenes (2.738Å, 2.847 Å, 2.841 Å, 2.872 Å). H···H interaction only exists in phenyl unit with the distance of 2.364 Å.

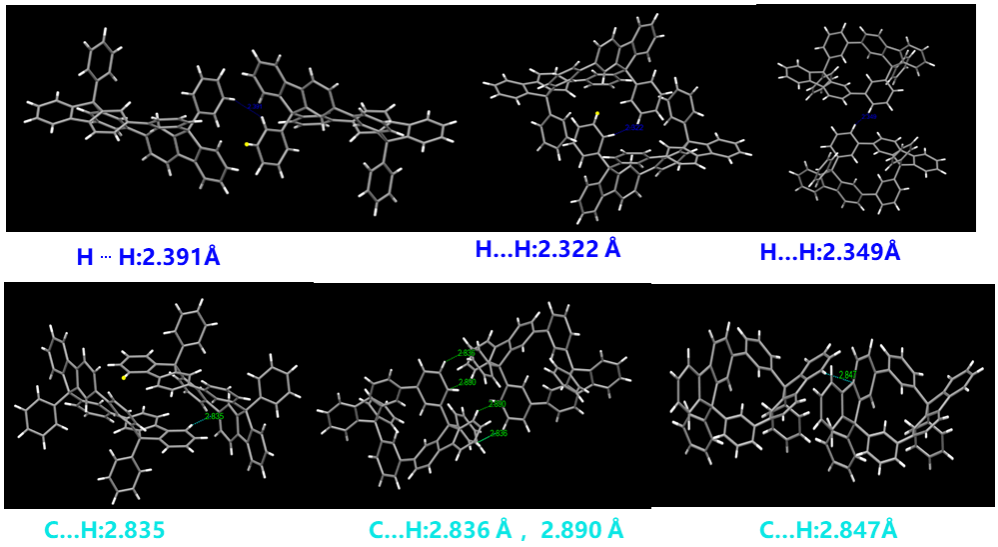


Supplementary Fig. 29 | The distances between the overlapping fluorene units of TWGs. these distance are7.5~7.7 Å in *cis-trans*-TWG1, and 6.6~7.0 Å in *cis-cis*-

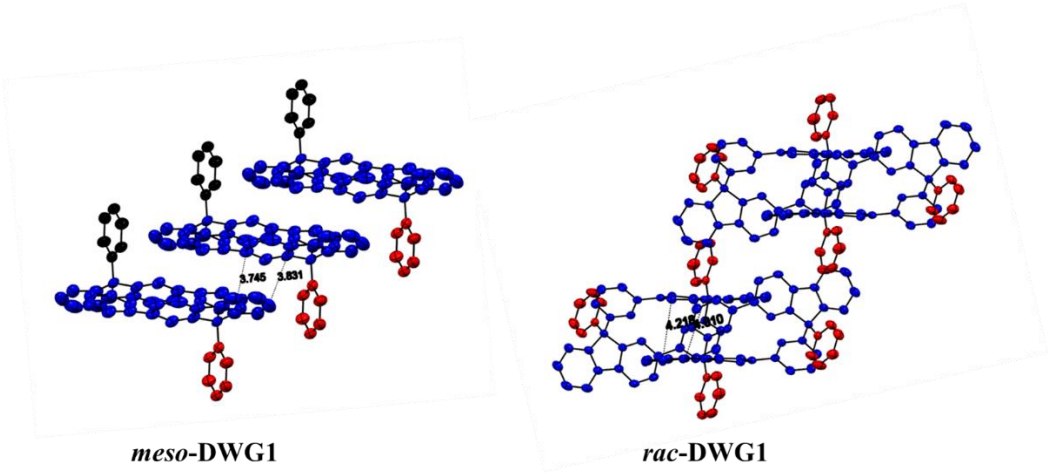
TWG1.



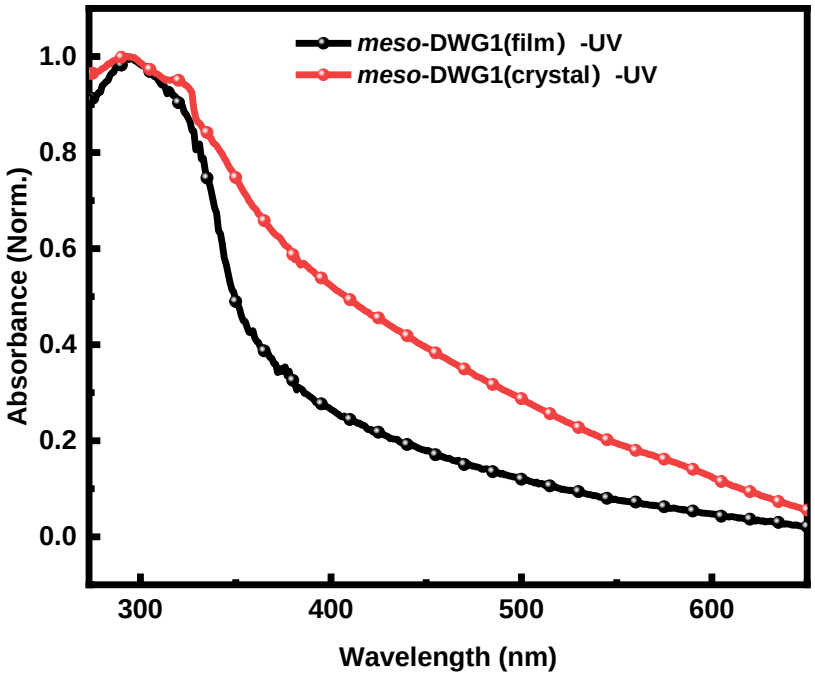
Supplementary Fig. 30 | The intermolecular interactions for *meso*-DWG1. In the intermolecular interactions of *meso*-DWG, interactions include only one typr of C–H···π interactions (2.841 Å, 2.874 Å). C–H···π interactions mainly exist between branched phenyl and phenyl (2.841 Å) and the vertexes between adjacent fluorenes and phenyl (2.847 Å).



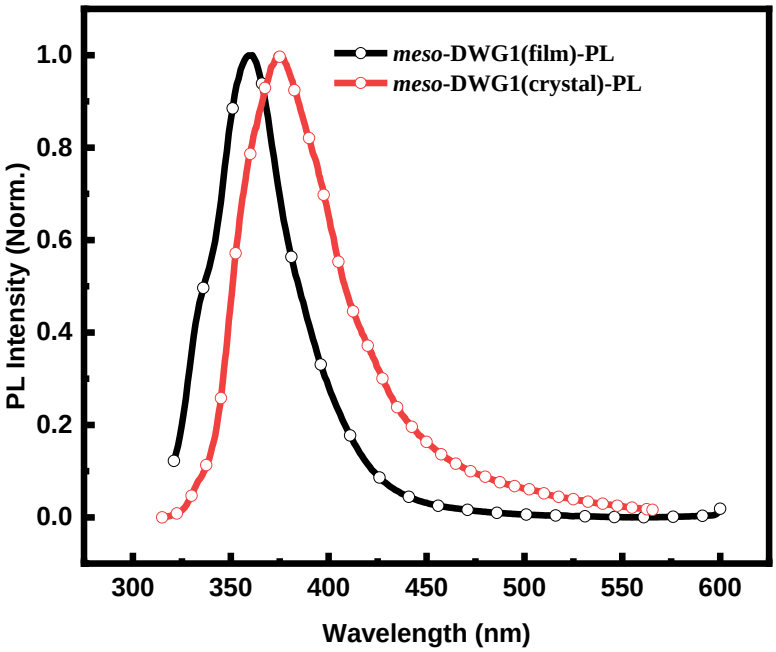
Supplementary Fig. 31 | The intermolecular interactions for *rac*-DWG1. The intermolecular interactions for *rac*-DWG1. In the intermolecular interactions of *rac*-DWG1, interactions include C–H···π interactions (2.835Å, 2.836 Å, 2.890 Å, 2.847 Å) and H···H interaction (2.391 Å, 2.322 Å, 2.394 Å). C–H···π interactions mainly exist between fluorene and fluorene (2.835Å, 2.847 Å), branched phenyl and backbone phenyl (2.836 Å) and between backbone phenyl and fluorenes (2.349 Å). H···H interaction exists in branched phenyl and phenyl (2.391 Å, 2.322 Å) and between backbone phenyl and phenyl (2.349 Å).



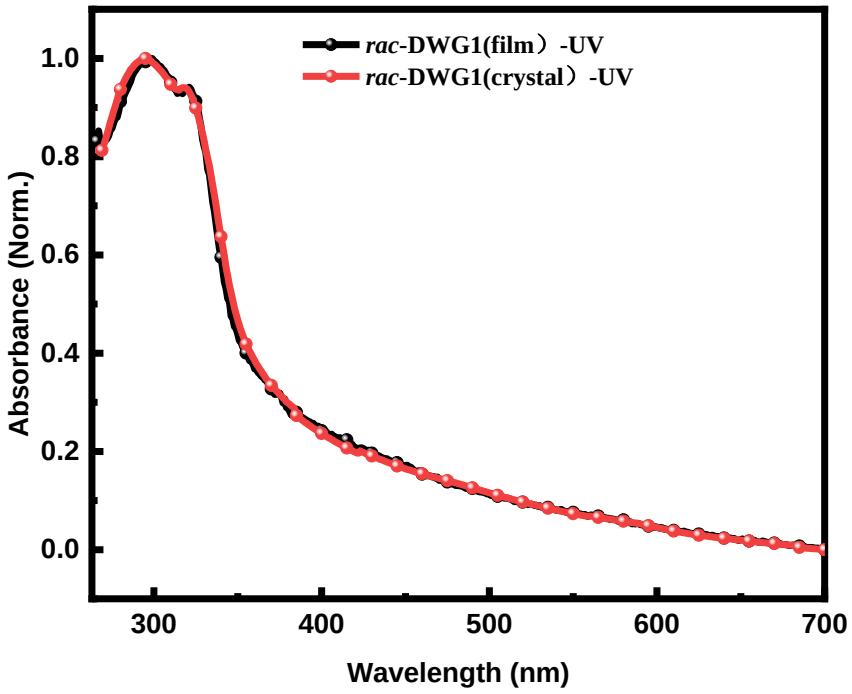
Supplementary Fig. 32 | The distances between the overlapping fluorene units of DWGs. these distance are 3.7~3.8 Å in *meso*-DWG1, 4.0~4.2Å in *rac*-DWG1.



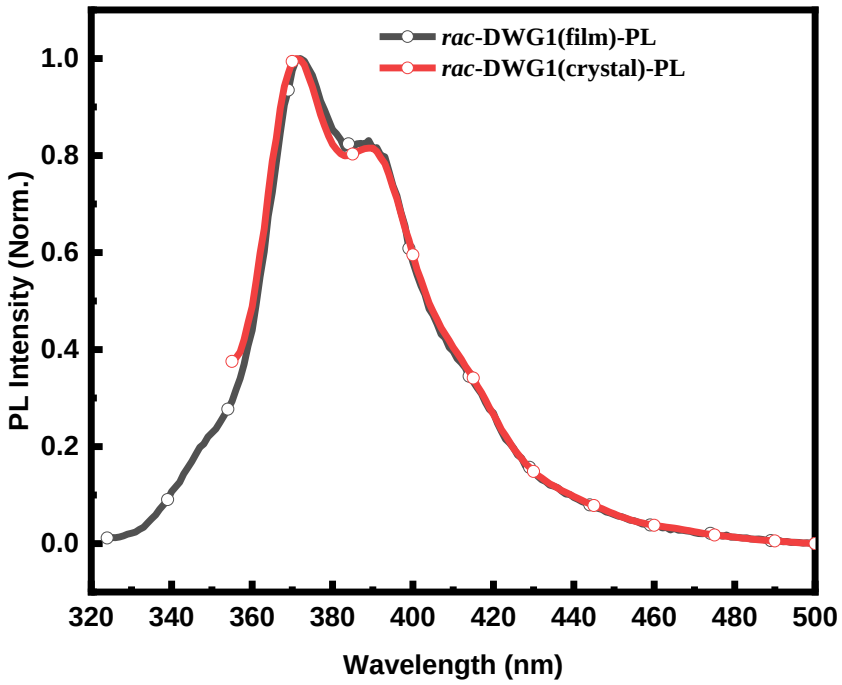
Supplementary Fig. 33 | UV-vis absorbance spectra of *meso*-DWG1 in single crystal and film.



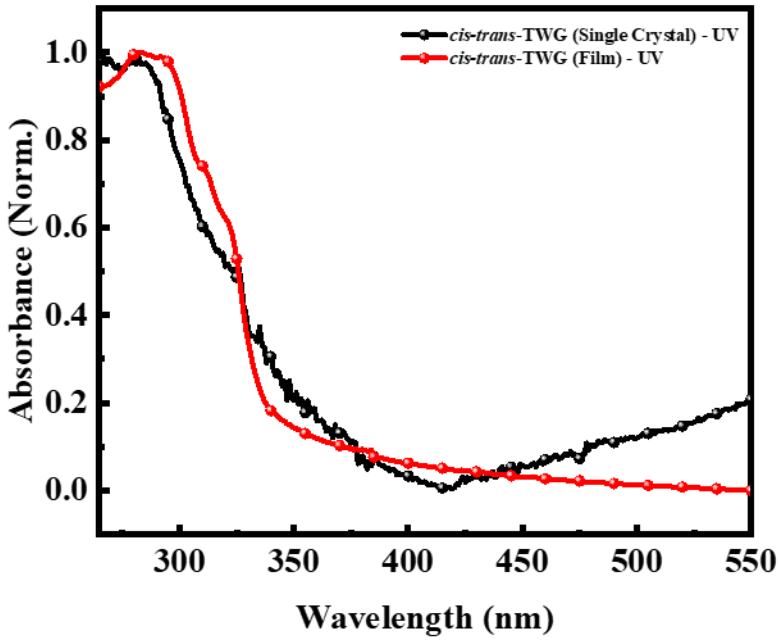
Supplementary Fig. 34 | PL spectra of *meso*-DWG1 in single crystal and film.



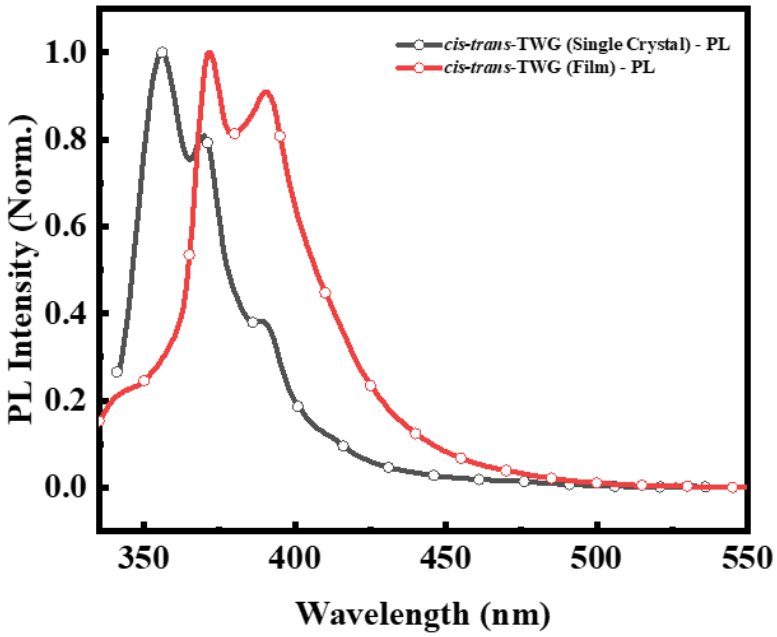
Supplementary Fig. 35 | UV-vis absorbance spectra of *rac*-DWG1 in single crystal and film.



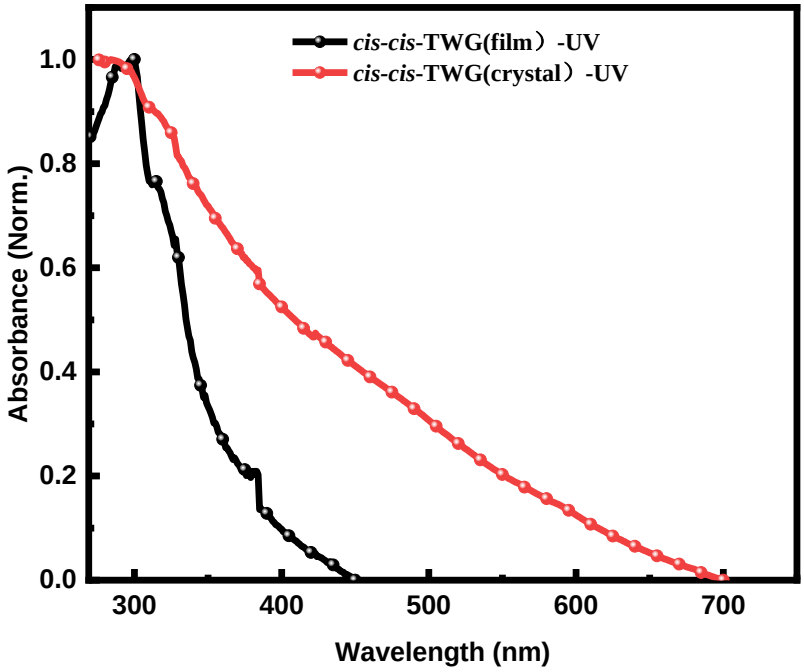
Supplementary Fig. 36 | PL spectra of *rac*-DWG1 in single crystal and film.



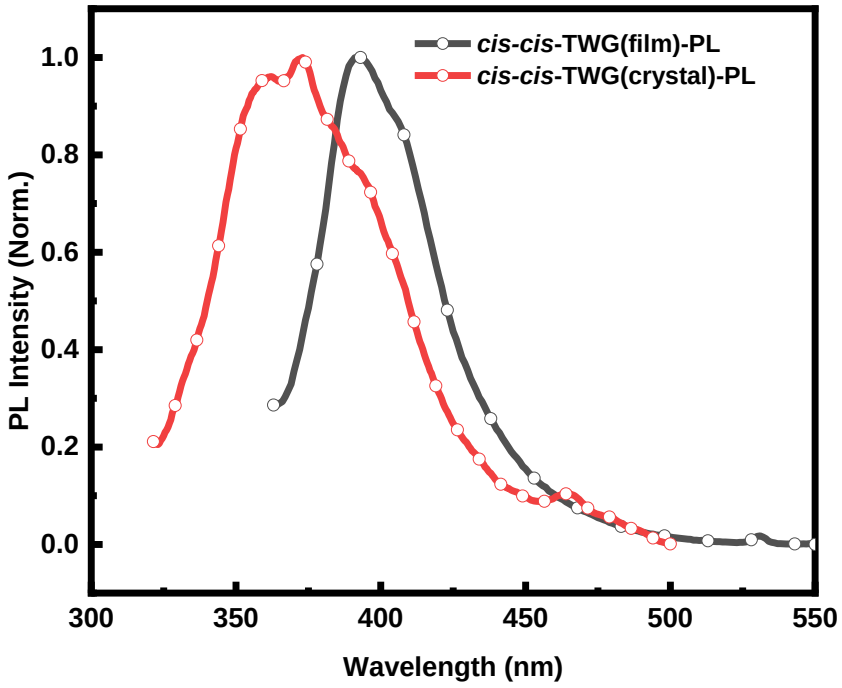
Supplementary Fig. 37 | UV-vis absorbance spectra of *cis-trans*-TWG1 in single crystal and film.



Supplementary Fig. 38 | PL spectra of *cis-trans*-TWG1 in single crystal and film.

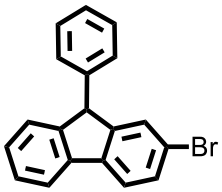


Supplementary Fig. 39 | UV-vis absorbance spectra of *cis-cis*-TWG1 in single crystal and film.

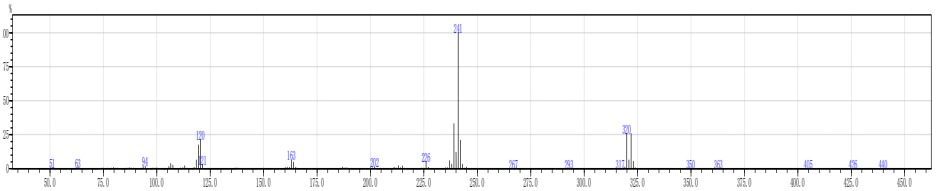


Supplementary Fig. 40 ｜PL spectra of *cis-cis*-TWG1 in single crystal and film.

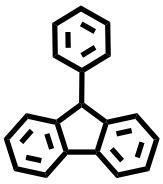
Section 7. GC-MS, MALDI-TOF-MS and NMR spectra for all substrates and products.



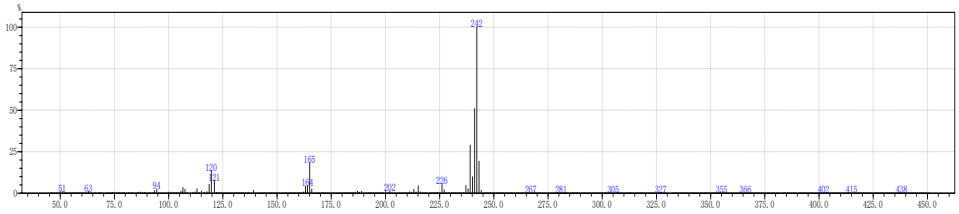
1a



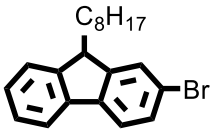
Supplementary Figure. 41 ｜GC-MS spectrum of 1a.

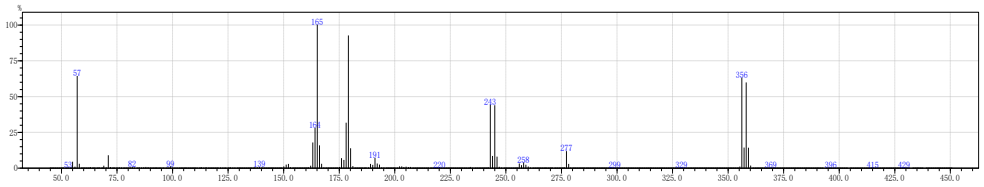


2a

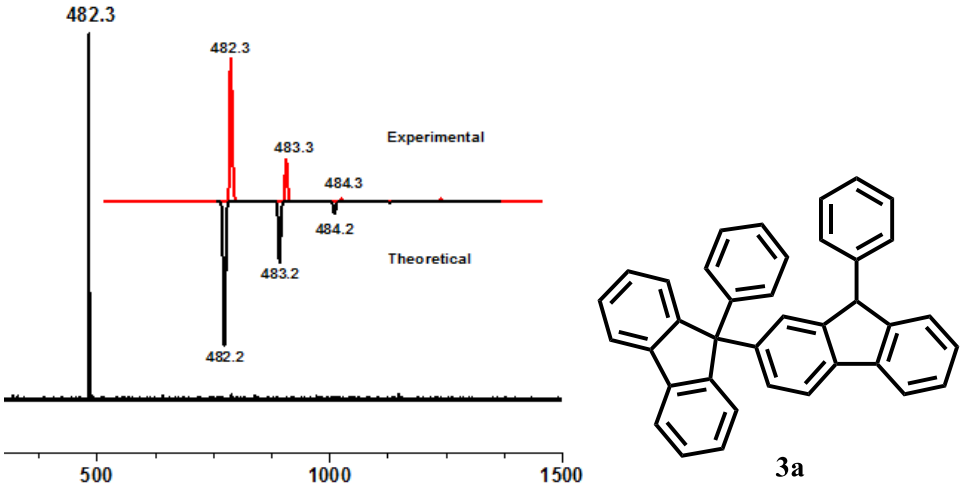


Supplementary Figure. 42 ｜GC-MS spectrum of 9-phenyl-fluorene.

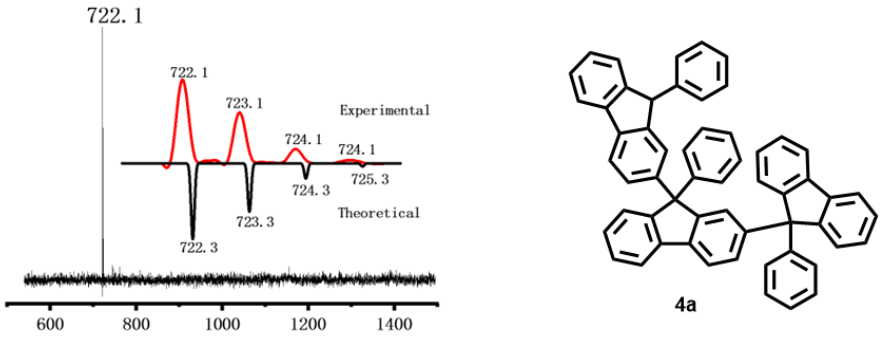




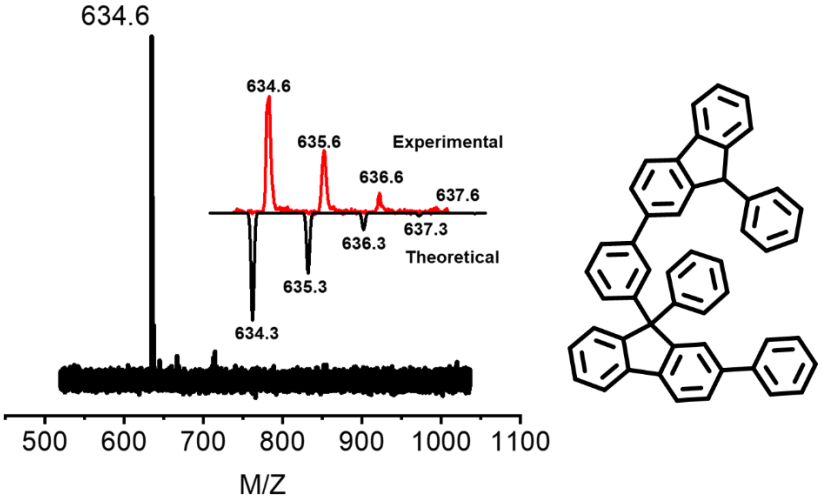
Supplementary Supplementary Fig. 43 ｜GC-MS spectrum of 2-bromo-9-octylfluorene**.**



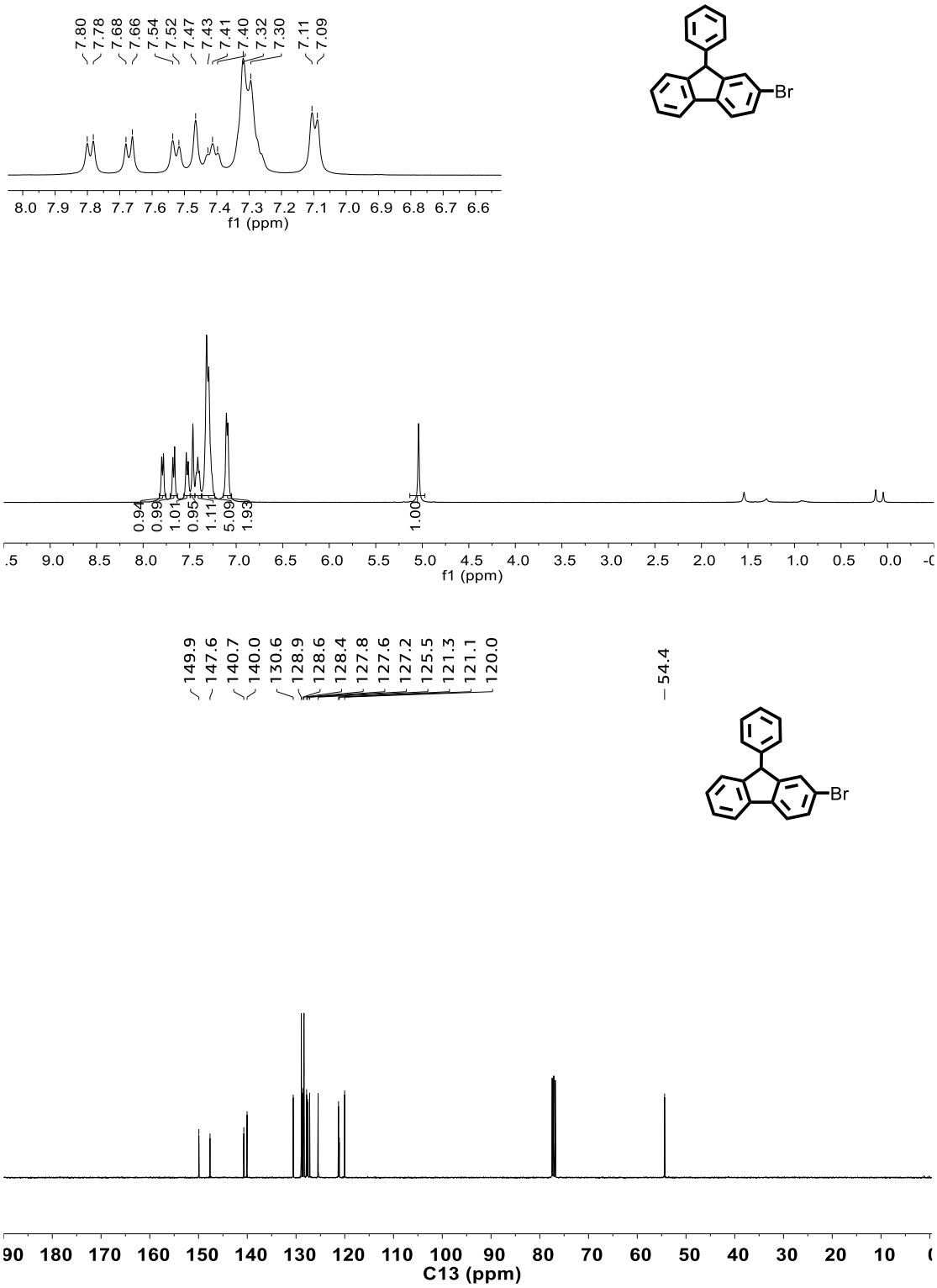
Supplementary Supplementary Fig. 44 ｜MALDI-TOF-MS spectrum of 9-9'-diphenyl-9*H*,9'*H*-2,9'-bifluorene.



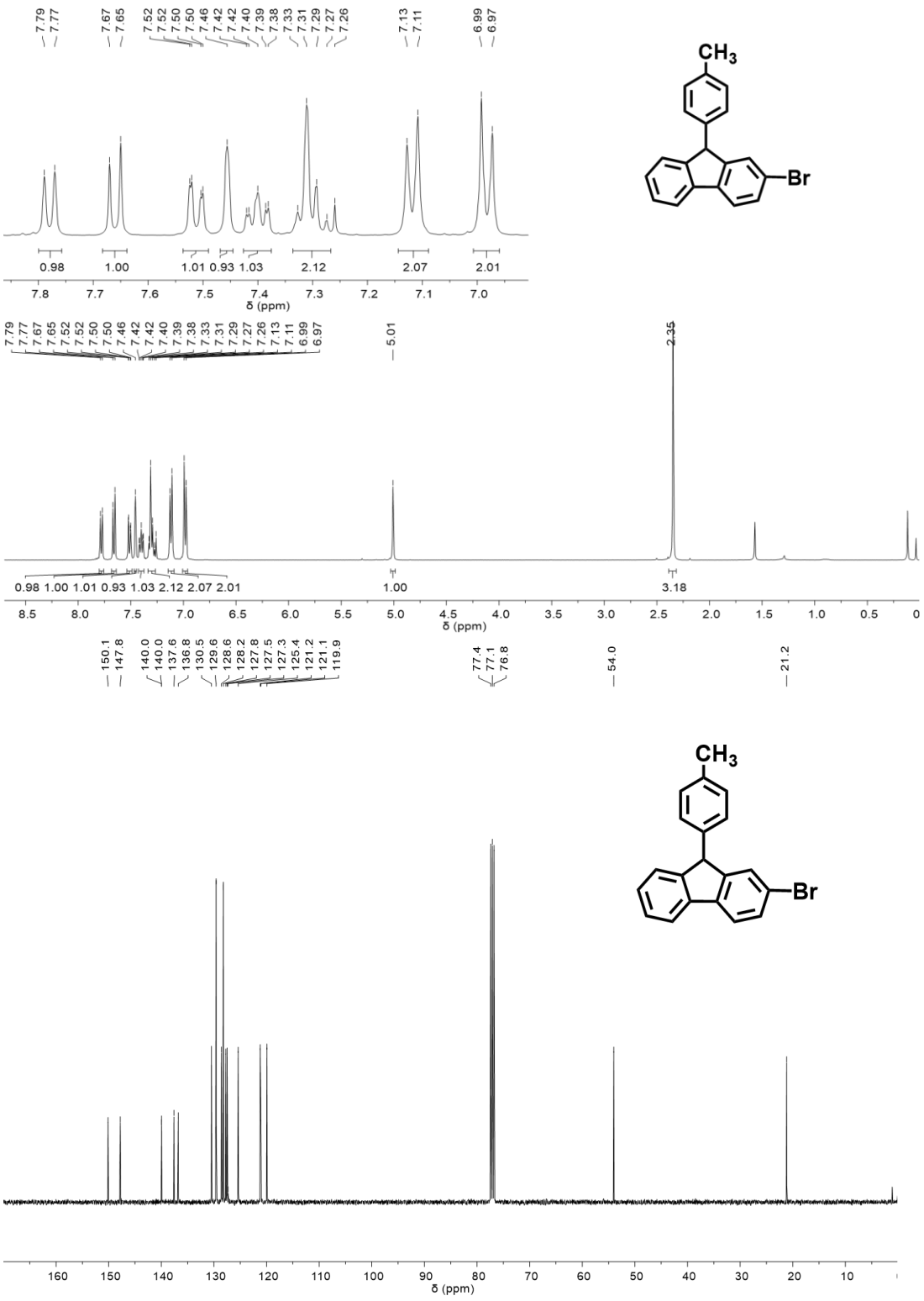
Supplementary Supplementary Fig. 45 | MALDI-TOF spectrum of trimerized product (4a).



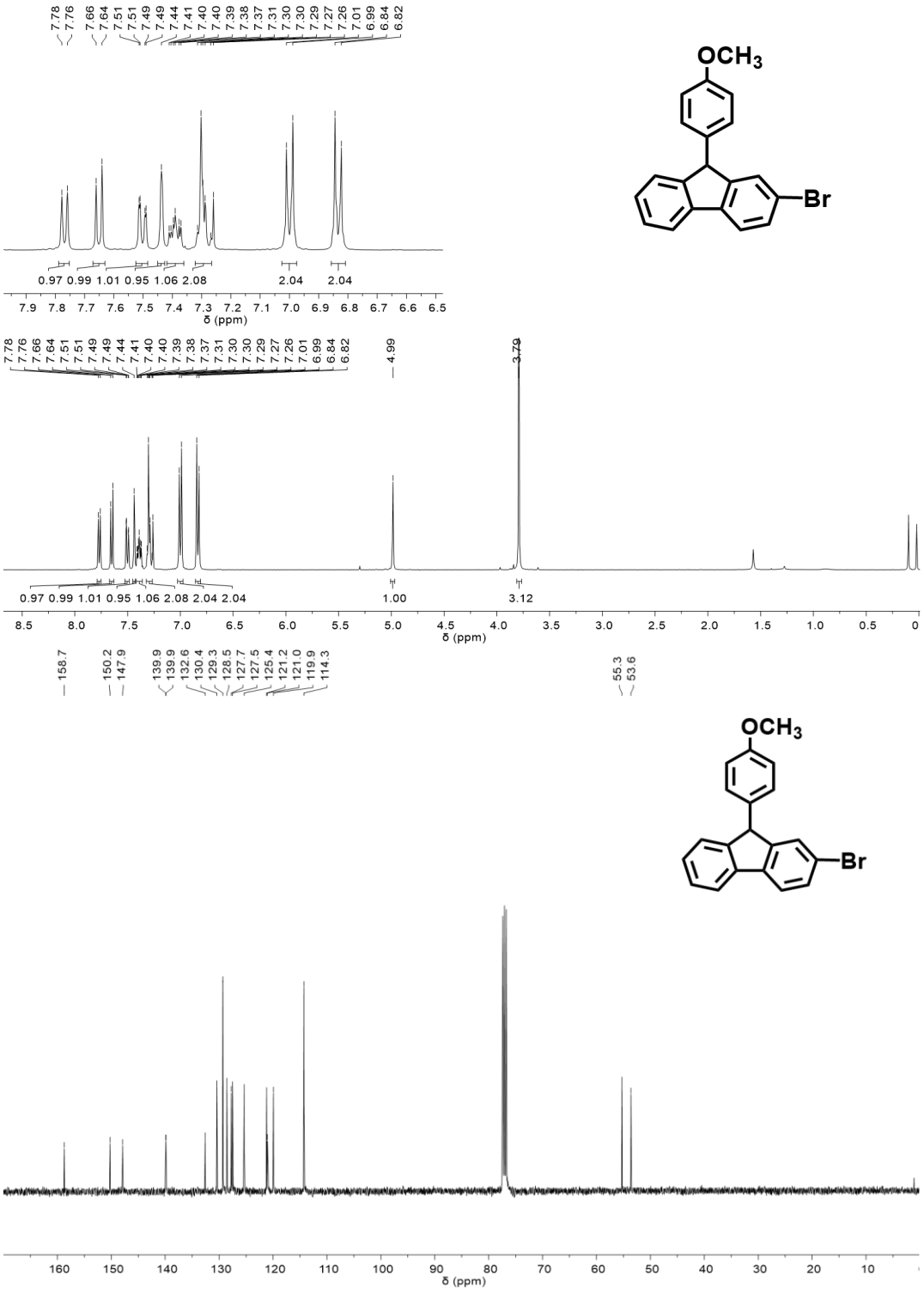
Supplementary Supplementary Fig. 46 | MALDI-TOF spectrum of trimerized product (3h).



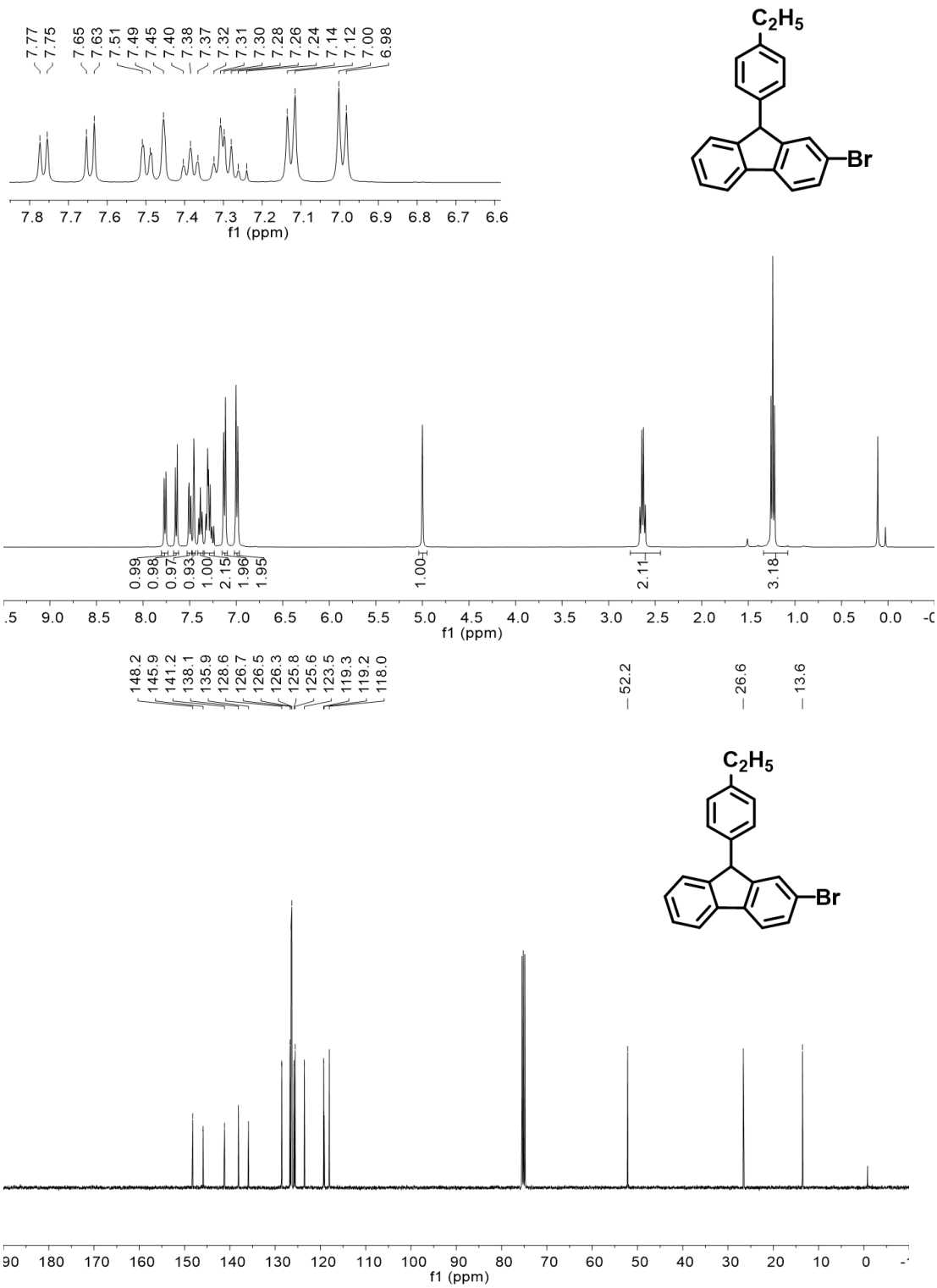
Supplementary Figure. 47 | ^{1}H and ^{13}C-NMR Spectra of 1a.



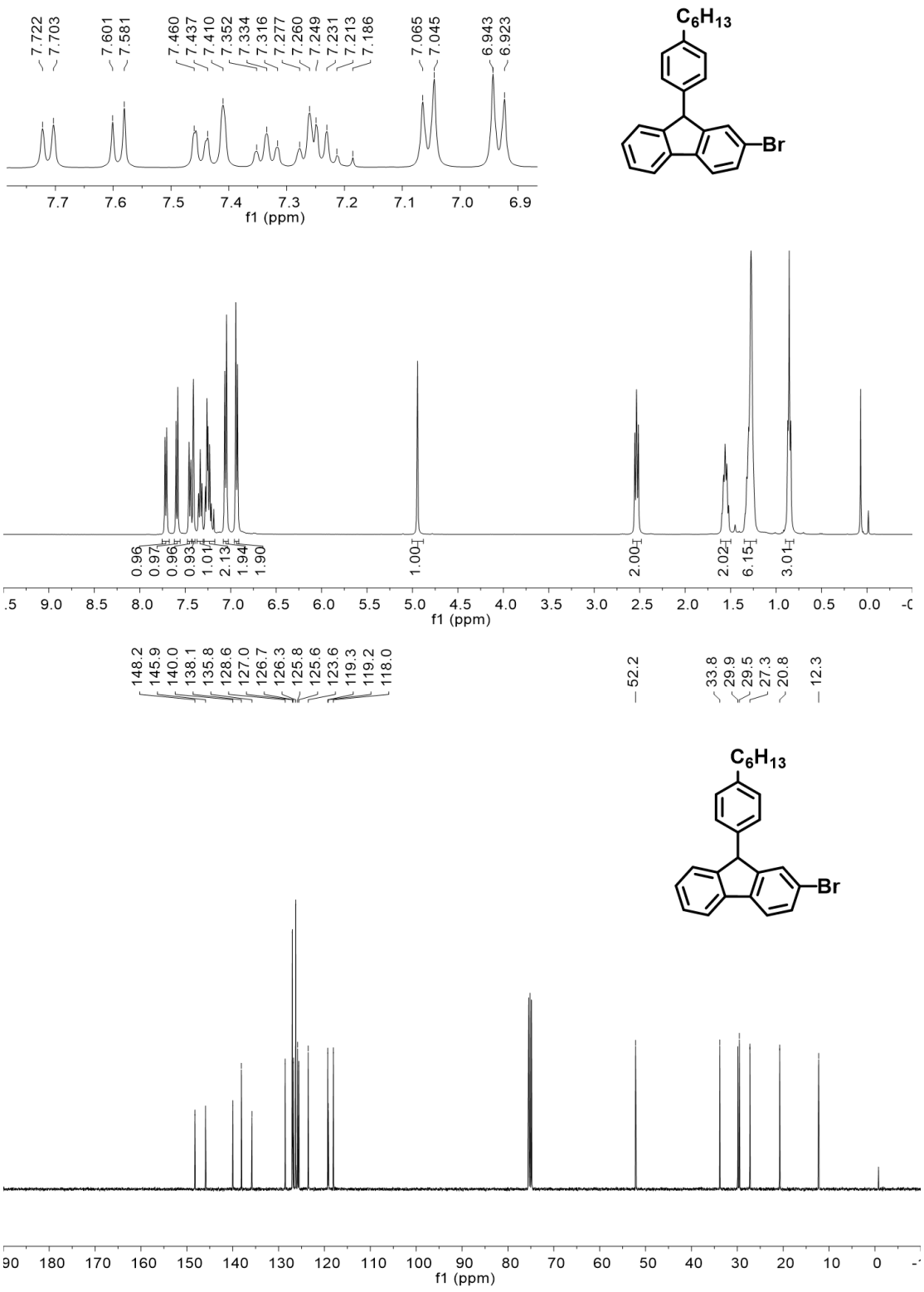
Supplementary Figure. 48 ｜ ^{1}H and ^{13}C-NMR Spectra of 1b.



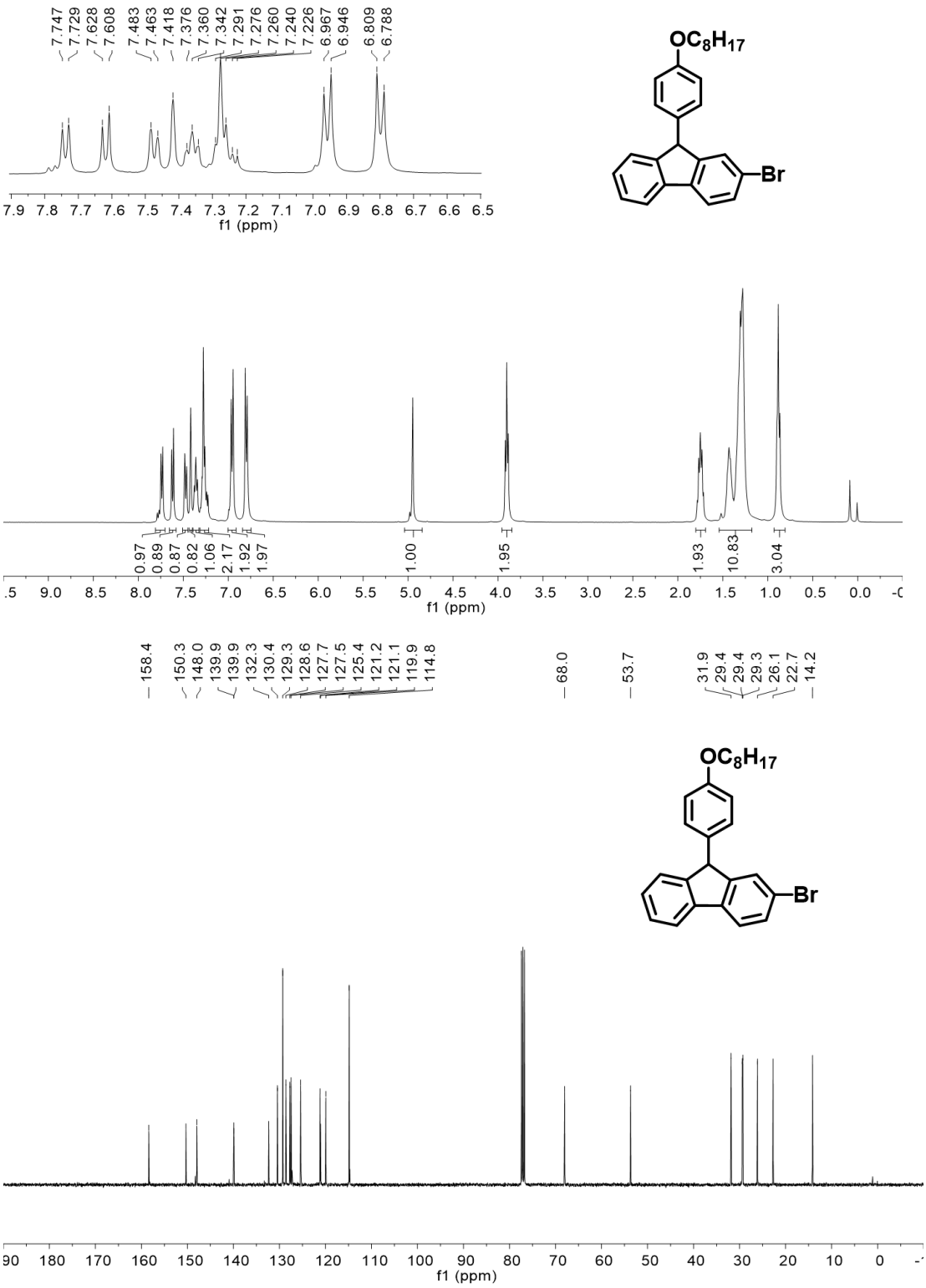
Supplementary Figure. 49 ｜ ^{1}H and ^{13}C-NMR Spectra of 1c.



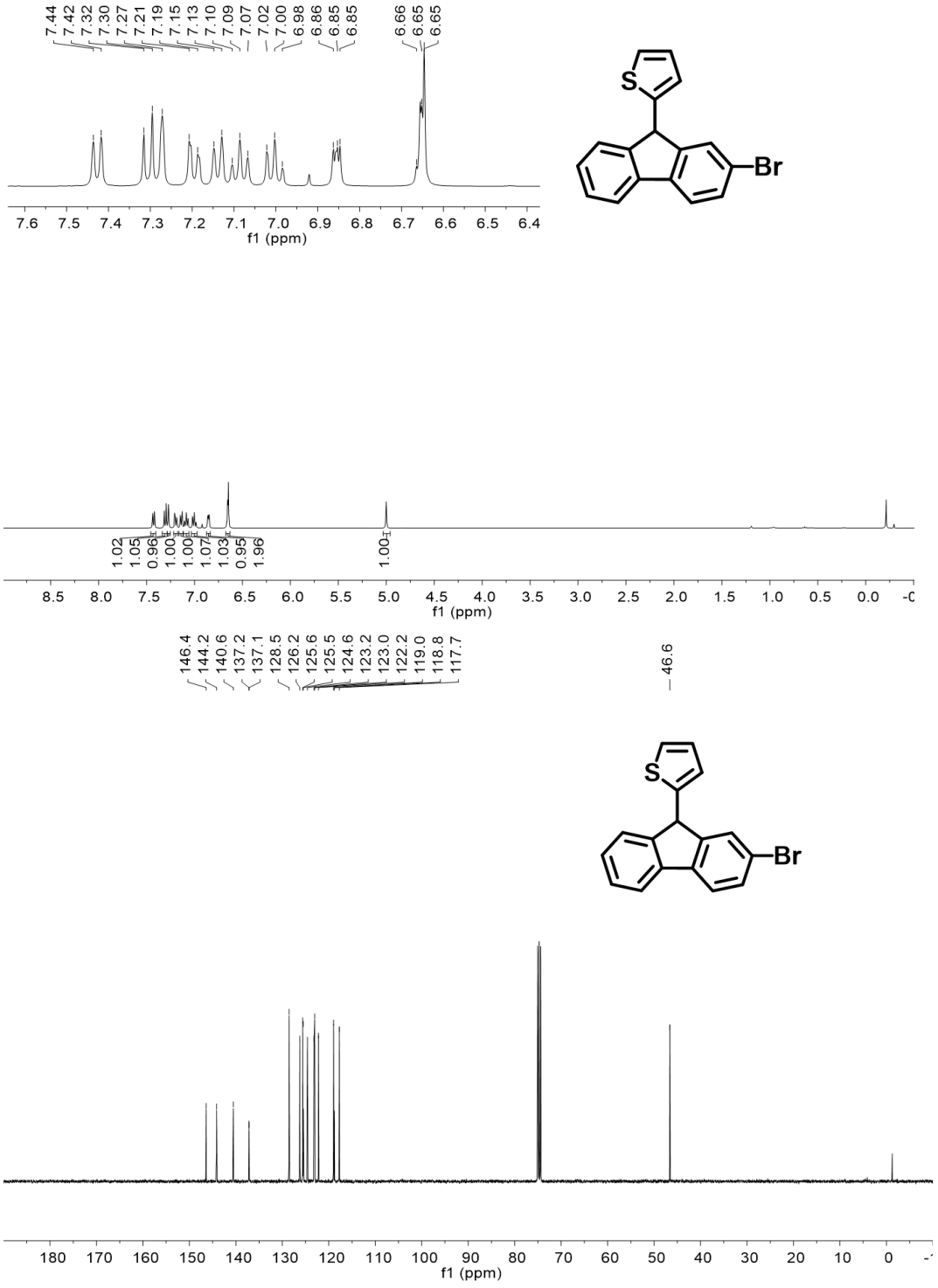
Supplementary Figure. 50 ｜ ^{1}H and ^{13}C-NMR Spectra of 1d.



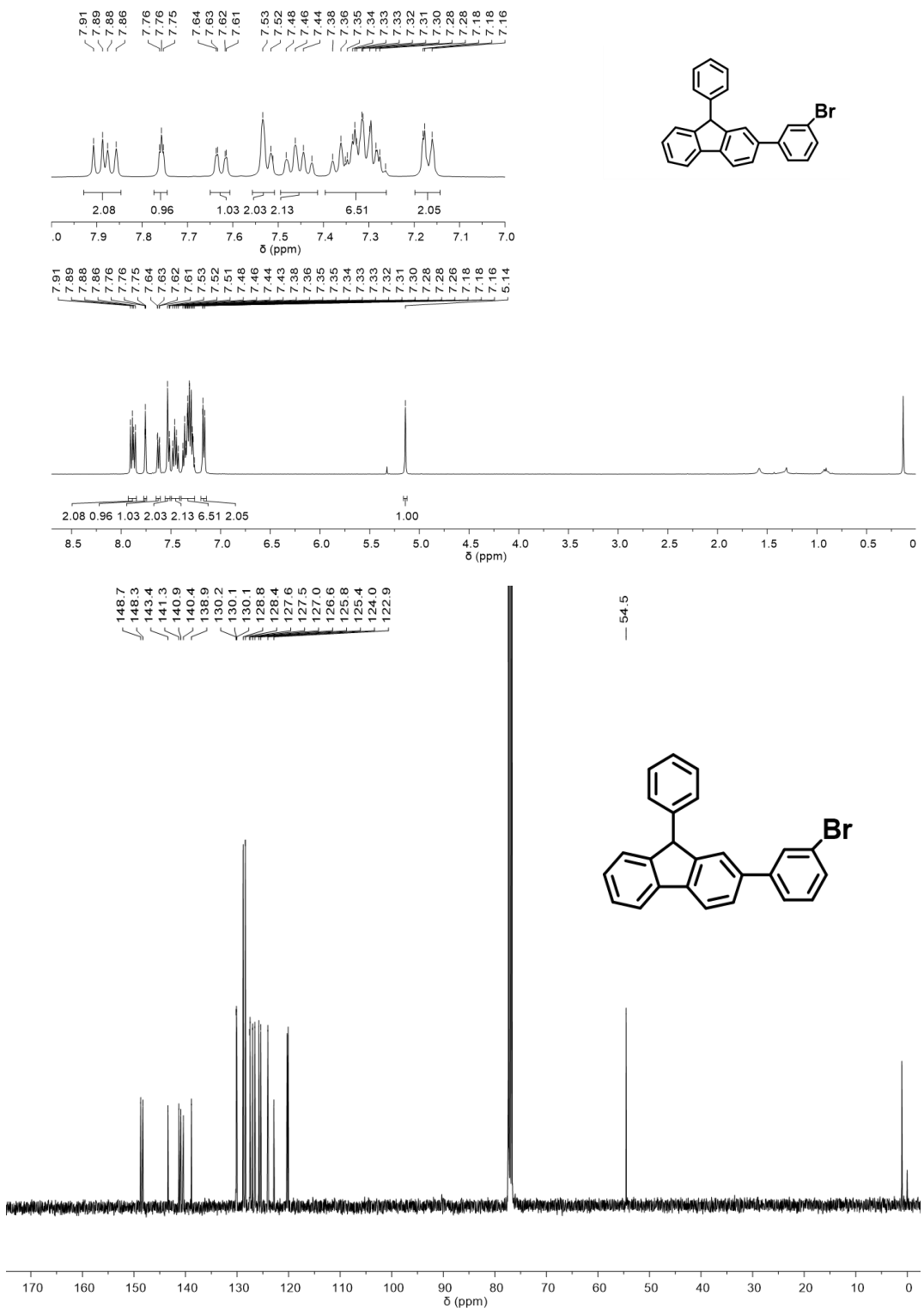
Supplementary Figure. 51 ｜ ^{1}H and ^{13}C-NMR Spectra of 1e.



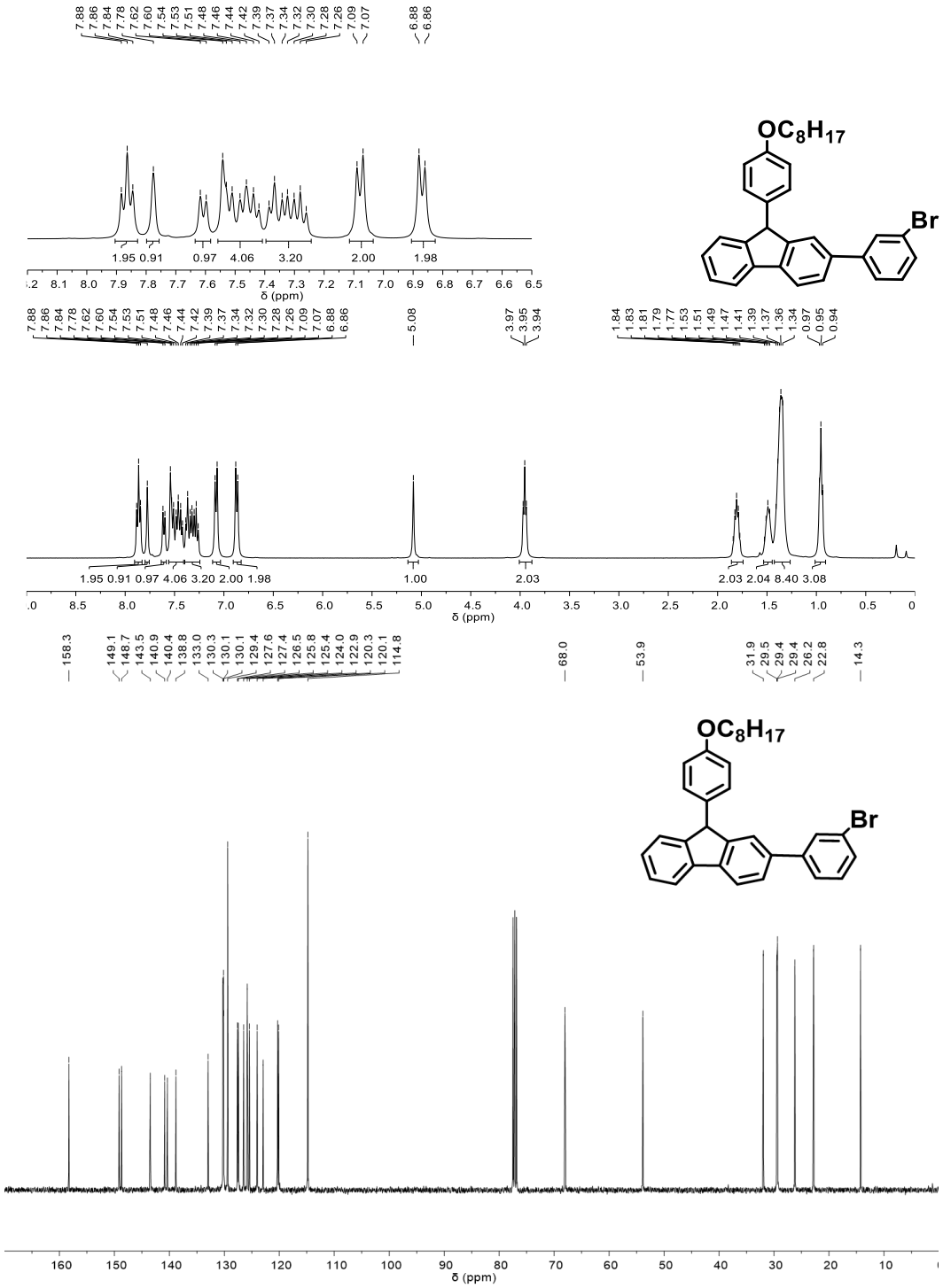
Supplementary Figure. 52 ｜ ^{1}H and ^{13}C-NMR Spectra of 1f.



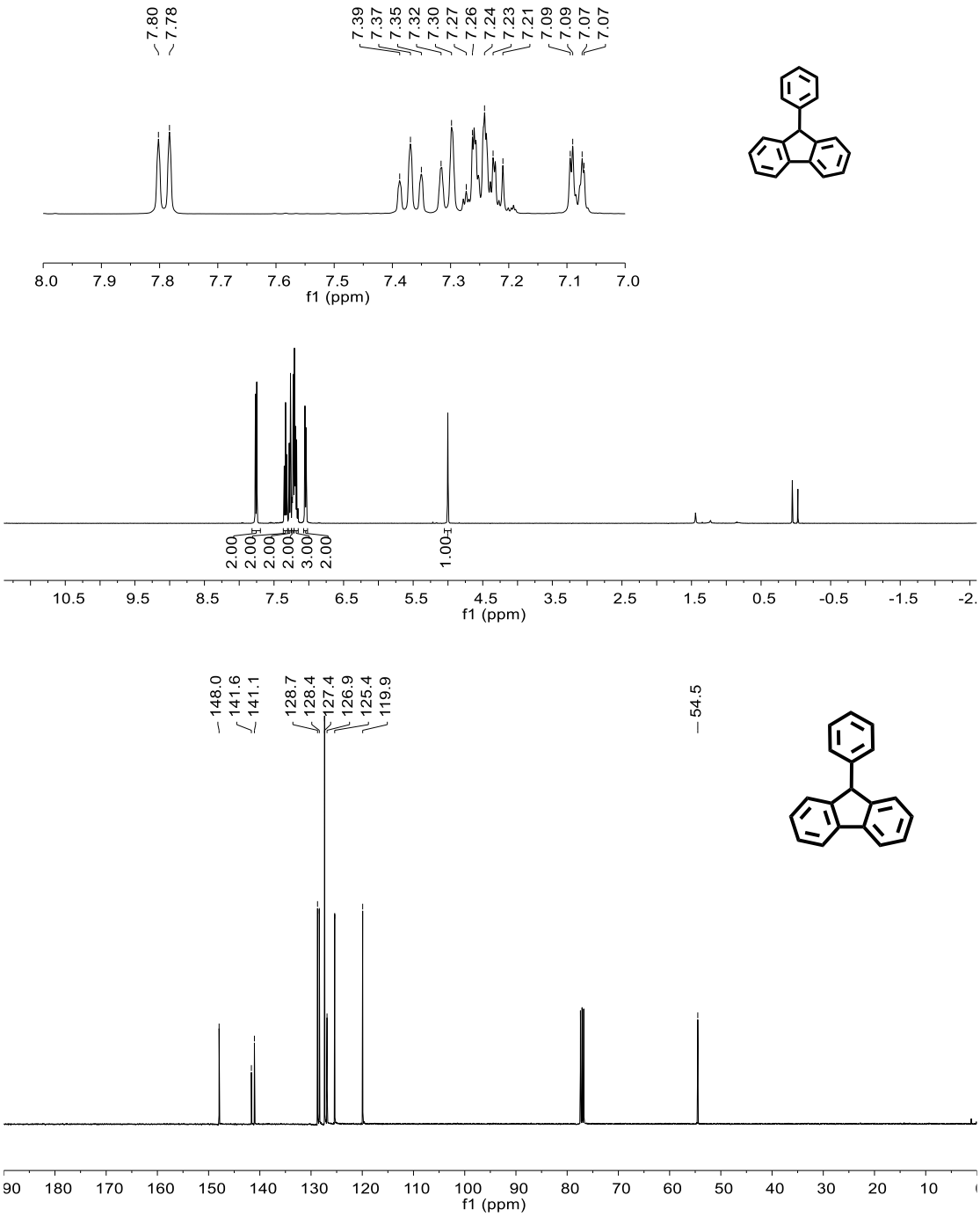
Supplementary Figure. 53 | ^{1}H and ^{13}C-NMR Spectra of 1g.



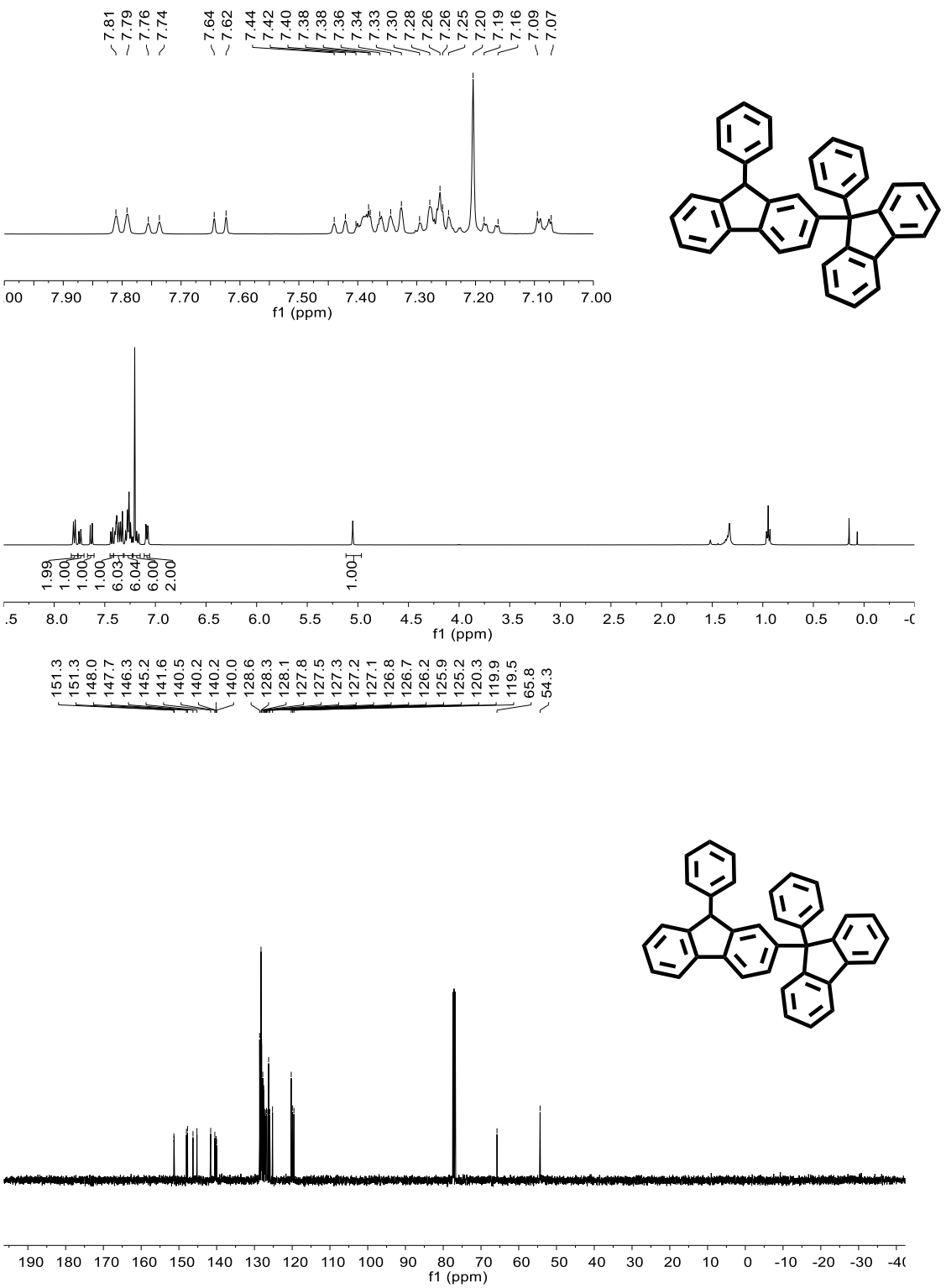
Supplementary Figure. 54 | ^{1}H and ^{13}C-NMR Spectra of 1h.



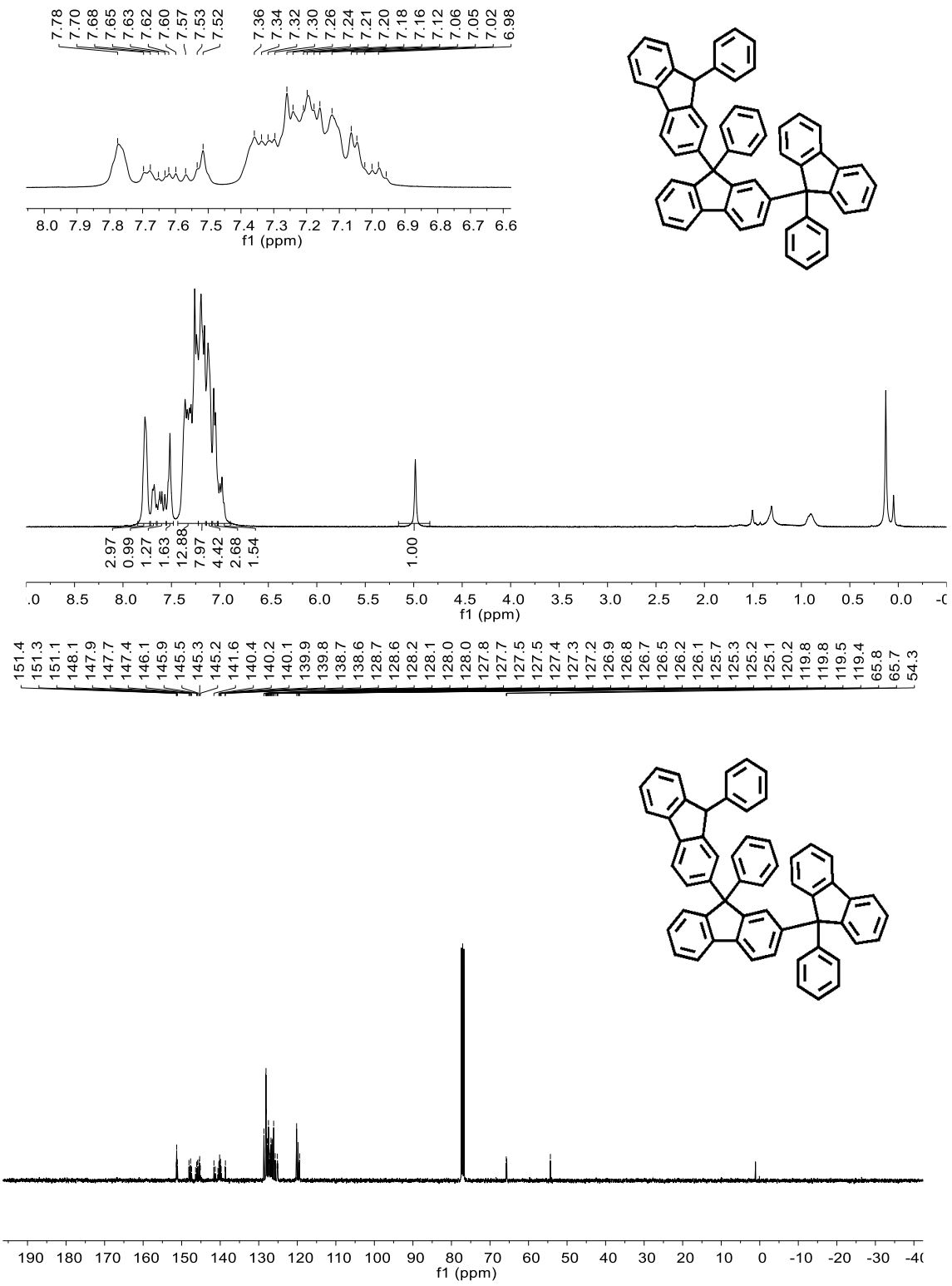
Supplementary Figure. 55 | ^{1}H and ^{13}C-NMR Spectra of 1i.



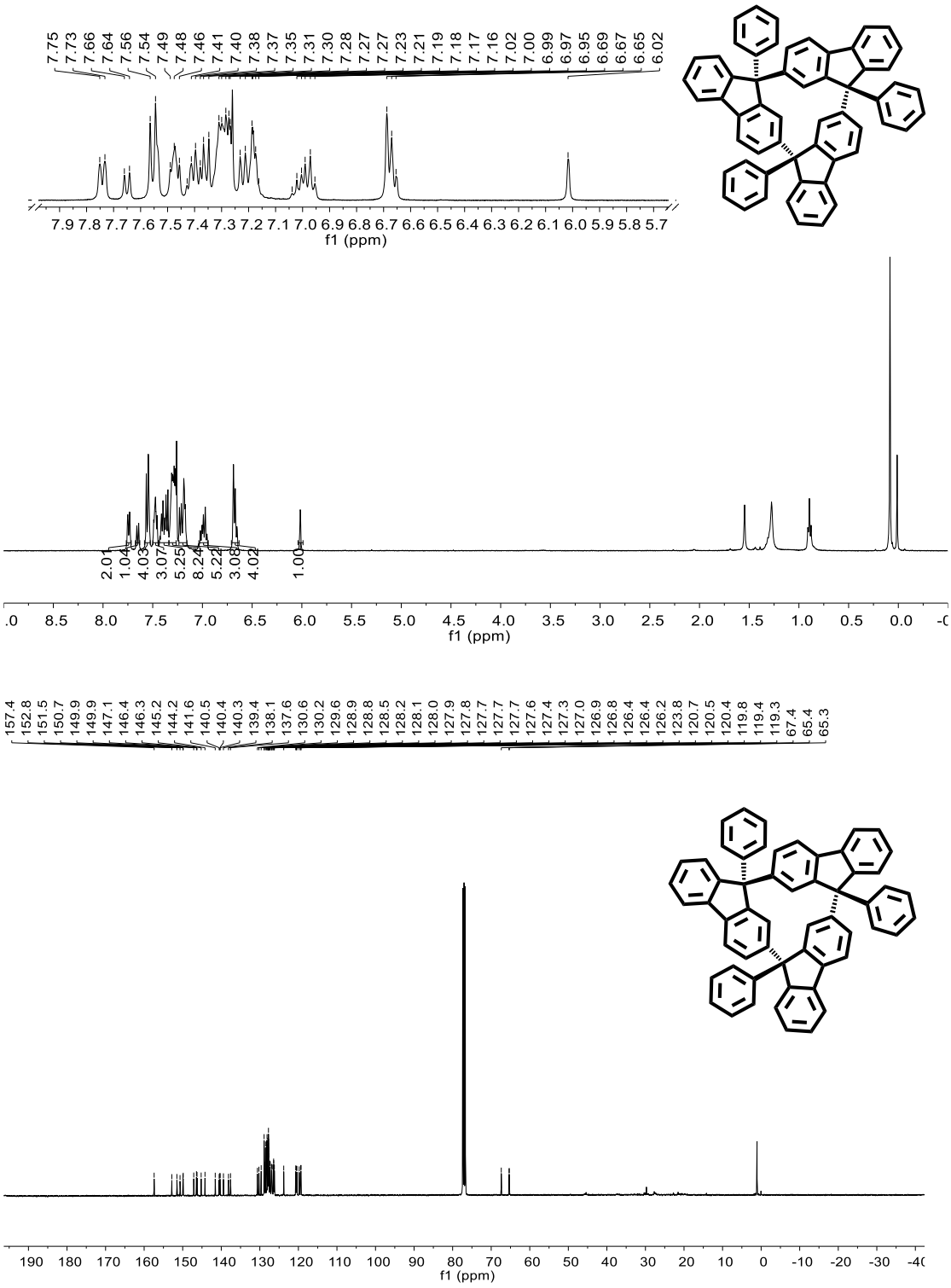
Supplementary Figure. 56 | ^{1}H and ^{13}C-NMR Spectra of 9 9-phenyl-*9H*-fluorene （2a）.



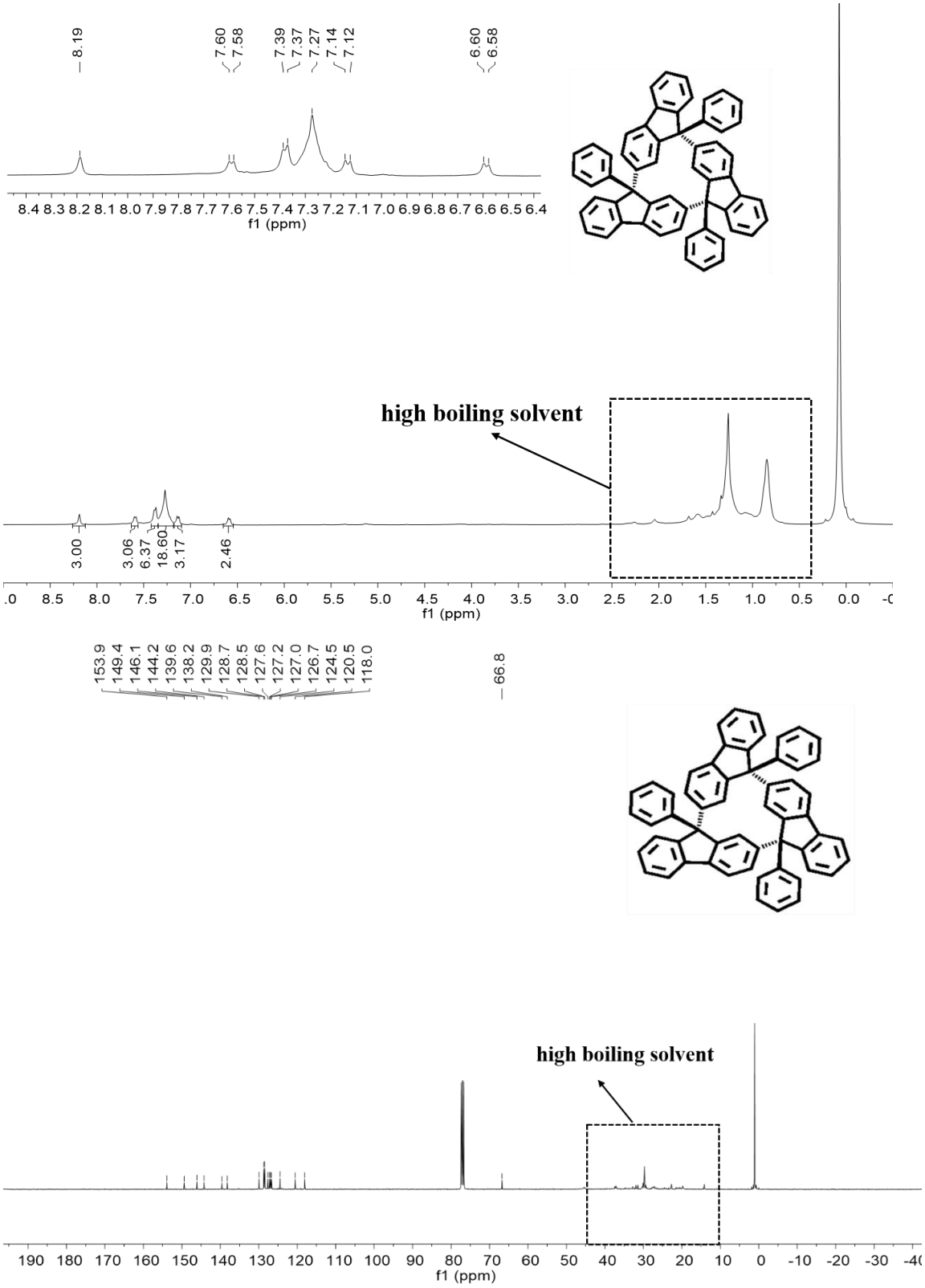
Supplementary Figurev. 57 ｜^{1}H and ^{13}C-NMR Spectra of 9-9'-diphenyl-9*H*,9'*H*-2,9'-bifluorene（3a）.



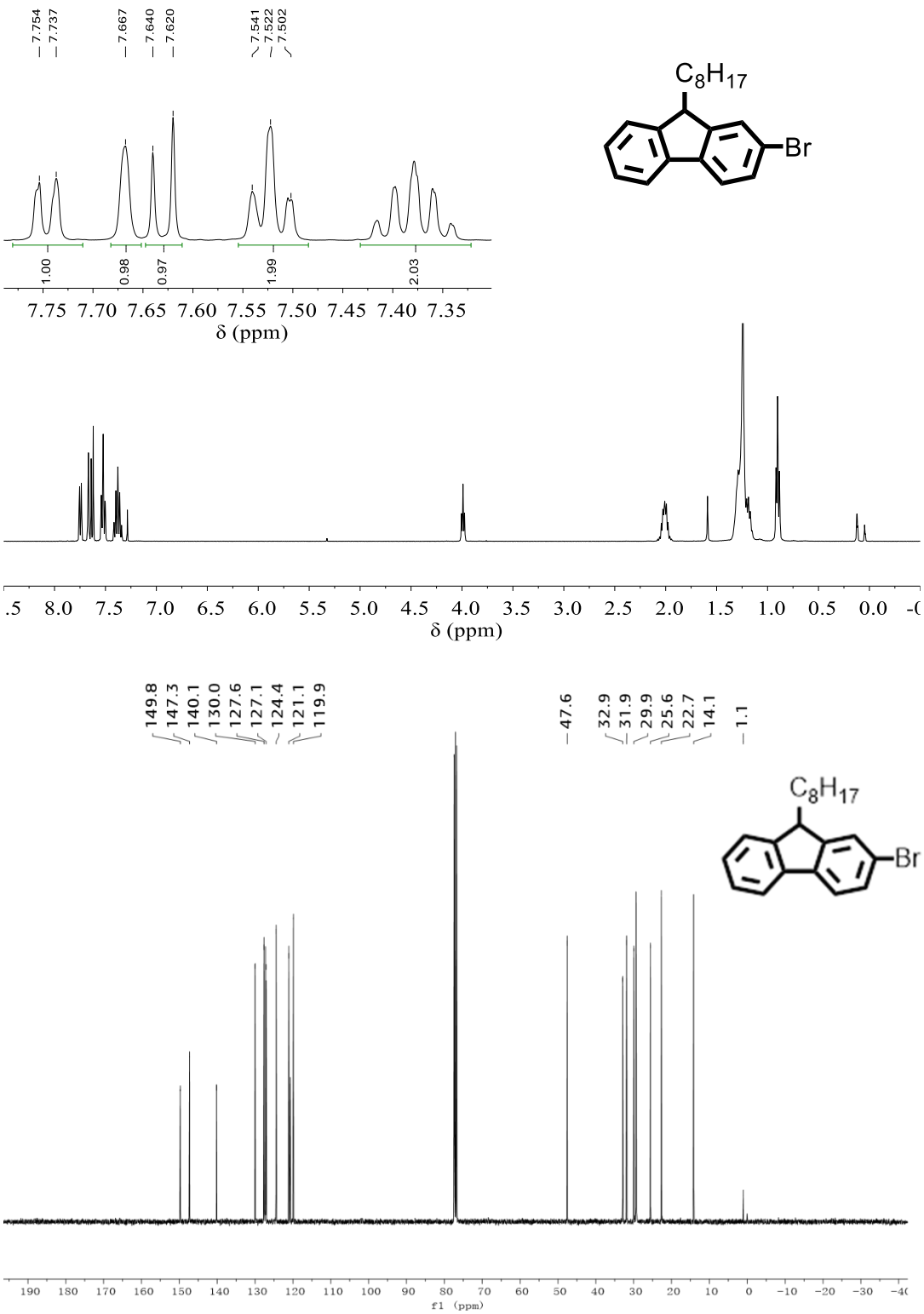
Supplementary Figure. 58 | ^{1}H and ^{13}C-NMR Spectra of 4a.



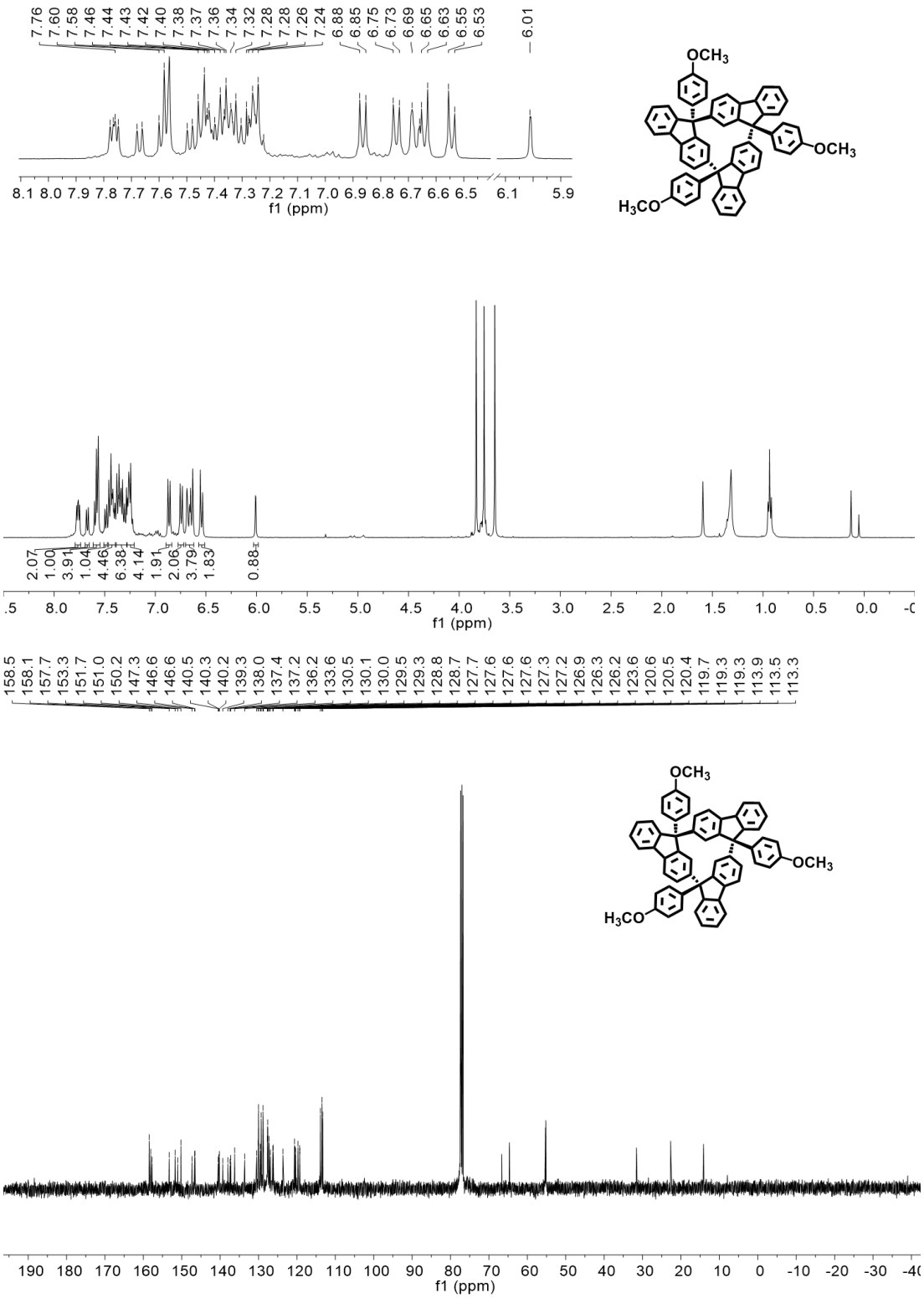
Supplementary Figure. 59 | ^{1}H and ^{13}C-NMR Spectra of *cis-trans*-TWG1.



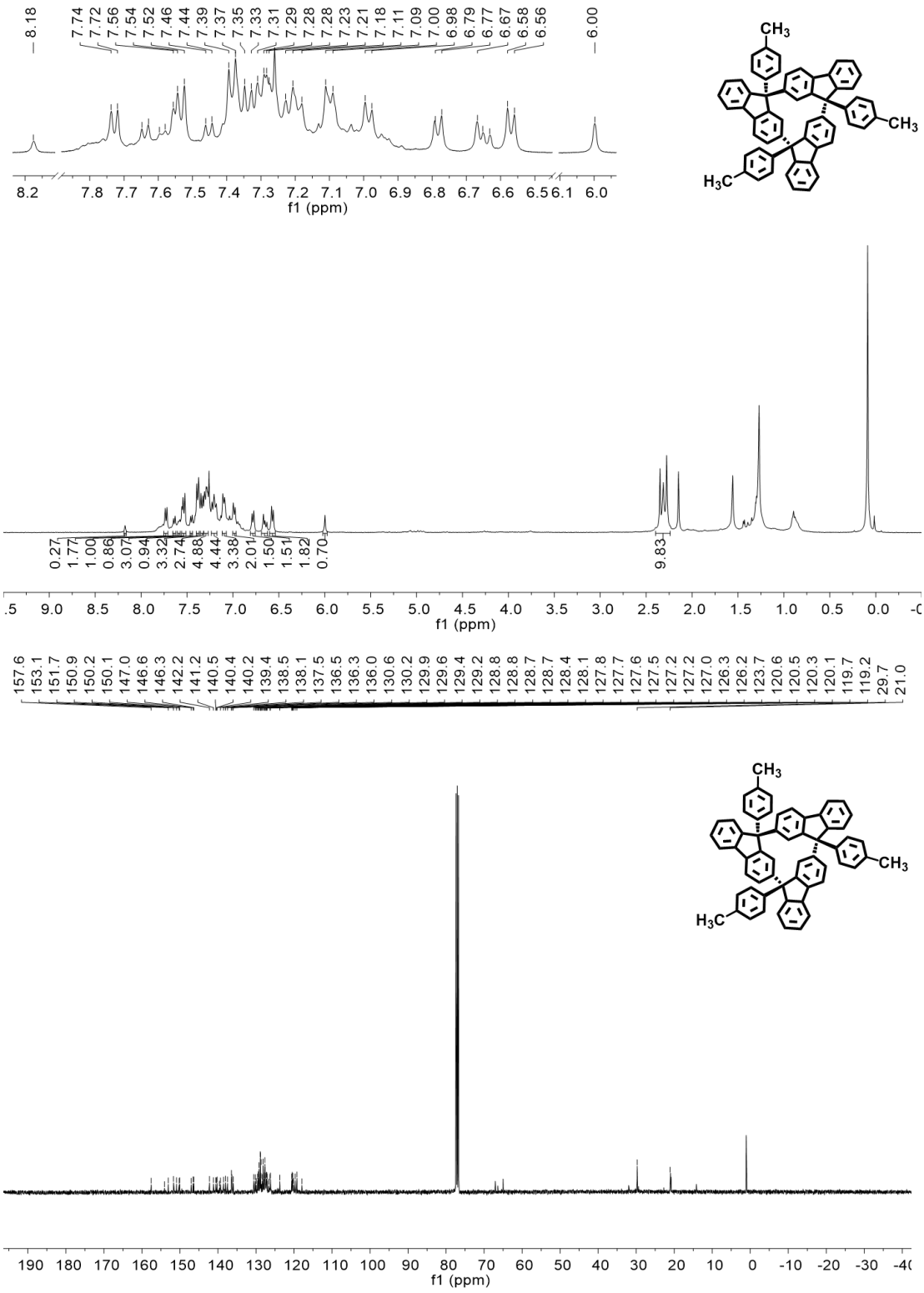
Supplementary Figure. 60 | ^{1}H and ^{13}C-NMR Spectra of *cis-cis*-TWG1.



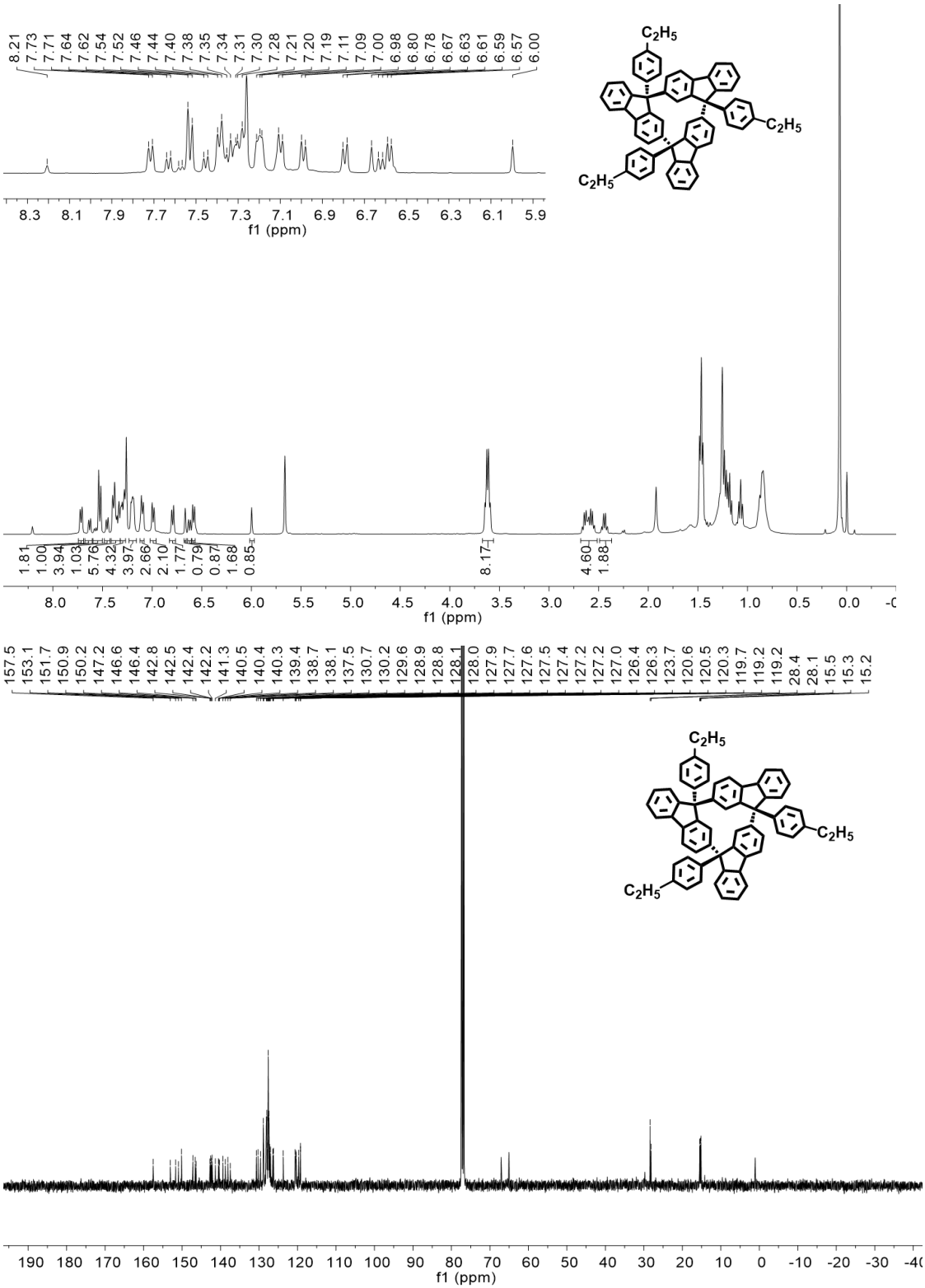
Supplementary Figure. 61 | ^{1}H and ^{13}C-NMR Spectra of 2-bromo-9-octyl-9*H*-fluorene**.**



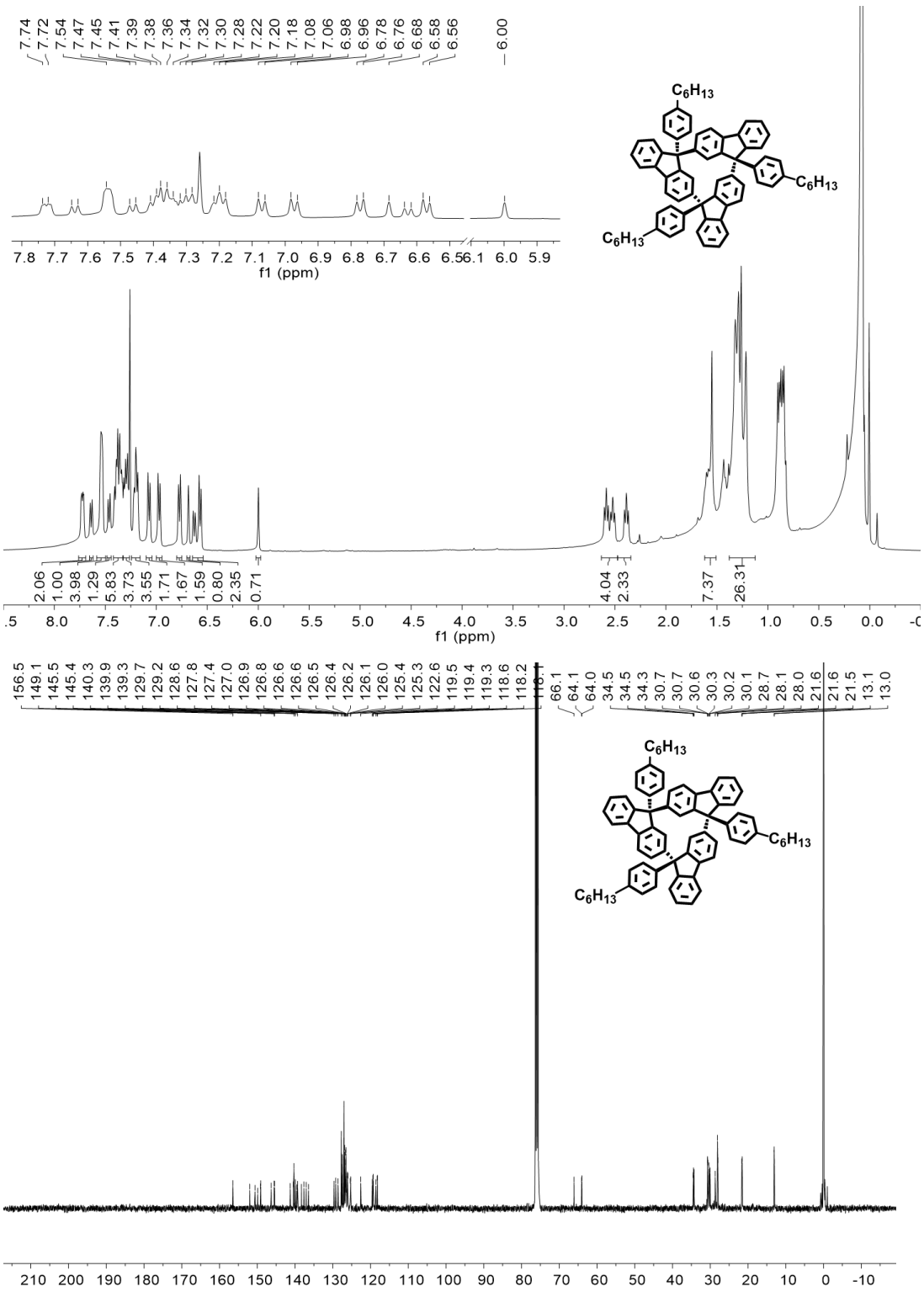
Supplementary Figure. 62 ｜ ^{1}H and ^{13}C-NMR Spectra of TWGs2.



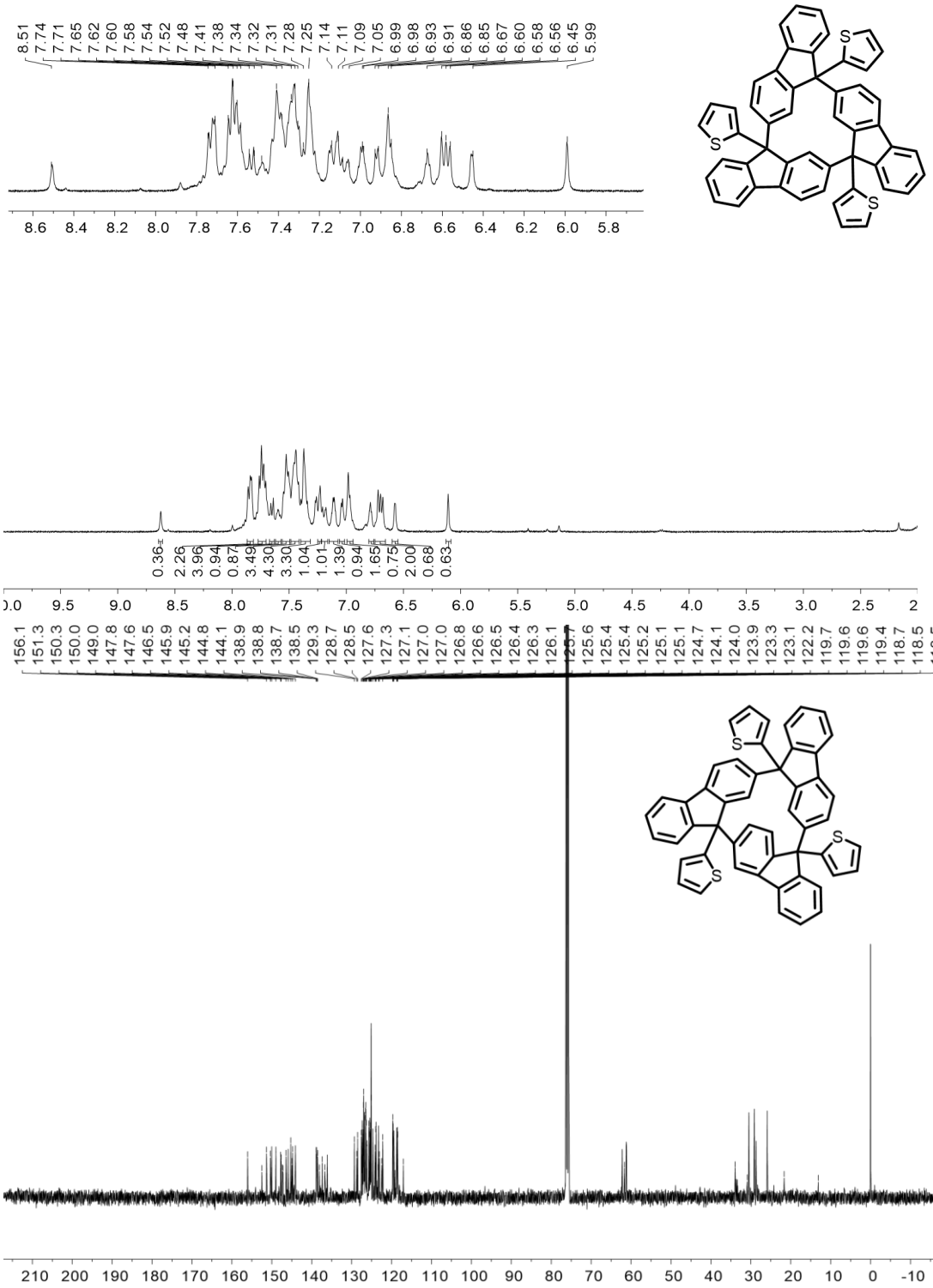
Supplementary Figure. 63 ｜ ^{1}H and ^{13}C-NMR Spectra of TWGs3.



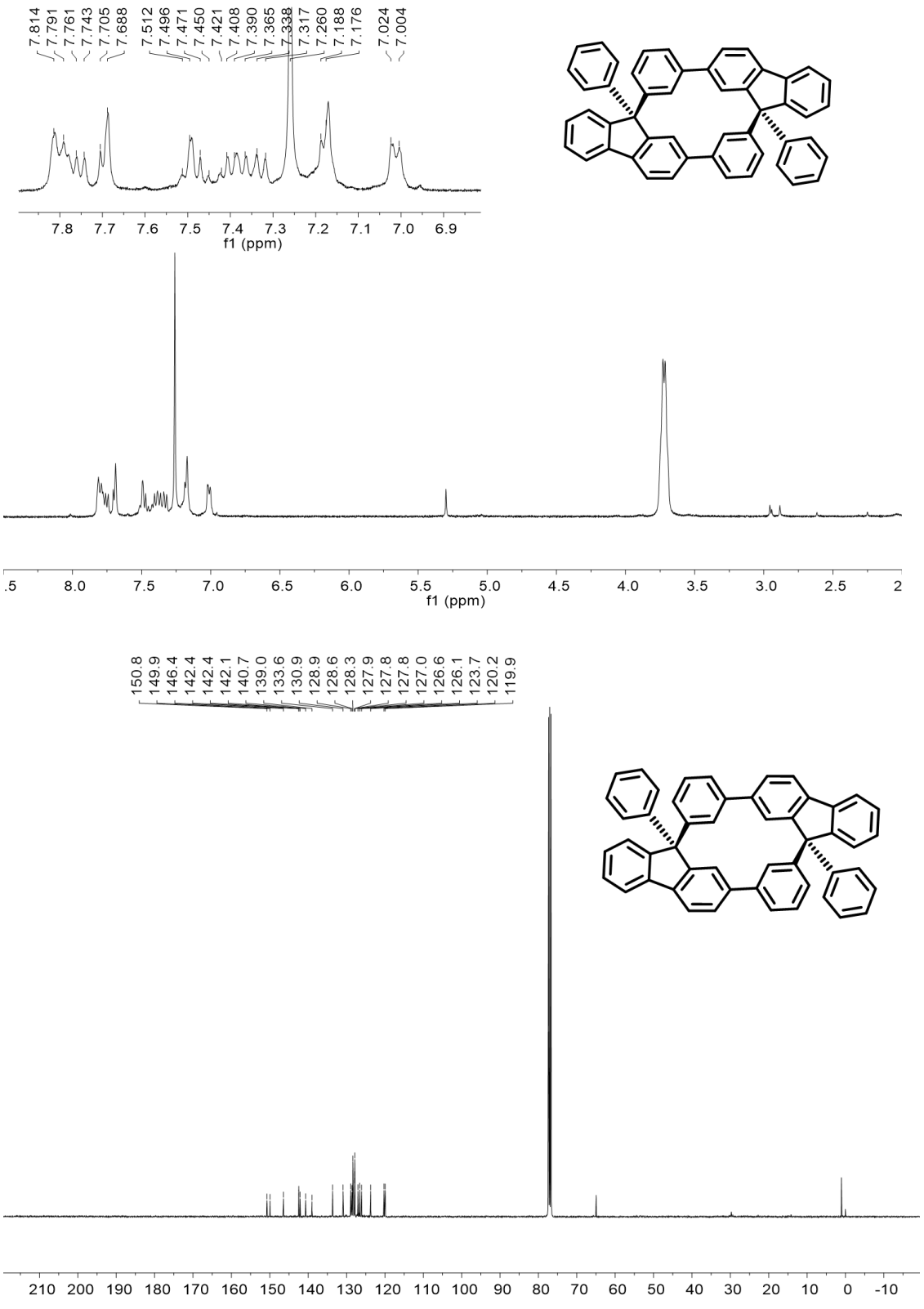
Supplementary Figure. 64 ｜ ^{1}H and ^{13}C-NMR Spectra of TWG4.



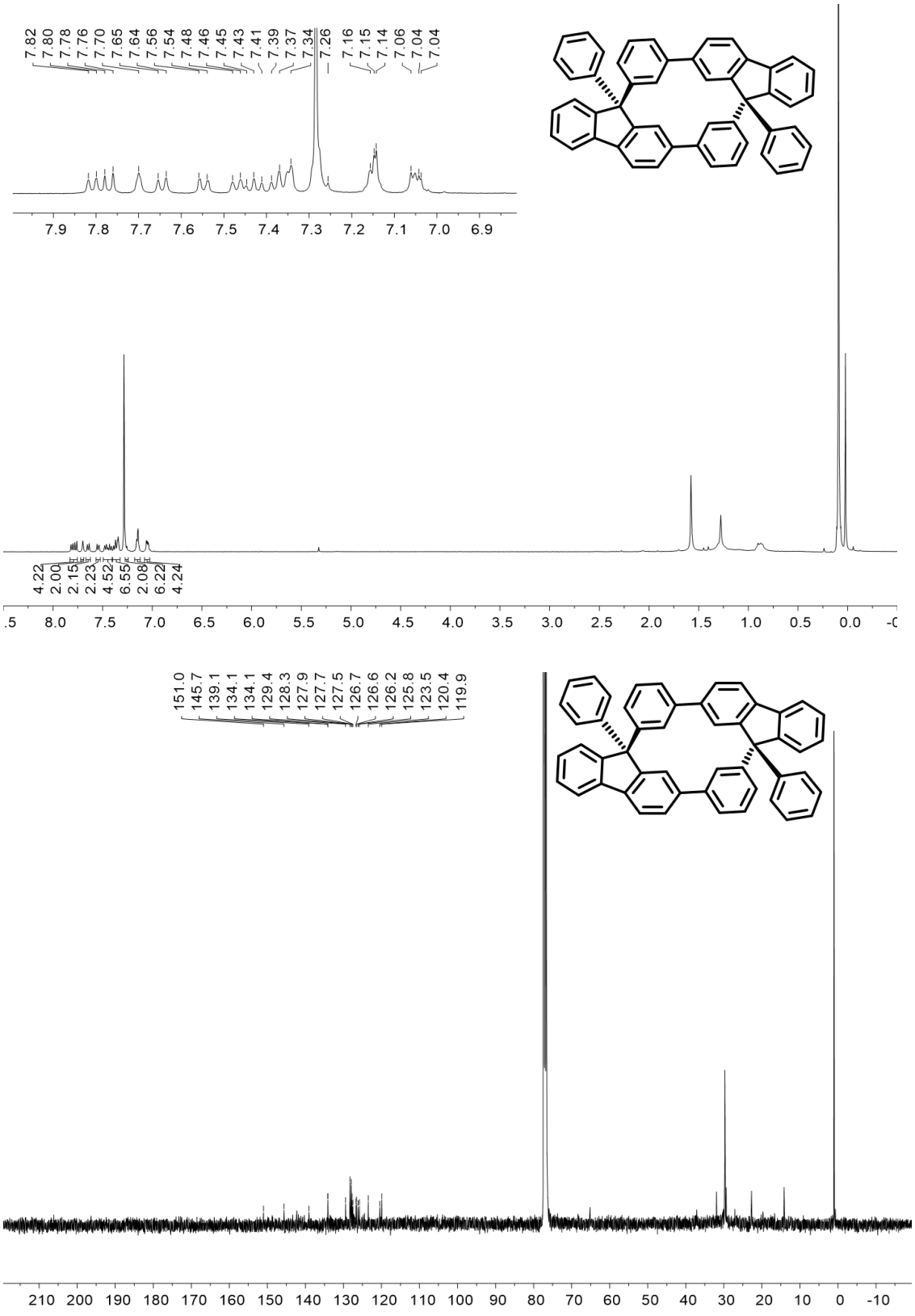
Supplementary Figure. 65 | ^{1}H and ^{13}C-NMR Spectra of TWG5.



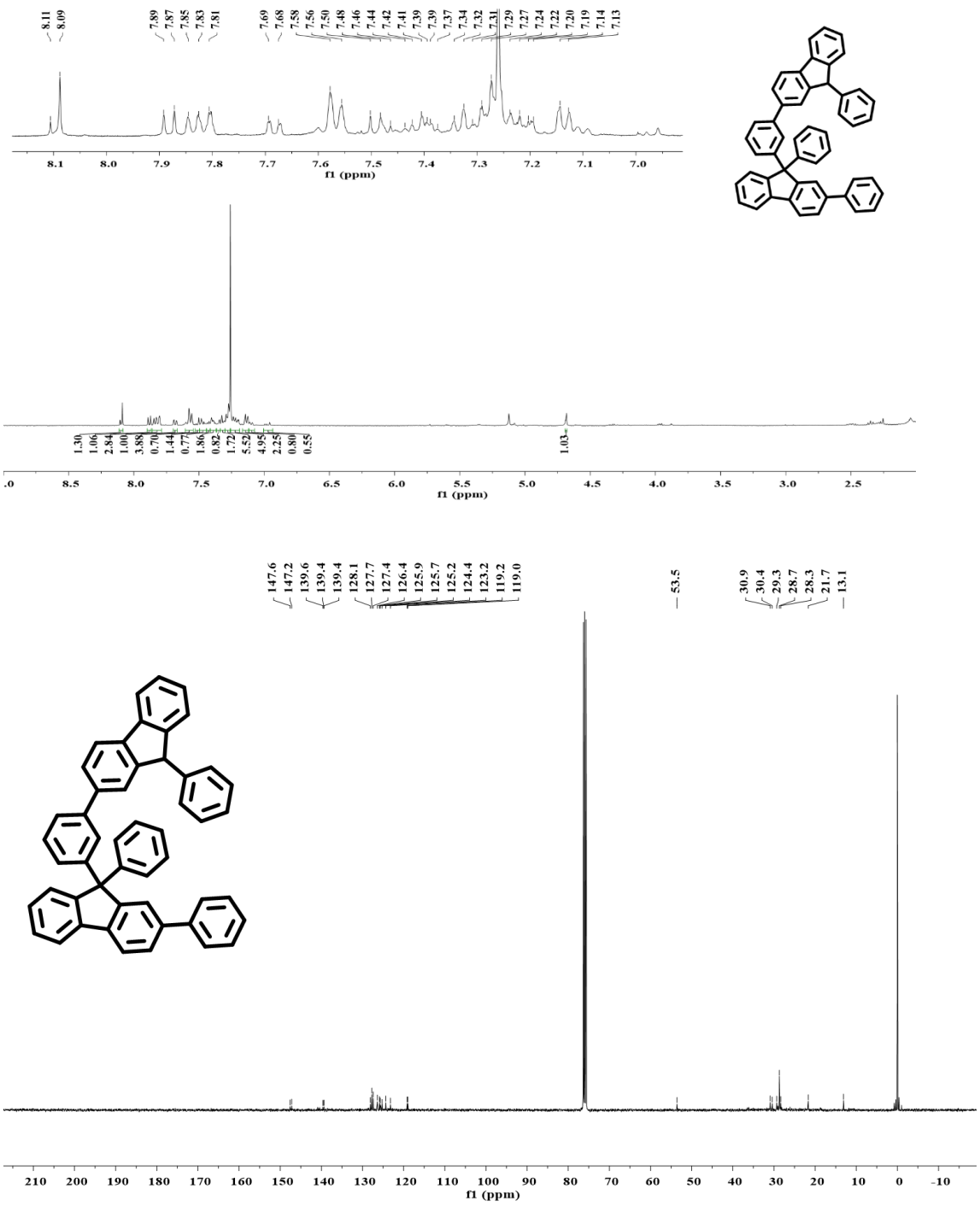
Supplementary Figure. 66 ｜ ^{1}H and ^{13}C-NMR Spectra of TWG6.



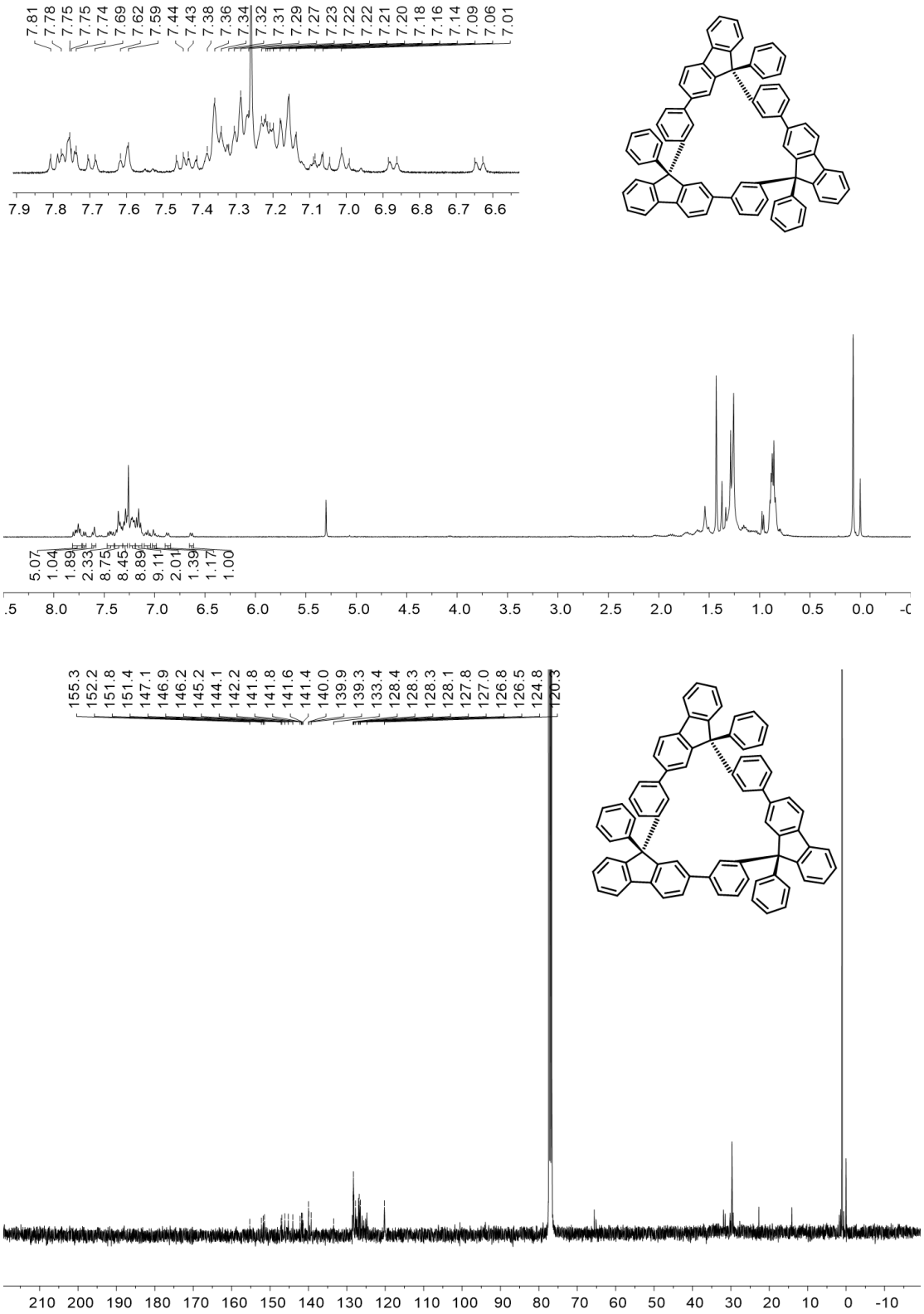
Supplementary Figure. 67 | ^{1}H and ^{13}C-NMR Spectra of *rac*-DWG1.



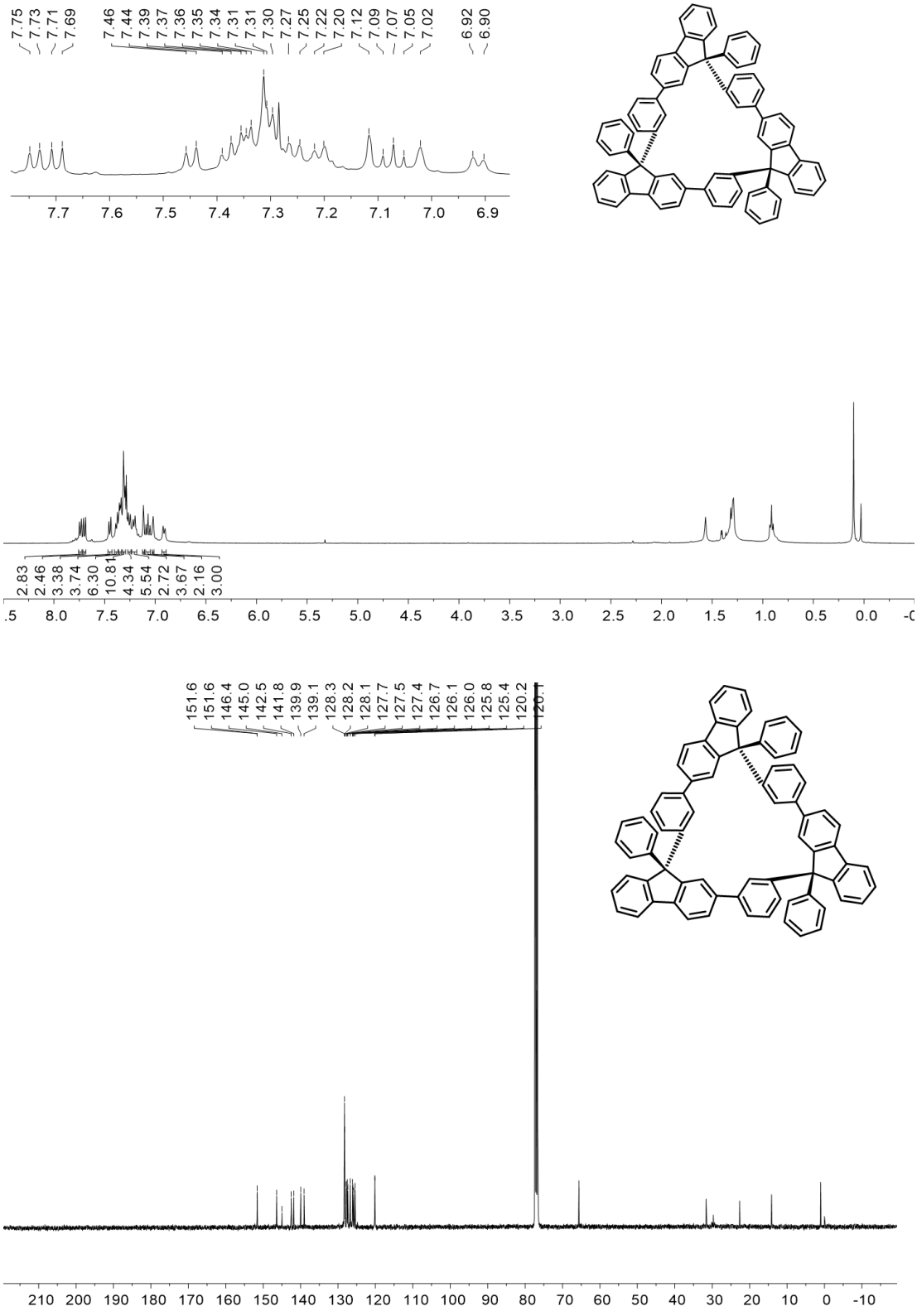
Supplementary Figure. 68 | ^{1}H and ^{13}C-NMR Spectra of *meso*-DWG1.



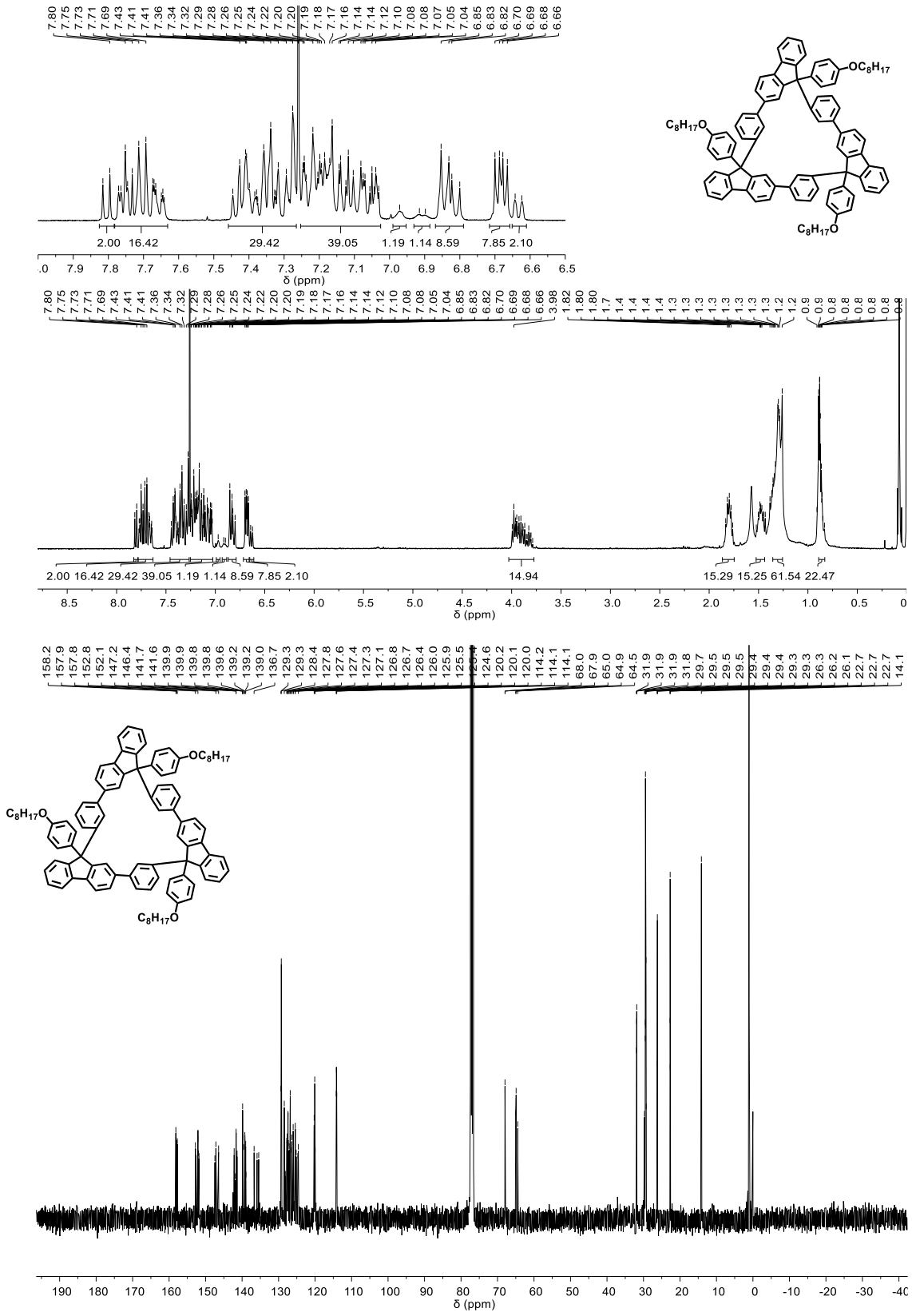
Supplementary Figure. 69 ｜ ^{1}H and ^{13}C-NMR Spectra of 3h.



Supplementary Figure. 70 ｜ ^{1}H and ^{13}C-NMR Spectra of *cis-cis*-TWG8



Supplementary Figure. 71 ｜ ^{1}H and ^{13}C-NMR Spectra of *cis-trans*-TWG8



Supplementary Figure. 72 | ^{1}H and ^{13}C-NMR Spectra of TWGs9

Supplementary References

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