SUPPORTING INFORMATION

Lemniscular Carbon Nanohoops with Contiguous Conjugation from Planar Chiral [2.2]Paracyclophane: Influence of the Regioselective Synthesis on Topological Chirality

Jing He,[†] Mo-Han Yu,[‡] Zhe Lian,[†] Yan-Qing Fan,[†] Sheng-Zhu Guo,[†] Xiao-Nan Li,[†] Wen-Guang Wang,[†] Ying Wang,[†] Zhi-Yun Cheng,[§] Hua Jiang*[,†].

[†]College of Chemistry, Beijing Normal University, Beijing 100875 (P.R. China)
[‡]College of Chemistry and Chemical Engineering, Liaoning Normal University, Dalian 116029 (P.R. China)
[§]School of Mathematical Sciences, Beijing Normal University, Beijing 100875 (P.R. China)

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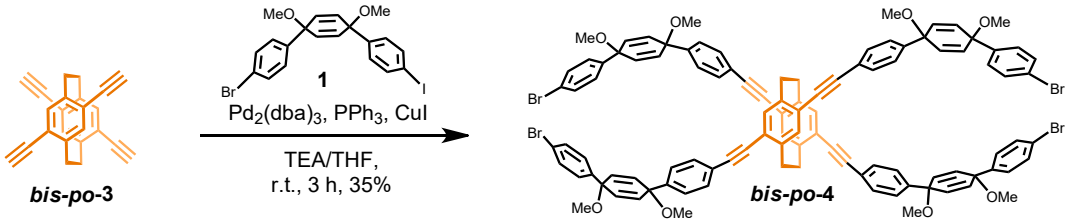
1. Experimental Procedures

1.1 General Procedures and Materials.

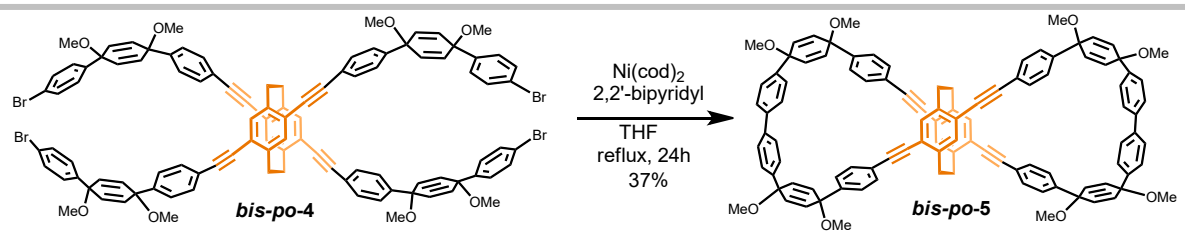
All starting chemicals were obtained from commercial sources and used without further purification, unless indicated otherwise. Per-deuterated solvents for NMR spectroscopy were obtained from Cambridge Isotope Laboratories. Anhydrous triethylamine (TEA) was distilled over calcium hydride (CaH_2) under Ar. Anhydrous tetrahydrofuran (THF) was distilled over sodium (Na) and benzophenone under Ar. Compound **1**,[S1] ***bis-po-3***,[S2] ***bis-pm-3***,[S3] were prepared according to the literatures. Columns for HPLC are specified in the corresponding sections. Column chromatography was carried out on flash grade silica gel, using 0 - 20 psig pressure. Analytical TLC was carried out using tapered silica plates with a preadsorbent zone. NMR spectra were obtained with JEOL Delta (400 MHz and 600 MHz) using chloroform-*d* ($CDCl_3$) as solvent. The chemical shift references were as follows: (^{1}H) chloroform-*d*, 7.26 ppm; (^{13}C) chloroform-*d*, 77.00 ppm (chloroform-*d*). Mass spectra (ESI, MALDI) were acquired on GCT and FTICR spectrometer (Bruker Daltonics Inc. APEXII, BIFLEX III), respectively. Fluorescence spectra were measured on FS5 and FLS980, and UV-Vis spectra were recorded on Shimadzu UV-3600. CD spectra were recorded on a ChirascanTM Circular Dichroism spectrometer (Applied Photophysics Ltd, Surrey, United Kingdom). CPL spectra were gained with Chirascan-CPL, Applied Photophysics.

1.2 Synthetic Procedures



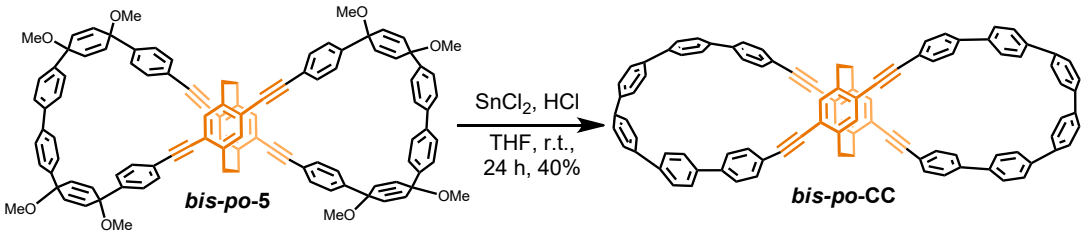
Compound ***bis-po-3*** (200.00 mg, 0.658 mmol), Compound **1** (1307.9 mg, 2.632 mmol), $Pd_2(dba)_3$ (60.26 mg, 0.066 mmol, 0.1 equiv), PPh_3 (69.27 mg, 0.263 mmol), CuI (25.00 mg, 0.132 mmol) were added to a dried flask. The flask was evacuated and backfilled with Ar three times. After cooling to 0^{o}C, the dried THF (44 mL) and TEA (11 mL) was added to the reaction. The mixture was stirred for 12 h on room temperature. The reaction was quenched with water and extracted with ethyl acetate three times. The combined organic layer was washed with brine, dried with Na_2SO_4, and evaporated under reduce pressure. The crude solid was purified by column chromatography on silica gel (EA/PE, 1/6, v/v) to get ***bis-po-4*** as a yellow powder (406.1 mg, 35%).

R_f = 0.25 (EA/PE = 1/3, v/v). M.p. = 76-77 ^{o}C.
^{1}H NMR (400 MHz, $CDCl_3$, 298 K) δ = 7.53 (d, J = 8.3 Hz, 8H), 7.46 (d, J = 8.5 Hz, 8H), 7.41 (d, J = 8.4 Hz, 8H), 7.29 (d, J = 8.5 Hz, 8H), 7.12 (s, 4H), 6.18-6.06 (m, 16H), 3.56 (s, 4H), 3.44 (d, J = 4.5 Hz, 24H), 3.08 (s, 4H). ^{13}C NMR (150 MHz, $CDCl_3$, 298 K), δ = 143.6, 142.5, 142.1, 134.7, 133.5, 133.4, 133.3, 131.7, 131.7, 131.6, 131.0, 128.9, 127.9, 126.2, 126.2, 125.2, 123.1, 121.8, 94.5, 89.6, 77.3, 77.1, 76.9, 74.8, 74.6, 65.6, 52.1 32.8. HRMS (MALDI-TOF) calculated for $C_{104}H_{85}Br_4O_8$ $[M]^+$: 1778.2967, found 1778.2982.



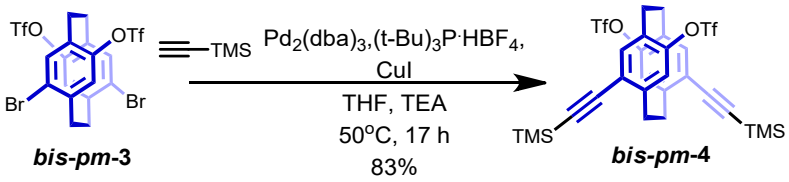
In a nitrogen-filled glove bag, ***bis-po*-4** (456 mg, 0.26 mmol), $Ni(cod)_2$ (352 mg, 1.3 mmol), 2,2'-bipyridyl (200 mg, 1.3 mmol) were added to a 500 mL two-necked flask containing a magnetic stirring bar and equipped with a condenser. The flask was sealed with a septum and transferred out of glove bag. After dry THF (270 mL) was added to the flask via syringe through a septum, the mixture was refluxed for 24 h. The reaction mixture was cooled down to room temperature and filtered through a short pad of silica gel with ethyl acetate/$CHCl_3$. The solvent was evaporated under reduce pressure to give a crude product, and then was purified by column chromatography on silica gel (PE/ EA, 5/1, v/v) to get a white solid (140.6 mg, 37%).

R_f = 0.22 (EA/PE = 1/2, v/v). M.p. = 232-233 °C.
^{1}H NMR (400 MHz, Chloroform-*d*, 298K) δ = 7.56 (d, *J* = 8.4 Hz, 8H), 7.49 (d, *J* = 8.3 Hz, 8H), 7.43 (d, *J* = 8.4 Hz, 8H), 7.36 (d, *J* = 8.3 Hz, 8H), 7.04 (s, 4H), 6.31 (dd, *J* = 10.3, 2.0 Hz, 4H), 6.18 – 6.09 (m, 12H), 3.69-3.61 (m, 4H), 3.48 (d, *J* = 7.3 Hz, 24H), 3.19-3.07 (m, 4H). ^{13}C NMR (100 MHz, Chloroform-*d*, 298K) δ = 143.2, 142.5, 141.8, 140.2, 135.2, 134.1, 133.0, 132.1, 131.6, 127.1, 126.7, 126.5, 124.6, 123.0, 94.5, 89.2, 77.4, 77.1, 76.8, 75.5, 75.4, 52.3, 52.1, 29.8. HRMS (MALDI-TOF) calculated for $C_{104}H_{84}O_8$ $[M]^+$: 1461.6200, found 1461.6221.



A H_2SnCl_4/THF solution was freshly prepared by dissolving anhydrous $SnCl_2$ (521.5 mg, 2.75 mmol) in 9 ml anhydrous THF under nitrogen atmosphere and then adding concentrated HCl (aq) (0.4 ml) to the solution. The resulting solution was deoxygenated and stirred for 15 minutes before use. ***Bis-po*-5** (80.2 mg, 0.055 mmol) was dissolved in anhydrous THF (15 ml) under a nitrogen atmosphere and the freshly prepared H_2SnCl_4/THF solution (9.4 ml) was added to this solution. The reaction mixture was stirred at room temperature. The reaction mixture was stirred at room temperature. The reaction mixture was stirred at room temperature for 36 h before being quenched with NaOH/H_2O solution. The aqueous layer was extracted with dichloromethane and the organic layers were combined and dried with anhydrous Na_2SO_4. The crude mixture was purified by column chromatography (SiO_2, DCM/ petroleum ether, 1/5) to get ***bis-po*-CC** as a light yellow solid (26.7 mg, 40%).

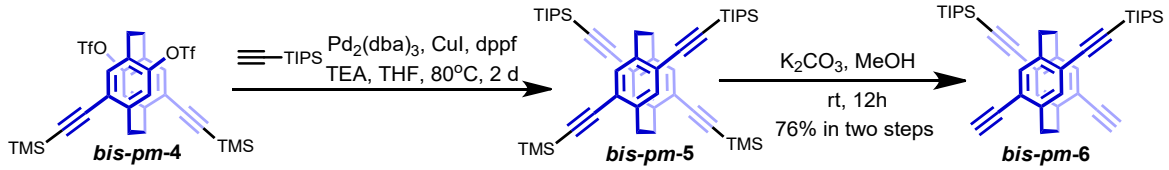
R_f = 0.20 (DCM/PE = 1/2, v/v). M.p. > 300 °C.
^{1}H NMR (600 MHz, Chloroform-*d*, 298K) δ = 7.61 (m, *J* = 8.7 Hz, 4H), 7.53 (m, 20H), 7.45 (d, *J* = 8.7 Hz, 8H), 7.40 (d, *J* = 8.4 Hz, 8H), 7.37 (d, *J* = 8.4 Hz, 8H), 6.98 (s, 4H), 3.56 (m,, 4H), 3.11 – 3.01 (m, 4H). ^{13}C NMR (150 MHz, Chloroform-*d*, 298K) δ = 141.6, 140.0, 139.6, 138.9, 138.2, 137.8, 136.7, 131.9, 127.7, 127.0, 123.9, 122.4, 91.9, 89.6, 34.8, 33.7. HRMS (MALDI-TOF) calculated for $C_{96}H_{60}$ $[M]^+$: 1213.4729, found 1213.4770.



A mixture of ***bis-pm*-3**[S3](3.14 g, 4.74 mmol), $Pd_2(dba)_3$ (869.9 mg, 0.95 mmol), t-$Bu_3P{\cdot}HBF_4$ (549.8 mg, 1.89 mmol), CuI (180.5 mg, 0.95 mmol), THF (65 mL) and Et_3N (65 mL) was placed in a round-bottom flask equipped with a magnetic stirring bar. After degassing the reaction mixture several times, (trimethylsilyl)acetylene (9.5 mL 68.77 mmol) was added to the mixture. The reaction was carried out at 50 °C with stirring for 17 h. After the reaction mixture was cooled to room temperature, precipitates were removed by filtration, and the solvent was removed with a rotary evaporator. The residue was purified by column chromatography on SiO_2 (CH_2Cl_2/hexane = 1/100 v/v as an eluent) to afford ***bis-pm*-4** as a light yellow solid (2.74 g, 83%).

R_f = 0.20 (PE). M.p. = 81-82 °C.

^{1}H NMR (600 MHz, Chloroform-*d*, 298K) δ = 7.00 (s, 2H), 6.78 (s, 2H), 3.38 (m, 4H), 2.93 (m, 4H), 0.31 (s, 18H).^{13}C NMR (150 MHz, Chloroform-d, 298K) δ =147.9, 145.6, 136.9, 132.0, 126.1, 125.0, 121.9, 119.8, 117.7, 115.6, 113.8, 102.5, 101.0, 31.9, 29.7. HRMS (MALDI-TOF) calculated for $C_{28}H_{30}F_6O_6S_2Si_2$ $[M]^+$: 696.0927, found 696.0923.

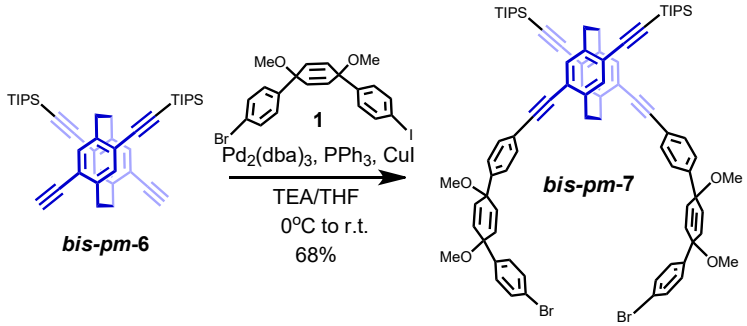


A mixture of ***bis-pm*-4** (2.74 g, 3.93 mmol), $Pd_2(dba)_3$ (720.61 mg, 0.79 mmol), dppf (871.5 mg, 1.57 mmol), CuI (149.4 mg, 0.79 mmol), THF (92 mL) and Et_3N (92 mL) was placed in a round-bottom flask equipped with a magnetic stirring bar. After degassing the reaction mixture several times, triisopropylsilylacetylene (9.0 mL, 39.3 mmol) was added to the mixture via syringe. The reaction was carried out at 80 °C for 2 d with stirring. After the reaction mixture was cooled to room temperature, precipitates were removed by filtration, and the solvent was removed with a rotary evaporator. The residue was purified by column chromatography on SiO_2 (hexane as an eluent) to afford ***bis-pm*-5**.

K_2CO_3 (3.7 g, 27 mmol) was added to a suspension of ***bis-pm*-5** (3.93 mmol) in MeOH (1600 mL) and CH_2Cl_2 (160 mL). After the mixture was stirred for 12 h at room temperature, H_2O was added to the reaction mixture. The organic layer was extracted with $CHCl_3$ and washed with brine. The combined organic layer was dried over Na_2SO_4. Na_2SO_4 was removed by filtration, and the solvent was removed with a rotary evaporator. The residue was purified by column chromatography on SiO_2 (hexane as an eluent) to afford ***bis-pm*-6** as a white solid (2.3 g, 76% in two steps).

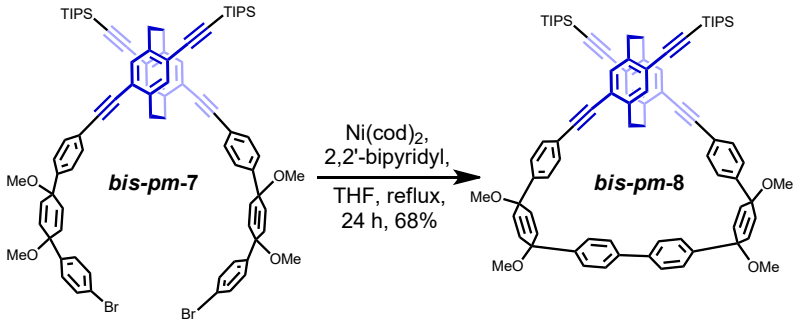
R_f = 0.30 (PE). M.p. = 76-77 °C.

^{1}H NMR (400 MHz, Chloroform-*d*, 298 K) δ = 7.08 (s, 2H), 7.02 (s, 2H), 3.51-3.34 (m, 4H), 3.30 (s, 2H), 3.05-2.90 (m, 4H), 1.18 (s, 42H). ^{13}C NMR (100 MHz, Chloroform-*d*, 298 K) δ = 142.5, 142.2, 135.1, 134.9, 126.0, 124.1, 106.3, 96.0, 83.0, 81.9, 32.3, 32.1, 18.9, 18.9, 11.6. HRMS (MALDI-TOF) calculated for $C_{42}H_{56}Si_2$ $[M]^+$: 616.3921, found 616.3915.



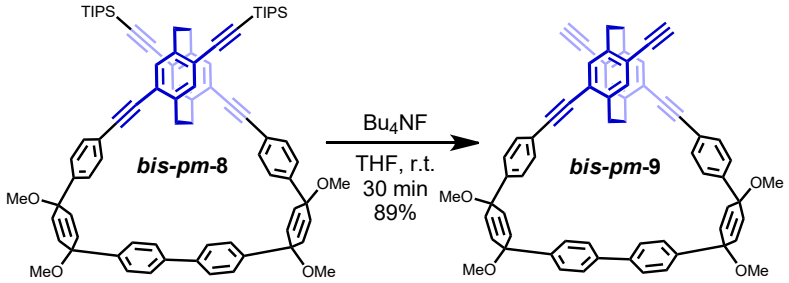
Compound ***bis-pm-6*** (1.0 g, 1.62 mmol), compound **1** (2.0 g, 4.05 mmol), $Pd_2(dba)_3$ (148.3 mg, 0.16 mmol), PPh_3 (170.6 mg, 0.65 mmol), CuI (61.6 mg, 0.32 mmol) were added to a dried flask. The flask was evacuated and backfilled with Ar three times. After cooling to 0°C, the dried THF (64 mL) and TEA (16 mL) was added to the reaction. The mixture was stirred for 3 h on room temperature. The reaction was quenched with water and extracted with ethyl acetate three times. The combined organic layer was washed with brine, dried with sodium sulfate, and evaporated under reduce pressure. The crude product was purified by column chromatography on silica gel (EA/PE, 1/10, v/v) to get a yellow solid ***bis-pm-7*** (1.5 g, 68%).

R_f = 0.23 (EA/PE = 1/5, v/v). M.p. = 81-82 °C.
^{1}H NMR (600 MHz, Chloroform-*d*, 298K) δ = 7.51 (d, *J* = 8.3 Hz, 4H), 7.46 (d, *J* = 8.5 Hz, 4H), 7.39 (d, *J* = 8.2 Hz, 4H), 7.29 (d, *J* = 8.5 Hz, 4H), 7.09 (d, *J* = 17.4 Hz, 4H), 6.12 (m, 8H), 3.57-3.46 (m, 5H), 3.45 (d, *J* = 9.2 Hz, 11H), 3.10-2.99 (m, 4H), 1.20 (s, 42H). ^{13}C NMR (100 MHz, Chloroform-*d*, 298K) δ = 143.6, 142.6, 142.5, 142.1, 135.3, 134.3, 133.7, 133.6, 133.5, 133.3, 131.8, 131.6, 128.0, 126.2, 125.4, 125.3, 123.1, 121.9, 106.7, 95.8, 94.5, 89.5, 74.6, 52.2, 32.8, 32.5, 19.1, 11.7. HRMS (MALDI-TOF) calculated for $C_{82}H_{90}Br_2O_4Si_2$ $[M]^+$: 1354.4724, found 1354.4701.



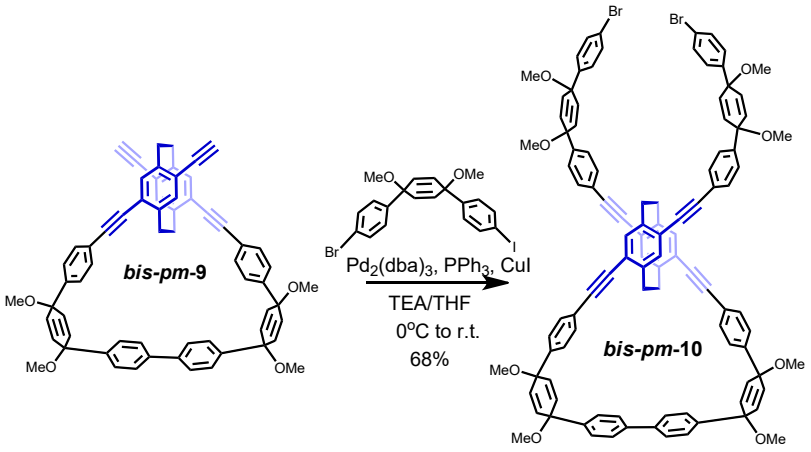
In a nitrogen-filled glove bag, ***bis-pm-7*** (860 mg, 0.64 mmol), $Ni(cod)_2$ (440 mg, 1.61 mmol), 2,2'-bipyridyl (249 mg, 1.61 mmol) were added to a 1000 mL two-necked flask containing a magnetic stirring bar and equipped with a condenser. The flask was sealed with a septum and transferred out of glove bag. After dry THF (640 mL) was added to the flask via syringe through a septum, the mixture was refluxed for 24 h. The reaction mixture was cooled down to room temperature and filtered through a short pad of silica gel with ethyl acetate/$CHCl_3$. The solvent was evaporated under reduce pressure to give a crude product, and then was purified by column chromatography on silica gel (PE/ EA, 5/1, v/v) to get ***bis-pm-8*** as a white solid (520.4 mg, 68%).

R_f = 0.22 (EA/PE = 1/5, v/v). M.p. = 166-167 °C.
^{1}H NMR (400 MHz, Chloroform-*d*, 298K) δ = 7.62 (d, *J* = 8.4 Hz, 4H), 7.50 (d, *J* = 8.4 Hz, 4H), 7.44 (d, *J* = 8.4 Hz, 4H), 7.38 (d, *J* = 8.4 Hz, 4H), 7.06 (s, 2H), 6.99 (s, 2H), 6.27 (m, 2H), 6.19 (m, 2H), 6.12 (m, 4H), 3.49 (d, *J* = 14.1 Hz, 16H), 3.11-2.92 (m, 4H), 1.23 (s, 42H). ^{13}C NMR (100 MHz, Chloroform-*d*, 298K) δ = 143.7, 143.4, 142.5, 140.0, 135.7, 134.6, 134.2, 133.3, 132.9, 131.9, 131.3, 127.0, 126.5, 125.2, 123.0, 106.9, 96.5, 96.1, 91.2, 75.6, 75.0, 52.3, 52.1, 33.0, 32.5, 19.1, 11.7. HRMS (MALDI-TOF) calculated for $C_{82}H_{90}O_4Si_2$ $[M]^+$: 1194.6318, found 1194.6368.



Compound ***bis-pm*-8** (518.4 mg, 0.43 mmol) was dissolved in THF (30 mL), followed by the addition of Bu_4NF (1.0 M THF solution, 4.3 mL). The reaction was carried out at room temperature for 30 min. H_2O was added to the reaction mixture. The organic layer was extracted three times with EA and washed with brine, and dried over Na_2SO_4. Na_2SO_4 was removed by filtration. The solvent was evaporated under reduce pressure to give a crude product. The solvent was evaporated under reduce pressure to give a crude product, and then was purified by column chromatography on silica gel (PE/ EA, 5/1, v/v) to get ***bis-pm*-9** as a yellow solid (338 mg, 89%).

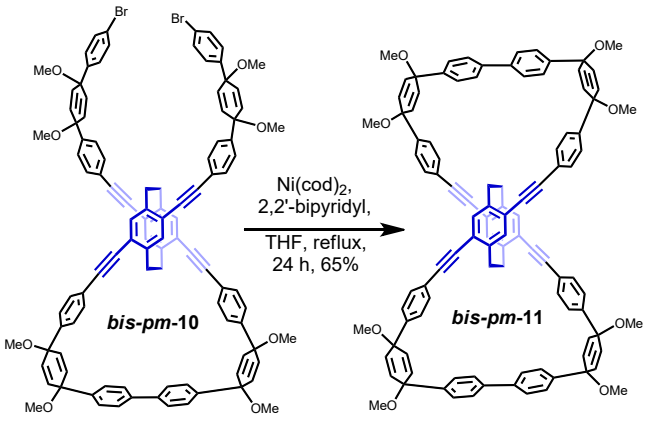
R_f = 0.19 (EA/PE = 1/5, v/v). M.p. = 193-194 °C.
^{1}H NMR (400 MHz, Chloroform-*d*, 298K) δ = 7.61 (d, J = 8.3 Hz, 4H), 7.49 (m, 8H), 7.40 (d, J = 8.3 Hz, 4H), 7.04 (s, 2H), 6.95 (s, 2H), 6.25 (m, 2H), 6.22 – 6.17 (m, 2H), 6.15 – 6.08 (m, 4H), 3.46 (m, 16H), 3.41 (s, 2H), 3.10 – 2.98 (m, 4H). ^{13}C NMR (150 MHz, Chloroform-*d*, 298K) δ = 143.8, 143.7, 143.0, 142.5, 139.7, 135.3, 134.2, 134.0, 133.4, 133.1, 132.0, 131.3, 127.0, 126.9, 126.5, 125.5, 123.7, 122.6, 96.6, 90.6, 83.1, 82.7, 75.5, 74.9, 68.6, 52.2, 52.1, 33.0, 32.3, 27.8, 22.2. HRMS (MALDI-TOF) calculated for $C_{64}H_{50}O_4$ $[M]^+$: 882.3709, found 882.3701.



Compound ***bis-pm*-9** (338 mg, 0.38 mmol), compound **1** (476 mg, 0.96 mmol), $Pd_2(dba)_3$ (35.1 mg, 0.038 mmol), PPh_3 (40.3 mg, 0.15 mmol), CuI (14.6 mg, 0.08 mmol) were added to a dried flask. The flask was evacuated and backfilled with Ar three times. After cooling to 0°C, the dried THF (16 mL) and TEA (4 mL) was added to the reaction. The mixture was stirred for 3 h on room temperature. The reaction was quenched with water and extracted with ethyl acetate three times. The combined organic layer was washed with brine, dried with sodium sulfate, and evaporated under reduce pressure. The crude product was purified by column chromatography on silica gel (EA/PE, 1/5, v/v) to get a yellow solid ***bis-pm*-10** (419.1 mg, 68%).

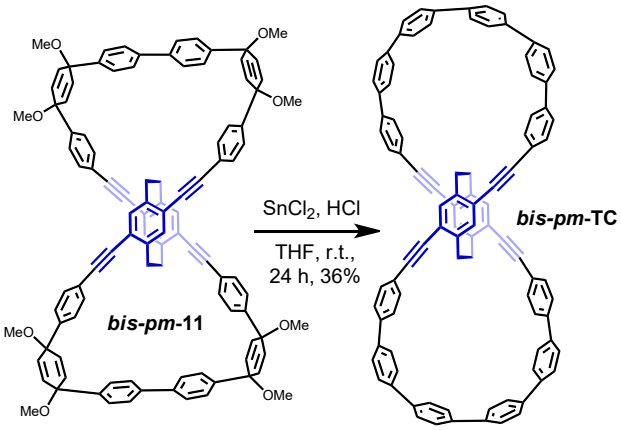
R_f = 0.21 (EA/PE = 1/2, v/v). M.p. = 165-166 °C.
^{1}H NMR (400 MHz, Chloroform-*d*, 298K) δ = 7.62 (d, J = 8.1 Hz, 4H), 7.55 (d, J = 7.9 Hz, 4H), 7.53-7.45 (m, 12H), 7.41 (t, J = 8.1 Hz, 8H), 7.30 (d, J = 8.6 Hz, 4H), 7.06 (s, 2H), 6.98 (s, 2H), 6.25 (m, 2H), 6.22-6.14 (m, 3H), 6.14 – 6.08 (m, 11H), 3.59-3.51 (m, 4H), 3.49 (d, J = 0.7 Hz, 6H), 3.47 – 3.44 (m, 12H), 3.43 (s, 6H), 3.15-3.00 (m, 4H). ^{13}C NMR (150 MHz, Chloroform-*d*, 298K) δ = 143.9, 143.6, 143.5, 142.6, 142.5, 142.4, 134.8, 134.3, 134.0, 133.6, 133.5, 133.5, 133.4, 133.4, 133.1, 132.3, 131.7, 131.34, 128.0, 127.0, 127.0, 126.5, 126.3, 125.0, 124.8, 123.0, 122.9, 121.9, 96.5,

94.5, 91.1, 89.6, 75.6, 75.0, 74.8, 74.6, 52.3, 52.2, 52.1, 33.1, 33.0. HRMS (MALDI-TOF) calculated for $C_{104}H_{84}Br_2O_8$ $[M]^+$: 1621.4546, found 1621.4411.



In a nitrogen-filled glove bag, ***bis-pm*-10** (419.1 mg, 0.26 mmol), $Ni(cod)_2$ (177.6 mg, 0.65 mmol), 2,2'-bipyridyl (101.0 mg, 0.65 mmol) were added to a 500 mL two-necked flask containing a magnetic stirring bar and equipped with a condenser. The flask was sealed with a septum and transferred out of glove bag. After dry THF (260 mL) was added to the flask via syringe through a septum, the mixture was refluxed for 24 h. The reaction mixture was cooled down to room temperature and filtered through a short pad of silica gel with ethyl acetate/$CHCl_3$. The solvent was evaporated under reduce pressure to give a crude product, and then was purified by column chromatography on silica gel (PE/ EA, 5/1, v/v) to get ***bis-pm*-11** as a white solid (247.0 mg, 65%).

R_f = 0.20 (EA/PE = 1/2, v/v). M.p. = 240-241 °C.
^{1}H NMR (400 MHz, Chloroform-*d*, 298K) δ = 7.63 (d, J = 8.4 Hz, 8H), 7.52 (d, J = 8.9 Hz, 16H), 7.41 (d, J = 8.3 Hz, 8H), 6.96 (s, 4H), 6.26 (m, 4H), 6.21 (m, 4H), 6.13 (m, 8H), 3.51 (s, 12H), 3.48 (s, 12H), 3.51 – 3.42 (m, 4H), 3.16 – 3.04 (m, 4H). ^{13}C NMR (100 MHz, Chloroform-*d*, 298K) δ = 144.0, 143.5, 142.5, 139.0, 134.2, 134.0, 133.4, 133.1, 132.4, 131.4, 127.0, 126.9, 126.4, 124.7, 122.9, 96.4, 91.0, 75.5, 75.0, 52.3, 52.2, 33.2, 29.8. HRMS (MALDI-TOF) calculated for $C_{104}H_{84}O_8$ $[M]^+$: 1460.6166, found 1460.6153.



A H_2SnCl_4/THF solution was freshly prepared by dissolving anhydrous $SnCl_2$ (409 mg, 2.15 mmol) in 9 ml anhydrous THF under nitrogen atmosphere and then adding concentrated HCl (aq) (0.32 ml) to the solution. The resulting solution was deoxygenated and stirred for 15 minutes before use. *Bis-pm*-**11** (63 mg, 0.043 mmol) was dissolved in anhydrous THF (8 ml) and toluene (8 ml) under a nitrogen atmosphere and the freshly prepared H_2SnCl_4/THF solution (9.3 ml) was added to this solution. The reaction mixture was stirred at room temperature. The reaction mixture was stirred at room

temperature for 17 h before being quenched with $NaOH/H_2O$ solution. The aqueous layer was extracted with dichloromethane and the organic layers were combined and dried with anhydrous Na_2SO_4. The crude mixture was purified by column chromatography (SiO_2, DCM/ petroleum ether, 1/10) to get ***bis-pm*-TC** as a light yellow solid (18.8 mg, 36%).

R_f = 0.20 (DCM/PE = 1/2, v/v). M.p. > 300 °C.
^{1}H NMR (400 MHz, Chloroform-*d*, 298K) δ = 7.57-7.53 (m, 22H), 7.49 (d, J = 8.7 Hz, 10H), 7.43 (s, 16H), 6.84 (s, 4H), 2.90-2.76 (m, 4H), 2.69-2.56 (m, 4H). 13C NMR (100 MHz, Chloroform-*d*, 298K) δ = 144.83, 140.58, 138.9, 138.2, 137.8, 137.3, 131.5, 131.5, 127.7, 127.6, 127.2, 121.9, 96.5, 93.0, 31.51, 30.3. HRMS (MALDI-TOF) calculated for $C_{96}H_{60}$ $[M]^+$: 1213.4729, found 1213.4731.

2. Results and Discussion

2.1 Planar chiral 4,7,12,15-tetrasubstituted [2.2]PCP

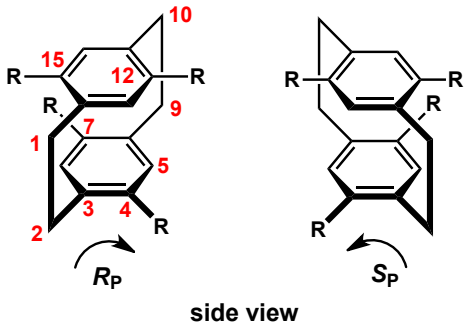


Fig. S1 *R*p-and *S*p- describe the planar chirality of 4,7,12,15-tetrasubstituted [2.2]PCP.

2.2 Topological transformation

2.2.1 semi-macrocycles PCP-[n]CPP

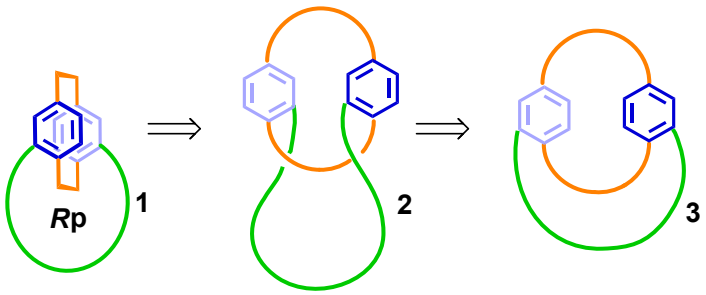
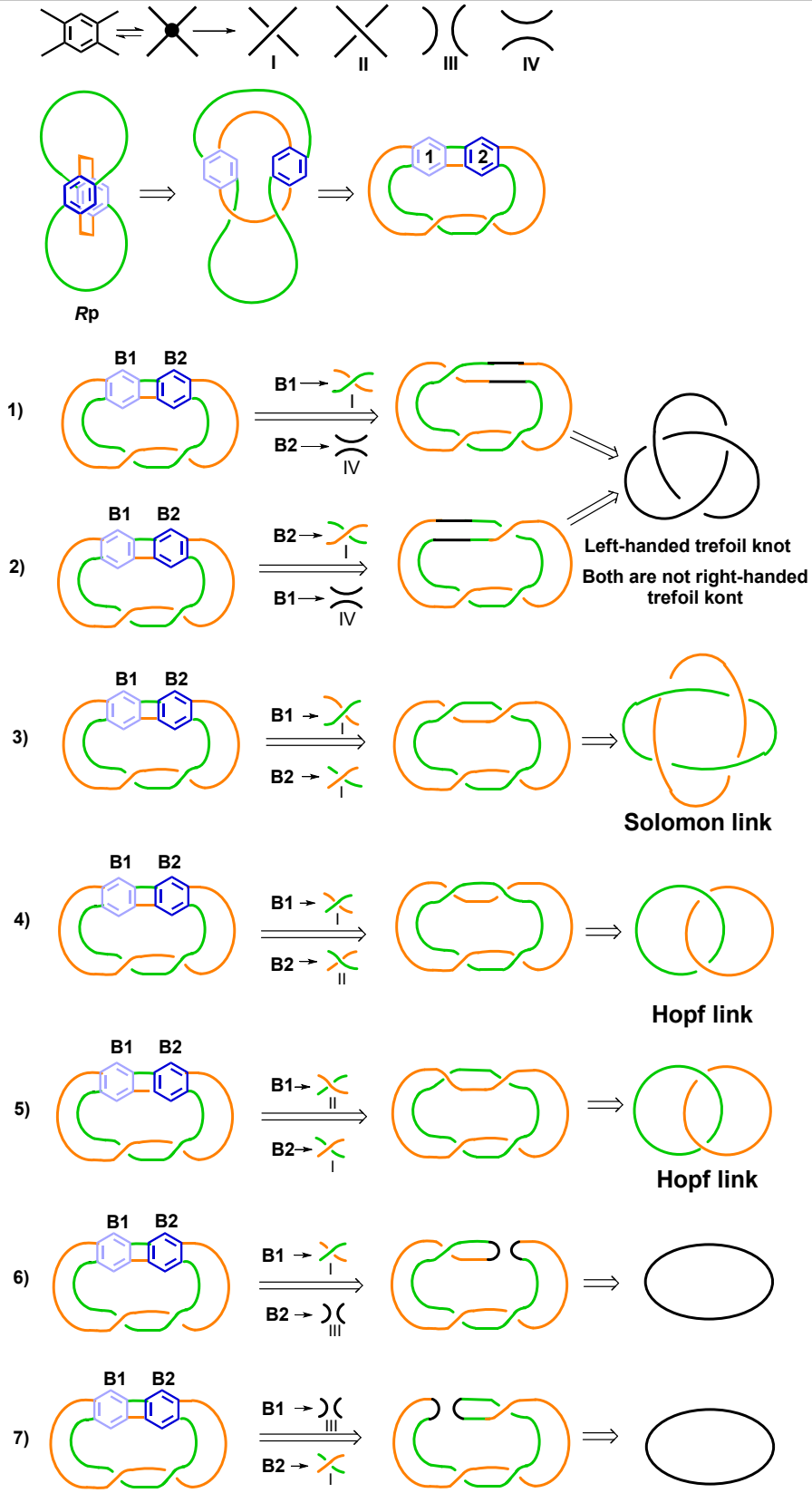


Fig. S2 Topological transformation of semi-macrocycles including ***bis-pm-8***, ***bis-pm-10*** and **PCP-[n]CPP** to be planar molecular graph, which demonstrates it is topologically achiral.

2.2.2 Rp-bis-pm-TC


I
II
III
IV
1
2
Rp
B1
B2
1)
2)
3)
4)
5)
6)
7)
Left-handed trefoil knot
Both are not right-handed trefoil kont
Solomon link
Hopf link
Hopf link

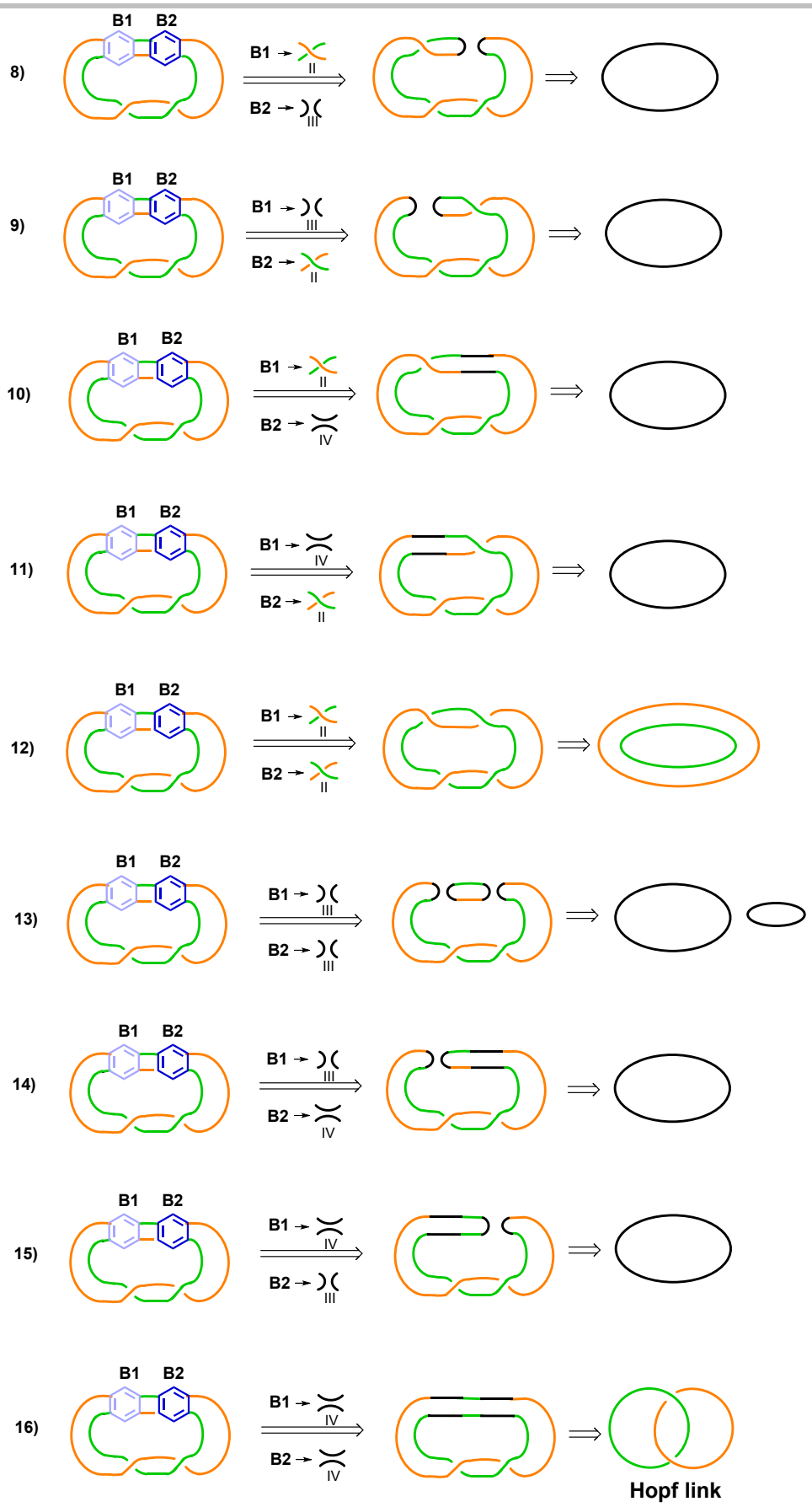


Fig. S3 Topological transformation of *R*p-***bis-pm*-TC** into all topological trivial and nontrivial species.

Table S1. All topological trival and nontrival species of *R*p-***bis-pm*-TC**.

B1 / B2	I	II	III	IV
I				
II				
III				
IV				

2.2.3 Sp-bis-pm-TC

Topological transformation of *S*p-***bis-pm*-TC** taking the transformation to be right-handed trefoil knot as an example.

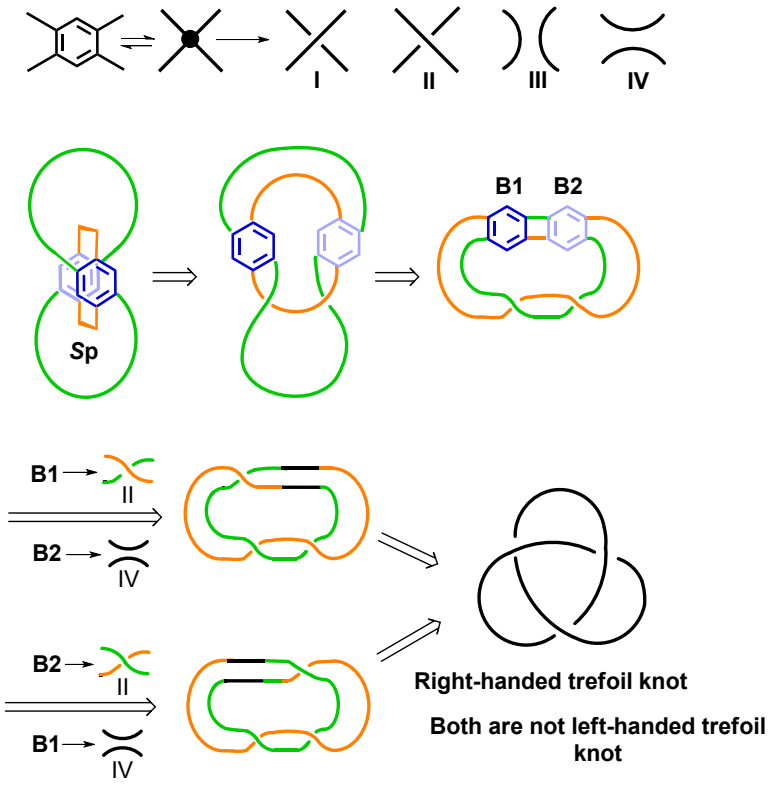
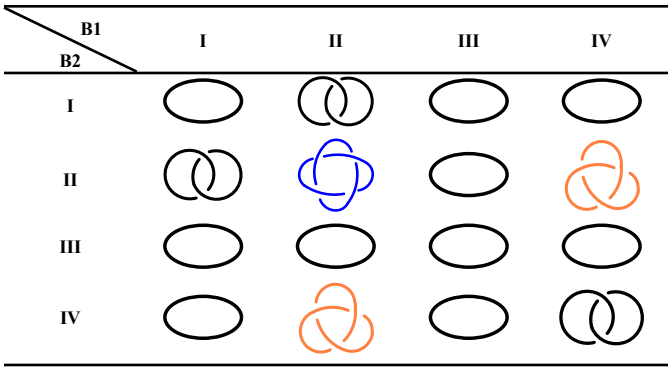


Fig. S4 Topological transformation of *S*p-***bis-pm*-TC** by taking the transformation to a trefoil knot subgraph as an example.

Table S2. All topological trival and nontrival species of *Sp*-***bis-pm-TC***.



2.2.4 bis-po-CC

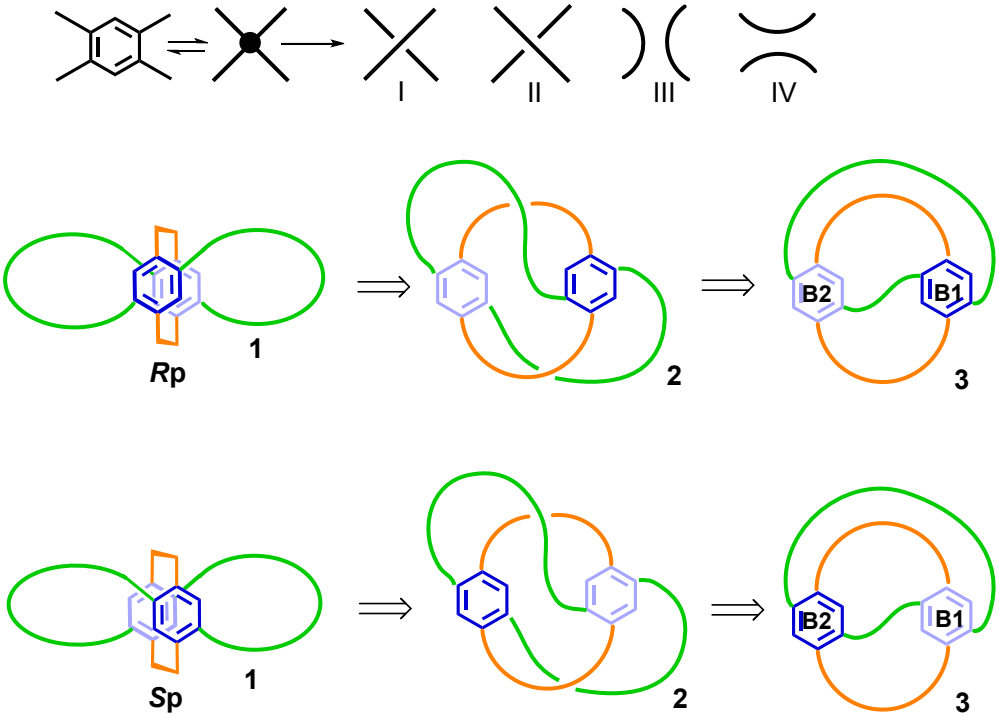
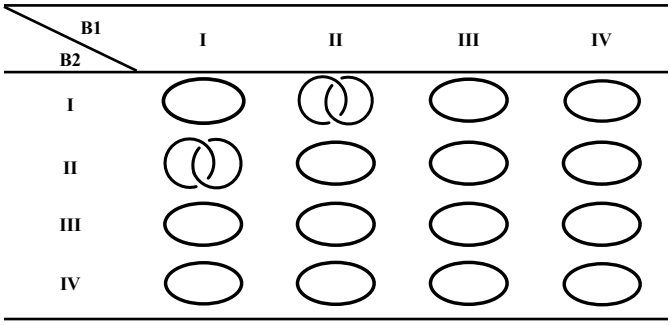


Fig. S5 Topological deformation of ***bis-po*-CC**.

Table S3. All topological trival and nontrival species of *Sp*-***bis-po*-CC**.



2.3 Comparison of the ^{1}H NMR spectra

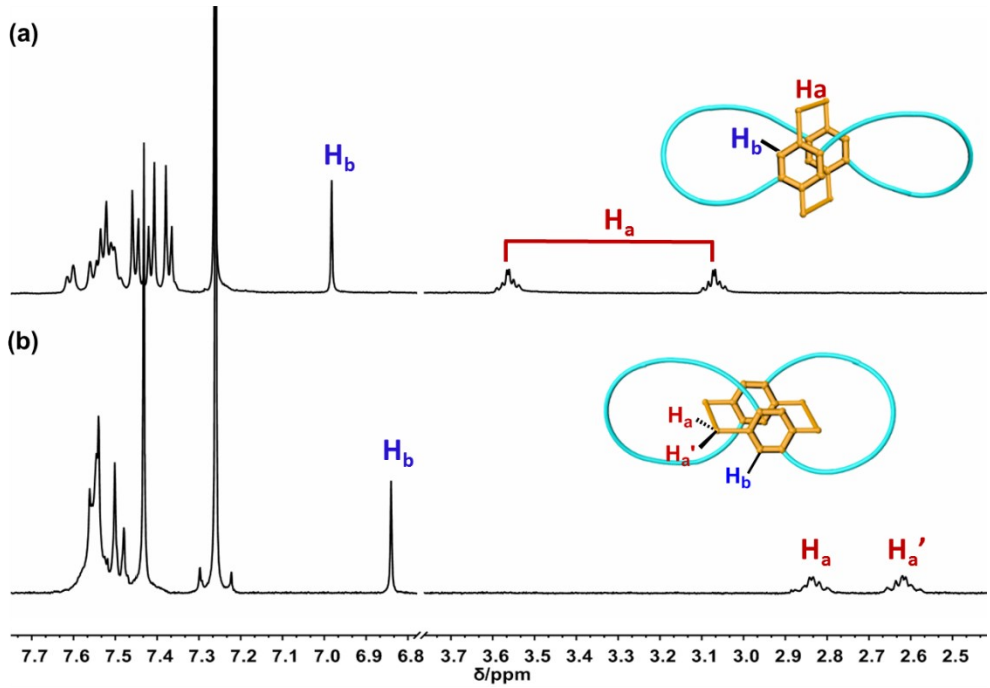


Fig. S6 Comparison of the ^{1}H NMR spectra (600 MHz, $CDCl_3$, 298 K) of (a) ***bis-po*-CC** and (b) ***bis-pm*-TC**.

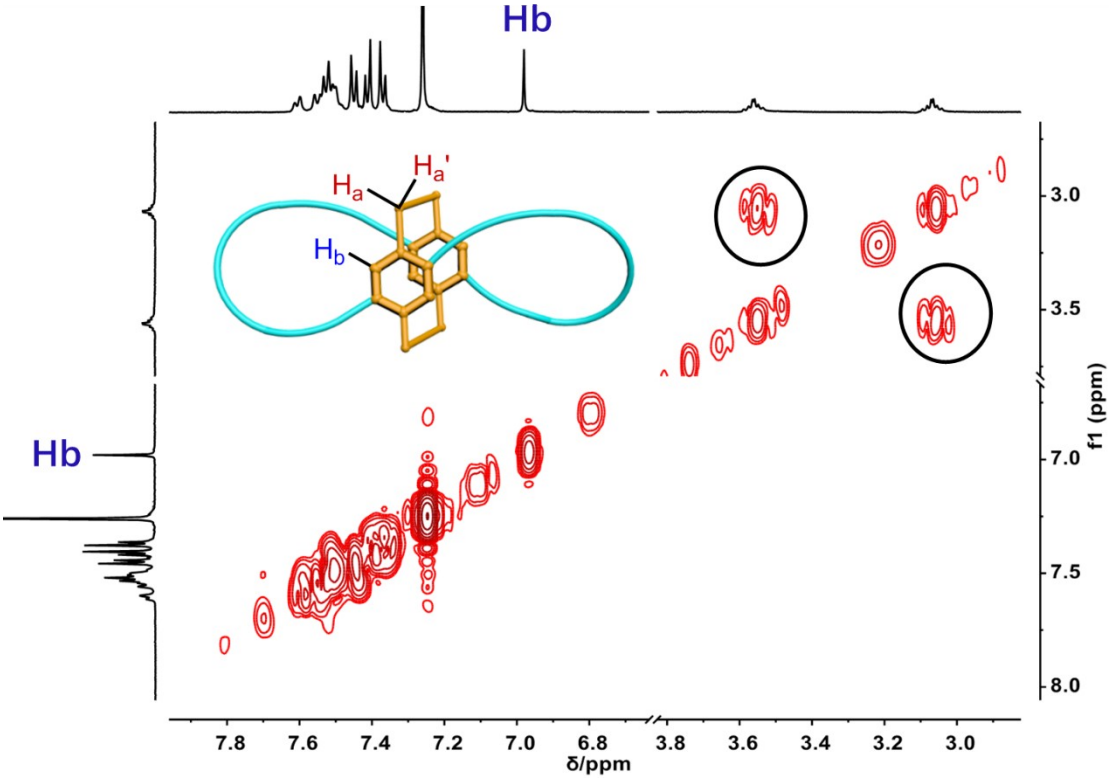


Fig. S7 ^{1}H–^{1}H COSY spectra of ***bis-po*-CC** (600 MHz, $CDCl_3$, 298 K).

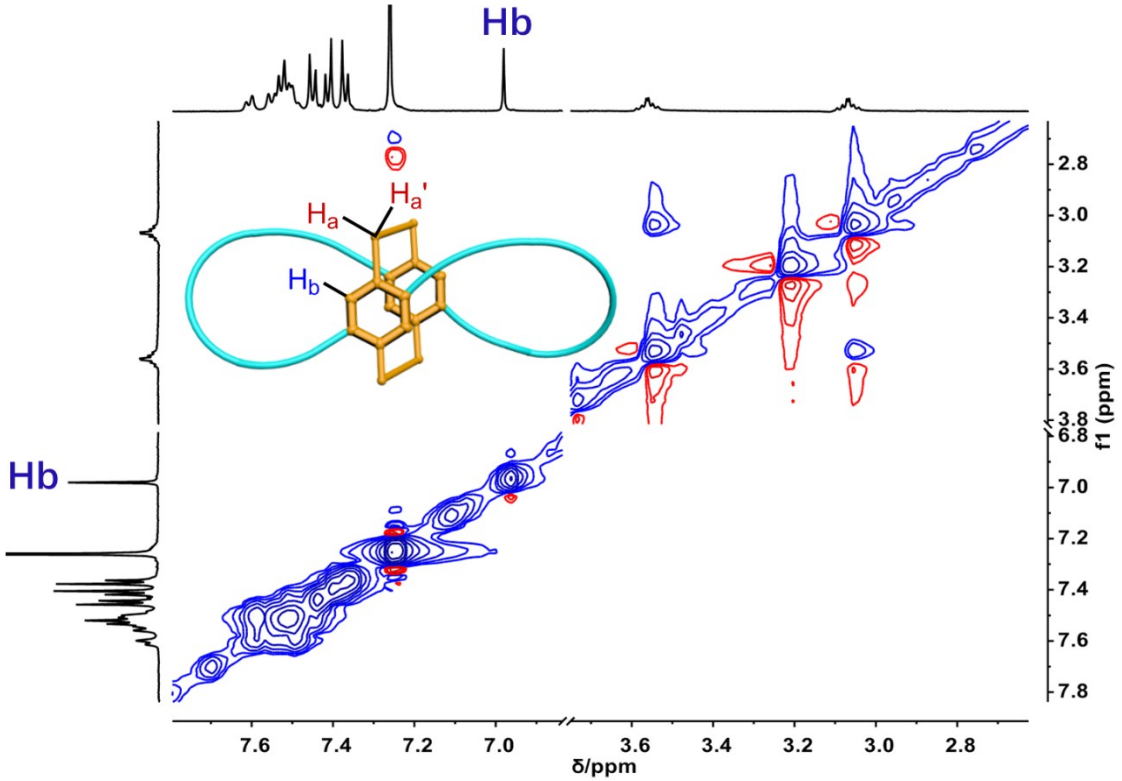


Fig. S8 NOESY spectra of ***bis-po*-CC** (600 MHz, $CDCl_3$, 298 K).

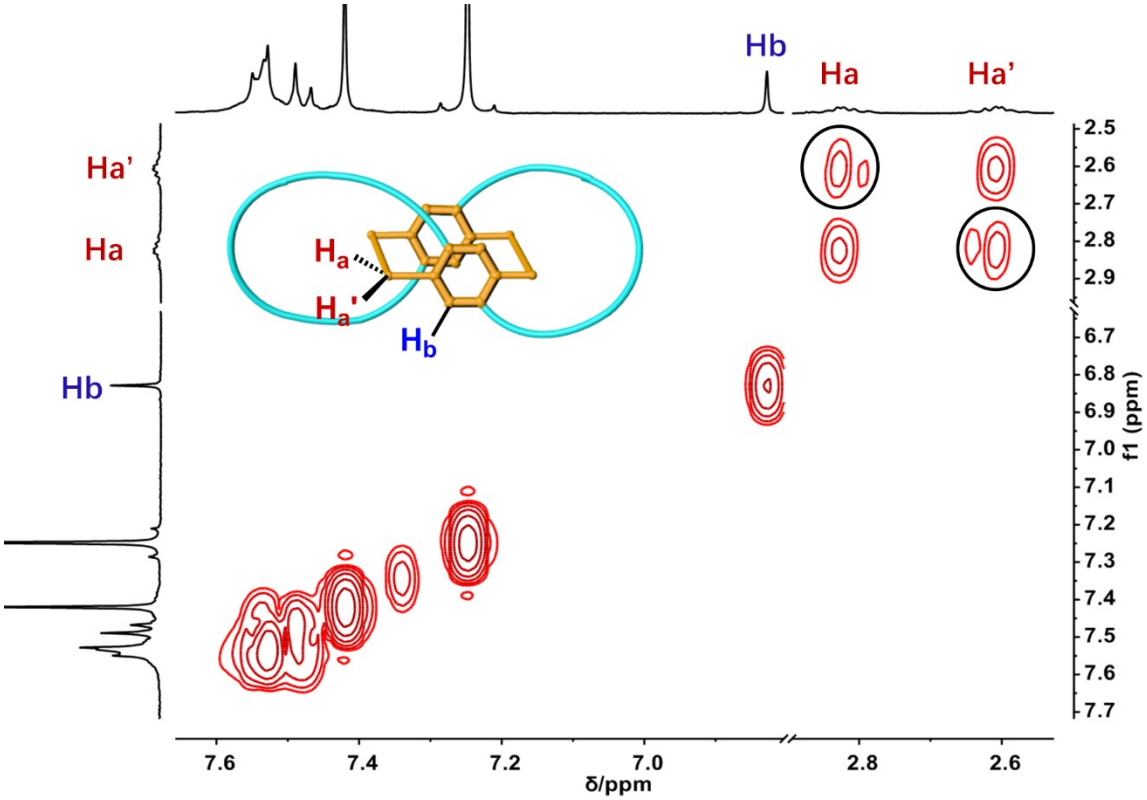


Fig. S9 ^1H–^1H COSY spectra of ***bis-pm*-TC** (600 MHz, $CDCl_3$, 298 K).

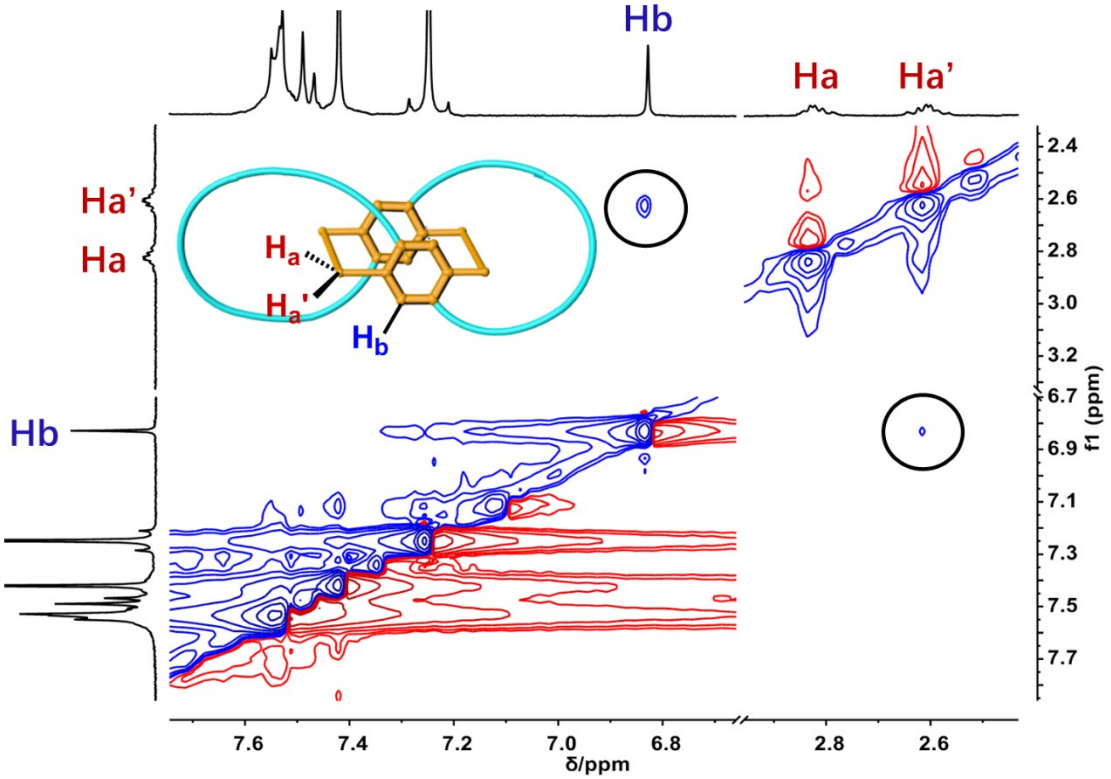


Fig. S10 NOESY spectra of ***bis-pm*-TC** (600 MHz, $CDCl_3$, 298 K).

2.4 X-ray Crystallography

Crystals suitable for X-ray analysis were obtained by vapor diffusion of hexane into chloroform solution of ***bis-pm*-11** and ***bis-pm*-TC**, respectively. Single crystal X-ray diffraction data were collected on a Rigaku Super Nova, Dual, Cu at zero, AtlasS2 diffractometer. The crystal was kept at 100.00(10) K during data collection. Using Olex2[S4], the structure was solved with the ShelXT[S5] structure solution program using Direct Methods and refined with the ShelXL[S6] refinement package using Least Squares minimization. The disordered solvent molecules were removed with the SQUEEZE routine in PLATON[S7] and the solvent-free model was employed for the final refinement. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were positioned by geometric idealization. Details of the crystal data and a summary of the intensity data collection parametersare listed in Table S4-S5. Crystallographic data were deposited at the Cambridge Crystallographic Data Center (CCDC **2173517** for ***bis-pm*-11**, **2173519** for ***bis-pm*-TC**). The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures.

Crystal Structure Data of compound ***bis-pm*-11** (CCDC number: 2173517).

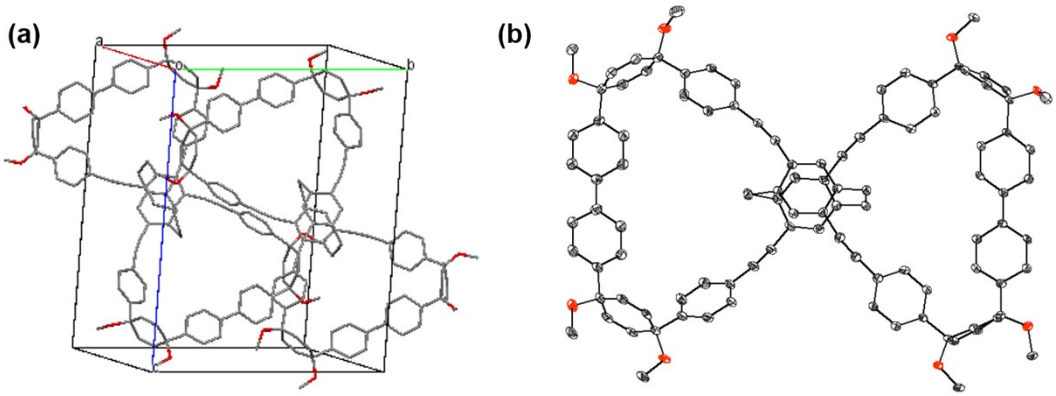


Fig. S11 Crystal structure of ***bis-pm*-11** was obtained by slow diffusion of hexane into chloroform solution. (a) Crystal cell (b) ORTEP drawing. Hydrogen atoms are omitted for clarity. Thermal ellipsoids are drawn at the 50% probability level.

Table S4. Crystal data and structure refinement for compound ***bis-pm*-11.**

	***bis-pm*-11**
CCDC	2173517
Empirical formula	$C_{104}H_{84}O_8$
Formula weight	1461.71
Temperature/K	99.99(10)
Crystal system	triclinic
Space group	P-1
a/Å	13.7107(2)
b/Å	16.2983(3)
c/Å	21.2715(3)
α/°	94.4940(10)
β/°	95.4560(10)
γ/°	112.361(2)
Volume/Å^3	4342.01(13)

Z	2
ρ_{calc}g/cm^3	1.118
μ/mm^{-1}	0.545
F(000)	1544.0
Crystal size/mm^3	0.2 × 0.05 × 0.02
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.816 to 152.694
Index ranges	-17 ≤ h ≤ 17, -20 ≤ k ≤ 20, -26 ≤ l ≤ 26
Reflections collected	55712
Independent reflections	17529 [R_{int} = 0.0823, R_{sigma} = 0.0622]
Data/restraints/parameters	17529/0/1017
Goodness-of-fit on F^2	1.104
Final R indexes [I>=2σ (I)]	R_1 = 0.0913, wR_2 = 0.2200
Final R indexes [all data]	R_1 = 0.1037, wR_2 = 0.2275
Largest diff. peak/hole / e Å^{-3}	0.66/-0.41

Crystal Structure Data of compound ***bis-pm*-TC** (CCDC number: **2173519**).

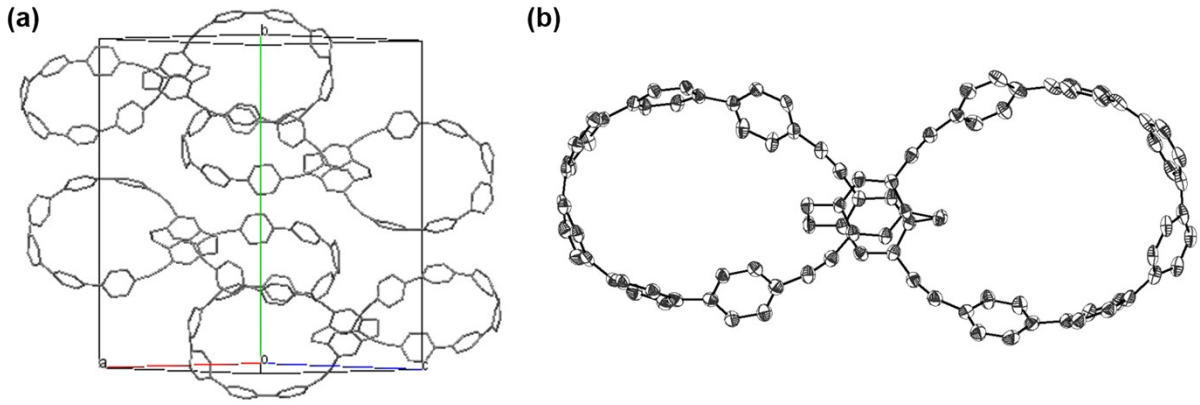


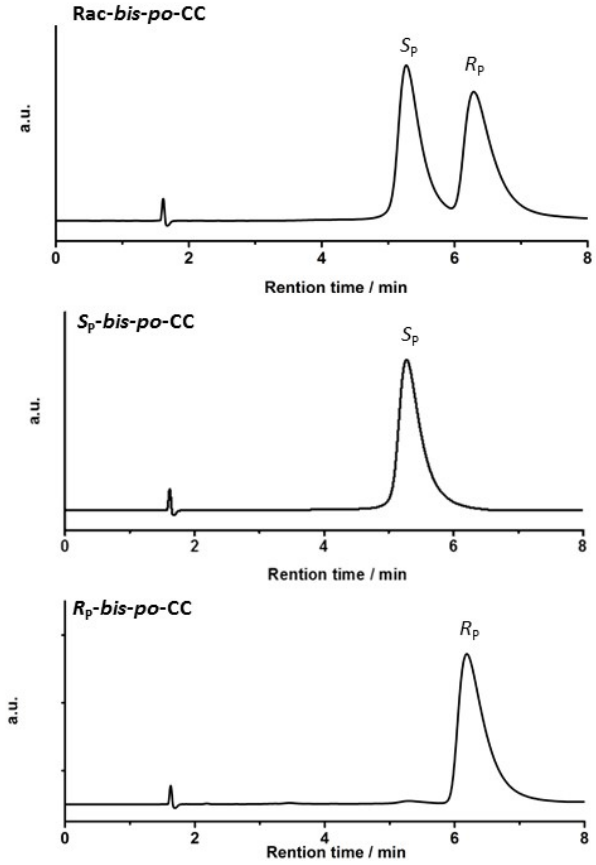
Fig. S12 Crystal structure of ***bis-pm*-TC** was obtained by slow diffusion of hexane into chloroform solution. (a) Crystal cell (b) ORTEP drawing. Hydrogen atoms are omitted for clarity. Thermal ellipsoids are drawn at the 50% probability level.

Table S5. Crystal data and structure refinement for compound ***bis-pm*-TC.**

	***bis-pm*-TC**
CCDC	2173519
Empirical formula	$C_{99}H_{60}$
Formula weight	1249.47
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	15.8108(10)
b/Å	27.4612(19)

c/Å	18.3586(11)
α/°	90
β/°	104.885(7)
γ/°	90
Volume/Å^3	7703.5(9)
Z	4
ρ_{calc}g/cm^3	1.077
μ/mm^{-1}	0.464
F(000)	2616.0
Crystal size/mm^3	0.1 × 0.1 × 0.1
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.438 to 154.418
Index ranges	-20 ≤ h ≤ 19, -21 ≤ k ≤ 34, -21 ≤ l ≤ 23
Reflections collected	55423
Independent reflections	15468 [R_{int} = 0.1441, R_{sigma} = 0.1322]
Data/restraints/parameters	15468/0/865
Goodness-of-fit on F^2	0.925
Final R indexes [I>=2σ (I)]	R_1 = 0.0874, wR_2 = 0.2233
Final R indexes [all data]	R_1 = 0.1494, wR_2 = 0.2625
Largest diff. peak/hole / e Å^{-3}	0.63/-0.26

2.5 Details of HPLC Experiments



Peak	Ret.Time	Area%
1	5.230	47.1767
2	6.119	49.6415

Peak	Ret.Time	Area%
1	5.456	97.3687

Peak	Ret.Time	Area%
1	6.187	95.1677

Fig. S13 HPLC charts of the enantiomers of ***bis-po*-CC**.

Resolution of racemic ***bis-po*-CC** by HPLC. ***Bis-po*-CC** (10 mg) was subjected to high-pressure liquid chromatography (HPLC) (Chiralpak IB column, 4.6 mm Φ × 250 mmL) equipped with a UV-vis detector.

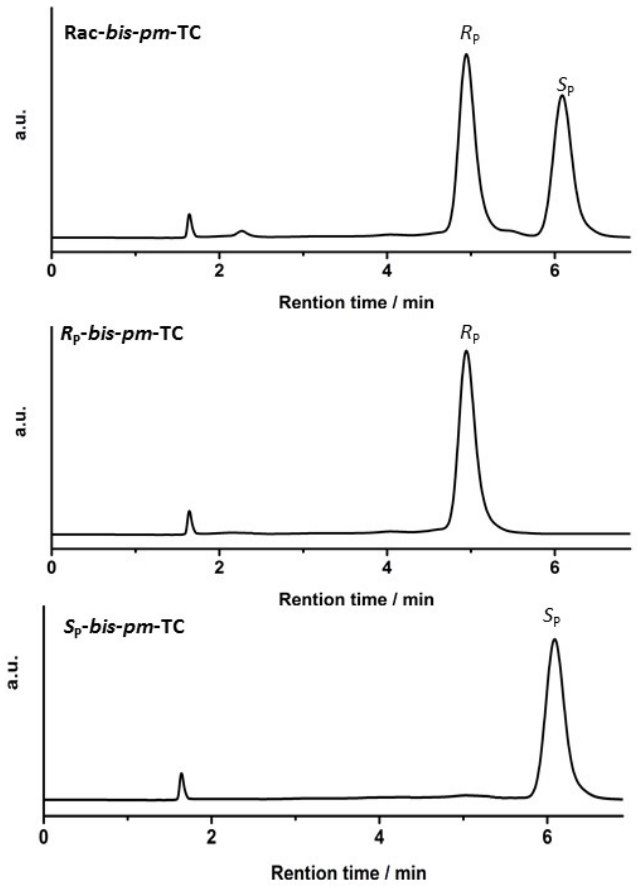
Single injection volume: 10μL. Sample concentration: 1 mg/mL. Chromatography condition: DCM/Hexane (v/v, 28:72) with a flow rate of 2.0 mL/min.

Peak 1:

Assigned as R_P-***bis-po*-CC**, retention time: 5.2 min, isolated total: 4.7 mg, 47%

Peak 2:

Assigned as S_P-***bis-po*-CC**, retention time: 6.1 min, isolated total: 4.9 mg, 49%



Peak	Ret.Time	Area%
1	4.873	47.7162
2	5.960	45.7891

Peak	Ret.Time	Area%
1	4.873	96.562

Peak	Ret.Time	Area%
1	5.982	95.8182

Fig. S14 HPLC charts of the enantiomers of ***bis-pm*-TC**.

Resolution of racemic compound ***bis-pm*-TC** by HPLC. ***Bis-pm*-TC** (10 mg) was subjected to high-pressure liquid chromatography (HPLC) (Chiralpak IB column, 4.6 mm Φ × 250 mmL) equipped with a UV-vis detector.

Single injection volume: 10μL. Sample concentration: 1 mg/mL. Chromatography condition: DCM/MeOH (v/v, 42:58) with a flow rate of 2.0 mL/min.

Peak 1:

Assigned as R_P-***bis-pm*-TC**, retention time: 4.8 min, isolated total: 4.8 mg, 48%

Peak 2:

Assigned as S_P-***bis-pm*-TC**, retention time: 5.9 min, isolated total: 4.6 mg, 46%

2.6 Photophysical Properties

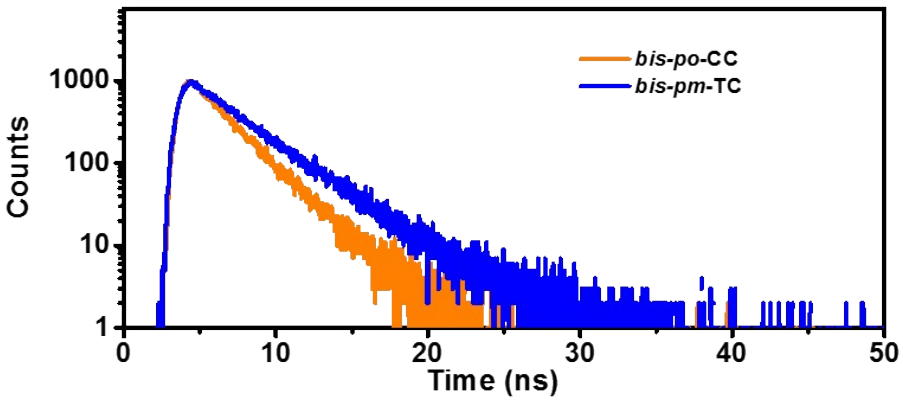


Fig. S15 Emission lifetime of ***bis-po*-CC** and ***bis-pm*-TC** in CH_2Cl_2 (c = 1.0×10^{-5} M).

2.7 Comparison of $|g_{lum}|$ of some CPL-active organic molecules

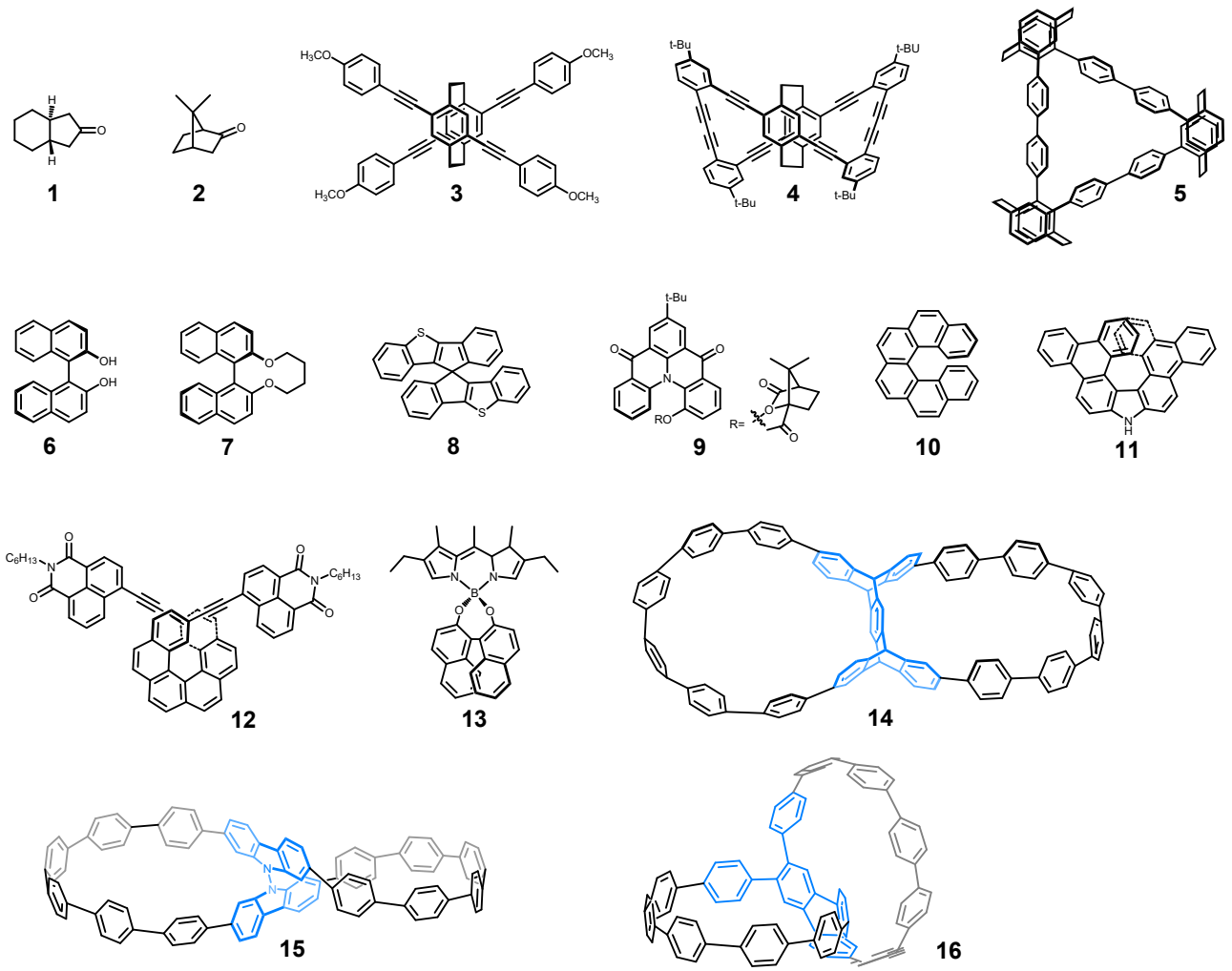


Fig. S16. Representative examples of CPL-active organic molecules.

Table S6. Comparison of the CPL dissymmetry factors of some CPL-active organic molecules.

Compounds	$g_{lum} \times 10^3$	Ref.
1	35	*Chem. Phys. Lett.* 1967, 1, 129.
2	≈2.4	*J. Am. Chem. Soc.* 1976, 98, 2210.
3	1.4	*Chem. Eur. J.* 2016, 22, 2291.
4	11	*J. Am. Chem. Soc.* 2014, 136, 3350.
5	1.6	*Chem.-Eur. J.* 2021, 27, 16225.
6	0.47	*Chem. Lett.* 2015, 44, 1607.
7	1.4	*Chem. Asian J.* 2012, 7, 2836.
8	1.5	*Org. Lett.* 2017, 19, 5082.
9	1.0	*J. Am. Chem. Soc.* 2003, 125, 11808.
10	0.14	*J. Chem. Theory Comput.* 2016, 12, 2799.
11	1.9	*Angew. Chem. Int. Ed.* 2020, 59, 7813.
12	3.2	*Chem. Sci.* 2020, 11, 567.
13	0.85	*J. Am. Chem. Soc.* 2014, 136, 3346.

14	3.4	*Angew. Chem. Int. Ed.* 2019, 58, 3943.
15	3.7	*J. Am. Chem. Soc.* 2019, 141, 7421.
16	6.5 19	*Nat. Commun.* 2022, 13, 3543.

2.8 Computational details and results

All theoretical calculations were performed by the density functional theory (DFT)[S8] and time-dependent DFT (TD DFT)[S9] with B3LYP functional in dichloromethane.[S10] The geometries of ground state of ***bis-po*-CC**, ***bis-pm*-TC**, ***po*-PCP-[6]CPP**, and ***pm*-PCP-[6]CPP** were optimized at the B3LYP/6-31G (d, p) level. The UV-vis curves were calculated at TD PBE0(D3BJ)/6-31G (d, p) level. The ECD curves were predicted at the TD B3LYP/6-311G (d, p) level with a key word of IOP (9/40=4). The conductor-like polarizable continuum model (CPCM) with dielectric constant of 8.93 were employed to consider the effect of the polar solvent dichloromethane. Orbital localization analyses were carried out using Multiwfn3.4. LOL-π isosurfaces for the molecules are illustrated at isovalue = 0.30. LOL-π isosurfaces for the molecules are illustrated at isovalue = 0.60. All of these calculations were performed by Gaussian09 program package.[S11]

2.8.1 Simulated UV-vis spectra

To investigate the absorption behavior, we employed time-dependent (TD) calculations on ***bis-po*-CC** and ***bis-pm*-TC** at TD PBE0(D3BJ)/6-31G (d, p) level in dichloromethane.

TD-DFT calculation results reveal that the S_9 and S_{11} states make the major contribution to the observed peak (λ_{abs}= 334 nm, $\lambda_{TD\text{-}DFT}$ = 328.2 nm, Fig. S18) in the compound ***bis-po*-CC** (Table S7), which corresponds to the transitions of HOMO-2→ LUMO+2 (Table S9). S_3 state makes the major contribution to the observed peak (λ_{abs}= 361 nm, $\lambda_{TD\text{-}DFT}$ = 367 nm, Fig. S18) in the compound ***bis-po*-CC** (Table S8), which corresponds to the transitions of HOMO-2→ LUMO (Table S9).

TD-DFT calculation results reveal that the S_3 and S_6 states make the major contribution to the observed peak (λ_{abs}= 338 nm, $\lambda_{TD\text{-}DFT}$ = 341.2 nm, Fig. S19) in the compound ***bis-pm*-TC** (Table S10), which corresponds to the transitions of HOMO → LUMO and HOMO-2→ LUMO+1 (Table S11). The simulated UV-vis spectra depicted in Fig. S18 and Fig. S19 matches well with the experimental ones.

LUMO+2

-1.60

-1.67

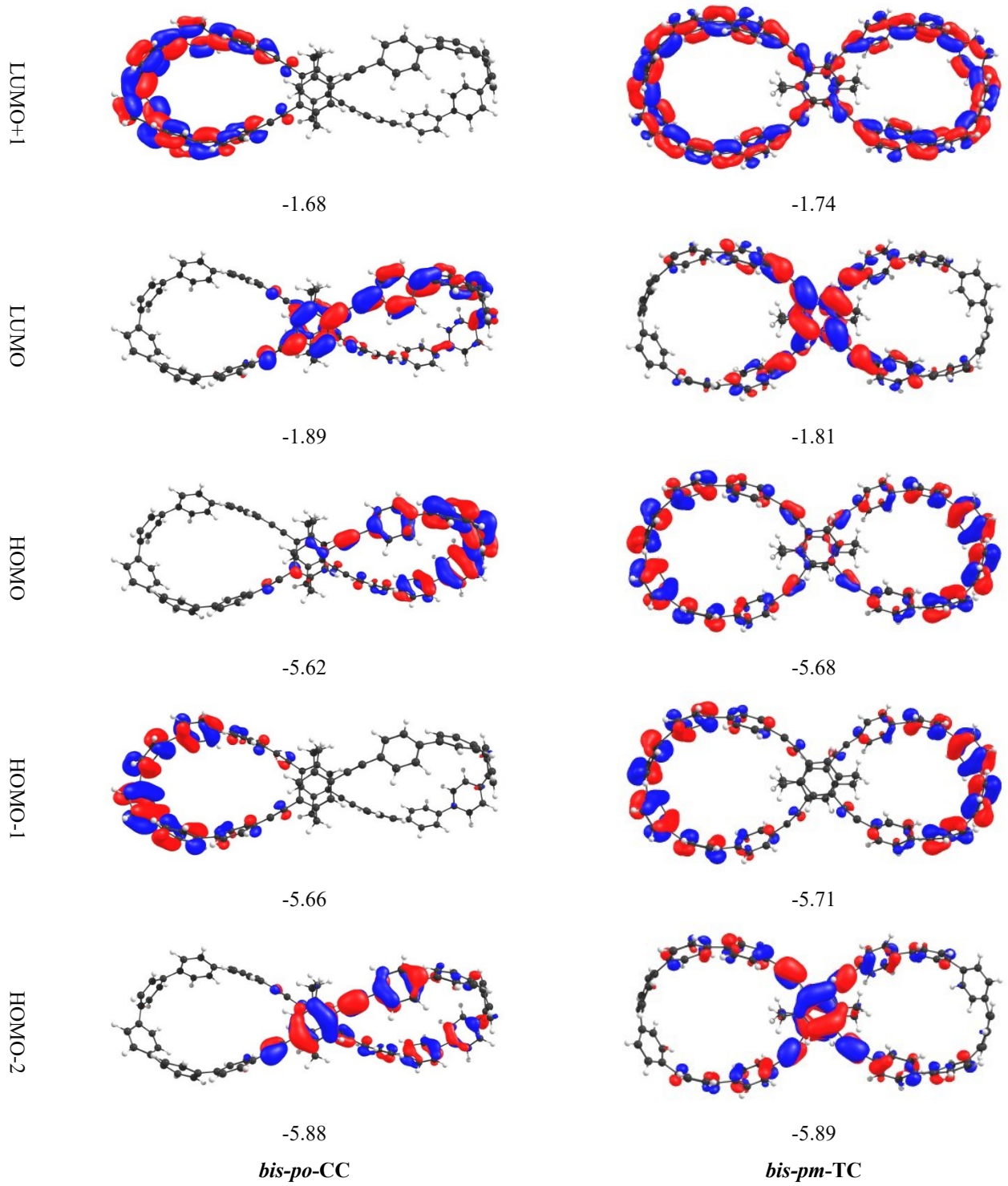


Fig. S17 The TD B3LYP/6-311+G (d, p) predicted frontier molecular orbital and energies (eV) of ***bis-po*-CC** and ***bis-pm*-TC** in dichloromethane.

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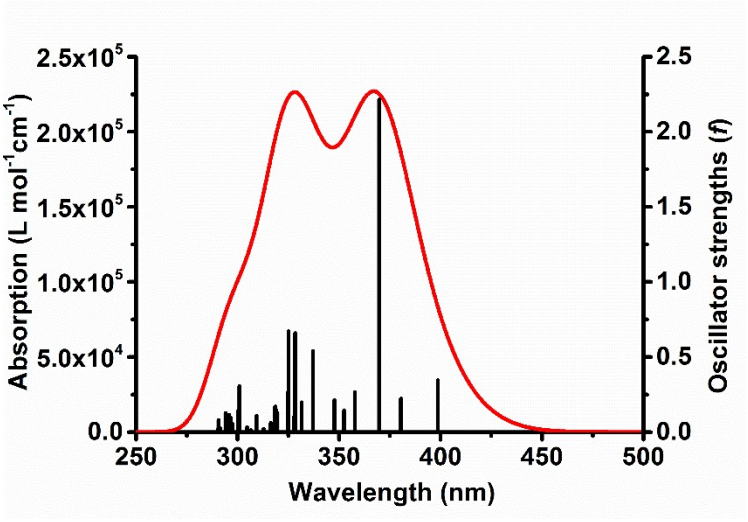


Fig. S18 Simulated UV-vis spectra of ***bis-po*-CC** in dichloromethane.

Table S7. Main contribution of individual transition to the peak of ***bis-po*-TC** (λ=328.2 nm)

Transition	Contribution
S_9	22.4%
S_{11}	22.2%
S_7	14.6%

Table S8. Main contribution of individual transition to the peak of ***bis-po*-TC** (λ=367.0 nm)

Transition	Contribution
S_3	74.1%

Table S9. The TD DFT calculated absorption maxima (λ_{max}, nm), oscillator strengths (f), and major transition in dichloromethane of ***bis-po*-TC**.

state	Energy	λ_{max}	f	Description
S_3	3.3534	370	2.22	HOMO-2→LUMO(0.488)
				HOMO-1→LUMO(0.34)
				HOMO-1→LUMO+1(0.14)
				HOMO→LUMO+2(0.30)
S_7	3.6769	337	0.54	HOMO-3→LUMO(0.17)
				HOMO-2→LUMO+1(0.20)
				HOMO-2→LUMO+3(0.14)
				HOMO-1→LUMO+1(0.12)
				HOMO→LUMO+1(0.42)
				HOMO→LUMO+3(0.39)
				HOMO→LUMO+4(0.12)

S_9	3.7749	328	0.66	HOMO-4→LUMO(0.26) HOMO-3→LUMO(0.12) HOMO-3→LUMO+3(0.11) HOMO-2→LUMO+1(0.11) HOMO-2→LUMO+2(0.39) HOMO-2→LUMO+3(0.14) HOMO-1→LUMO+2(0.31) HOMO-1→LUMO+4(0.15) HOMO→LUMO+2(0.15) HOMO→LUMO+3(0.11)
S_{11}	3.8132	325	0.67	HOMO-2→LUMO+1(0.22) HOMO-2→LUMO+2(0.37) HOMO-2→LUMO+3(0.24) HOMO-1→LUMO+4(0.36) HOMO→LUMO+1(0.18) HOMO→LUMO+3(0.11)

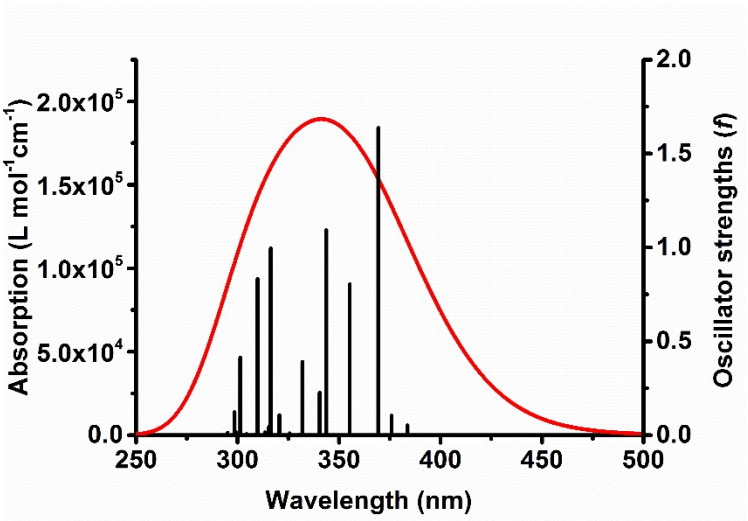


Fig. S19 Simulated UV-vis spectra of ***bis-pm*-TC** in dichloromethane.

Table S10. Main contribution of individual transition to the peak of ***bis-pm*-TC** (λ=341.2 nm)

Transition	Contribution
S_6	23.2%
S_3	21.6%
S_4	15.1%
S_{14}	12.8%

Table S11. The TD DFT calculated absorption maxima (λ_{max}, nm), oscillator strengths (*f*), and major transition in dichloromethane of ***bis-pm*-TC**.

state	Energy	λ_{max}	*f*	Description
S_3	3.3566	369	1.64	HOMO-3→LUMO (0.32)
				HOMO-2→LUMO+1(0.11)
				HOMO-1→LUMO+3(0.10)
				HOMO→LUMO(0.60)
S_4	3.4896	355	0.80	HOMO-2→LUMO(0.60)
				HOMO-1→LUMO+2(0.20)
				HOMO→LUMO+1(0.28)
S_6	3.6062	344	1.09	HOMO-7→LUMO(0.11)
				HOMO-3→LUMO(0.31)
				HOMO-2→LUMO+1(0.54)
				HOMO-2→LUMO+4(0.21)
S_{14}	3.9190	316	1.00	HOMO-7→LUMO(0.10)
				HOMO-2→LUMO+1(0.13)
				HOMO-1→LUMO+3(0.55)
				HOMO→LUMO+5(0.37)

2.8.2 Simulated ECD spectra

To confirm the absolute configuration of ***bis-po*-CC** and ***bis-pm*-TC**, we calculated the ECD of *R*p- configuration of ***bis-po*-CC** and ***bis-pm*-TC** in dichloromethane by TD-DFT at B3LYP/6-311G (d, p) level. The calculated major transitions, related rotatory strengths and oscillator strengths are shown in Table S11 and Table S12. The calculated ECD curves are shown in Fig. S20. For both of them, we found similar orbital shapes and transitions. HOMO and LUMO are delocalized over the two rings, all these transitions are π→π* transitions. The transition density of S_1 excitation is shown in Fig. S21. For ***bis-po*-CC**, the calculated positive rotatory strengths at 419 nm (MO318 to MO319) are associated with the experimentally observed positive cotton effect (CE) at 391 *nm*. The negative rotatory strength at 393 *nm* (MO318 to MO321) are associated with the experimentally observed negative CE at 335 *nm*. Therefore, it was considered that the short dashed line was the configuration of R_P.

For ***bis-pm*-TC**, the calculated positive rotatory strengths at 377 nm (MO316 to MO320) are associated with the experimentally observed positive cotton effect (CE) at 337 *nm*. The negative rotatory strength at 412 *nm* (MO317 to MO320) are associated with the experimentally observed negative CE at 384 *nm*. Therefore, it was considered that the short dashed line was the configuration of R_P.

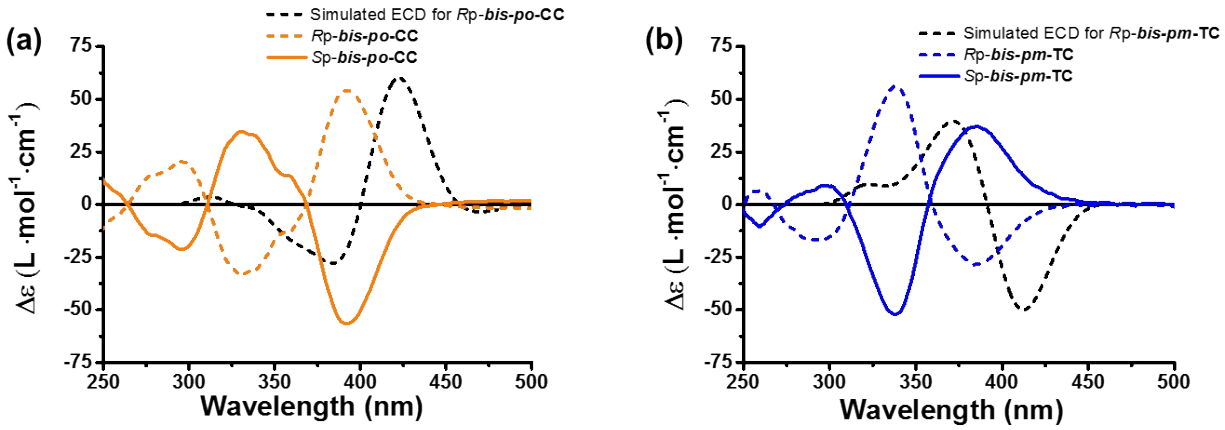


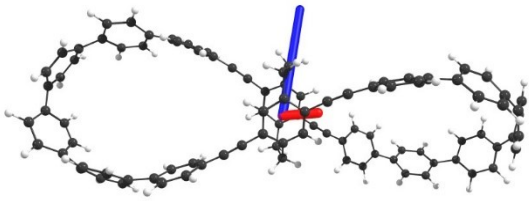
Fig. S20 The calculated and experimental ECD curves in dichloromethane of (a) ***bis-po*-CC** and (b) ***bis-pm*-TC.**

Table S12. The TD B3LYP/6-311G (d, p) calculated excitation energy (*ΔE,* eV), wavelength (*λ*, nm), oscillator strengths (*f*), rotatory strength in velocity form (R_{vel}, 10^{-4} cgs), rotatory strength in length form (R_{len}, 10^{-4} cgs) and major transition in of dichloromethane of ***bis-po*-CC**.

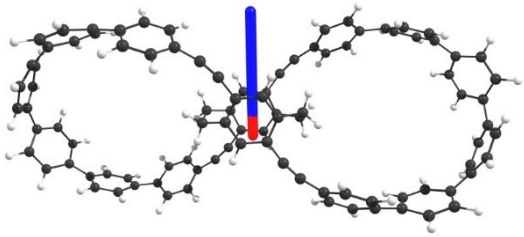
state	major transition	*ΔE* (eV)	λ (nm)	*f*	R_{vel} (10^{-4} cgs)	R_{len} (10^{-4} cgs)
1	318→319(0.63462)	2.82	440	0.36	-481.0	-487.4
2	317→320(0.59744)	2.96	419	0.22	2260.5	2268.7
3	317→319(0.57086)	3.05	407	0.98	-691.2	-698.6
4	318→321(0.45314)	3.15	393	1.35	-504/1	-507.6
14	314→319(0.43813)	3.53	351	0.39	-205.9	-208.0
16	316→322(0.47339)	3.60	344	0.08	179.5	183.7
24	313→321(-0.27736)	3.85	322	0.13	-313.1	-317.3
28	317→324(0.50462)	3.91	317	0.03	182.7	185.8

Table S13. The TD B3LYP/6-311G (d, p) calculated excitation energy (*ΔE,* eV), wavelength (*λ*, nm), oscillator strengths (*f*), rotatory strength in velocity form (R_{vel}, 10^{-4} cgs), rotatory strength in length form (R_{len}, 10^{-4} cgs) and major transition in of dichloromethane of ***bis-pm*-TC**.

state	major transition	*ΔE* (eV)	λ (nm)	*f*	R_{vel} (10^{-4} cgs)	R_{len} (10^{-4} cgs)
1	318→320(0.51613)	2.95	420	0.10	1542.5	1546.0
2	317→320(0.51228)	3.00	412	0.11	-4014.8	-4031.4
6	316→320(0.66614)	3.29	377	2.10	607.5	615.3
14	317→322(0.59531)	3.58	346	0.69	244.5	246.8
24	316→323(0.54587)	3.81	325	0.02	47.1	48.7



***bis-po*-CC**
S_1 transition dipole moments
$|\mu| = 5.46 \times 10^{-17}\ esu\ cm$
$|m| = 7.32 \times 10^{-20}\ erg\ G^{-1}$
$\theta_{\mu,m} = 97°$



***bis-pm*-TC**
S_1 transition dipole moments
$|\mu| = 2.91 \times 10^{-18}\ esu\ cm$
$|m| = 5.30 \times 10^{-20}\ erg\ G^{-1}$
$\theta_{\mu,m} = 0°$

Fig. S21 Transition dipole moments of ***bis-po*-CC** and ***bis-pm*-TC**. For the dipole moments, the EDTM vector is in red, and the MDTM vector is in blue.

2.8.3 LOL-π isosurfaces

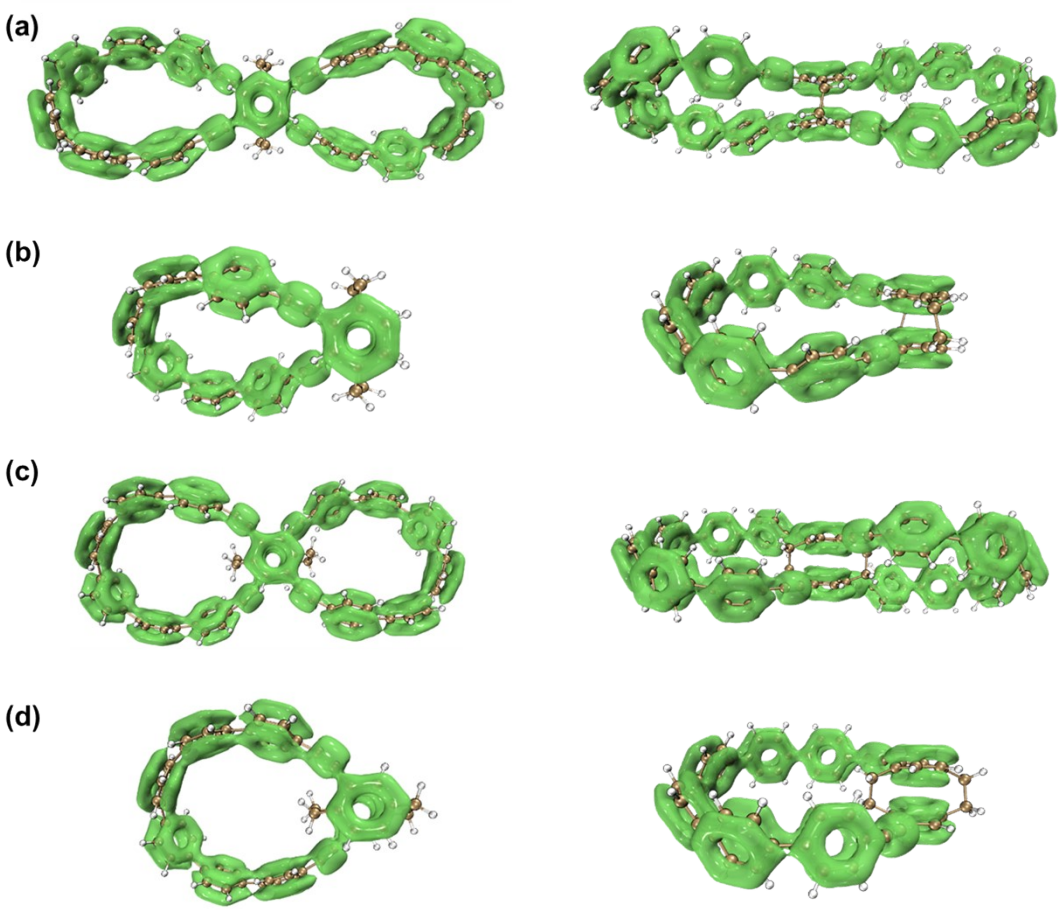


Fig. S22 (a) LOL-π isosurfaces (isovalue = 0.30) for (a) ***bis-po*-CC**, (b) semi-macrocycle ***po*-PCP-[6]CPP**, (c) ***bis-pm*-TC** and (d) semi-macrocycle ***pm*-PCP-[6]CPP**.

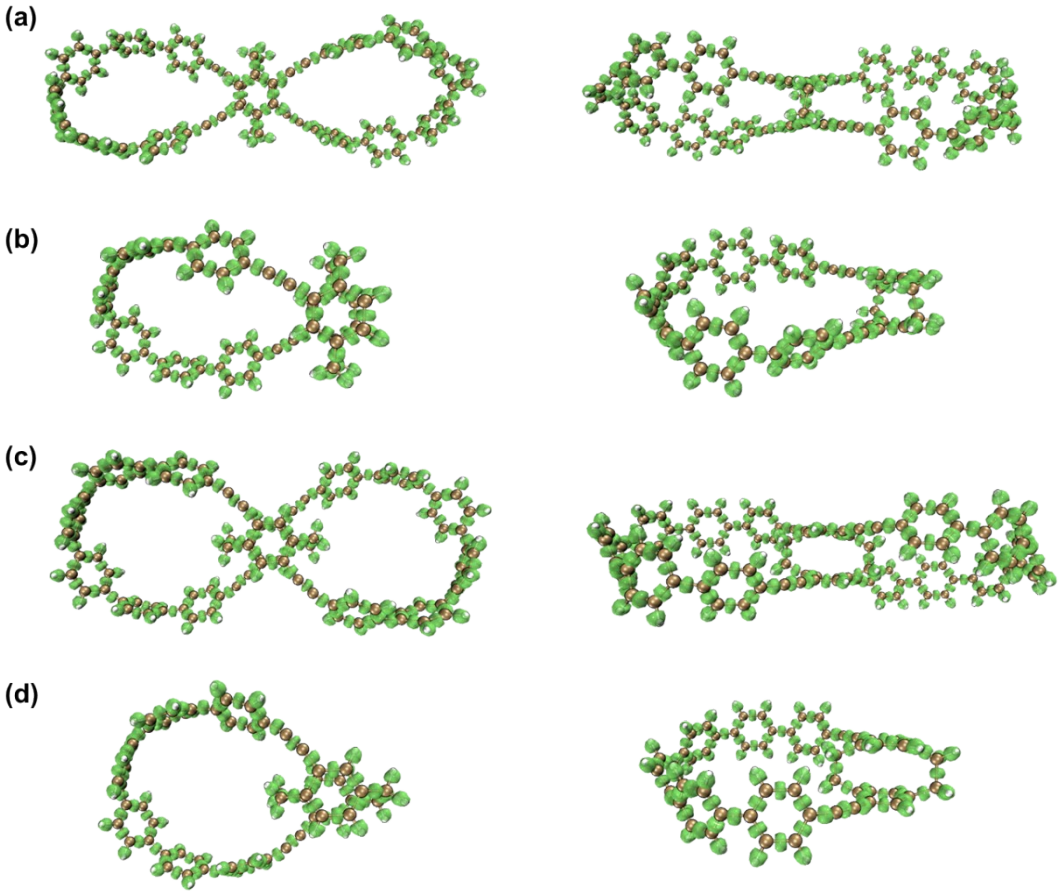


Fig. S23 (a) LOL- σ isosurfaces (isovalue = 0.60) for (a) **bis-po-CC**, (b) semi-macrocycle **po-PCP-[6]CPP**, (c) **bis-pm-TC** and (d) semi-macrocycle **pm-PCP-[6]CPP**.

2.8.4 Cartesian coordinates of optimized species.

Optimized S_0 geometry of compound ***bis-po*-CC**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.448056	1.638068	1.852517
2	6	0	2.295182	-1.486644	-1.595137
3	6	0	3.502076	2.233815	1.994157
4	6	0	3.316329	-2.121098	-1.796037
5	6	0	-1.191715	0.901957	-1.395110
6	6	0	-1.276672	-0.503655	-1.326646
7	6	0	-0.018564	1.557144	1.580985
8	6	0	-1.168068	0.795342	1.788559
9	6	0	-1.134819	-0.614295	1.849232
10	6	0	0.100128	-1.273935	1.619775

11	6	0	1.226646	0.903512	1.765147
12	6	0	1.258188	-0.506258	1.744516
13	6	0	0.162937	-2.658377	1.009543
14	6	0	-0.258486	-2.673392	-0.535581
15	6	0	-0.147009	-1.309991	-1.185093
16	6	0	0.077377	1.513753	-1.238235
17	6	0	1.197241	0.701990	-1.423469
18	6	0	1.109541	-0.705287	-1.440241
19	6	0	-0.112924	2.923240	0.933674
20	6	0	0.224679	2.894275	-0.632184
21	6	0	-2.388055	1.675680	-1.498467
22	1	0	-2.262030	-0.954076	-1.254258
23	1	0	-2.137764	1.283735	1.770361
24	6	0	-2.349217	-1.341691	2.011878
25	1	0	-0.489566	-3.363038	1.533805
26	1	0	1.186082	-3.034294	1.092070
27	1	0	-1.293957	-3.016083	-0.608082
28	1	0	0.369420	-3.414561	-1.039036
29	1	0	2.184823	1.153437	-1.425795
30	1	0	0.567965	3.640796	1.401264
31	1	0	-1.129505	3.304557	1.060349
32	1	0	1.254819	3.233001	-0.770148
33	1	0	-0.429078	3.623232	-1.120431
34	6	0	-3.428638	2.289127	-1.661130
35	6	0	-3.395978	-1.936887	2.204978
36	1	0	2.226173	-0.995704	1.692865
37	6	0	-4.680430	-2.514811	2.427788
38	6	0	-4.715465	2.889269	-1.825608
39	6	0	-5.614833	-1.838130	3.239059
40	6	0	-6.919289	-2.298380	3.350965
41	6	0	-7.355502	-3.445164	2.658755
42	6	0	-5.085073	-3.714343	1.806426
43	6	0	-6.396339	-4.165299	1.921324
44	6	0	-8.810976	-3.720109	2.566877
45	6	0	-9.707000	-3.376782	3.597908
46	6	0	-11.070398	-3.242772	3.352385
47	6	0	-11.597438	-3.430097	2.059202
48	6	0	-9.369268	-4.114546	1.338516
49	6	0	-10.730217	-3.970824	1.090457
50	6	0	-12.846759	-2.766940	1.600688
51	6	0	-13.493205	-3.111922	0.396267
52	6	0	-14.191133	-2.158205	-0.339685
53	6	0	-14.262414	-0.818603	0.096005
54	6	0	-13.187970	-1.523639	2.164881
55	6	0	-13.881483	-0.570152	1.428618
56	6	0	-5.171989	3.334514	-3.083047
57	6	0	-6.491936	3.740887	-3.258179
58	6	0	-7.409835	3.718398	-2.191481
59	6	0	-5.605205	2.952082	-0.735897

60	6	0	-6.919700	3.356869	-0.920367
61	6	0	-8.875806	3.860877	-2.377153
62	6	0	-9.507647	3.372401	-3.536541
63	6	0	-10.871434	3.092545	-3.550610
64	6	0	-11.660959	3.265658	-2.396913
65	6	0	-9.710880	4.256753	-1.316545
66	6	0	-11.068970	3.961002	-1.323875
67	6	0	-12.879397	2.452135	-2.139717
68	6	0	-12.971171	1.179238	-2.733562
69	6	0	-13.647396	0.141663	-2.103808
70	6	0	-14.260951	0.329752	-0.850592
71	6	0	-13.749465	2.704284	-1.058643
72	6	0	-14.428155	1.664828	-0.427869
73	6	0	4.792737	2.823270	2.165548
74	6	0	4.571796	-2.757723	-2.043482
75	1	0	-5.318233	-0.922462	3.739963
76	1	0	-7.633478	-1.715362	3.923023
77	1	0	-4.373058	-4.269505	1.204355
78	1	0	-6.686047	-5.076755	1.407284
79	1	0	-9.325952	-3.152641	4.589937
80	1	0	-11.718124	-2.911893	4.158713
81	1	0	-8.718917	-4.408824	0.520829
82	1	0	-11.093096	-4.147021	0.083340
83	1	0	-13.360926	-4.104151	-0.025257
84	1	0	-14.579699	-2.433822	-1.315715
85	1	0	-12.757235	-1.224685	3.114710
86	1	0	-13.958016	0.433316	1.833473
87	1	0	-4.493687	3.323526	-3.930041
88	1	0	-6.818958	4.051802	-4.245717
89	1	0	-5.271152	2.627038	0.243969
90	1	0	-7.598769	3.315338	-0.075848
91	1	0	-8.911816	3.099660	-4.402142
92	1	0	-11.298976	2.635903	-4.437871
93	1	0	-9.281484	4.720883	-0.434091
94	1	0	-11.645516	4.161642	-0.427048
95	1	0	-12.363434	0.939564	-3.599305
96	1	0	-13.532087	-0.859990	-2.503783
97	1	0	-13.814411	3.701824	-0.634282
98	1	0	-14.996982	1.883311	0.471255
99	6	0	5.139448	-2.746202	-3.334437
100	6	0	6.438421	-3.194545	-3.542675
101	6	0	7.229937	-3.661985	-2.476184
102	6	0	6.620544	-3.765274	-1.210599
103	6	0	5.319562	-3.325925	-0.994068
104	6	0	8.699300	-3.831263	-2.601429
105	6	0	9.444148	-4.671355	-1.751407
106	6	0	10.819429	-4.511075	-1.603843
107	6	0	11.511516	-3.491990	-2.288269
108	6	0	10.796360	-2.796541	-3.281906

109	6	0	9.425044	-2.962481	-3.435496
110	6	0	12.774929	-2.896163	-1.778760
111	6	0	13.007555	-2.898943	-0.390982
112	6	0	13.734943	-1.880647	0.214198
113	6	0	14.284022	-0.987553	-1.941123
114	6	0	13.556326	-2.008408	-2.546814
115	6	0	14.257299	-0.813915	-0.542164
116	6	0	5.435217	2.792038	3.420616
117	6	0	6.760096	3.191857	3.549925
118	6	0	7.503789	3.628277	2.436916
119	6	0	6.824582	3.752896	1.209354
120	6	0	5.497564	3.362275	1.071884
121	6	0	8.983197	3.743744	2.474556
122	6	0	9.724982	2.850645	3.267892
123	6	0	11.078112	2.635115	3.035117
124	6	0	11.758386	3.302367	1.998525
125	6	0	11.064326	4.344680	1.352049
126	6	0	9.706715	4.554838	1.579177
127	6	0	12.967791	2.660960	1.418115
128	6	0	13.758343	1.743919	2.141191
129	6	0	14.412525	0.697822	1.496202
130	6	0	14.300443	0.527136	0.101108
131	6	0	13.776028	1.613568	-0.625160
132	6	0	13.121985	2.657175	0.019405
133	1	0	4.564637	-2.348626	-4.164477
134	1	0	6.855966	-3.147667	-4.543560
135	1	0	7.200820	-4.117157	-0.363945
136	1	0	4.895208	-3.362991	0.003955
137	1	0	8.935661	-5.421138	-1.152352
138	1	0	11.344158	-5.136981	-0.888218
139	1	0	11.285789	-2.010876	-3.847461
140	1	0	8.898317	-2.308232	-4.122668
141	1	0	12.471473	-3.593974	0.246708
142	1	0	13.730201	-1.821748	1.297457
143	1	0	14.777902	-0.252791	-2.570515
144	1	0	13.510104	-2.043860	-3.631302
145	1	0	4.896288	2.417231	4.284639
146	1	0	7.234022	3.131116	4.524605
147	1	0	7.366022	4.082454	0.328641
148	1	0	5.016338	3.414271	0.100684
149	1	0	9.216415	2.217128	3.987408
150	1	0	11.571396	1.834048	3.575184
151	1	0	11.568335	4.950392	0.604867
152	1	0	9.191363	5.321695	1.008265
153	1	0	13.775222	1.779662	3.226475
154	1	0	14.913980	-0.055279	2.097245
155	1	0	13.708561	1.556649	-1.706447
156	1	0	12.577210	3.372453	-0.587765

Optimized S_0 geometry of compound ***bis-pm*-TC**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.777905	-3.838395	-1.950557
2	6	0	-4.241171	-4.759079	-0.990036
3	6	0	-5.565981	-5.188145	-1.003479
4	6	0	-6.478552	-4.716299	-1.966986
5	6	0	-4.649482	-3.478785	-2.999557
6	6	0	-5.968101	-3.910417	-3.003542
7	1	0	-3.575924	-5.085888	-0.197325
8	1	0	-5.907430	-5.857567	-0.219843
9	1	0	-4.302415	-2.793551	-3.765851
10	1	0	-6.637371	-3.531877	-3.768810
11	6	0	-6.477801	4.716279	1.967000
12	6	0	-5.565217	5.187907	1.003398
13	6	0	-5.967422	3.910341	3.003547
14	6	0	-4.648889	3.478445	2.999466
15	6	0	-3.777334	3.837830	1.950372
16	6	0	-4.240497	4.758570	0.989854
17	1	0	-3.575258	5.085195	0.197061
18	1	0	-5.906601	5.857356	0.219757
19	1	0	-6.636701	3.531962	3.768886
20	1	0	-4.301895	2.793169	3.765756
21	6	0	-7.950869	-4.812964	-1.796334
22	6	0	-8.502168	-4.742151	-0.504623
23	6	0	-9.824799	-4.359207	-0.308684
24	6	0	-10.656608	-4.027400	-1.394664
25	6	0	-8.843409	-4.696003	-2.880071
26	6	0	-10.167405	-4.313696	-2.684100
27	6	0	-11.973233	-2.023648	-2.041526
28	6	0	-12.568799	-0.840268	-1.620572
29	6	0	-11.795489	-3.102596	-1.156023
30	6	0	-12.478790	-3.032397	0.073897
31	6	0	-13.082468	-1.849362	0.492141
32	6	0	-13.017964	-0.681870	-0.295894
33	1	0	-7.858943	-4.848130	0.362962
34	1	0	-10.165935	-4.174496	0.704706
35	1	0	-8.482270	-4.837073	-3.894444
36	1	0	-10.803790	-4.159511	-3.550584
37	1	0	-11.496891	-2.042887	-3.016307
38	1	0	-12.530460	0.016264	-2.285134
39	1	0	-12.460590	-3.880457	0.752398
40	1	0	-13.520146	-1.810735	1.485144
41	6	0	-13.082274	1.850335	-0.491652
42	6	0	-12.478419	3.033294	-0.073451

43	6	0	-12.568588	0.841181	1.621028
44	6	0	-11.972849	2.024488	2.041941
45	6	0	-11.795025	3.103410	1.156422
46	6	0	-10.655999	4.028057	1.394974
47	6	0	-9.824215	4.359723	0.308933
48	6	0	-10.166666	4.314300	2.684372
49	6	0	-8.842598	4.696406	2.880248
50	6	0	-7.950112	4.813203	1.796449
51	6	0	-8.501510	4.742460	0.504775
52	1	0	-7.858325	4.848314	-0.362855
53	1	0	-12.460151	3.881348	-0.751959
54	1	0	-12.530310	-0.015355	2.285589
55	1	0	-10.165448	4.175046	-0.704431
56	1	0	-10.803016	4.160226	3.550902
57	1	0	-8.481369	4.837434	3.894594
58	1	0	-11.496438	2.043669	3.016689
59	6	0	-1.654885	2.293650	1.712364
60	6	0	-2.551145	3.115623	1.809057
61	6	0	-1.655081	-2.294707	-1.712736
62	6	0	-2.551531	-3.116480	-1.809349
63	6	0	3.777869	-3.838552	1.950291
64	6	0	4.241204	-4.759285	0.989851
65	6	0	5.566011	-5.188352	1.003414
66	6	0	6.478513	-4.716460	1.966963
67	6	0	4.649367	-3.478899	2.999342
68	6	0	5.967984	-3.910537	3.003448
69	1	0	3.576019	-5.086114	0.197096
70	1	0	5.907518	-5.857804	0.219829
71	1	0	4.302245	-2.793623	3.765574
72	1	0	6.637199	-3.531956	3.768745
73	6	0	6.477847	4.716399	-1.966946
74	6	0	5.565216	5.187963	-1.003357
75	6	0	5.967516	3.910539	-3.003575
76	6	0	4.648982	3.478646	-2.999590
77	6	0	3.777378	3.837951	-1.950510
78	6	0	4.240496	4.758623	-0.989905
79	1	0	3.575221	5.085184	-0.197115
80	1	0	5.906563	5.857356	-0.219652
81	1	0	6.636832	3.532212	-3.768908
82	1	0	4.302025	2.793423	-3.765944
83	6	0	1.654958	2.293712	-1.712654
84	6	0	2.551198	3.115713	-1.809283
85	6	0	0.804085	-1.151745	1.610358
86	6	0	-0.599164	-1.246683	1.569572
87	6	0	1.407212	-0.120261	-1.406352
88	6	0	0.599221	-1.246620	-1.570007
89	6	0	-0.804024	-1.151680	-1.610797
90	6	0	-1.407316	0.119236	-1.406203
91	6	0	0.803901	1.150680	-1.610735

92	6	0	-0.599344	1.245616	-1.569805
93	6	0	-2.772970	0.245474	-0.760228
94	6	0	-2.772875	-0.246601	0.760154
95	6	0	-1.407152	-0.120314	1.405975
96	6	0	1.407378	0.119181	1.405830
97	6	0	0.599405	1.245553	1.569485
98	6	0	-0.803837	1.150616	1.610419
99	6	0	2.772934	-0.246578	-0.760540
100	6	0	2.773030	0.245447	0.759861
101	1	0	-1.049338	-2.234138	1.527172
102	1	0	1.049391	-2.234079	-1.527645
103	1	0	-1.049514	2.233068	-1.527308
104	1	0	-3.536213	-0.332513	-1.289825
105	1	0	-3.077351	1.294684	-0.785027
106	1	0	-3.536073	0.331367	1.289835
107	1	0	-3.077223	-1.295820	0.784993
108	1	0	1.049572	2.233009	1.527008
109	1	0	3.536134	0.331408	-1.290195
110	1	0	3.077281	-1.295798	-0.785413
111	1	0	3.077411	1.294657	0.784692
112	1	0	3.536276	-0.332558	1.289432
113	6	0	1.655147	-2.294775	1.712221
114	6	0	2.551534	-3.116607	1.808917
115	6	0	7.950843	-4.813104	1.796398
116	6	0	8.502208	-4.742299	0.504712
117	6	0	9.824836	-4.359316	0.308834
118	6	0	10.656578	-4.027470	1.394854
119	6	0	8.843324	-4.696102	2.880178
120	6	0	10.167322	-4.313766	2.684268
121	6	0	11.973097	-2.023674	2.041762
122	6	0	12.568653	-0.840278	1.620837
123	6	0	11.795439	-3.102629	1.156256
124	6	0	12.478797	-3.032414	-0.073634
125	6	0	13.082460	-1.849362	-0.491851
126	6	0	13.017886	-0.681873	0.296187
127	1	0	7.859029	-4.848303	-0.362903
128	1	0	10.166024	-4.174609	-0.704540
129	1	0	8.482140	-4.837170	3.894535
130	1	0	10.803660	-4.159546	3.550781
131	1	0	11.496682	-2.042916	3.016509
132	1	0	12.530231	0.016262	2.285385
133	1	0	12.460672	-3.880492	-0.752116
134	1	0	13.520219	-1.810720	-1.484818
135	6	0	13.082193	1.850331	0.491981
136	6	0	12.478358	3.033299	0.073775
137	6	0	13.017797	0.682842	-0.296072
138	6	0	12.568558	0.841200	-1.620726
139	6	0	11.972841	2.024519	-2.041644
140	6	0	11.795007	3.103433	-1.156122

141	6	0	10.656001	4.028099	-1.394708
142	6	0	9.824158	4.359727	-0.308698
143	6	0	10.166748	4.314405	-2.684122
144	6	0	8.842696	4.696541	-2.880058
145	6	0	7.950149	4.813299	-1.796306
146	6	0	8.501469	4.742483	-0.504602
147	1	0	7.858232	4.848300	0.362993
148	1	0	13.519941	1.811736	1.484954
149	1	0	12.460098	3.881361	0.752272
150	1	0	12.530262	-0.015337	-2.285285
151	1	0	10.165335	4.175001	0.704676
152	1	0	10.803148	4.160358	-3.550620
153	1	0	8.481529	4.837621	-3.894419
154	1	0	11.496433	2.043703	-3.016395
155	6	0	-13.017861	0.682836	0.296381
156	1	0	-13.520020	1.811759	-1.484627

2.8.5 Cartesian coordinates of optimized species of LOL- isosurfaces.

Optimized S_0 geometry of compound ***bis-po*-CC**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.449218	-1.666704	-1.843806
2	6	0	2.284917	1.492668	1.568694
3	6	0	3.501193	-2.268668	-1.968909
4	6	0	3.302051	2.135974	1.758480
5	6	0	-1.192554	-0.912290	1.378106
6	6	0	-1.282633	0.492413	1.302844
7	6	0	-0.017862	-1.574097	-1.590883
8	6	0	-1.163786	-0.808903	-1.803482
9	6	0	-1.125797	0.600043	-1.869350
10	6	0	0.111405	1.254673	-1.640993
11	6	0	1.230562	-0.927053	-1.772108
12	6	0	1.266835	0.482357	-1.757551
13	6	0	0.175628	2.640605	-1.033240
14	6	0	-0.268493	2.661637	0.504715
15	6	0	-0.155688	1.302194	1.163192
16	6	0	0.079741	-1.518473	1.230058
17	6	0	1.195873	-0.701589	1.413192
18	6	0	1.102940	0.705130	1.422974
19	6	0	-0.117473	-2.936301	-0.935272
20	6	0	0.232196	-2.900383	0.627200
21	6	0	-2.386178	-1.689798	1.471766

22	1	0	-2.270654	0.936339	1.219602
23	1	0	-2.136598	-1.291947	-1.779520
24	6	0	-2.337172	1.332170	-2.027759
25	1	0	-0.462972	3.349973	-1.570378
26	1	0	1.204281	3.007967	-1.099362
27	1	0	-1.309374	2.995006	0.558302
28	1	0	0.345582	3.411790	1.014167
29	1	0	2.186771	-1.146952	1.414361
30	1	0	0.554321	-3.662498	-1.405073
31	1	0	-1.139414	-3.310221	-1.050023
32	1	0	1.267488	-3.230641	0.756200
33	1	0	-0.412296	-3.633564	1.123717
34	6	0	-3.426070	-2.305895	1.624937
35	6	0	-3.380120	1.936143	-2.211337
36	1	0	2.237716	0.966363	-1.698881
37	6	0	-4.662860	2.519683	-2.423806
38	6	0	-4.716139	-2.900776	1.773738
39	6	0	-5.607854	1.848312	-3.226311
40	6	0	-6.911291	2.313483	-3.326498
41	6	0	-7.337445	3.461471	-2.631342
42	6	0	-5.058514	3.720535	-1.800366
43	6	0	-6.368654	4.176747	-1.903274
44	6	0	-8.790661	3.740198	-2.524861
45	6	0	-9.695593	3.428030	-3.557327
46	6	0	-11.058092	3.296455	-3.306308
47	6	0	-11.576319	3.455610	-2.006502
48	6	0	-9.338940	4.104854	-1.283693
49	6	0	-10.698798	3.963695	-1.030567
50	6	0	-12.826691	2.791700	-1.554139
51	6	0	-13.478842	3.131344	-0.351896
52	6	0	-14.179529	2.174933	0.377423
53	6	0	-14.248360	0.837074	-0.062261
54	6	0	-13.162629	1.549666	-2.122035
55	6	0	-13.858698	0.593539	-1.392368
56	6	0	-5.154608	-3.439524	3.000105
57	6	0	-6.475746	-3.845248	3.168925
58	6	0	-7.412144	-3.733036	2.125465
59	6	0	-5.628913	-2.864983	0.702608
60	6	0	-6.943064	-3.272047	0.879547
61	6	0	-8.875843	-3.884607	2.317160
62	6	0	-9.502284	-3.434532	3.493942
63	6	0	-10.865562	-3.153261	3.522171
64	6	0	-11.659758	-3.287792	2.367373
65	6	0	-9.715393	-4.244174	1.248178
66	6	0	-11.072734	-3.947907	1.270577
67	6	0	-12.874078	-2.461777	2.134896
68	6	0	-12.936738	-1.190014	2.732823
69	6	0	-13.609620	-0.141290	2.118989
70	6	0	-14.249282	-0.315833	0.877873

71	6	0	-13.766588	-2.697478	1.069194
72	6	0	-14.441745	-1.646675	0.454191
73	6	0	4.791593	-2.860863	-2.125985
74	6	0	4.554715	2.779468	1.997875
75	1	0	-5.316772	0.931066	-3.728853
76	1	0	-7.636154	1.732341	-3.888525
77	1	0	-4.337369	4.272279	-1.204814
78	1	0	-6.652209	5.090685	-1.388329
79	1	0	-9.319864	3.228849	-4.557601
80	1	0	-11.715867	2.991084	-4.115823
81	1	0	-8.678659	4.367753	-0.462286
82	1	0	-11.054899	4.109145	-0.015442
83	1	0	-13.349191	4.124345	0.070886
84	1	0	-14.575375	2.445267	1.353000
85	1	0	-12.719348	1.253360	-3.067706
86	1	0	-13.926100	-0.411802	-1.795994
87	1	0	-4.458200	-3.500860	3.830896
88	1	0	-6.790325	-4.231801	4.134693
89	1	0	-5.309155	-2.459662	-0.252430
90	1	0	-7.642123	-3.152161	0.058127
91	1	0	-8.898798	-3.188094	4.363200
92	1	0	-11.291846	-2.723553	4.424546
93	1	0	-9.285708	-4.677673	0.349357
94	1	0	-11.654144	-4.112197	0.368640
95	1	0	-12.302242	-0.962204	3.583252
96	1	0	-13.467141	0.859499	2.514061
97	1	0	-13.852480	-3.694720	0.645469
98	1	0	-15.031729	-1.851806	-0.435482
99	6	0	5.111086	2.809441	3.292952
100	6	0	6.408609	3.262774	3.498756
101	6	0	7.209959	3.697172	2.426617
102	6	0	6.612359	3.759643	1.153637
103	6	0	5.313698	3.313415	0.939362
104	6	0	8.678041	3.868631	2.556674
105	6	0	9.425893	4.708628	1.710139
106	6	0	10.801455	4.548754	1.567240
107	6	0	11.491519	3.530088	2.253002
108	6	0	10.772524	2.833539	3.242005
109	6	0	9.401019	2.999343	3.391232
110	6	0	12.754948	2.931735	1.748383
111	6	0	12.973240	2.902941	0.359460
112	6	0	13.702353	1.876943	-0.229489
113	6	0	14.279644	1.038574	1.938469
114	6	0	13.549943	2.067156	2.527917
115	6	0	14.242007	0.832950	0.544624
116	6	0	5.429596	-2.871705	-3.383166
117	6	0	6.755312	-3.271083	-3.503957
118	6	0	7.504392	-3.668274	-2.380868
119	6	0	6.830366	-3.752031	-1.147902

120	6	0	5.503352	-3.359786	-1.018664
121	6	0	8.983538	-3.779202	-2.416943
122	6	0	9.721591	-2.882920	-3.208705
123	6	0	11.073204	-2.661011	-2.974922
124	6	0	11.756547	-3.325250	-1.939491
125	6	0	11.066612	-4.369680	-1.293394
126	6	0	9.710301	-4.585832	-1.521068
127	6	0	12.961128	-2.675719	-1.359846
128	6	0	13.765989	-1.778617	-2.091088
129	6	0	14.417014	-0.722295	-1.460159
130	6	0	14.287807	-0.520214	-0.071262
131	6	0	13.745216	-1.586224	0.670109
132	6	0	13.094485	-2.639899	0.039623
133	1	0	4.525996	2.437502	4.128449
134	1	0	6.819758	3.248505	4.504355
135	1	0	7.204750	4.080293	0.301928
136	1	0	4.898326	3.314672	-0.063810
137	1	0	8.916456	5.459368	1.111551
138	1	0	11.331597	5.175592	0.855015
139	1	0	11.260953	2.042736	3.802605
140	1	0	8.868318	2.340973	4.071045
141	1	0	12.418032	3.575282	-0.287249
142	1	0	13.681614	1.787159	-1.311093
143	1	0	14.787759	0.320955	2.577747
144	1	0	13.513094	2.130009	3.612402
145	1	0	4.883734	-2.527008	-4.256069
146	1	0	7.228365	-3.243099	-4.481649
147	1	0	7.380267	-4.045600	-0.258727
148	1	0	5.025568	-3.375422	-0.043799
149	1	0	9.206339	-2.248470	-3.923796
150	1	0	11.563368	-1.852874	-3.508634
151	1	0	11.576106	-4.973151	-0.546774
152	1	0	9.195256	-5.355395	-0.951898
153	1	0	13.797333	-1.841534	-3.175728
154	1	0	14.933262	0.015931	-2.068694
155	1	0	13.656565	-1.499110	1.748504
156	1	0	12.529350	-3.334951	0.652830

Optimized S_0 geometry of compound ***bis-pm*-TC**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.772440	3.842476	1.932816

2	6	0	-4.231528	4.771537	0.978970
3	6	0	-5.556154	5.200833	0.988914
4	6	0	-6.473855	4.722742	1.943414
5	6	0	-4.650426	3.475235	2.973263
6	6	0	-5.968592	3.907348	2.974195
7	1	0	-3.560015	5.104386	0.193130
8	1	0	-5.895581	5.878639	0.210317
9	1	0	-4.305166	2.781928	3.733935
10	1	0	-6.645402	3.519912	3.729462
11	6	0	-6.474403	-4.722783	-1.943522
12	6	0	-5.556823	-5.201032	-0.988983
13	6	0	-5.968966	-3.907429	-2.974249
14	6	0	-4.650741	-3.475496	-2.973224
15	6	0	-3.772866	-3.842892	-1.932739
16	6	0	-4.232138	-4.771923	-0.978951
17	1	0	-3.560716	-5.104890	-0.193082
18	1	0	-5.896387	-5.878817	-0.210428
19	1	0	-6.645678	-3.519875	-3.729543
20	1	0	-4.305342	-2.782212	-3.733854
21	6	0	-7.944964	4.819673	1.767828
22	6	0	-8.492140	4.724928	0.476720
23	6	0	-9.814772	4.341932	0.283270
24	6	0	-10.651759	4.033725	1.371196
25	6	0	-8.841647	4.724415	2.849608
26	6	0	-10.165712	4.341875	2.656118
27	6	0	-11.952051	2.025976	2.027878
28	6	0	-12.548143	0.841237	1.612914
29	6	0	-11.790526	3.107074	1.143220
30	6	0	-12.488366	3.035106	-0.077815
31	6	0	-13.093144	1.850687	-0.489686
32	6	0	-13.014989	0.682633	0.295322
33	1	0	-7.841871	4.807176	-0.389128
34	1	0	-10.152909	4.131909	-0.726928
35	1	0	-8.481252	4.885431	3.862200
36	1	0	-10.808393	4.205689	3.522083
37	1	0	-11.456362	2.045041	2.993741
38	1	0	-12.491754	-0.019717	2.271538
39	1	0	-12.481639	3.886531	-0.753712
40	1	0	-13.545783	1.809595	-1.476861
41	6	0	-13.093421	-1.849819	0.489236
42	6	0	-12.488784	-3.034321	0.077392
43	6	0	-12.548175	-0.840439	-1.613335
44	6	0	-11.952223	-2.025258	-2.028270
45	6	0	-11.790891	-3.106380	-1.143607
46	6	0	-10.652243	-4.033188	-1.371530
47	6	0	-9.815360	-4.341529	-0.283561
48	6	0	-10.166165	-4.341387	-2.656429
49	6	0	-8.842142	-4.724110	-2.849849
50	6	0	-7.945535	-4.819513	-1.768019

51	6	0	-8.492772	-4.724711	-0.476941
52	1	0	-7.842564	-4.807061	0.388943
53	1	0	-12.482208	-3.885748	0.753287
54	1	0	-12.491635	0.020510	-2.271954
55	1	0	-10.153525	-4.131472	0.726621
56	1	0	-10.808777	-4.205093	-3.522429
57	1	0	-8.481713	-4.885157	-3.862423
58	1	0	-11.456487	-2.044390	-2.994108
59	6	0	-1.654690	-2.295007	-1.704647
60	6	0	-2.546403	-3.122085	-1.794062
61	6	0	-1.654460	2.294296	1.704901
62	6	0	-2.546068	3.121495	1.794240
63	6	0	3.772550	3.842215	-1.932992
64	6	0	4.231706	4.771465	-0.979362
65	6	0	5.556331	5.200760	-0.989484
66	6	0	6.473964	4.722487	-1.943959
67	6	0	4.650462	3.474773	-2.973429
68	6	0	5.968628	3.906888	-2.974542
69	1	0	3.560251	5.104462	-0.193535
70	1	0	5.895814	5.878713	-0.211041
71	1	0	4.305151	2.781311	-3.733937
72	1	0	6.645386	3.519297	-3.729776
73	6	0	6.474322	-4.722546	1.943944
74	6	0	5.556738	-5.200892	0.989456
75	6	0	5.968879	-3.907137	2.974624
76	6	0	4.650637	-3.475253	2.973599
77	6	0	3.772753	-3.842752	1.933158
78	6	0	4.232038	-4.771830	0.979422
79	1	0	3.560603	-5.104894	0.193605
80	1	0	5.896306	-5.878733	0.210952
81	1	0	6.645589	-3.519516	3.729886
82	1	0	4.305224	-2.781944	3.734201
83	6	0	1.654432	-2.295060	1.705078
84	6	0	2.546223	-3.122053	1.794501
85	6	0	0.804292	1.150841	-1.608770
86	6	0	-0.598757	1.245313	-1.568476
87	6	0	1.407002	0.119349	1.406624
88	6	0	0.598772	1.245336	1.568708
89	6	0	-0.804283	1.150970	1.609012
90	6	0	-1.407029	-0.120138	1.406674
91	6	0	0.804262	-1.151738	1.609104
92	6	0	-0.598794	-1.246108	1.568847
93	6	0	-2.772911	-0.246353	0.760376
94	6	0	-2.772925	0.245677	-0.759992
95	6	0	-1.407072	0.119394	-1.406340
96	6	0	1.406943	-0.120301	-1.406375
97	6	0	0.598624	-1.246218	-1.568495
98	6	0	-0.804426	-1.151747	-1.608757
99	6	0	2.772868	0.245493	0.760278

100	6	0	2.772818	-0.246587	-0.760075
101	1	0	-1.047557	2.233768	-1.521568
102	1	0	1.047645	2.233756	1.521755
103	1	0	-1.047669	-2.234532	1.522005
104	1	0	-3.537377	0.331523	1.290204
105	1	0	-3.077627	-1.296551	0.783124
106	1	0	-3.537442	-0.332152	-1.289795
107	1	0	-3.077582	1.295893	-0.782722
108	1	0	1.047424	-2.234673	-1.521600
109	1	0	3.537333	-0.332386	1.290104
110	1	0	3.077617	1.295682	0.782977
111	1	0	3.077463	-1.296807	-0.782787
112	1	0	3.537324	0.331218	-1.289922
113	6	0	1.654550	2.294104	-1.704690
114	6	0	2.546200	3.121244	-1.794167
115	6	0	7.945083	4.819440	-1.768481
116	6	0	8.492333	4.724923	-0.477389
117	6	0	9.814969	4.341938	-0.283948
118	6	0	10.651889	4.033524	-1.371867
119	6	0	8.841701	4.723976	-2.850297
120	6	0	10.165773	4.341453	-2.656816
121	6	0	11.952118	2.025659	-2.028299
122	6	0	12.548188	0.840962	-1.613183
123	6	0	11.790642	3.106884	-1.143789
124	6	0	12.488502	3.035068	0.077243
125	6	0	13.093248	1.850686	0.489270
126	6	0	13.015045	0.682525	-0.295576
127	1	0	7.842116	4.807335	0.388482
128	1	0	10.153162	4.132087	0.726268
129	1	0	8.481249	4.884811	-3.862897
130	1	0	10.808400	4.205094	-3.522794
131	1	0	11.456410	2.044604	-2.994155
132	1	0	12.491764	-0.020082	-2.271687
133	1	0	12.481805	3.886585	0.753023
134	1	0	13.545901	1.809717	1.476444
135	6	0	13.093422	-1.849950	-0.489156
136	6	0	12.488752	-3.034384	-0.077166
137	6	0	13.015089	-0.681802	0.295696
138	6	0	12.548182	-0.840288	1.613280
139	6	0	11.952197	-2.025040	2.028362
140	6	0	11.790845	-3.106270	1.143834
141	6	0	10.652172	-4.033024	1.371862
142	6	0	9.815280	-4.341464	0.283927
143	6	0	10.166094	-4.341083	2.656794
144	6	0	8.842069	-4.723774	2.850257
145	6	0	7.945455	-4.819276	1.768441
146	6	0	8.492687	-4.724608	0.477351
147	1	0	7.842477	-4.807048	-0.388523
148	1	0	13.546115	-1.808936	-1.476309

149	1	0	12.482163	-3.885898	-0.752952
150	1	0	12.491654	0.020746	2.271788
151	1	0	10.153445	-4.131520	-0.726278
152	1	0	10.808713	-4.204719	3.522777
153	1	0	8.481644	-4.884727	3.862848
154	1	0	11.456451	-2.044035	2.994197
155	6	0	-13.015066	-0.681774	-0.295767
156	1	0	-13.546107	-1.808668	1.476387

Optimized S_0 geometry of compound ***po*-PCP-[6]CPP**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.419187	-1.584778	-0.902950
2	6	0	-0.801567	-4.403611	-0.104258
3	6	0	5.359094	-0.400715	-1.666703
4	1	0	4.379247	-0.010832	-1.928844
5	6	0	4.213451	-2.286364	-0.603736
6	6	0	1.885754	-3.499686	-0.320520
7	6	0	3.171894	-2.892628	-0.422956
8	6	0	-2.267507	-4.574788	0.047579
9	6	0	-0.300488	-3.884055	-1.313209
10	1	0	-0.973407	-3.750980	-2.154884
11	6	0	-2.901811	-4.139959	1.223439
12	1	0	-2.302125	-3.869000	2.087605
13	6	0	6.504299	0.353896	-1.941710
14	6	0	6.665429	-1.987225	-0.360343
15	6	0	1.417322	-4.101650	0.864482
16	1	0	2.085204	-4.188336	1.716351
17	6	0	-4.266664	-3.874624	1.246013
18	1	0	-4.687667	-3.393636	2.123554
19	6	0	1.008992	-3.439909	-1.422948
20	1	0	1.356844	-2.993591	-2.349354
21	6	0	0.100915	-4.541499	0.966405
22	1	0	-0.240171	-4.975837	1.902375
23	6	0	5.358391	0.400970	1.666705
24	1	0	4.378444	0.011157	1.928570
25	6	0	7.740841	-0.262678	-1.706307
26	1	0	8.661148	0.236847	-2.001699
27	6	0	5.418744	1.585057	0.902988
28	6	0	-5.061980	-4.033995	0.095981
29	6	0	-3.097452	-4.931643	-1.032512
30	1	0	-2.656129	-5.359966	-1.928648

31	6	0	7.811981	-1.407964	-0.912824
32	1	0	8.787983	-1.767541	-0.593853
33	6	0	-7.045568	-2.794036	1.094245
34	1	0	-7.002566	-3.362338	2.019987
35	6	0	-6.298403	-3.218208	-0.022492
36	6	0	-6.520920	-2.526545	-1.226588
37	1	0	-6.000769	-2.835741	-2.127994
38	6	0	-7.201773	-1.315426	-1.241297
39	1	0	-7.180028	-0.727833	-2.153524
40	6	0	-7.692090	-0.742268	-0.053236
41	6	0	-7.733836	-1.584091	1.077419
42	1	0	-8.210049	-1.240230	1.991890
43	6	0	6.400589	1.843207	-2.215345
44	1	0	5.378143	2.077273	-2.528663
45	1	0	7.064753	2.150466	-3.032301
46	6	0	6.503441	-0.353807	1.941861
47	6	0	4.213111	2.286751	0.603609
48	6	0	-7.201892	1.315088	1.241363
49	1	0	-7.180053	0.727492	2.153587
50	6	0	-4.464580	-4.673308	-1.007243
51	1	0	-5.060679	-4.899198	-1.887613
52	6	0	-2.267952	4.574791	-0.047710
53	6	0	6.753166	-2.752066	0.942084
54	1	0	7.772504	-3.134928	1.061598
55	1	0	6.079181	-3.615131	0.954061
56	6	0	-6.521160	2.526275	1.226619
57	1	0	-6.000994	2.835535	2.127995
58	6	0	-7.692193	0.741878	0.053317
59	6	0	-7.734113	1.583710	-1.077326
60	1	0	-8.210350	1.239807	-1.991769
61	6	0	3.171582	2.893031	0.422700
62	6	0	-5.062376	4.033810	-0.096061
63	6	0	-2.902207	4.139770	-1.223519
64	1	0	-2.302484	3.868759	-2.087645
65	6	0	6.399423	-1.843143	2.215338
66	1	0	5.376617	-2.077091	2.527560
67	1	0	7.062678	-2.150556	3.032985
68	6	0	-6.298767	3.217949	0.022501
69	6	0	6.665119	1.987333	0.360562
70	6	0	-4.465031	4.673315	1.007084
71	1	0	-5.061153	4.899278	1.887418
72	6	0	7.811509	1.407896	0.913203
73	1	0	8.787606	1.767337	0.594372
74	6	0	7.740107	0.262619	1.706663
75	1	0	8.660318	-0.236994	2.002214
76	6	0	-7.045986	2.793738	-1.094184
77	1	0	-7.003124	3.362065	-2.019918
78	6	0	-4.267047	3.874355	-1.246077
79	1	0	-4.688009	3.393236	-2.123568

80	6	0	-3.097915	4.931723	1.032339
81	1	0	-2.656604	5.360154	1.928429
82	6	0	6.753124	2.752267	-0.941762
83	1	0	7.772264	3.135804	-1.060778
84	1	0	6.078544	3.614848	-0.953979
85	6	0	-0.801995	4.403672	0.104160
86	6	0	-0.301024	3.883553	1.312923
87	1	0	-0.974048	3.750021	2.154440
88	6	0	1.008483	3.439509	1.422606
89	1	0	1.356290	2.992783	2.348830
90	6	0	1.885396	3.499961	0.320317
91	6	0	1.417045	4.102433	-0.864442
92	1	0	2.085005	4.189599	-1.716200
93	6	0	0.100586	4.542178	-0.966320
94	1	0	-0.240433	4.976919	-1.902130

Optimized S_0 geometry of compound ***pm*-PCP-[6]CPP**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.135384	-4.319565	0.006016
2	6	0	-4.455768	0.525757	-1.310517
3	6	0	-4.455564	-0.526120	1.310548
4	6	0	-5.079920	-1.761867	0.988934
5	6	0	0.584923	-5.100070	-0.292550
6	6	0	-5.080579	1.761251	-0.988865
7	6	0	-5.255556	0.455645	1.901500
8	1	0	-4.790876	1.377898	2.242079
9	6	0	-4.244902	-2.849584	0.579801
10	6	0	4.776307	-4.279062	-0.070811
11	6	0	-6.485208	-1.822315	0.936429
12	1	0	-6.947700	-2.717386	0.527782
13	6	0	-0.221603	-5.640338	0.727475
14	1	0	0.209995	-6.330277	1.447410
15	6	0	-1.551507	-5.257140	0.880742
16	1	0	-2.128934	-5.632180	1.720344
17	6	0	-5.255397	-0.456296	-1.901499
18	1	0	-4.790367	-1.378356	-2.242123
19	6	0	-4.245991	2.849301	-0.579730
20	6	0	-3.356192	-3.638354	0.306528
21	6	0	-2.136742	4.319613	-0.006032
22	6	0	-7.274349	-0.702547	1.230951
23	6	0	-6.646251	-0.370995	-1.876054

24	1	0	-7.235860	-1.221739	-2.211329
25	6	0	2.068631	-5.155787	-0.271404
26	6	0	-3.084142	0.151980	-0.785490
27	1	0	-2.342883	0.935617	-0.969629
28	1	0	-2.745416	-0.748695	-1.306558
29	6	0	5.894301	-3.309052	0.070537
30	6	0	2.766907	-5.211351	0.949467
31	1	0	2.237366	-5.467451	1.862404
32	6	0	-3.357557	3.638371	-0.306432
33	6	0	-7.274618	0.701131	-1.230916
34	6	0	-3.084081	-0.151848	0.785501
35	1	0	-2.342532	-0.935209	0.969643
36	1	0	-2.745681	0.748955	1.306556
37	6	0	0.583552	5.100191	0.292398
38	6	0	-6.646384	0.369824	1.876066
39	1	0	-7.236305	1.220361	2.211320
40	6	0	5.981190	-2.539461	1.245549
41	1	0	5.431441	-2.840350	2.131135
42	6	0	4.092057	-4.798892	1.044693
43	1	0	4.562080	-4.785951	2.023765
44	6	0	-1.552877	5.257028	-0.880921
45	1	0	-2.130317	5.631940	-1.720573
46	6	0	6.668078	-2.871274	-1.023630
47	1	0	6.730993	-3.480216	-1.921406
48	6	0	-1.377265	-3.896510	-1.103512
49	1	0	-1.816801	-3.199023	-1.810105
50	6	0	-6.485896	1.821184	-0.936370
51	1	0	-6.948718	2.716079	-0.527710
52	6	0	6.582852	-1.287431	1.246151
53	1	0	6.475790	-0.662351	2.127445
54	6	0	7.121937	-0.739142	0.068736
55	6	0	2.833313	-4.880274	-1.419876
56	1	0	2.368349	-4.917300	-2.400801
57	6	0	-0.222973	5.640263	-0.727724
58	1	0	0.208595	6.330123	-1.447756
59	6	0	4.148416	-4.441624	-1.320921
60	1	0	4.647723	-4.103700	-2.223627
61	6	0	-1.378622	3.896758	1.103587
62	1	0	-1.818182	3.199439	1.810328
63	6	0	-0.049925	-4.273889	-1.241107
64	1	0	0.531041	-3.833609	-2.044663
65	6	0	7.264306	-1.613031	-1.026751
66	1	0	7.767124	-1.270775	-1.927760
67	6	0	-0.051293	4.274190	1.241122
68	1	0	0.529665	3.834131	2.044806
69	6	0	7.121695	0.740206	-0.068571
70	6	0	2.067263	5.155953	0.271247
71	6	0	6.582537	1.288326	-1.246024
72	1	0	6.475729	0.663215	-2.127330

73	6	0	4.775060	4.279516	0.070788
74	6	0	5.893272	3.309744	-0.070480
75	6	0	7.263709	1.614139	1.026930
76	1	0	7.766571	1.272051	1.927978
77	6	0	4.147117	4.442122	1.320863
78	1	0	4.646442	4.104381	2.223625
79	6	0	2.831960	4.880631	1.419749
80	1	0	2.366991	4.917722	2.400672
81	6	0	2.765536	5.211413	-0.949631
82	1	0	2.235984	5.467352	-1.862609
83	6	0	-8.646270	-0.522460	0.608273
84	1	0	-9.384203	-0.172862	1.340848
85	1	0	-9.003648	-1.489836	0.238476
86	6	0	4.090737	4.799100	-1.044788
87	1	0	4.560760	4.786104	-2.023855
88	6	0	5.980493	2.540183	-1.245475
89	1	0	5.430739	2.840884	-2.131120
90	6	0	-8.646469	0.520509	-0.608243
91	1	0	-9.384262	0.170629	-1.340823
92	1	0	-9.004225	1.487745	-0.238445
93	6	0	6.667096	2.872194	1.023754
94	1	0	6.729780	3.481156	1.921529

2.9 ^{1}H and ^{13}C NMR Spectra

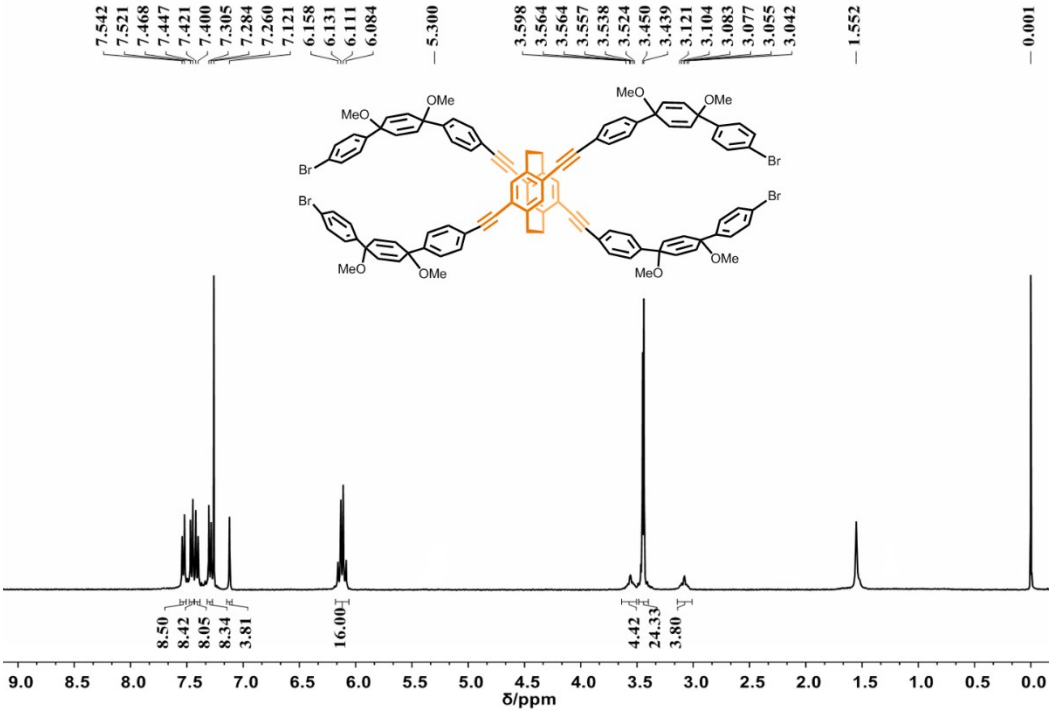


Fig. S24 ^{1}H NMR spectrum of compound ***bis-po*-4** in $CDCl_3$ (400 MHz, 298 K).

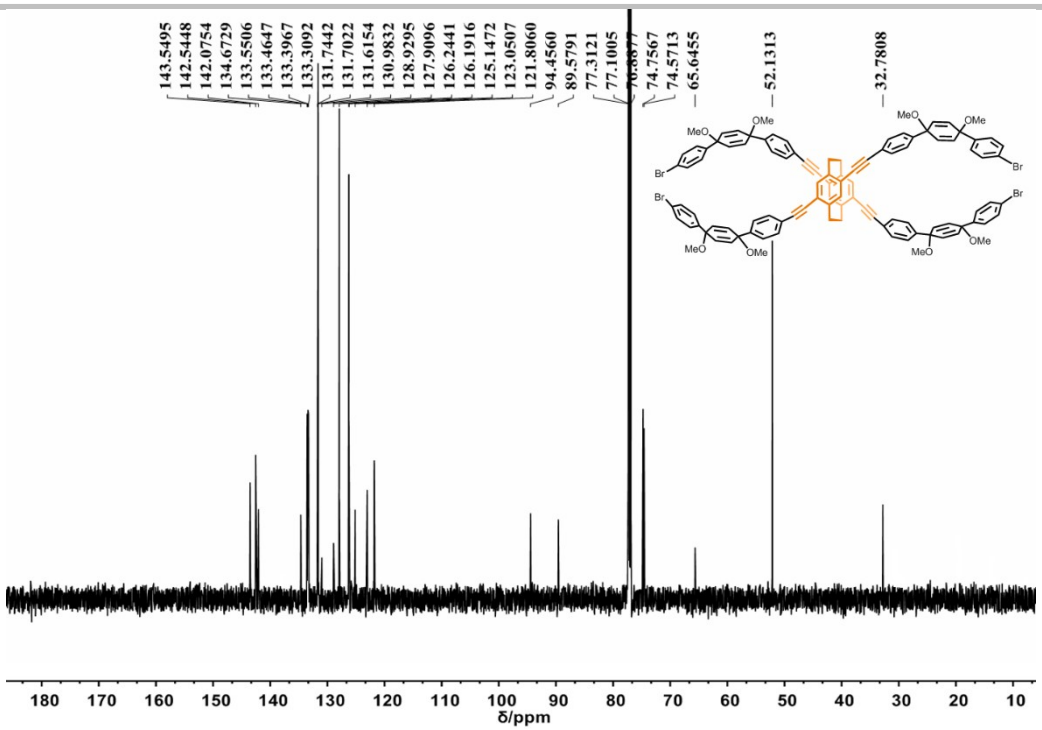


Fig. S25 ^{13}C NMR spectrum of compound ***bis-po*-4** in $CDCl_3$ (150 MHz, 298 K).

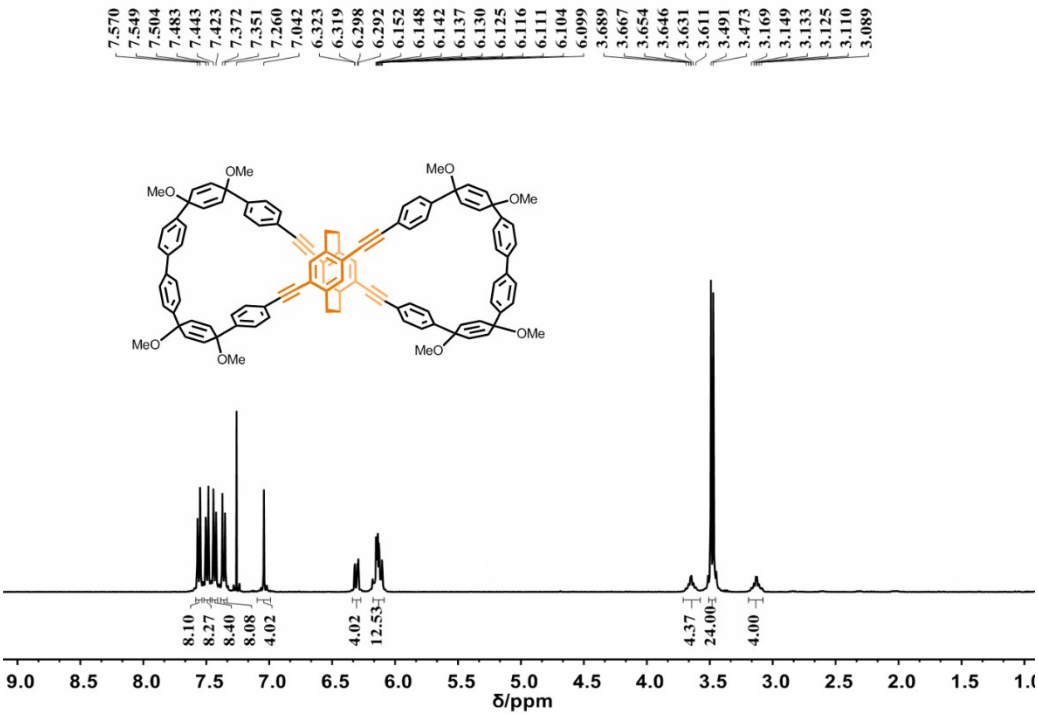


Fig. S26 ^{1}H NMR spectrum of compound ***bis-po*-5** in $CDCl_3$ (400 MHz, 298 K).

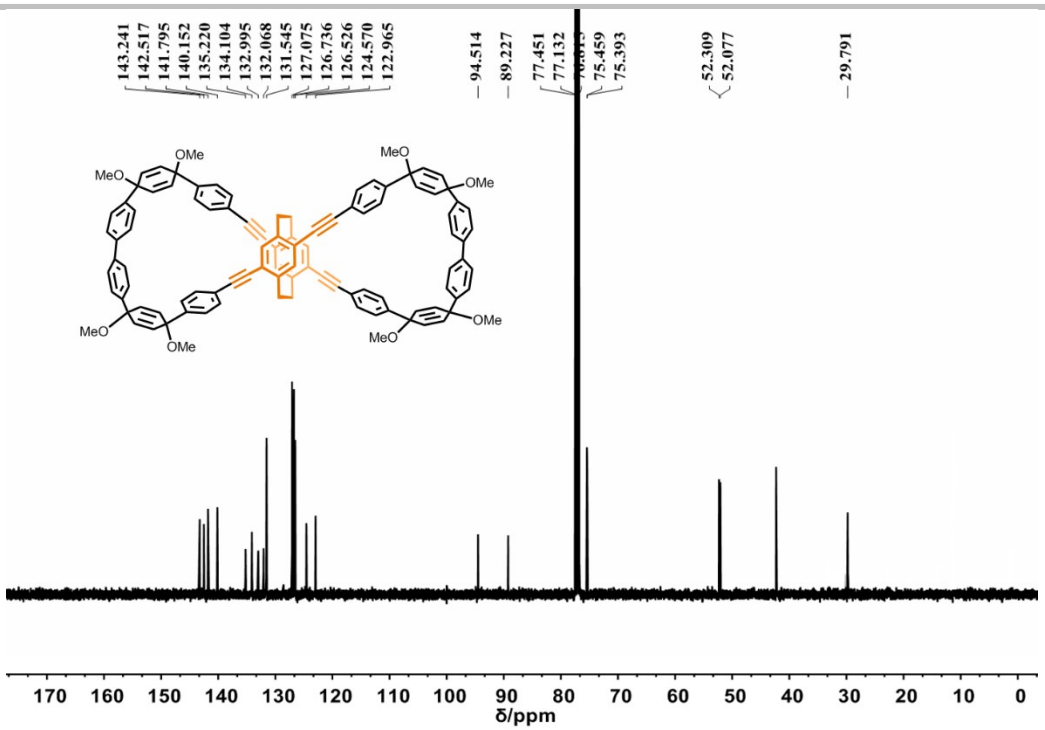


Fig. S27 ^{13}C NMR spectrum of compound ***bis-po*-5** in $CDCl_3$ (100 MHz, 298 K).

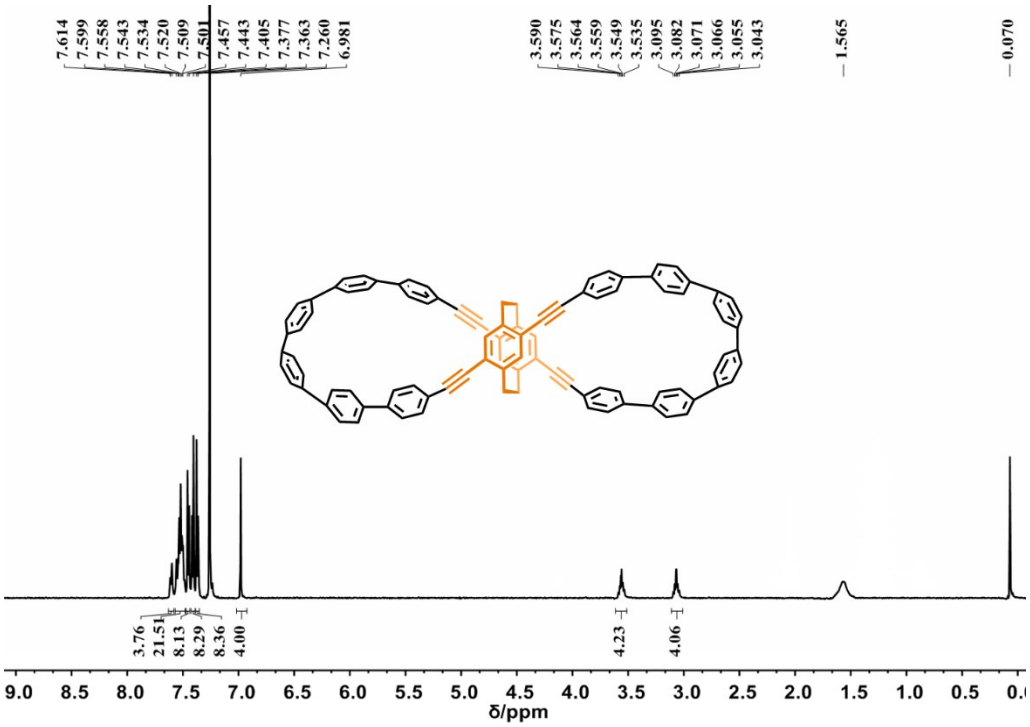


Fig. S28 ^{1}H NMR spectrum of compound ***bis-po*-CC** in $CDCl_3$ (600 MHz, 298 K).

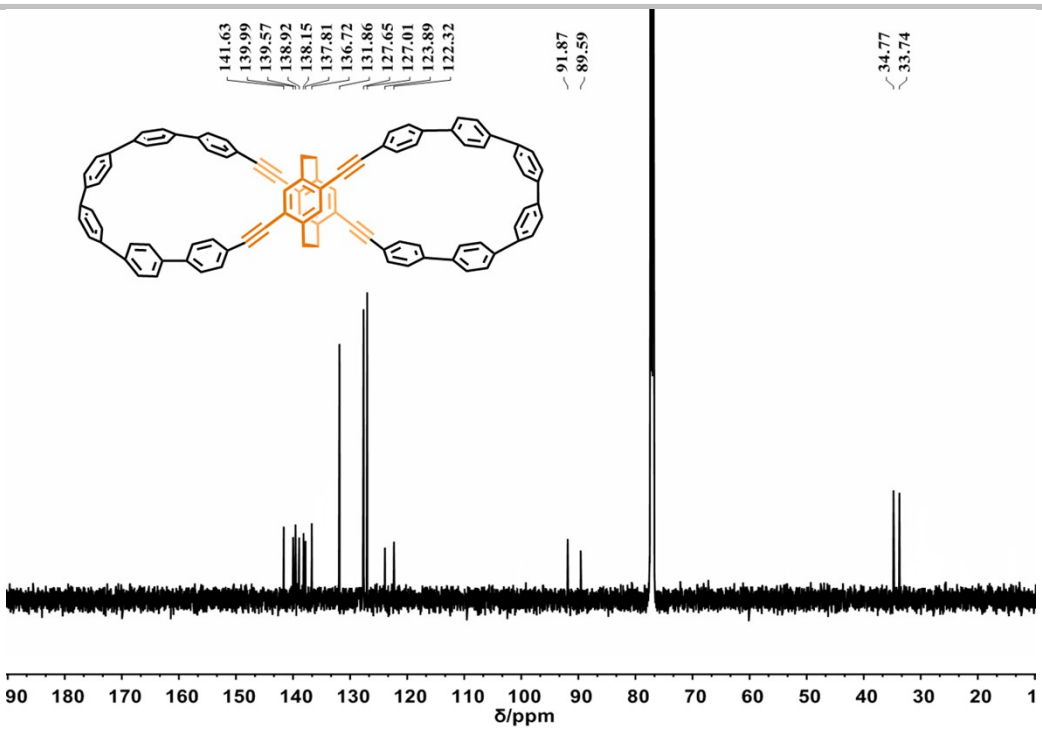


Fig. S29 ^{13}C NMR spectrum of compound ***bis-po*-CC** in $CDCl_3$ (150 MHz, 298 K).

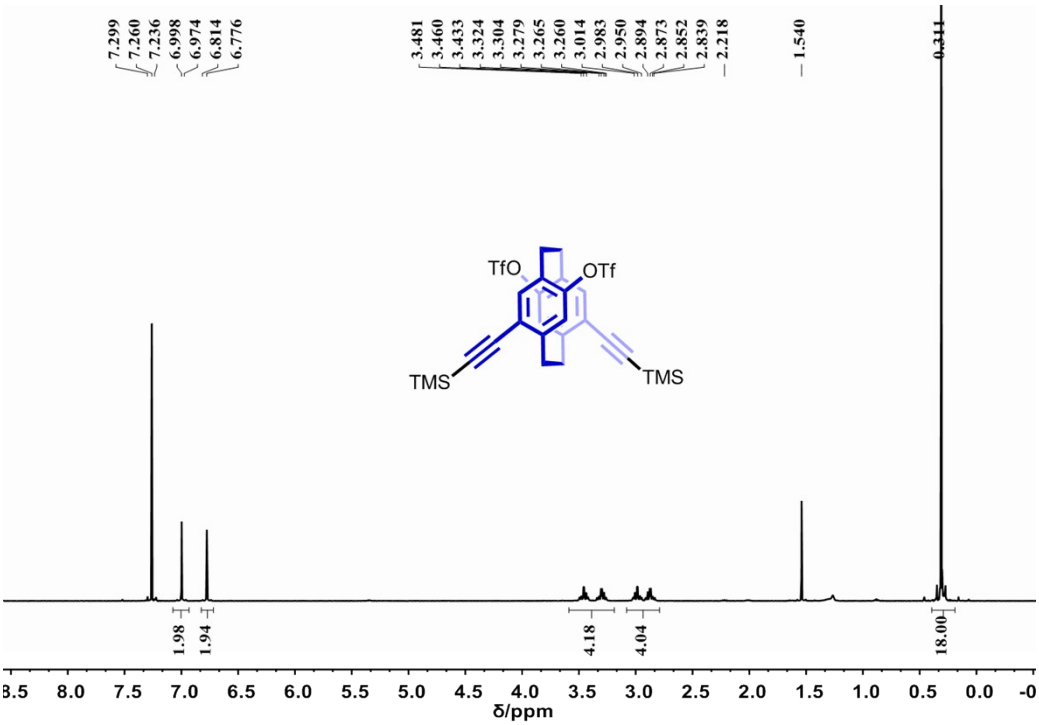


Fig. S30 ^{1}H NMR spectrum of compound ***bis-pm*-4** in $CDCl_3$ (600 MHz, 298 K).

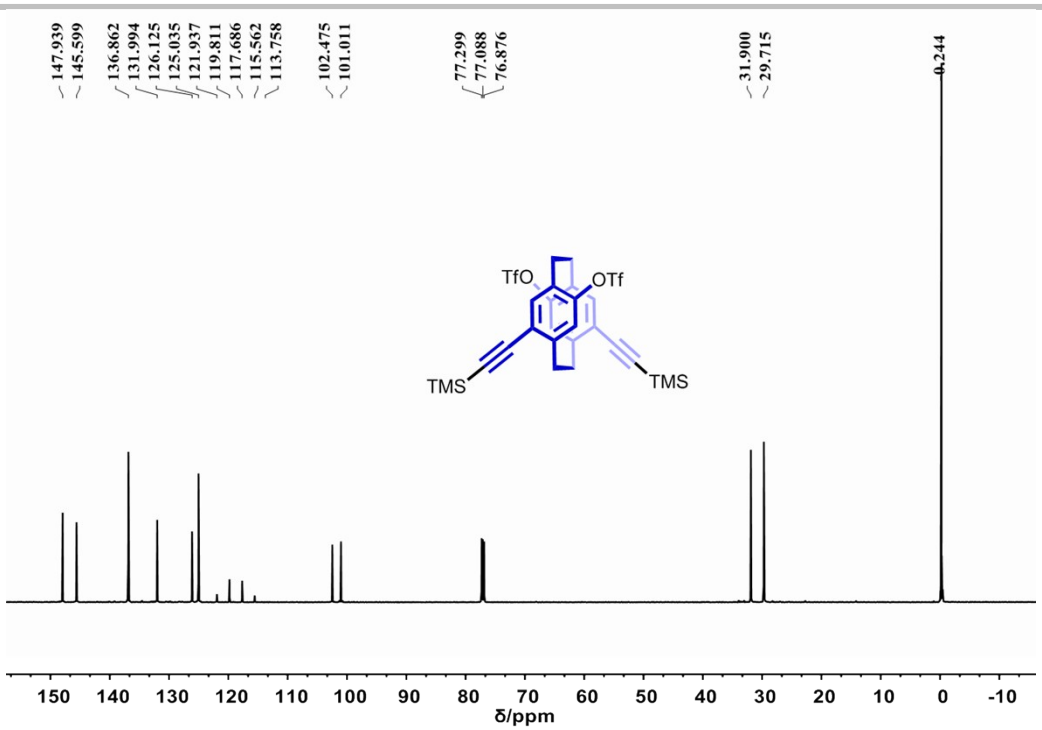


Fig. S31 ^{13}C NMR spectrum of compound ***bis-pm*-4** in $CDCl_3$ (150 MHz, 298 K).

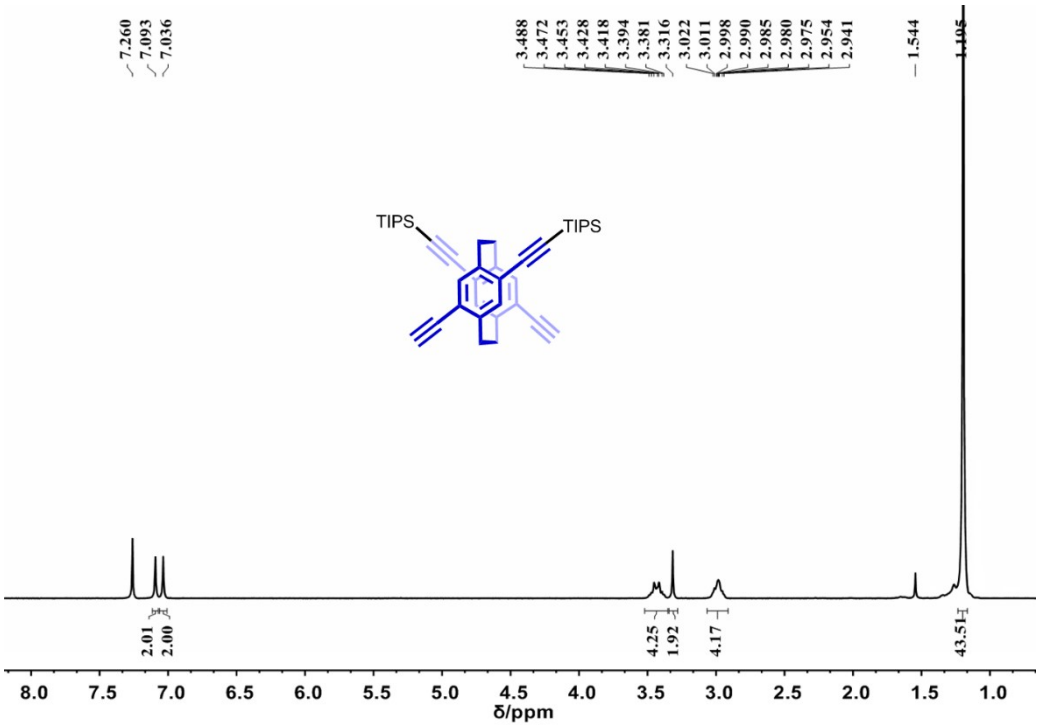


Fig. S32 ^{1}H NMR spectrum of compound ***bis-pm*-6** in $CDCl_3$ (400 MHz, 298 K).

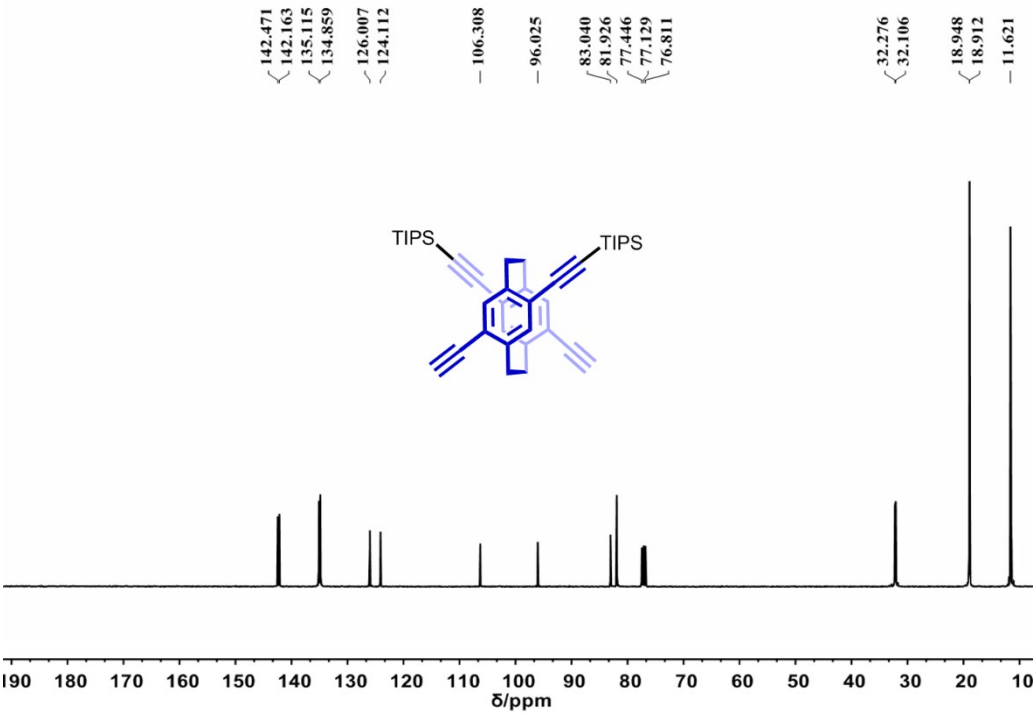


Fig. S33 ^{13}C NMR spectrum of compound ***bis-pm*-6** in $CDCl_3$ (100 MHz, 298 K).

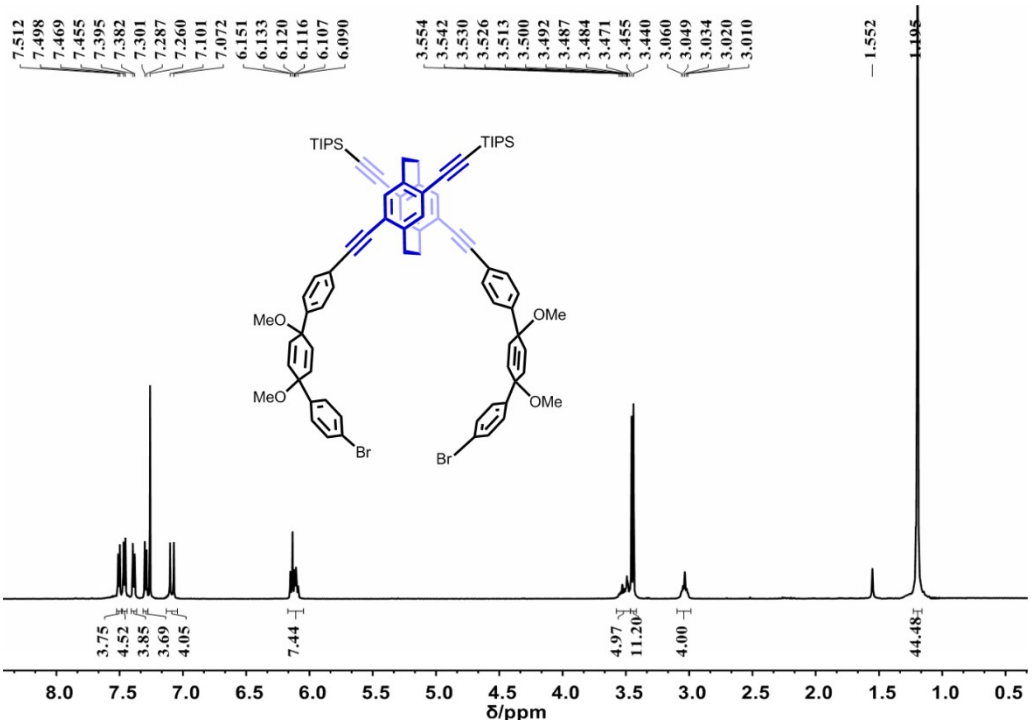


Fig. S34 ^{1}H NMR spectrum of compound ***bis-pm*-7** in $CDCl_3$ (600 MHz, 298 K).

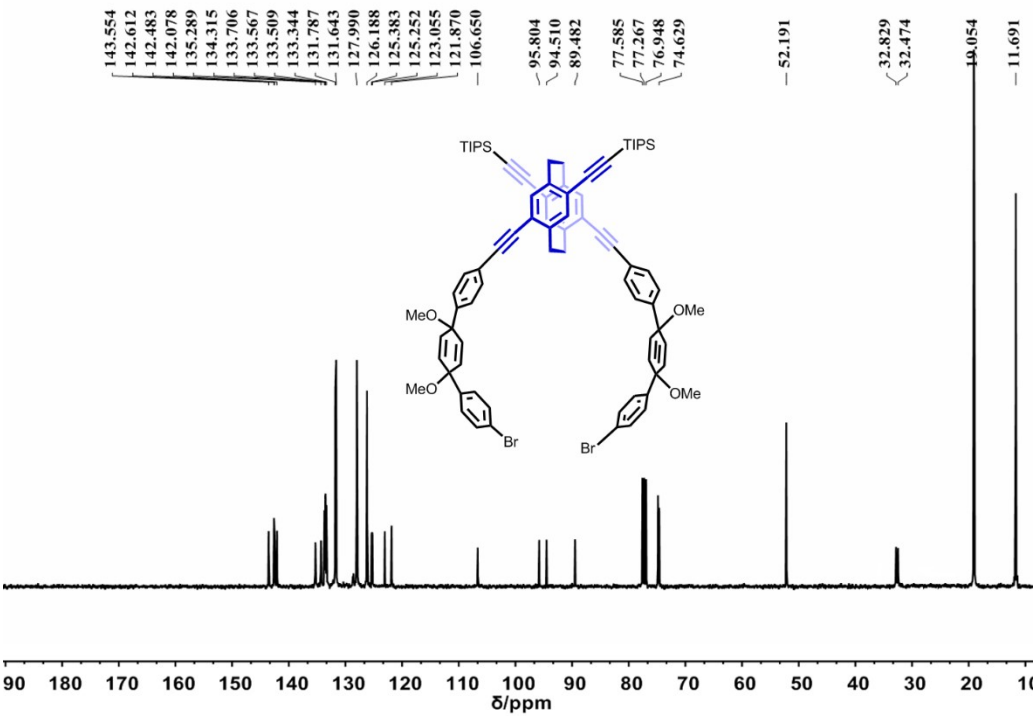


Fig. S35 ^{13}C NMR spectrum of compound ***bis-pm*-7** in $CDCl_3$ (100 MHz, 298 K).

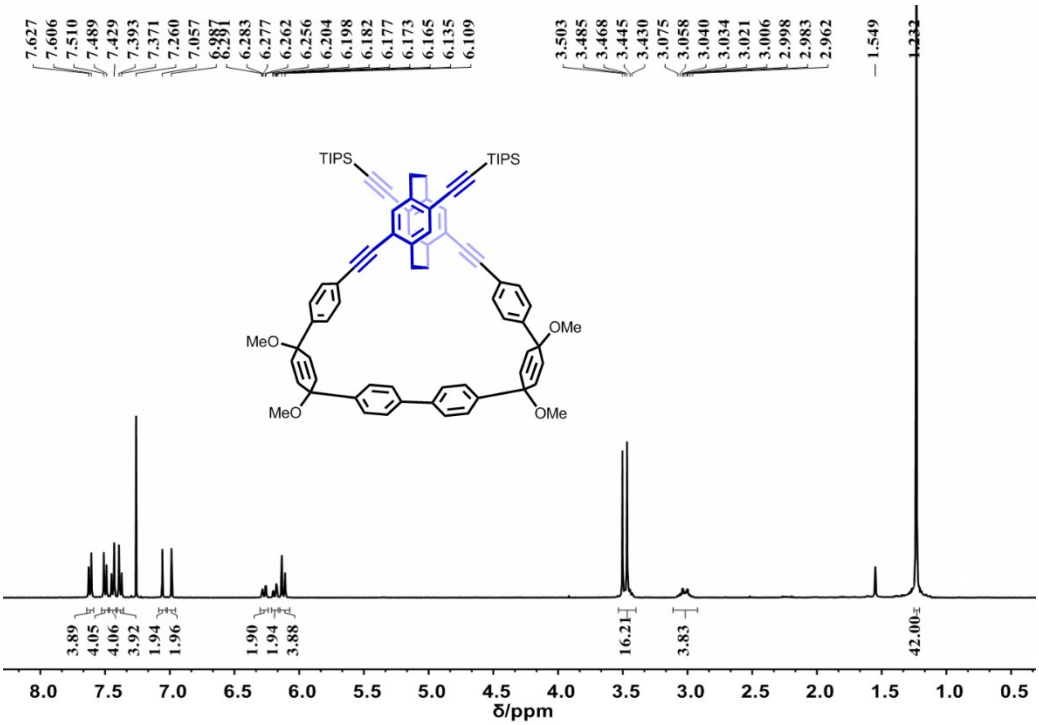


Fig. S36 ^{1}H NMR spectrum of compound ***bis-pm*-8** in $CDCl_3$ (600 MHz, 298 K).

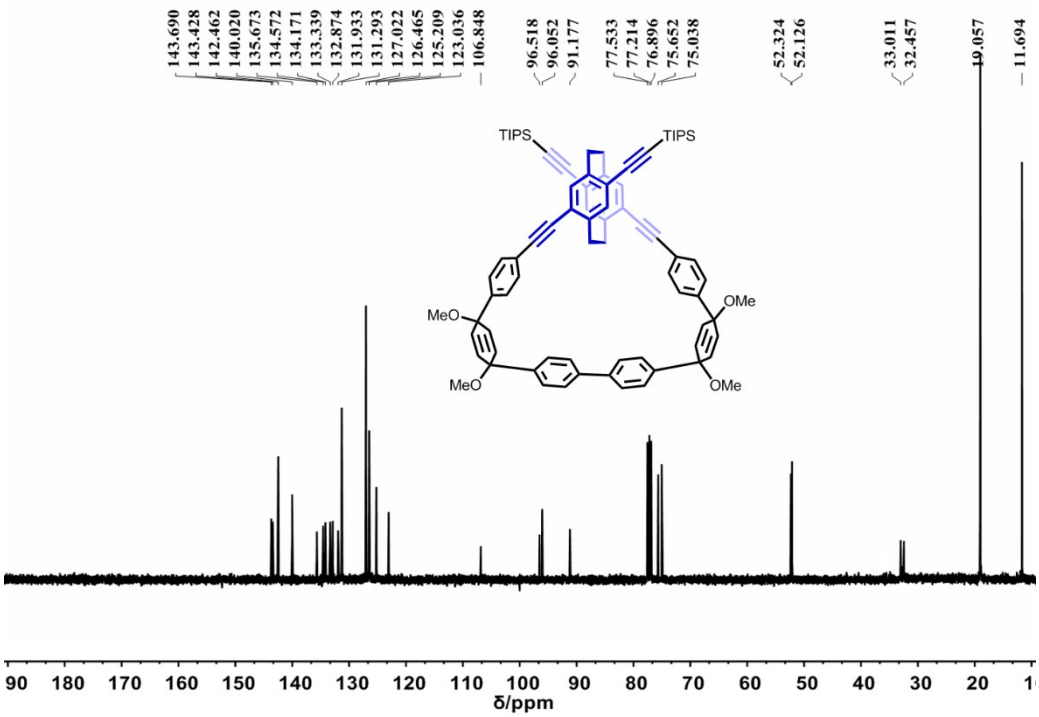


Fig. S37 ^{13}C NMR spectrum of compound ***bis-pm*-8** in $CDCl_3$ (100 MHz, 298 K).

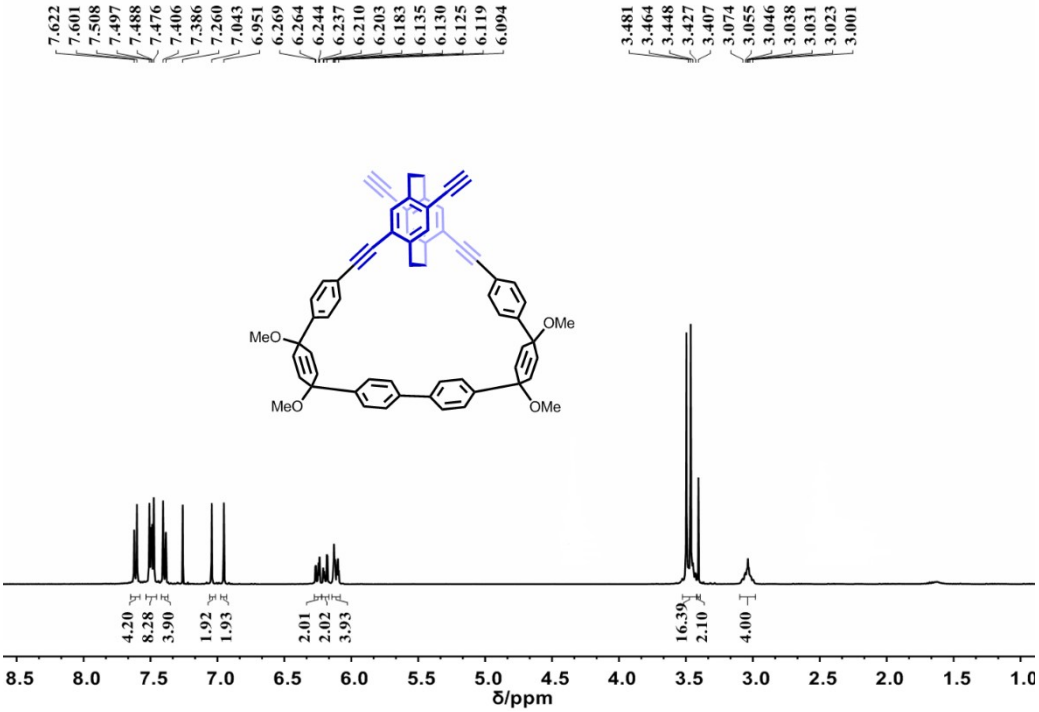


Fig. S38 ^{1}H NMR spectrum of compound ***bis-pm*-9** in $CDCl_3$ (400 MHz, 298 K).

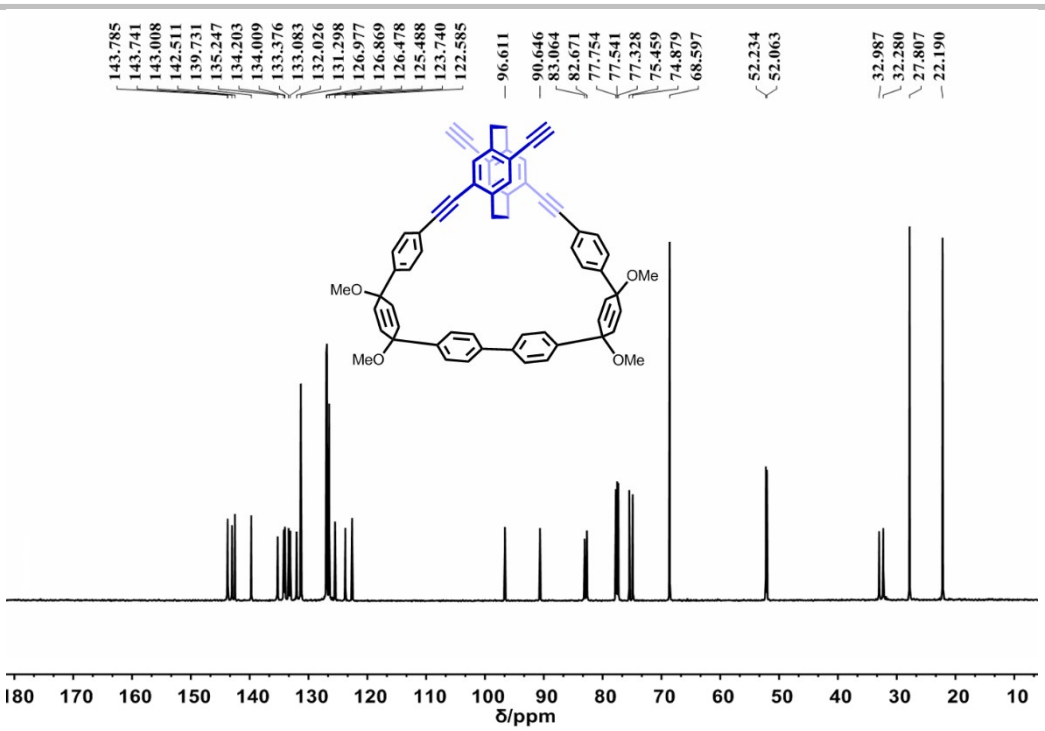


Fig. S39 ^{13}C NMR spectrum of compound ***bis-pm*-9** in $CDCl_3$ (150 MHz, 298 K).

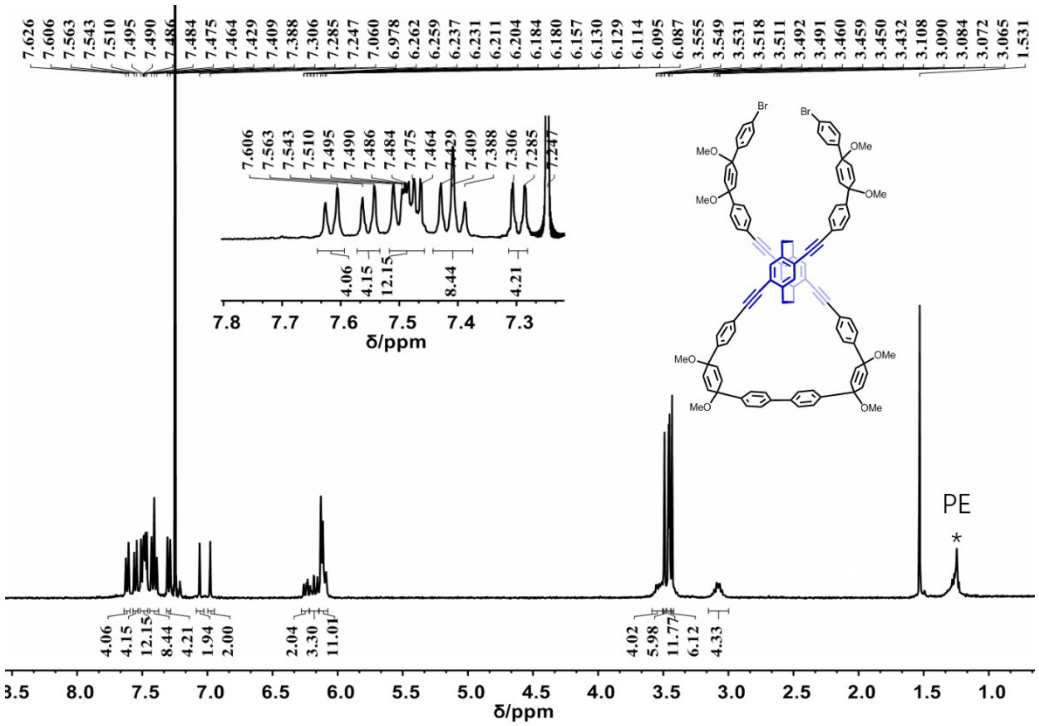


Fig. S40 ^{1}H NMR spectrum of compound ***bis-pm*-10** in $CDCl_3$ (400 MHz, 298 K).

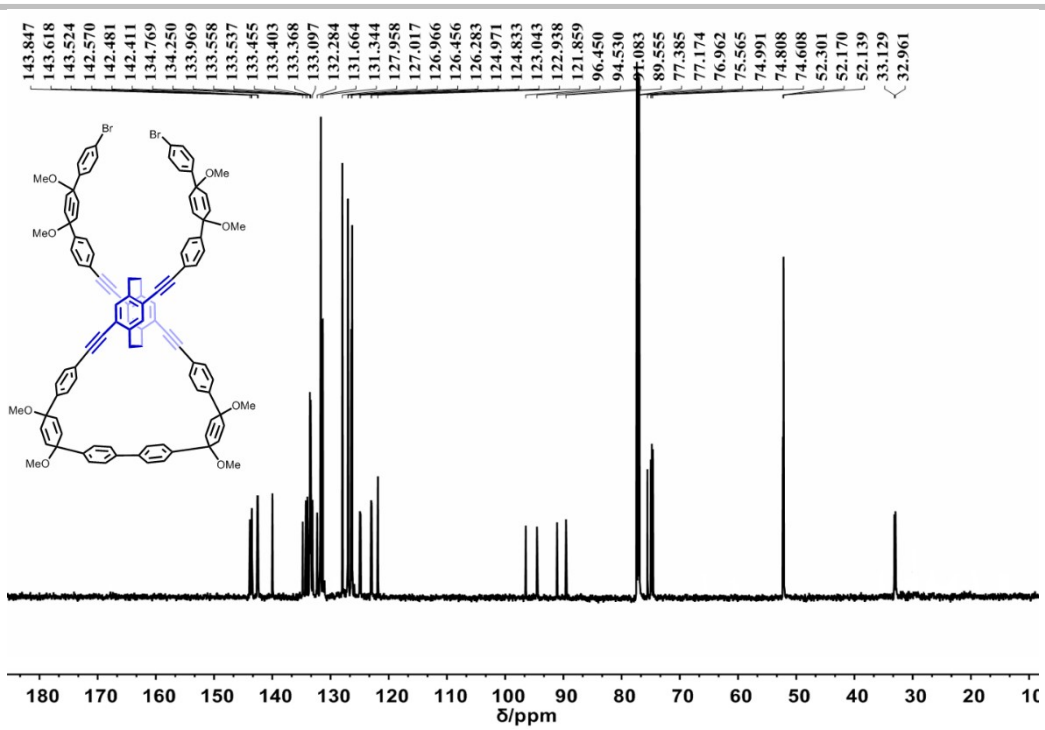


Fig. S41 ^{13}C NMR spectrum of compound ***bis-pm*-10** in $CDCl_3$ (150 MHz, 298 K).

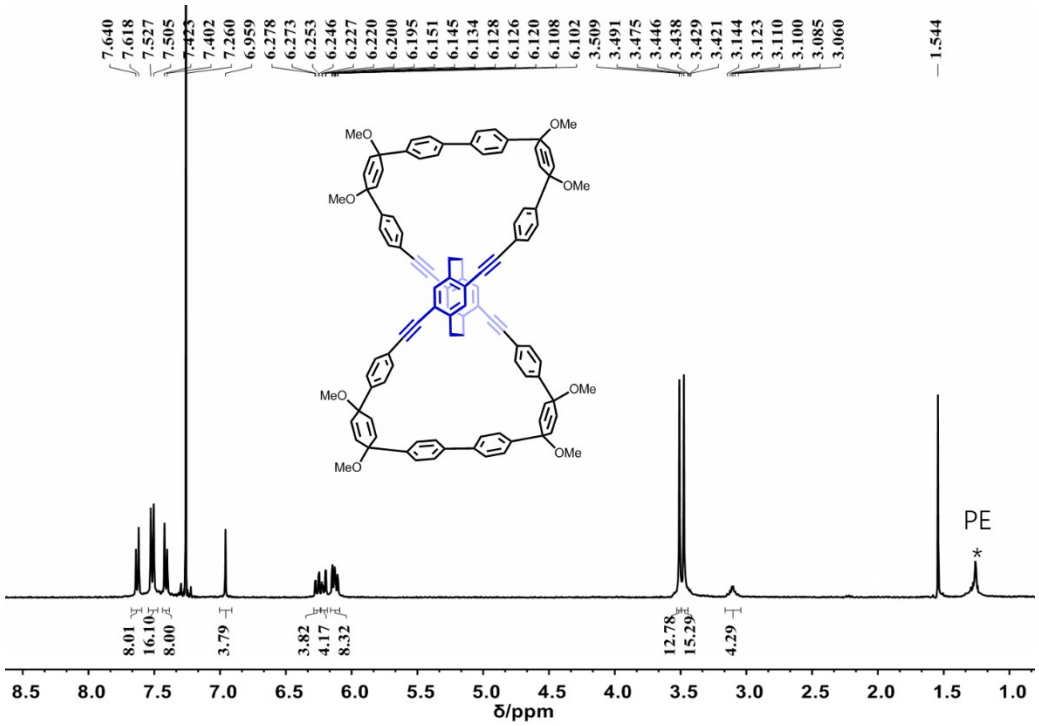


Fig. S42 ^{1}H NMR spectrum of compound ***bis-pm*-11** in $CDCl_3$ (400 MHz, 298 K).

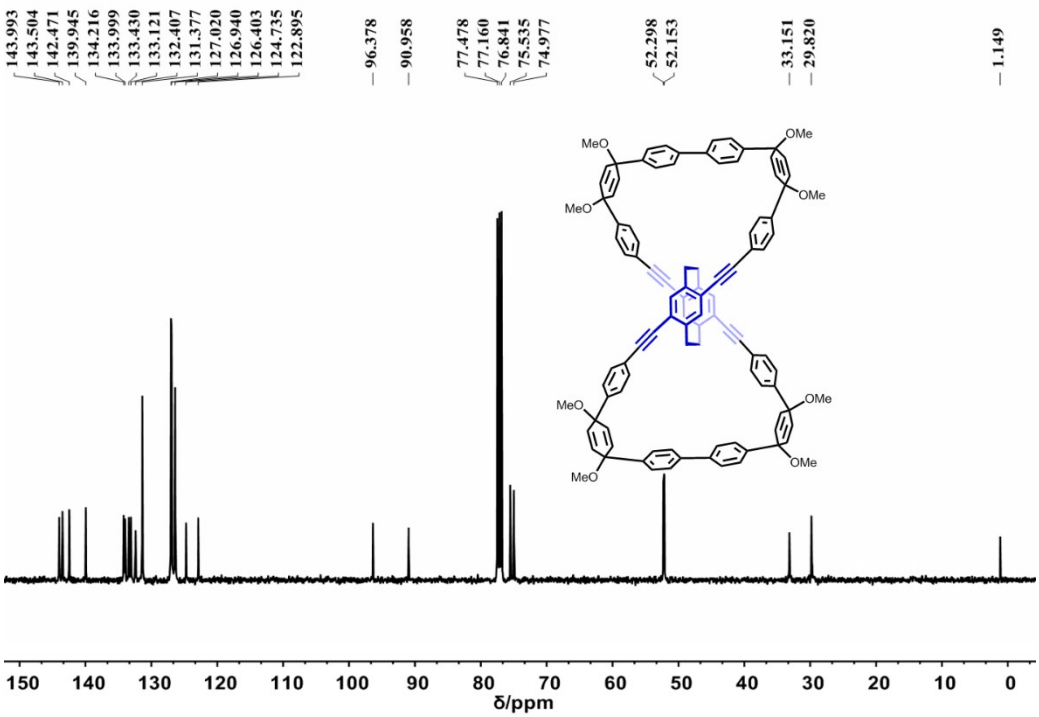


Fig. S43 ^{13}C NMR spectrum of compound ***bis-pm*-11** in $CDCl_3$ (100 MHz, 298 K).

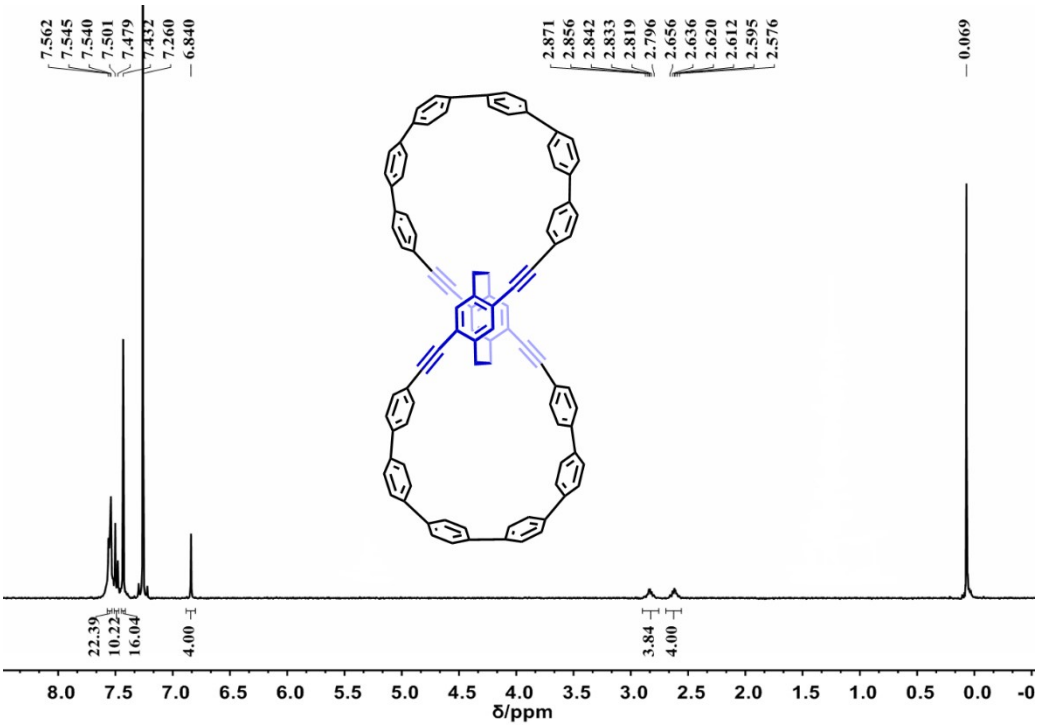


Fig. S44 ^{1}H NMR spectrum of compound ***bis-pm*-TC** in $CDCl_3$ (400 MHz, 298 K).

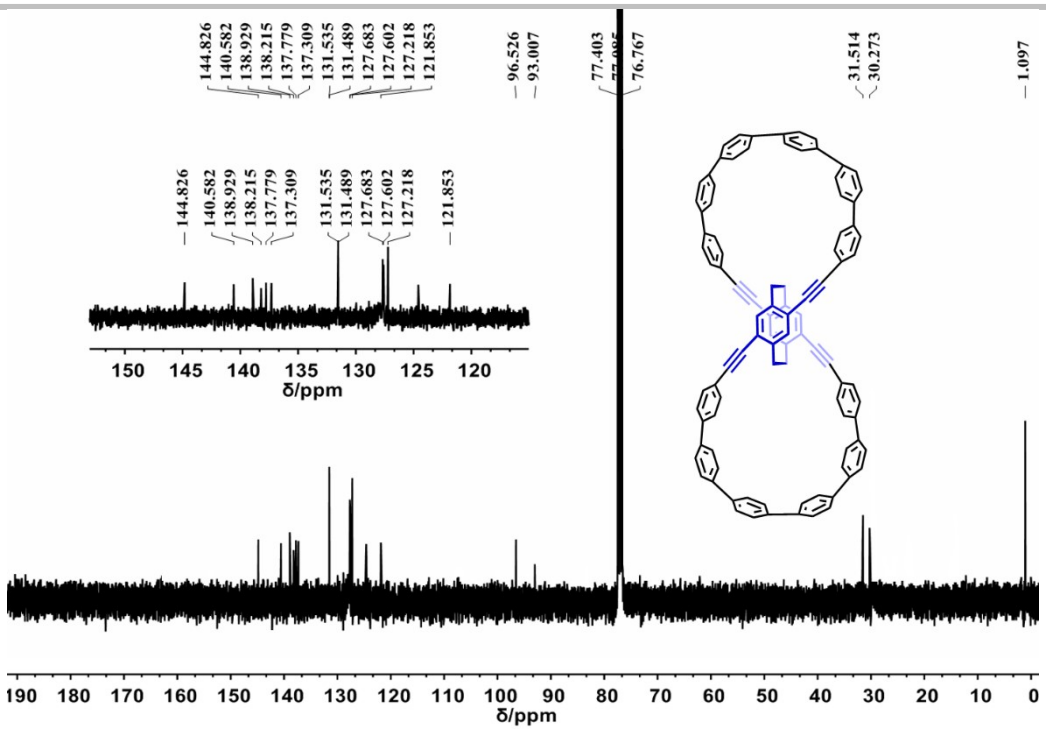


Fig. S45 ^{13}C NMR spectrum of compound ***bis-pm*-TC** in $CDCl_3$ (100 MHz, 298 K).

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