

Catalytic stereoselective synthesis of doubly, triply and quadruply twisted aromatic belts

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1. Synthetic experiments

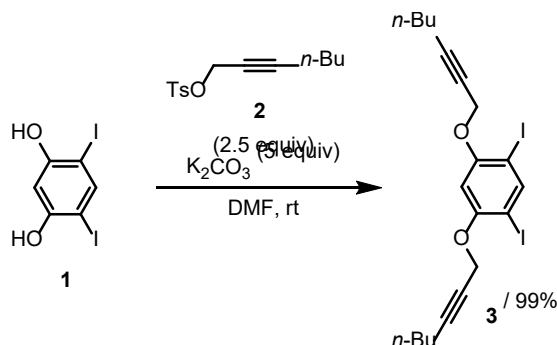
1.1. General experimental information

Dry degassed *i*-Pr₂NH (*N,N*-diisopropylamine, No. 471224, Sigma-Aldrich) for the synthesis of **5**, Dry degassed DMF (*N,N*-dimethylformamide, No. 044-32075, Wako Pure Chemical Industries) for the synthesis of macrocycles **9a**, **9b**, and **9c**, Anhydrous CH₂Cl₂ (No. 284505, Aldrich) for the synthesis of **10**, **11**, **12**, **13**, and **14** were used as received. Solvents for the synthesis of substrates were dried over Molecular Sieves 4Å (Wako) before use. H₈-BINAP and Segphos were obtained from Takasago International Corporation. [Rh(cod)₂]BF₄ was obtained from Umicore AG. 4,6-diiodobenzene-1,3-diol¹ (**1**), hept-2-yn-1-yl 4-methylbenzenesulfonate² (**2**), *tert*-butyldiphenyl(prop-2-yn-1-yloxy)silane³ (**4**), and 2,5-di(hex-1-yn-1-yl)benzene-1,4-diol⁴ (**8**) were prepared according to the literature. All other commercially available reagents were obtained from TCI Chemicals, Wako Pure Chemical Industries, Sigma-Aldrich, and Kanto Chemicals and used as received unless otherwise noted. Silica gel column chromatography was performed using silica gel [Silica Gel 60 N (spherical, neutral), Kanto Chemicals] and JIS (Japanese Industrial Standards) special grade solvents. Silica gel preparative thin layer chromatography (PTLC) was performed using silica gel (Wakogel® B-5F) and JIS special grade solvents. All reactions were carried out under an atmosphere of argon or nitrogen in oven-dried glassware with magnetic stirring.

1.2. General analytical information

All compounds were characterized by ¹H and ¹³C NMR spectroscopy. Copies of the ¹H and ¹³C NMR spectra for all new compounds can be found in section 7 “¹H, ¹³C, and 2D NMR Spectra of New Compounds” of the Supplementary Materials. All previously unreported compounds were additionally characterized by high-resolution mass spectrometry (HRMS). ¹H, ¹³C, COSY, NOESY, HMBC, and HSQC NMR data were collected on a Bruker AVANCE III HD 400 at ambient temperature. All ¹H NMR experiments are reported in δ units, parts per million (ppm), and were measured relative to the signals for residual chloroform (7.26 ppm). All ¹³C NMR spectra are reported in ppm relative to deuteriochloroform (77.01 ppm) and were obtained with ¹H decoupling. HRMS analyses were performed on a Bruker micrOTOF Focus II instrument. Melting points were determined on a Mettler MP50 or Yanaco MP-S3 and were uncorrected. Chiral HPLC analyses were performed on a JASCO HPCL 2000 series. A polarimetry measurement was performed using a JASCO P-2200 circular polarimeter. The UV/Vis absorption spectra were recorded on a JASCO V-630 spectrometer with a resolution of 1.0 nm. The emission spectra were recorded on a JASCO FP-6200 spectrometer with a resolution of 1.0 nm. The fluorescence quantum yields were measured on a Hamamatsu Photonics Absolute PL Quantum Yield Measurement System, C11347-01. The ECD spectra were obtained on a JASCO J-820 spectrodichrometer using a 10 mm quartz cell. The magnitude of the ECD signal is expressed in terms of molar circular dichroism $\Delta\epsilon/M^{-1} \text{ cm}^{-1}$.

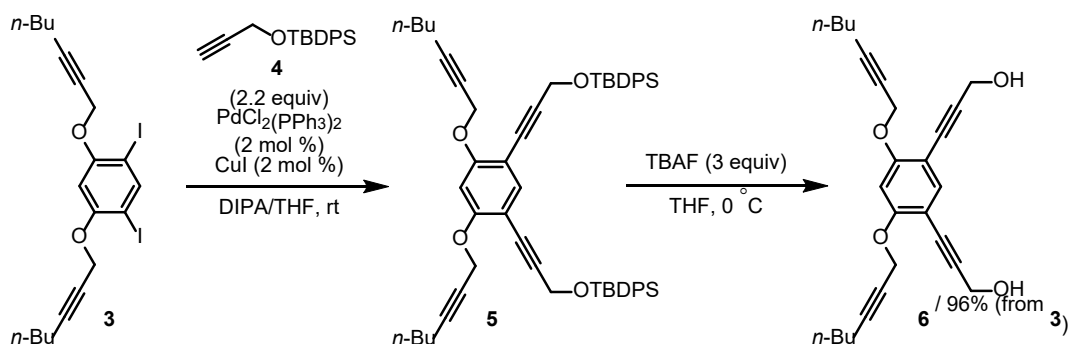
1.3. Synthesis of 1,5-bis(hept-2-yn-1-yloxy)-2,4-diiodobenzene (**3**)



To a solution of 4,6-diiodobenzene-1,3-diol¹ (**1**, 1.81 g, 5.00 mmol) and K_2CO_3 (3.46 g, 25.0 mmol) in dry DMF (20 mL) was added hept-2-yn-1-yl 4-methylbenzenesulfonate² (**2**, 3.33 g, 12.5 mmol). The mixture was stirred at room temperature for 12 h. The resulting mixture was quenched with water and extracted with Et_2O twice. The residue was purified by silica gel column chromatography (eluent: *n*-hexane/ $EtOAc$ = 20:1) to give **3** (2.73 g, 4.96 mmol, 99% yield).

Colorless solid; mp 65.0–66.5 °C; 1H NMR (400 MHz, $CDCl_3$) δ 8.06 (s, 1H), 6.82 (s, 1H), 4.73 (t, J = 2.1 Hz, 4H), 2.21 (tt, J = 2.1, 10.4 Hz, 4H), 1.53–1.43 (m, 4H), 1.43–1.31 (m, 4H), 0.89 (t, J = 7.3 Hz, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 158.0, 146.9, 100.5, 89.4, 77.3, 74.0, 58.1, 30.5, 21.9, 18.5, 13.5; HRMS (ESI) calcd for $C_{20}H_{24}I_2O_2Na$ $[M+Na]^+$ 572.9758, found 572.9744.

1.4. Synthesis of 3,3'-(4,6-bis(hept-2-yn-1-yloxy)-1,3-phenylene)bis(prop-2-yn-1-ol) (**6**)



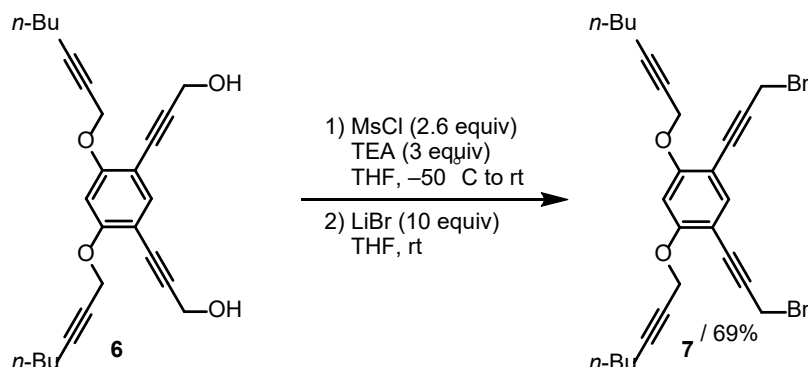
To a solution of **3** (1.93 g, 3.50 mmol), CuI (13.3 mg, 70.0 μ mol), and $Pd(PPh_3)_2Cl_2$ (49.1 mg, 70.0 μ mol) in *i*-Pr₂NH (10 mL) and THF (20 mL) was added a solution of tert-butyldiphenyl(prop-2-yn-1-yloxy)silane³ (**4**, 2.27 g, 7.70 mmol) in DIPA (10 mL). The mixture was stirred at room temperature for 12 h. The resulting mixture was filtered and concentrated. The residue was roughly purified by silica gel column chromatography (eluent: *n*-hexane/ $EtOAc$ = 5:1) to give crude **5**. The residue was used in the next step without further purification.

To a solution of this crude **5** in THF (20 mL) was added tetrabutylammonium fluoride (TBAF, 1.0 M in THF, 10.5 mL, 10.5 mmol) at 0 °C. The mixture was stirred at 0 °C for 1 h. The reaction was quenched with water and extracted with $EtOAc$ twice. The organic layer was washed with saturated aqueous NaCl, dried over Na_2SO_4 , and concentrated. The residue was purified by silica gel column chromatography (eluent: *n*-hexane/ $EtOAc$ = 1:1) to give **6** (1.41 g, 3.46 mmol, 96% yield in 2 steps).

Brown oil; 1H NMR (400 MHz, $CDCl_3$) δ 7.43 (s, 1H), 6.80 (s, 1H), 4.77 (t, J = 2.1 Hz, 4H), 4.51 (s, 4H), 2.21 (tt, J = 2.1, 10.4 Hz, 4H), 1.83 (br, 2H), 1.53–1.43 (m, 4H), 1.43–1.32 (m, 4H),

0.89 (t, $J = 7.2$ Hz, 6H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 159.7, 138.3, 105.4, 99.1, 90.6, 89.4, 80.9, 74.2, 57.5, 51.9, 30.5, 21.9, 18.5, 13.5; HRMS (ESI) calcd for $\text{C}_{26}\text{H}_{30}\text{O}_4\text{Na}$ $[\text{M}+\text{Na}]^+$ 429.2036, found 429.2019.

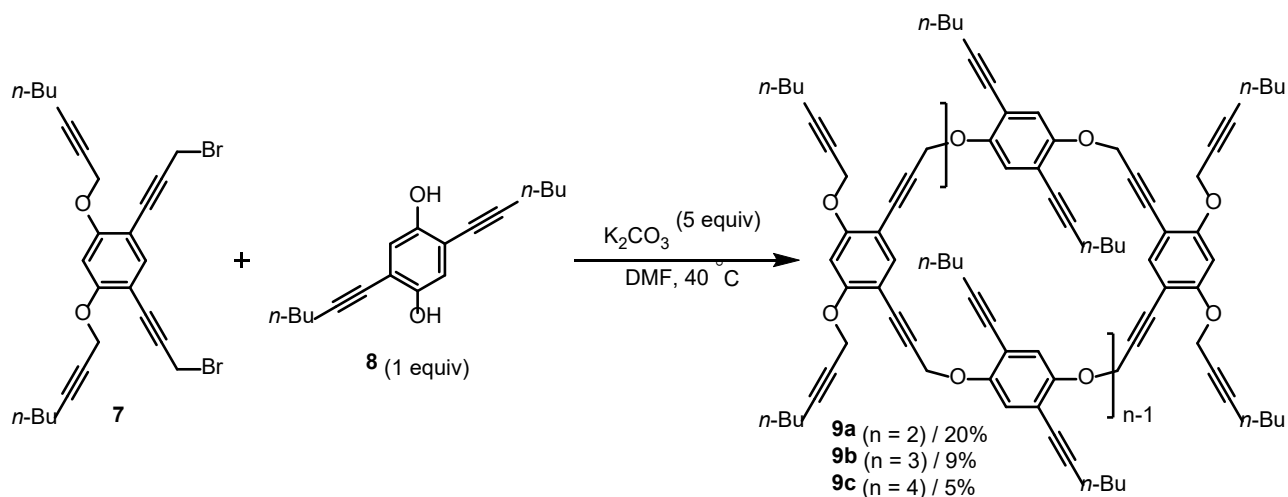
1.5. Synthesis of 1,5-bis(3-bromoprop-1-yn-1-yl)-2,4-bis(hept-2-yn-1-yloxy)benzene (7)



6 (2.86 g, 7.04 mmol) and TEA (2.93 ml, 21.1 mmol) were dissolved in THF (60 mL). Methanesulfonyl chloride (MsCl, 1.42 ml, 18.3 mmol) was added dropwise to the solution at -50°C , then the cooling bath was removed, and the pale yellow suspension was stirred at room temperature for 1 h. To the suspension was added lithium bromide (LiBr, 6.11 g, 70.4 mmol) in THF (60 ml) quickly. The mixture was stirred at room temperature for 2 h. The reaction was quenched with water and extracted with CH_2Cl_2 twice. The organic layer was washed with saturated aqueous NaCl, dried over Na_2SO_4 , and concentrated. The residue was purified by silica gel column chromatography (eluent: n -hexane/ $\text{CH}_2\text{Cl}_2 = 2:1$) to give **7** (2.58 g, 4.84 mmol, 69% yield).

Colorless solid; mp $54.2\text{--}56.2^\circ\text{C}$; ^1H NMR (400 MHz, CDCl_3) δ 7.47 (s, 1H), 6.79 (s, 1H), 4.76 (t, $J = 2.1$ Hz, 4H), 4.19 (s, 4H), 2.21 (tt, $J = 2.1, 10.4$ Hz, 4H), 1.52–1.43 (m, 4H), 1.43–1.33 (m, 4H), 0.89 (t, $J = 7.2$ Hz, 6H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 160.3, 138.7, 105.3, 99.4, 89.5, 87.5, 82.1, 74.1, 57.7, 30.5, 21.9, 18.5, 15.8, 13.5; HRMS (ESI) calcd for $\text{C}_{26}\text{H}_{28}\text{Br}_2\text{O}_2\text{Na}$ $[\text{M}+\text{Na}]^+$ 553.0348, found 553.0330.

1.6. Synthesis of cyclic polyynes 9a-c



To a Schlenk tube was added a solution of **7** (0.266 g, 0.500 mmol), 2,5-di(hex-1-yn-1-yl)benzene-1,4-diol⁴ (**8**, 0.135 g, 0.500 mmol), and K_2CO_3 (0.346 g, 2.50 mmol) in DMF (33 mL, 0.015 mol/L) at room temperature. The mixture was stirred at 40 °C for 48 h. The reaction was quenched with water and extracted with CH_2Cl_2 twice. The organic layer was washed with saturated aqueous NaCl, dried over Na_2SO_4 , and concentrated. The residue was dissolved in toluene and concentrated again. The resulting mixture was purified by GPC (eluent: $CHCl_3$) and silica gel preparative thin layer chromatography (PTLC, eluent: n -hexane/ CH_2Cl_2 = 1:1) to give **9a** (63.5 mg, 0.0495 mmol, 20% yield), **9b** (29.4 mg, 0.0153 mmol, 9% yield), and **9c** (15.0 mg, 0.00585 mmol, 5% yield).

Data for **9a**: Colorless solid; mp 135.6–137.4 °C; 1H NMR (400 MHz, $CDCl_3$) δ 7.41 (s, 2H), 7.08 (s, 4H), 6.80 (s, 2H), 4.94 (s, 8H), 4.77 (s, 8H), 2.44 (t, $J = 7.1$ Hz, 8H), 2.21 (tt, $J = 2.0, 10.5$ Hz, 8H), 1.61–1.53 (m, 8H), 1.51–1.33 (m, 24H), 0.89 (t, $J = 7.6$ Hz, 12H), 0.87 (t, $J = 7.7$ Hz, 12H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 159.7, 152.6, 139.1, 119.0, 114.4, 105.6, 99.3, 96.3, 89.3, 87.3, 82.8, 76.6, 74.2, 58.3, 57.6, 30.8, 30.5, 22.0, 21.9, 19.5, 18.5, 13.6, 13.5; HRMS (ESI) calcd for $C_{88}H_{96}O_8Na$ $[M+Na]^+$ 1303.6997, found 1303.7042.

Data for **9b**: Colorless oil; 1H NMR (400 MHz, $CDCl_3$) δ 7.40 (s, 3H), 7.12 (s, 6H), 6.82 (s, 3H), 4.92 (s, 12H), 4.76 (s, 12H), 2.45 (t, $J = 7.0$ Hz, 12H), 2.19 (tt, $J = 2.0, 10.4$ Hz, 12H), 1.65–1.52 (m, 12H), 1.52–1.41 (m, 24H), 1.41–1.32 (m, 12H), 0.89 (t, $J = 7.2$ Hz, 18H), 0.87 (t, $J = 7.2$ Hz, 18H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 160.0, 152.9, 138.5, 119.2, 114.6, 105.4, 99.4, 96.2, 89.2, 87.3, 82.7, 76.6, 74.3, 58.6, 57.6, 30.8, 30.5, 22.0, 21.9, 19.5, 18.5, 13.6, 13.5; HRMS (ESI) calcd for $C_{132}H_{144}O_{12}Na$ $[M+Na]^+$ 1944.0550, found 1944.0393.

Data for **9c**: Colorless oil; 1H NMR (400 MHz, $CDCl_3$) δ 7.41 (s, 4H), 7.12 (s, 8H), 6.83 (s, 4H), 4.91 (s, 16H), 4.76 (s, 16H), 2.46 (t, $J = 7.0$ Hz, 16H), 2.19 (tt, $J = 1.5, 7.0$ Hz, 16H), 1.67–1.53 (m, 16H), 1.53–1.41 (m, 32H), 1.41–1.30 (m, 16H), 0.90 (t, $J = 7.3$ Hz, 24H), 0.87 (t, $J = 7.2$ Hz, 24H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 160.1, 153.0, 138.3, 119.2, 114.6, 105.4, 99.5, 96.2, 89.2, 87.3, 82.7, 76.6, 74.4, 58.6, 57.6, 30.8, 30.5, 22.0, 21.9, 19.5, 18.5, 13.6, 13.5; HRMS (ESI) calcd for $C_{176}H_{192}O_{16}Na$ $[M+Na]^+$ 2584.4103, found 2584.3639, and $C_{176}H_{192}O_{16}Na_2$ $[M+2Na]^{2+}$ 1303.6997, found 1303.7111.

1.7. Synthesis of doubly twisted belts (*M,M*)-(–)-**10** and (*P,M*)-**11**

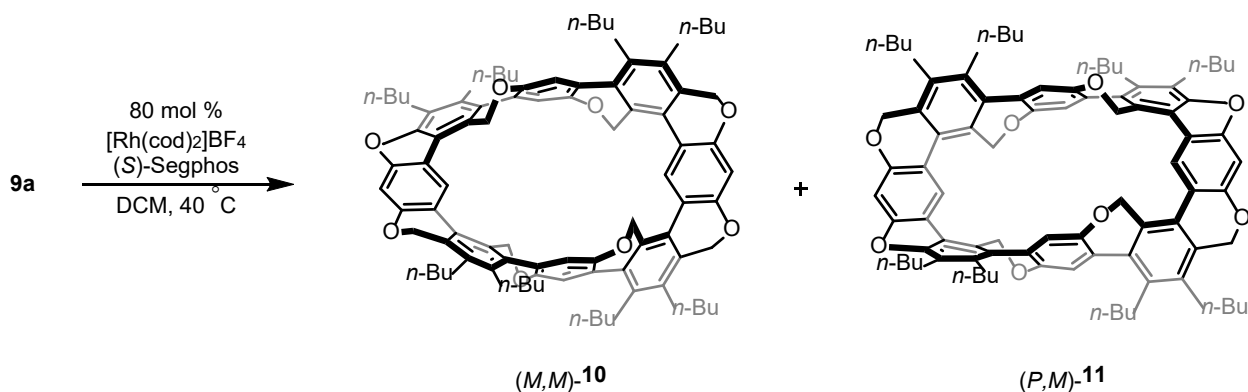
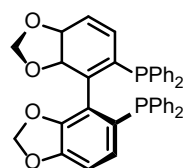
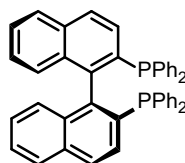


Table S1. Screening of ligands for rhodium-catalyzed [2+2+2] cycloaddition of **9a**.

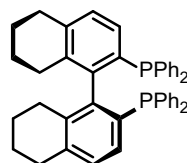
Ligand	yield (%) / er of (<i>M,M</i>)-(–)- 10	yield (%) of (<i>P,M</i>)- 11
(<i>S</i>)-Segphos	43 / 98:2	43
(<i>S</i>)-BINAP	30 / 96:4	51
(<i>S</i>)-H ₈ -BINAP	40 / 98:2	36



(*S*)-Segphos



(*S*)-BINAP



(*S*)-H₈-BINAP

(*S*)-Segphos (41.9 mg, 68.5 μmol) and $[\text{Rh}(\text{cod})_2]\text{BF}_4$ (27.8 mg, 68.5 μmol) were dissolved in CH_2Cl_2 (2.0 mL), and the mixture was stirred at room temperature for 10 min. H_2 was introduced to the resulting solution in a Schlenk tube. After stirring at room temperature for 30 min, the resulting mixture was concentrated to dryness. The residue was dissolved in CH_2Cl_2 (20 mL). To this solution was added a solution of **9a** (0.110 g, 85.6 μmol) in CH_2Cl_2 (22 mL). The mixture was stirred at 40 $^\circ\text{C}$ for 16 h. The resulting mixture was concentrated and purified by silica gel PTLC (eluent: *n*-hexane/ CH_2Cl_2 = 1:1) to give (*M,M*)-(–)-**10** (47.0 mg, 36.7 μmol , 43% yield, er = 98:2) and (*P,M*)-**10** (47.0 mg, 36.7 μmol , 43% yield).

Data for (*M,M*)-(–)-**10**: Colorless solid; mp 212.7 $^\circ\text{C}$ (decomposition); $[\alpha]_{\text{D}}^{25} -775^\circ$ [*c* 2.2 $\mu\text{g}/\text{cm}^3$, CH_2Cl_2 , er = 98:2]; ^1H NMR (400 MHz, CDCl_3) δ 7.22 (s, 4H), 6.80 (s, 2H), 6.19 (s, 2H), 5.43 (d, *J* = 13.9 Hz, 4H), 4.92 (d, *J* = 13.9 Hz, 4H), 4.68 (d, *J* = 13.3 Hz, 4H), 4.37 (d, *J* = 13.4 Hz, 4H), 3.08–2.92 (m, 4H), 2.91–2.77 (m, 4H), 2.75–2.53 (m, 8H), 1.62–1.37 (m, 32H), 1.00 (t, *J* = 6.9 Hz, 12H), 0.90 (t, *J* = 7.3 Hz, 12H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 156.9, 153.8, 135.8, 135.6, 132.7, 132.5, 132.0, 127.5, 126.5, 126.3, 118.5, 117.7, 104.8, 70.4, 68.1, 34.1, 33.3, 28.8, 28.3, 23.2, 23.0, 13.9, 13.8; HRMS (ESI) calcd for $\text{C}_{88}\text{H}_{96}\text{O}_8\text{Na}$ [*M*+*Na*] $^+$ 1303.6997, found 1303.7080; CHIRALPAK IG-3, *n*-hexane/ CH_2Cl_2 = 60:40, 1.0 mL min^{-1} , retention times: 5.64 min (major isomer) and 3.84 min (minor isomer).

Data for (*P,M*)-**11**: Colorless solid; mp 263.8 $^\circ\text{C}$ (decomposition); ^1H NMR (400 MHz, CDCl_3) δ 7.17 (s, 4H), 6.93 (s, 2H), 6.09 (s, 2H), 5.36 (d, *J* = 14.5 Hz, 4H), 5.23 (d, *J* = 12.7 Hz, 4H), 4.79 (d, *J* = 14.5 Hz, 4H), 4.53 (d, *J* = 12.8 Hz, 4H), 2.93–2.78 (m, 4H), 2.76–2.63 (m, 4H), 2.62–2.50 (m, 4H), 2.50–2.34 (m, 4H), 1.50–1.28 (m, 32H), 0.96 (t, *J* = 6.6 Hz, 12H), 0.87 (t, *J* = 7.2 Hz, 12H);

^{13}C NMR (CDCl_3 , 100 MHz) δ 155.5, 153.2, 135.6, 135.5, 133.7, 132.1, 131.4, 130.1, 127.8, 126.1, 123.1, 115.5, 111.1, 69.7, 69.1, 34.0, 32.5, 28.4, 28.1, 23.3, 22.9, 13.9, 13.8; HRMS (ESI) calcd for $\text{C}_{88}\text{H}_{96}\text{O}_8\text{Na}$ $[\text{M}+\text{Na}]^+$ 1303.6997, found 1303.7118.

1.8. Synthesis of triply twisted belts (M,M,M) -(-)-**12** and (P,M,M) -(-)-**13**

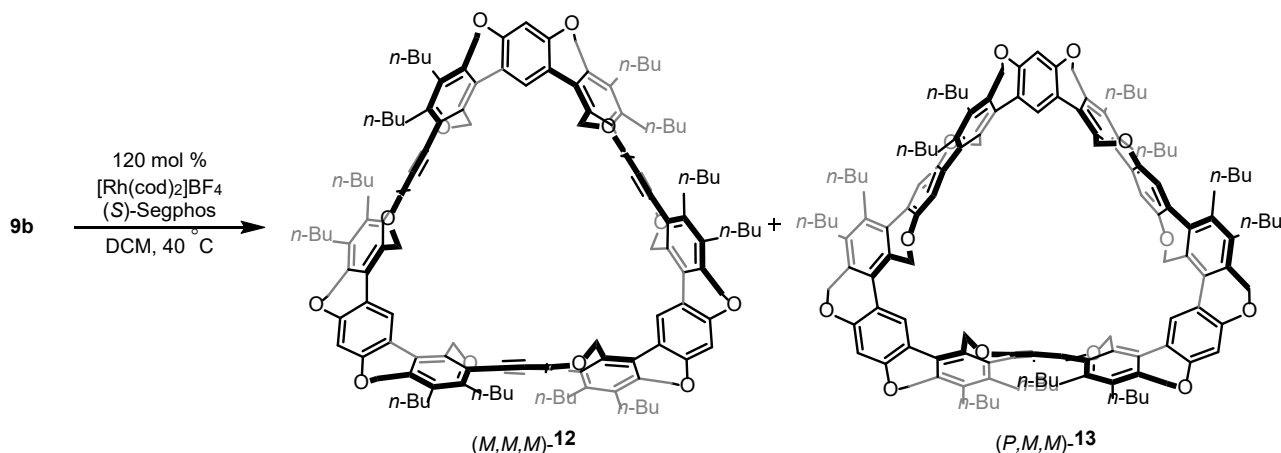
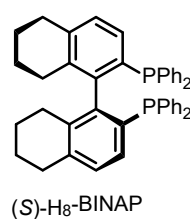
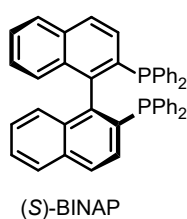
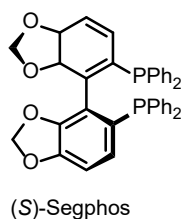


Table S2. Screening of ligands for rhodium-catalyzed [2+2+2] cycloaddition of **9b**.

Ligand	yield (%) / er of (M,M,M) -(-)- 12	yield (%) / er of (P,M,M) -(-)- 13
$(S)\text{-Segphos}$	21 / 93:7	25 / 87:13
$(S)\text{-BINAP}$	18 / 88:12	14 / 76:24
$(S)\text{-H}_8\text{-BINAP}$	25 / 82:18	23 / 33:67



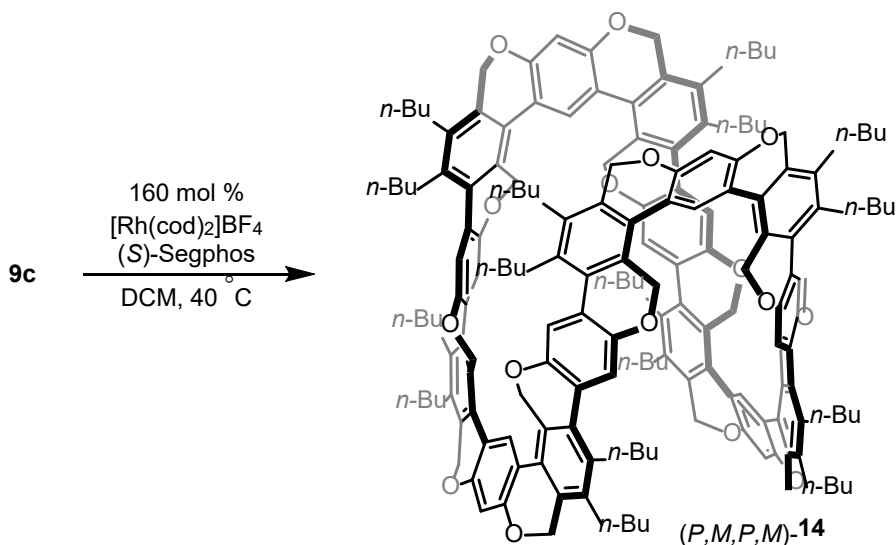
$(S)\text{-Segphos}$ (17.0 mg, 27.9 μmol) and $[\text{Rh}(\text{cod})_2]\text{BF}_4$ (11.3 mg, 27.9 μmol) were dissolved in CH_2Cl_2 (2.0 mL), and the mixture was stirred at room temperature for 10 min. H_2 was introduced to the resulting solution in a Schlenk tube. After stirring at room temperature for 30 min, the resulting mixture was concentrated to dryness. The residue was dissolved in CH_2Cl_2 (5.0 mL). To this solution was added a solution of **9b** (44.7 mg, 23.2 μmol) in CH_2Cl_2 (5.6 mL). The mixture was stirred at 40°C for 16 h. The resulting mixture was concentrated and purified by silica gel PTLC (eluent: $n\text{-hexane}/\text{CH}_2\text{Cl}_2 = 9:7$) to give (M,M,M) -(-)-**12** (8.95 mg, 4.66 μmol , 21% yield, er = 93:7) and (P,M,M) -(-)-**13** (11.1 mg, 5.77 μmol , 25% yield, er = 87:13).

Data for (M,M,M) -(-)-**12**: Colorless solid; mp 242.8°C (decomposition); $[\alpha]_D^{25} -664^\circ$ [c 3.0 $\mu\text{g}/\text{cm}^3$, CH_2Cl_2 , er = 93:7]; ^1H NMR (400 MHz, CDCl_3) δ 7.23 (s, 6H), 6.83 (s, 3H), 6.60 (s, 3H), 5.42 (d, $J = 13.3$ Hz, 6H), 5.15 (d, $J = 12.7$ Hz, 6H), 4.84 (d, $J = 13.3$ Hz, 6H), 4.66 (d, $J = 12.7$ Hz, 6H), 2.87–2.62 (m, 24H), 1.73–1.60 (m, 12H), 1.54–1.38 (m, 36H), 1.00 (t, $J = 6.9$ Hz, 18H), 0.94 (t, $J = 7.3$ Hz, 18H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 158.2, 151.4, 136.7, 136.6, 132.8, 130.2, 129.4, 127.5, 126.2, 124.9, 117.2, 114.8, 104.4, 67.9, 67.6, 34.1, 33.4, 29.4, 28.5, 23.3, 22.7, 13.9, 13.8; HRMS (ESI) calcd for $\text{C}_{132}\text{H}_{144}\text{O}_{12}\text{Na}$ $[\text{M}+\text{Na}]^+$ 1944.0550, found 1944.0412; CHIRALPAK IG-3, $n\text{-hexane}/\text{CH}_2\text{Cl}_2 = 70:30$, 1.0 mL min^{-1} , retention times: 5.41 min (major isomer) and 4.21 min

(minor isomer).

Data for (*P,M,M*)-(-)-**13**: Colorless solid; mp 211.9 °C (decomposition); $[\alpha]^{25}_{\text{D}} -34^{\circ}$ [*c* 3.7 $\mu\text{g}/\text{cm}^3$, CH_2Cl_2 , *er* = 87:13]; ^1H NMR (400 MHz, CDCl_3) δ 7.34 (s, 2H), 7.24 (s, 2H), 7.08 (s, 2H), 6.99 (s, 2H), 6.82 (s, 2H), 6.53 (s, 2H), 6.46 (s, 2H), 5.67 (d, *J* = 11.7 Hz, 2H), 5.56 (d, *J* = 12.3 Hz, 2H), 5.43 (d, *J* = 13.2 Hz, 2H), 5.40 (d, *J* = 14.0 Hz, 2H), 5.30 (d, *J* = 13.6 Hz, 2H), 4.93 (d, *J* = 12.1 Hz, 2H), 4.90 (d, *J* = 11.5 Hz, 2H), 4.88 (d, *J* = 12.6 Hz, 2H), 4.88 (d, *J* = 12.3 Hz, 2H), 4.88 (d, *J* = 12.6 Hz, 2H), 4.73 (d, *J* = 13.7 Hz, 2H), 4.38 (d, *J* = 12.2 Hz, 2H), 2.87–2.59 (m, *J* = 9.9 Hz, 20H), 2.54–2.40 (m, 4H), 1.66–1.40 (m, 40H), 1.40–1.23 (m, 8H), 1.03–0.93 (m, 30H), 0.88–0.82 (t, *J* = 7.3 Hz, 6H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 158.6, 157.2, 156.1, 152.3, 151.6, 150.9, 136.9, 136.6, 136.18, 136.17, 136.0, 135.9, 134.6, 133.9, 133.3, 130.8, 130.39, 130.38, 130.0, 129.6, 128.3, 127.5, 127.2, 126.9, 126.8, 126.7, 125.5, 124.7, 124.6, 120.4, 120.1, 117.5, 114.0, 113.8, 113.5, 109.1, 103.3, 69.0, 68.5, 68.3, 68.2, 68.1, 66.8, 34.58, 34.56, 34.1, 33.5, 32.7, 32.6, 29.2, 28.93, 28.86, 28.5, 28.4, 28.3, 23.33, 23.31, 23.31, 22.9, 22.8, 22.6, 13.89, 13.87, 13.85, 13.84, 13.79, 13.78; HRMS (ESI) calcd for $\text{C}_{132}\text{H}_{144}\text{O}_{12}\text{Na}$ $[\text{M}+\text{Na}]^+$ 1944.0550, found 1944.0397; CHIRALPAK IF-3, *n*-hexane/ CH_2Cl_2 = 60:40, 1.0 mL min^{-1} , retention times: 4.27 min (major isomer) and 5.52 min (minor isomer).

1.9. Synthesis of quadruply twisted belt (*P,M,P,M*)-14



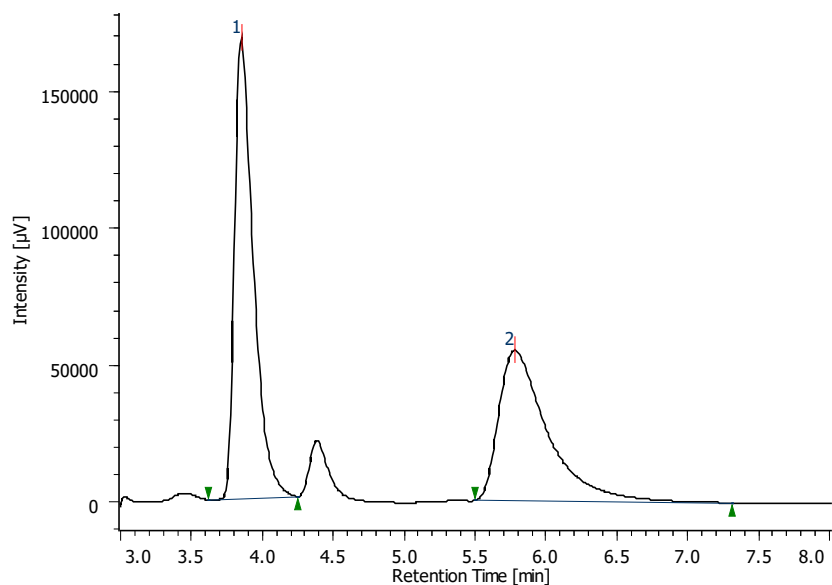
(*S*)-Segphos (4.59 mg, 7.52 μmol) and $[\text{Rh}(\text{cod})_2]\text{BF}_4$ (3.05 mg, 7.52 μmol) were dissolved in CH_2Cl_2 (2.0 mL), and the mixture was stirred at room temperature for 10 min. H_2 was introduced to the resulting solution in a Schlenk tube. After stirring at room temperature for 30 min, the resulting mixture was concentrated to dryness. The residue was dissolved in CH_2Cl_2 (2.0 mL). To this solution was added a solution of **9c** (12.0 mg, 4.70 μmol) in CH_2Cl_2 (2.7 mL). The mixture was stirred at 40 $^\circ\text{C}$ for 16 h. The resulting mixture was concentrated and purified by silica gel PTLC (eluent: *n*-hexane/ CH_2Cl_2 = 9:7) to give (*P,M,P,M*)-**14** (5.05 mg, 1.97 μmol , 42% yield).

Colorless solid; mp >300 $^\circ\text{C}$; ^1H NMR (400 MHz, CDCl_3) δ 7.39 (s, 8H), 6.90 (s, 4H), 6.69 (s, 4H), 5.77 (d, J = 12.6 Hz, 8H), 5.40 (d, J = 13.5 Hz, 8H), 5.00 (d, J = 12.8 Hz, 8H), 4.73 (d, J = 13.1 Hz, 8H), 2.97–2.82 (m, 16H), 2.77–2.69 (m, 8H), 2.66–2.57 (m, 8H), 1.74–1.65 (m, 16H), 1.53–1.41 (m, 48H), 1.00 (t, J = 6.9 Hz, 24H), 0.99 (t, J = 6.9 Hz, 24H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 157.2, 151.0, 137.1, 137.0, 133.0, 130.0, 129.8, 127.8, 126.1, 125.0, 118.0, 115.7, 107.0, 68.3, 67.5, 33.9, 33.2, 29.9, 28.6, 23.3, 22.8, 13.84, 13.80; HRMS (ESI) calcd for $\text{C}_{176}\text{H}_{192}\text{O}_{16}\text{Na}$ $[\text{M}+\text{Na}]^+$ 2584.4103, found 2584.3644, and $\text{C}_{176}\text{H}_{192}\text{O}_{16}\text{Na}_2$ $[\text{M}+2\text{Na}]^{2+}$ 1303.6997, found 1303.7126.

2. Chiral HPLC charts

(±)-**10**

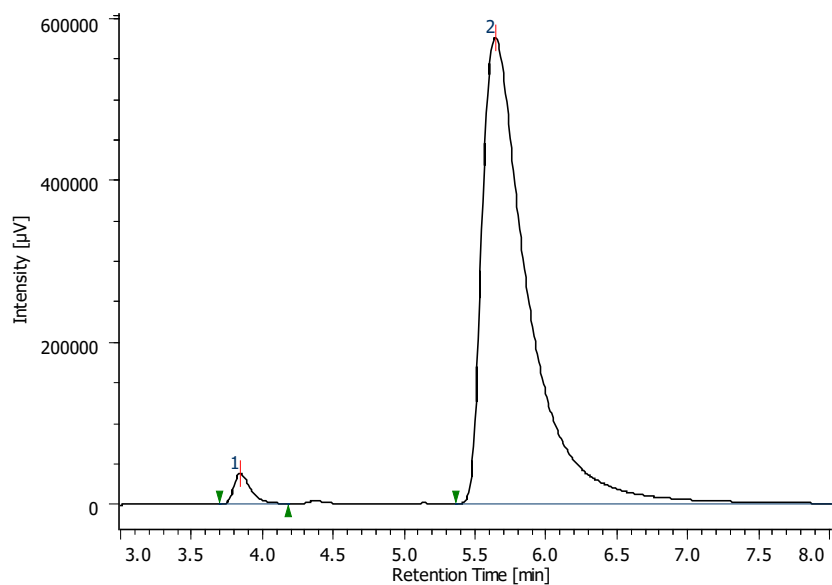
CHIRALPAK IG-3, *n*-hexane/CH₂Cl₂ = 60:40, 1.0 mL min⁻¹



Peak No.	Retention time (min)	Area (%)
1	3.850	53.851
2	5.775	46.149

(*M,M*)-(-)-**10** (er = 98:2)

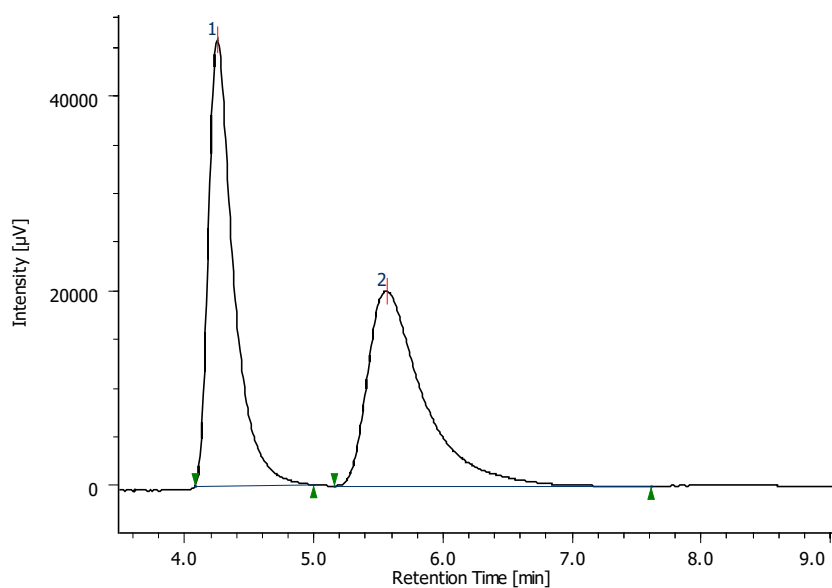
CHIRALPAK IG-3, *n*-hexane/CH₂Cl₂ = 60:40, 1.0 mL min⁻¹



Peak No.	Retention time (min)	Area (%)
1	3.842	2.362
2	5.642	97.638

(±)-**12**

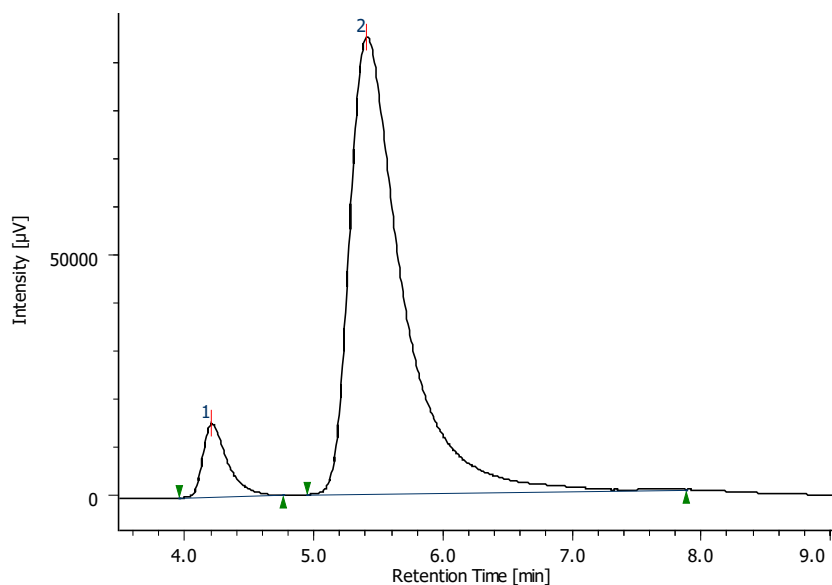
CHIRALPAK IG-3, *n*-hexane/CH₂Cl₂ = 70:30, 1.0 mL min⁻¹



Peak No.	Retention time (min)	Area (%)
1	4.250	50.928
2	5.558	49.072

(*M,M,M*)-(-)-**12** (er = 93:7)

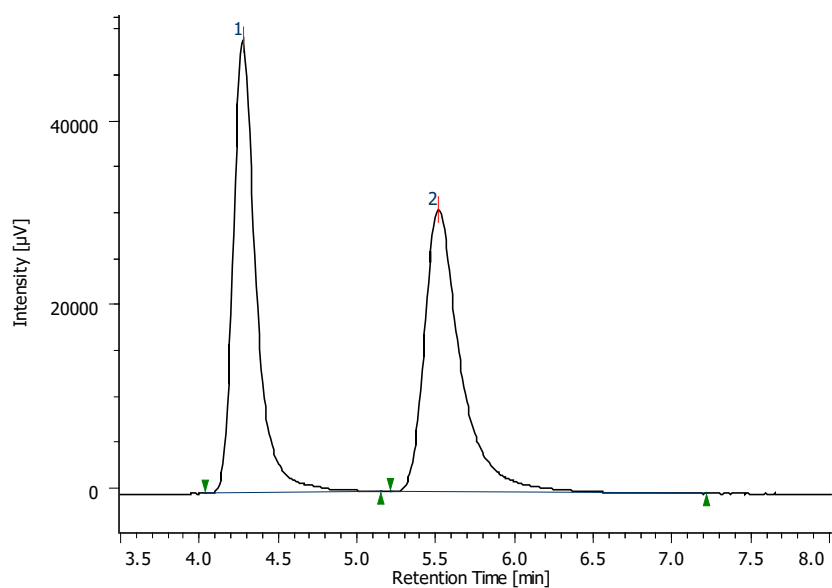
CHIRALPAK IG-3, *n*-hexane/CH₂Cl₂ = 70:30, 1.0 mL min⁻¹



Peak No.	Retention time (min)	Area (%)
1	4.208	6.915
2	5.408	93.085

(±)-**13**

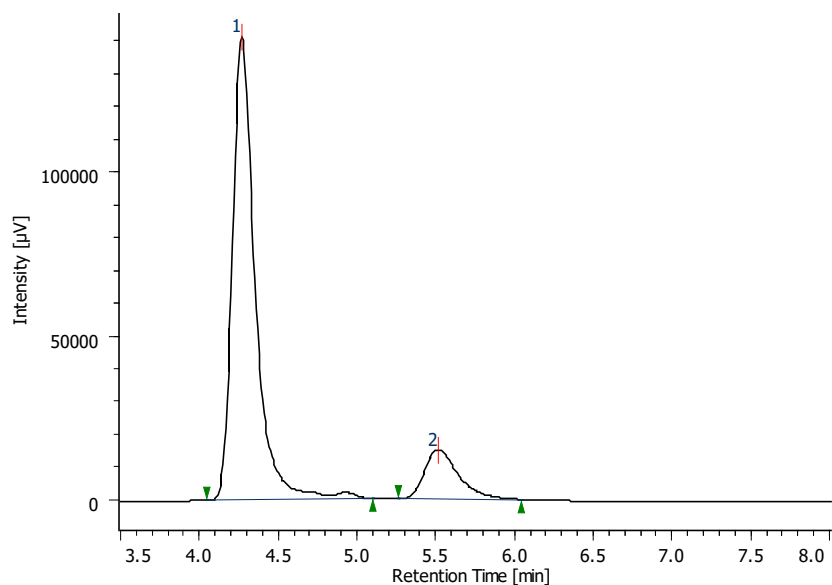
CHIRALPAK IF-3, *n*-hexane/CH₂Cl₂ = 60:40, 1.0 mL min⁻¹



Peak No.	Retention time (min)	Area (%)
1	4.275	50.481
2	5.517	49.519

(*P,M,M*)-(-)-**13** (er = 87:13)

CHIRALPAK IF-3, *n*-hexane/CH₂Cl₂ = 60:40, 1.0 mL min⁻¹



Peak No.	Retention time (min)	Area (%)
1	4.267	86.518
2	5.517	13.482

3. X-Ray crystallographic analysis

Details of the crystal data and the summaries of the intensity data collection parameters for (±)-**10**, (±)-**12**, and **14** are listed in Tables S3–S5.

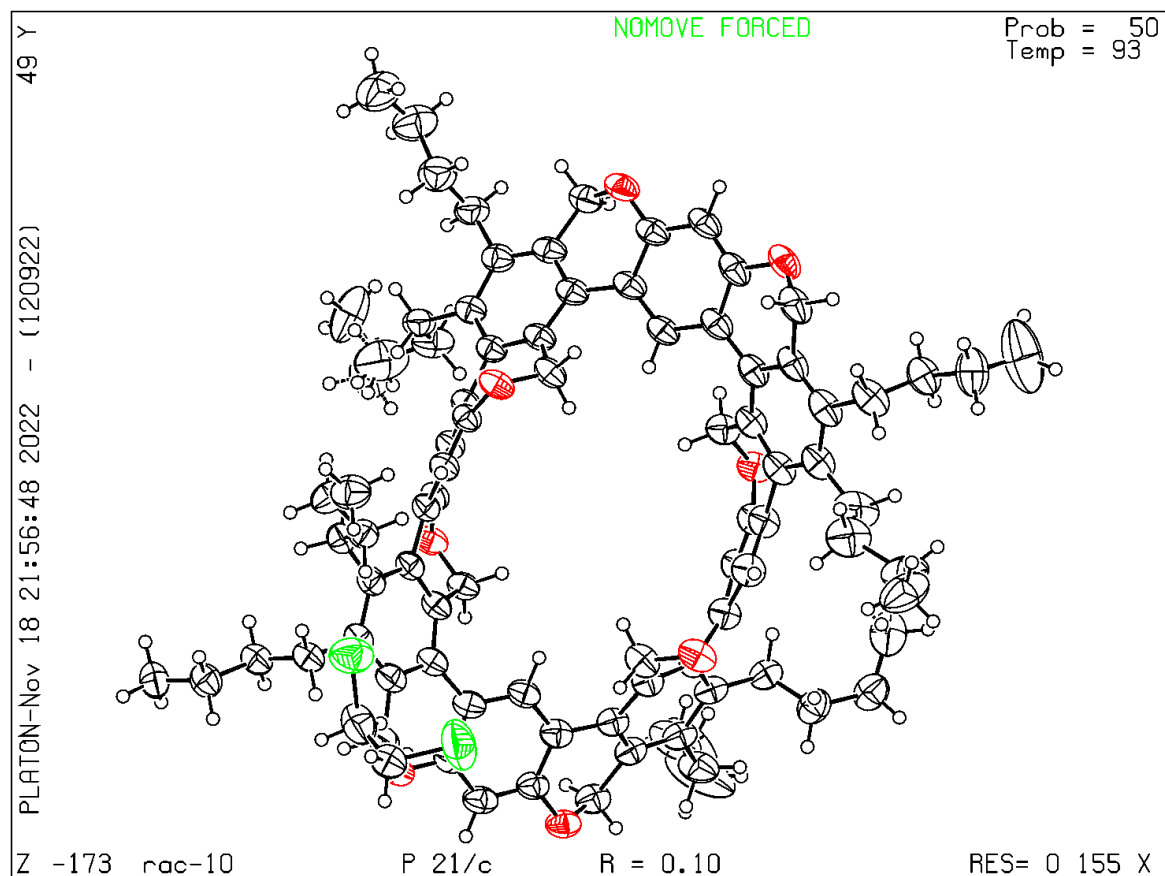
A colorless prism-shaped single crystal of **10**, $0.26 \times 0.10 \times 0.04$ mm³, was selected for diffraction measurements. The diffraction data were collected using a RIGAKU XtaLAB Synergy-S diffractometer equipped with a HyPix6000HE hybrid pixel array detector with CuK α radiation by an oscillation method about the ω -axis at 93 K. X-rays were monochromated and focused by a confocal mirror. Bragg spots were integrated, scaled, and averaged up to $\sin\theta/\lambda = 0.633$ Å^{−1} by the program CrysAlisPro⁵. Lorentz, polarization, and numerical absorption corrections were applied during the scaling processes. The number of measured and independent reflections, completeness, and R_{int} was 62500, 15131, 0.959, and 0.0699, respectively.

The initial structure of **10** was solved by a dual-space method using the program SHELXT-2018/2⁶, and refined by a full matrix least-squares method using the program SHELXL-2019/2⁷. All hydrogen atoms were put at geometrically calculated positions and refined as riding models. One of the eight butyl groups was disordered. The terminal methyl group in the disordered butyl group was separated into two positions and refined to be the same C–C distances with the SADI command. The temperature factor of the methyl group was constrained with the EADP and the RIGU commands being the same as each other. The occupancy factors of the disordered moiety were constrained to the sum of the corresponding parts to be 1. The total number of constraints was 7. The final R values against 10469 unique reflections ($\theta_{\text{max}} = 77.51^\circ$) with $I > 2\sigma(I)$ are 0.1043, 0.3026, and 1.028 for the $R(F)$, $wR(F^2)$, and S , respectively. Crystallographic data have been deposited with the Cambridge Crystallographic Data Centre: Deposition code CCDC 2220749.

Table S3. Crystallographic data and structure refinement details for (±)-**10** (CCDC 2220749).

Empirical formula	C ₉₀ H ₁₀₀ Cl ₂ O ₈
Formula weight	1380.59
Temperature/K	93
Crystal system	monoclinic
Space group	$P2_1/c$
$a/\text{\AA}$	27.6406(5)
$b/\text{\AA}$	16.9566(3)
$c/\text{\AA}$	16.2602(2)
$\beta/^\circ$	103.4185(17)
$V/\text{\AA}^3$	7412.9(2)
Z	4
$\rho_{\text{calc}}/\text{g cm}^{-3}$	1.237
μ/mm^{-1}	1.245
$F(000)$	2952.0
Crystal size/mm ³	$0.263 \times 0.100 \times 0.042$
Radiation	CuK α ($\lambda = 1.54184$ Å)
2θ range for data collection/ $^\circ$	6.162 to 155.018
Index ranges	$-34 \leq h \leq 34$, $-18 \leq k \leq 20$, $-20 \leq l \leq 17$
Reflections collected	62500

Independent reflections	15131 [$R_{\text{int}} = 0.0699$, $R_{\text{sigma}} = 0.0523$]
Data/restraints/parameters	15131/7/920
Goodness-of-fit on F^2	1.028
Final R indexes [$I \geq 2\sigma(I)$]	$R(F) = 0.1043$, $wR(F^2) = 0.3026$
Final R indexes [all data]	$R(F) = 0.1332$, $wR(F^2) = 0.3324$
Largest diff. peak/hole / $\text{e \AA}^{-3}$	0.991/-1.075



A colorless prism-shaped single crystal of **12**, $0.13 \times 0.06 \times 0.03 \text{ mm}^3$, was selected for diffraction measurements. The diffraction data were collected using a RIGAKU AFC-11 diffractometer equipped with a HyPix6000HE hybrid pixel array detector with MoK α radiation by an oscillation method about the ω -axis at 89.93(16) K. X-rays were monochromated and focused by a confocal mirror. Bragg spots were integrated, scaled, and averaged up to $\sin\theta/\lambda = 0.602 \text{ \AA}^{-1}$ by the program CrysAlisPro⁵. Lorentz, polarization, and multi-scan absorption corrections were applied during the scaling processes. The number of measured and independent reflections, completeness, and R_{int} was 309620, 23699, 1.000, and 0.0919, respectively.

The initial structure of **12** was solved by a dual-space method using the program SHELXT-2018/2⁶, and refined by a full matrix least-squares method using the program SHELXL-2018/3⁷. All hydrogen atoms were put at geometrically calculated positions and refined as riding models. Two of the twelve butyl groups and one of the four solvent molecules (methoxycyclopentane) were disordered although the main part of **12** was ordered. Each disordered moiety was separated into two parts and refined to be the same distances with the SADI command. The temperature factors of the disordered moieties were constrained with the EADP command for butyl groups and restrained with the SIMU command for the solvent being the same as each other. The occupancy factors of the disordered moieties were constrained to the sum of the corresponding parts to be unity. The total number of constraints was 158. The final R values against 14437 unique reflections ($\theta_{\text{max}} = 25.35^\circ$) with $I > 2\sigma(I)$ are 0.0850, 0.2153, and 1.040 for the $R(F)$, $wR(F^2)$, and S , respectively. Crystallographic data have been deposited with the Cambridge Crystallographic Data Centre: Deposition code CCDC 2220760.

Table S4. Crystallographic data and structure refinement details for ($\pm$)-**12** (CCDC 2220760).

Empirical formula	C ₁₅₆ H ₁₉₂ O ₁₆
Formula weight	2323.08
Temperature/K	89.93(16)
Crystal system	orthorhombic
Space group	<i>Pbca</i>
$a/\text{\AA}$	37.7343(5)
$b/\text{\AA}$	12.0991(3)
$c/\text{\AA}$	56.6781(8)
$V/\text{\AA}^3$	25876.4(8)
Z	8
$\rho_{\text{calc}}/\text{g cm}^{-3}$	1.193
μ/mm^{-1}	0.075
$F(000)$	10048.0
Crystal size/ mm^3	$0.125 \times 0.061 \times 0.026$
Radiation	MoK α ($\lambda = 0.71073 \text{ \AA}$)
2θ range for data collection/ $^\circ$	3.07 to 50.7
Index ranges	$-45 \leq h \leq 45$, $-14 \leq k \leq 14$, $-67 \leq l \leq 68$
Reflections collected	309620
Independent reflections	23699 [$R_{\text{int}} = 0.0919$, $R_{\text{sigma}} = 0.0537$]

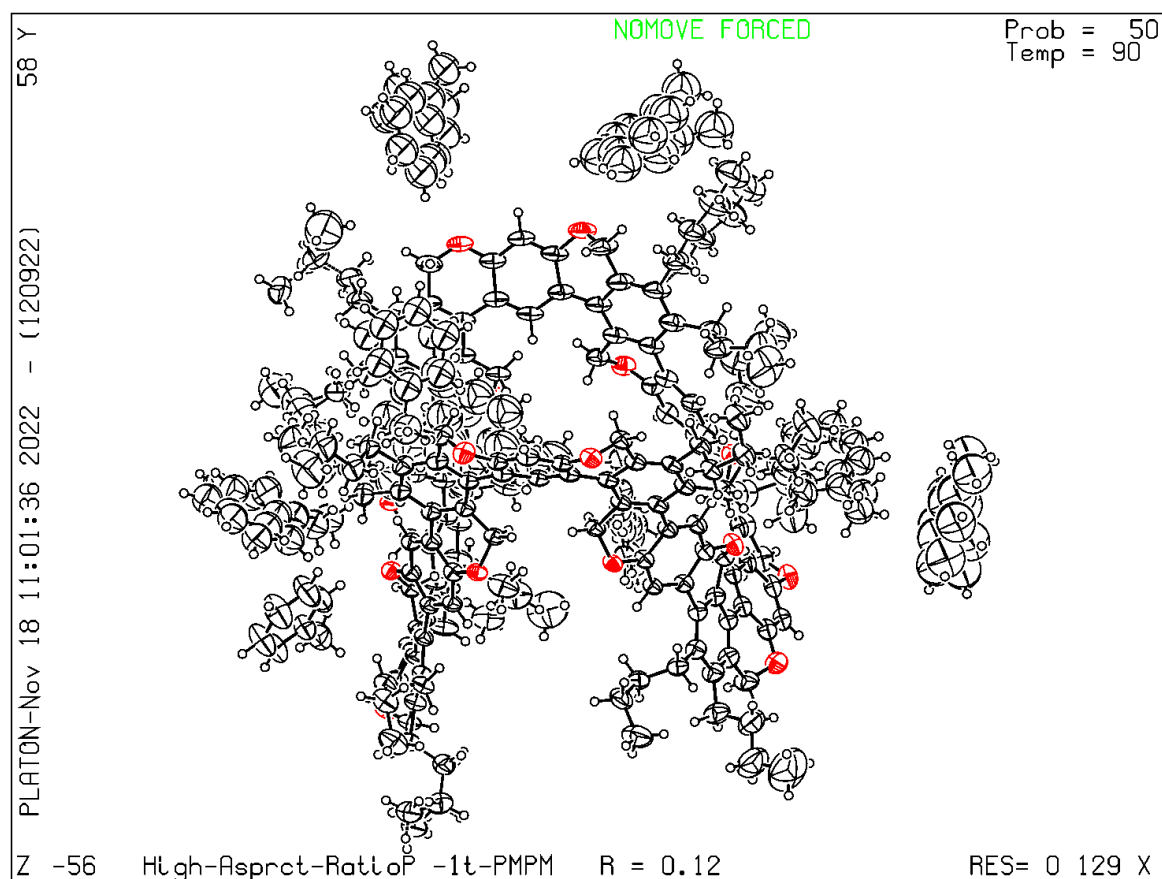
A colorless block-shaped single crystal of **14**, $0.56 \times 0.38 \times 0.31 \text{ mm}^3$, was selected for diffraction measurements. The diffraction data were collected using a RIGAKU AFC-11 diffractometer equipped with a HyPix6000HE hybrid pixel array detector with MoK α radiation by an oscillation method about the ω -axis at 89.9(4) K. X-rays were monochromated and focused by a confocal mirror. Bragg spots were integrated, scaled, and averaged up to $\sin\theta/\lambda = 0.595 \text{ \AA}^{-1}$ by the program CrysAlisPro⁵. Lorentz, polarization, and multi-scan absorption corrections were applied during the scaling processes. The number of measured and independent reflections, completeness, and R_{int} was 331951, 48000, 0.999, and 0.0576, respectively.

The initial structure of **14** was solved by a dual-space method using the program SHELXT-2018/2⁶, and refined by a full matrix least-squares method using the program SHELXL-2018/3⁷. All hydrogen atoms were put at geometrically calculated positions and refined as riding models. Seven of the sixteen butyl groups and eight of the nine solvent molecules (toluene) were disordered although the main part of **14** was ordered. The disordered butyl groups were separated into two parts and refined to be the C–C bond distance 1.53 Å with the DFIX command and to be the same bond angles with the SADI command. The temperature factors of the disordered butyl groups were restrained with the SIMU and RIGU commands and reduced anisotropy with the ISOR command. All the solvent toluene molecules were treated as a rigid body. The temperature factors of the carbon atoms in the disordered toluene molecules were restrained being the same with the SIMU and RIGU commands and reduced anisotropy with the ISOR command. The occupancy factors of the disordered moieties were constrained to the sum of the corresponding parts to be unity. After the refinements, the contribution of non-periodically aligned solvent molecules to the intensities of reflections was removed with the SQUEEZE program⁸. The solvent-accessible voids were surveyed with a void probe radius of 1.20 Å. The contribution of 1106 electrons/unit cell, which corresponds to 12 toluene molecules was removed from the reflection data. The refinements were performed using the reflection data after treatment of the SQUEEZE program with the same procedure described above being the structure converged. The total number of constraints was 3104. The final R values against 35064 unique reflections ($\theta_{\text{max}} = 25.03^\circ$) with $I > 2\sigma(I)$ are 0.1248, 0.2515, and 0.925 for the $R(F)$, $wR(F^2)$, and S , respectively. Crystallographic data have been deposited with the Cambridge Crystallographic Data Centre: Deposition code CCDC 2220761.

Table S5. Crystallographic data and structure refinement details for **14** (CCDC 2220761).

Empirical formula	C ₂₃₉ H ₂₆₄ O ₁₆
Formula weight	3392.49
Temperature/K	89.9(4)
Crystal system	triclinic
Space group	$P\bar{1}$
$a/\text{\AA}$	21.8090(4)
$b/\text{\AA}$	25.3669(4)
$c/\text{\AA}$	28.0379(4)
$\alpha/^\circ$	66.1939(15)
$\beta/^\circ$	75.0099(14)
$\gamma/^\circ$	77.4210(14)
$V/\text{\AA}^3$	13595.4(4)
Z	2

$\rho_{\text{calc}}/\text{g cm}^{-3}$	0.829
μ/mm^{-1}	0.051
$F(000)$	3652.0
Crystal size/ mm^3	$0.56 \times 0.38 \times 0.31$
Radiation	MoK α ($\lambda = 0.71073 \text{ \AA}$)
2θ range for data collection/ $^\circ$	3.062 to 50.054
Index ranges	$-25 \leq h \leq 25, -30 \leq k \leq 30, -33 \leq l \leq 33$
Reflections collected	331951
Independent reflections	48000 [$R_{\text{int}} = 0.0576, R_{\text{sigma}} = 0.0302$]
Data/restraints/parameters	48000/3104/2765
Goodness-of-fit on F^2	0.925
Final R indexes [$I \geq 2\sigma(I)$]	$R(F) = 0.1248, wR(F^2) = 0.2515$
Final R indexes [all data]	$R(F) = 0.1462, wR(F^2) = 0.2606$
Largest diff. peak/hole / $\text{e \AA}^{-3}$	1.951/−0.898



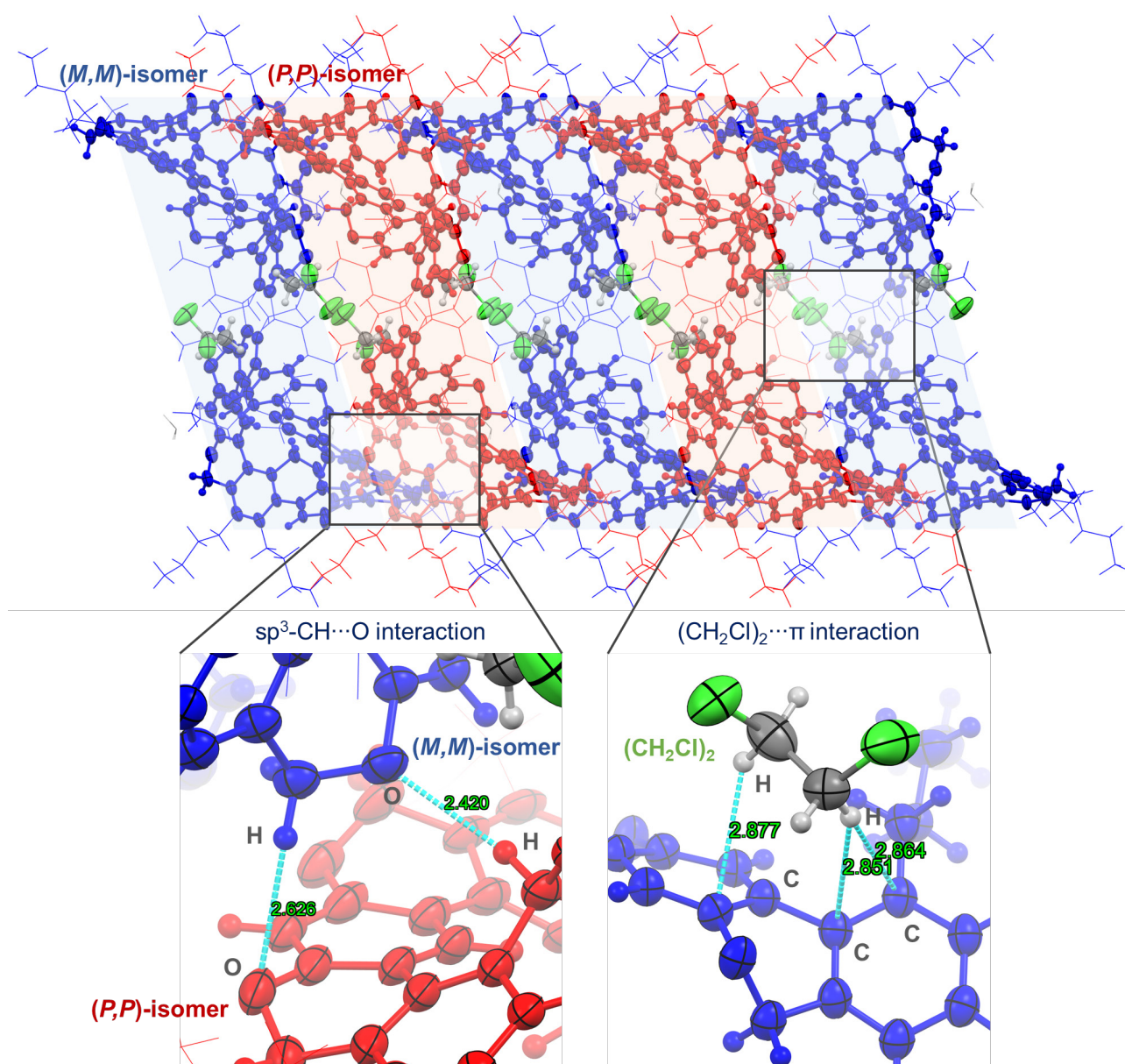


Figure S1. Detailed packing structure of (±)-10.

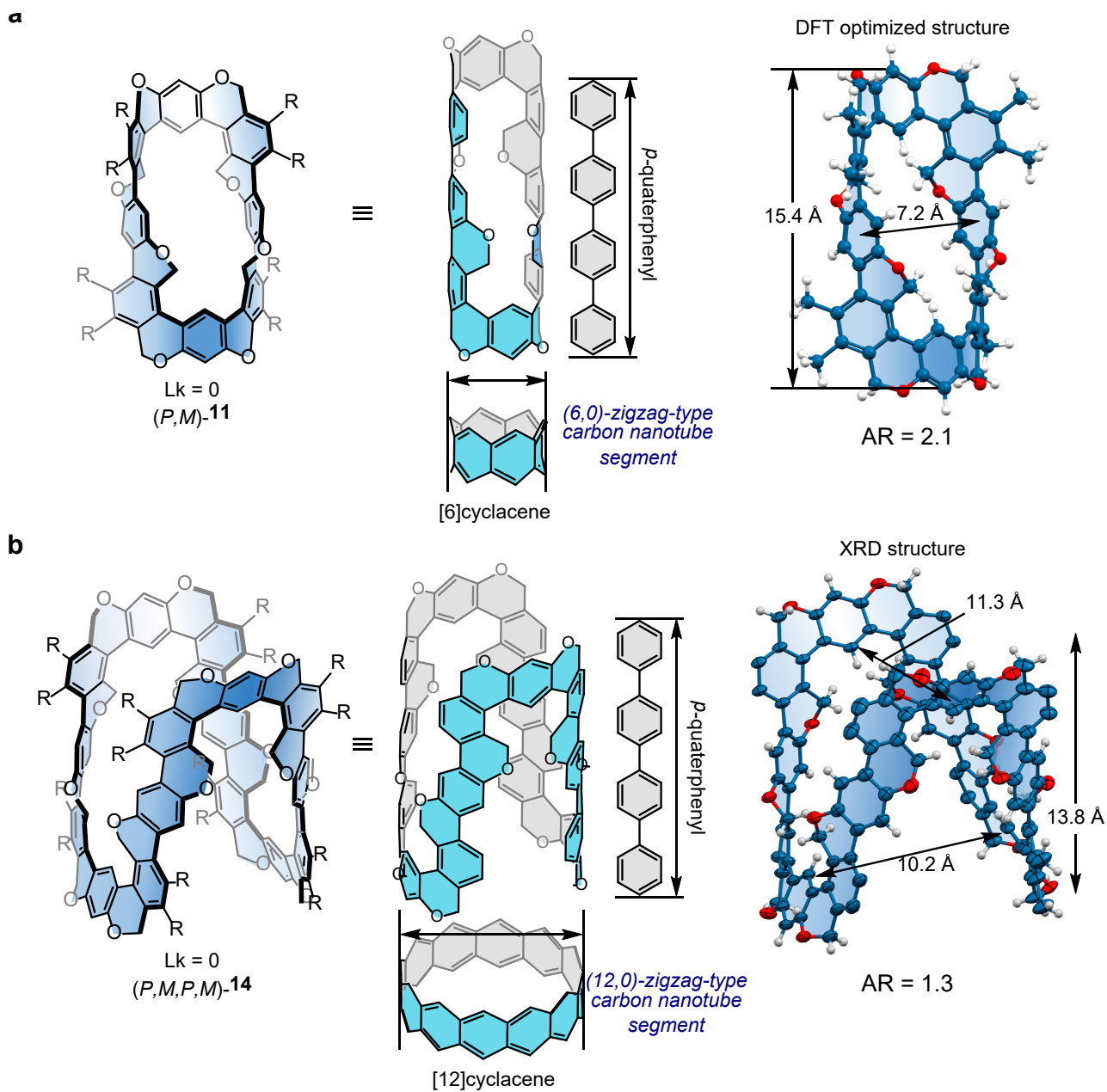


Figure S2. The aspect ratio⁹ (AR = height/diameter) of longitudinally extended belts with Lk = 0. AR of 11 (**a**) and 14 (**b**) are based on the DFT optimized structure and the XRD structure, respectively.

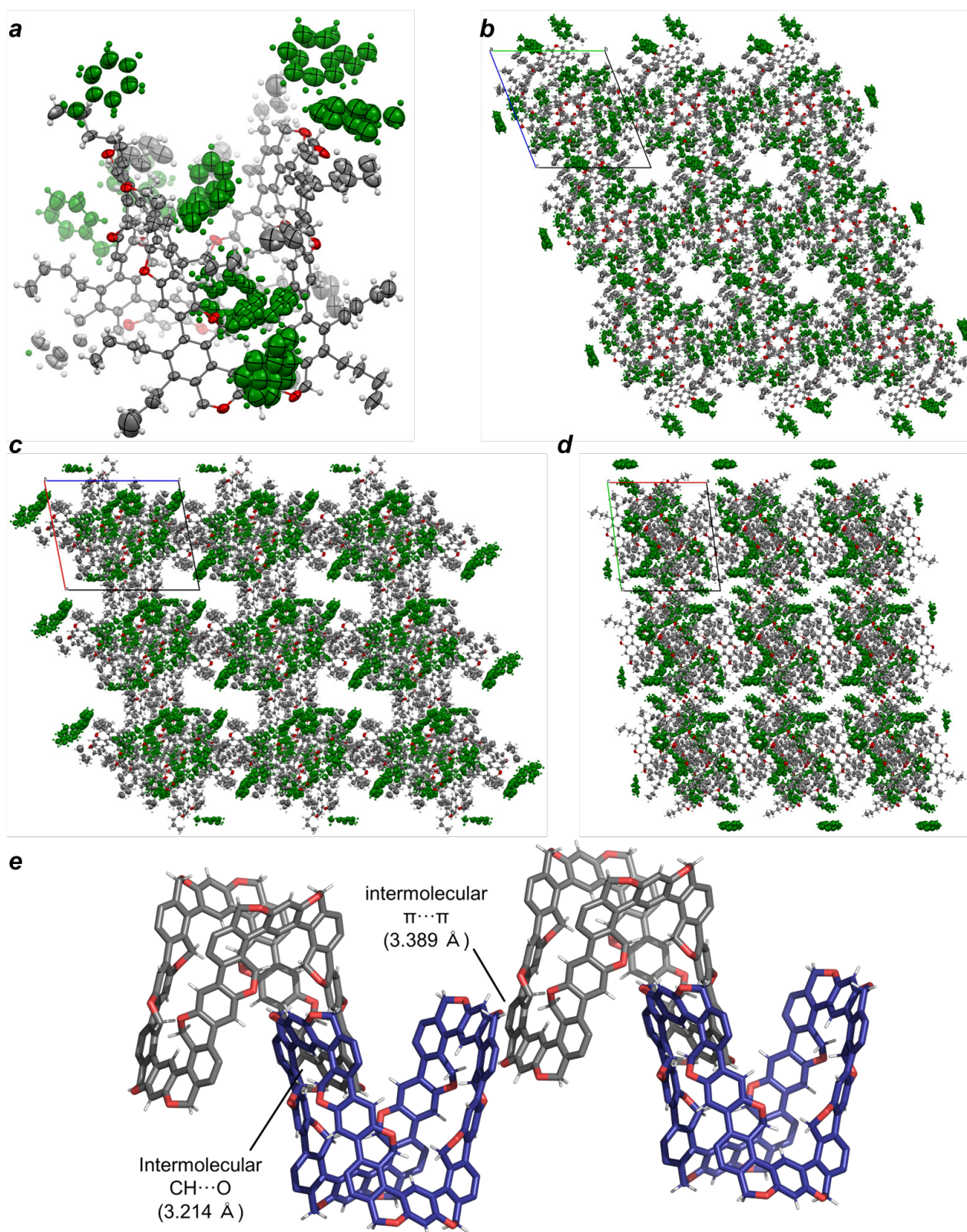


Figure S3. X-ray crystal structures of **14**. **a**, The unimolecular structure of **14** (gray) with some disordered solvent molecules (green) at 50% probability. **b-d**, Packing structures viewed from *a*-axis (**b**), *b*-axis (**c**), and *c*-axis (**d**). **e**, Intermolecular CH $\cdots$ O and $\pi \cdots \pi$ interactions.

4. Reaction mechanism of stereoselective [2+2+2] cycloaddition

A plausible reaction pathway from **9a** to (*M,M*)-**10** and (*P,M*)-**11** is shown in Fig. S4.

The first [2+2+2] cycloaddition of **9a** gives the intermediate **IM1** with single planar chirality, and this process determines the enantioselectivity of the products. The second cycloaddition provides three intermediates **IM2a-IM2c** from the corresponding three reaction sites **a-c** of **IM1**, and all of them have (*M,M*)- and (*P,M*)-rotamer pairs; (*M,M*)-**IM2a** /(*P,M*)-**IM2a** with a twist chirality, (*M,M*)-**IM2b** /(*P,M*)-**IM2b** with two planar chiralities, and (*M,M*)-**IM2c** /(*P,M*)-**IM2c** with a twist chirality. The diastereoselectivity is determined in this step because steric hindrance prevents the interconversion of rotamer pairs.

Finally, cycloadditions at the two remaining reaction sites give (*M,M*)-**10** and (*P,M*)-**11**. The very high enantioselectivity of (*M,M*)-**10** (er = 98:2) accounts for the perfect control of the planar chirality of **IM1** by the axial chiral ligand. Considering that such chirality-control is also operative for the generation of **IM2** from **IM1**, the formation of enantiomeric pairs in **IM2** [e.g., (*M,M*)-**IM2a** and (*P,M*)-**IM2a**] should be ruled out. Hence, it is reasonable to suppose that (*M,M*)-**10** and (*P,M*)-**11** are not derived from any rotamer pairs of **IM2**, but are generated from the other **IM2** pairs [e.g., (*M,M*)-**IM2a** and (*P,M*)-**IM2b**].

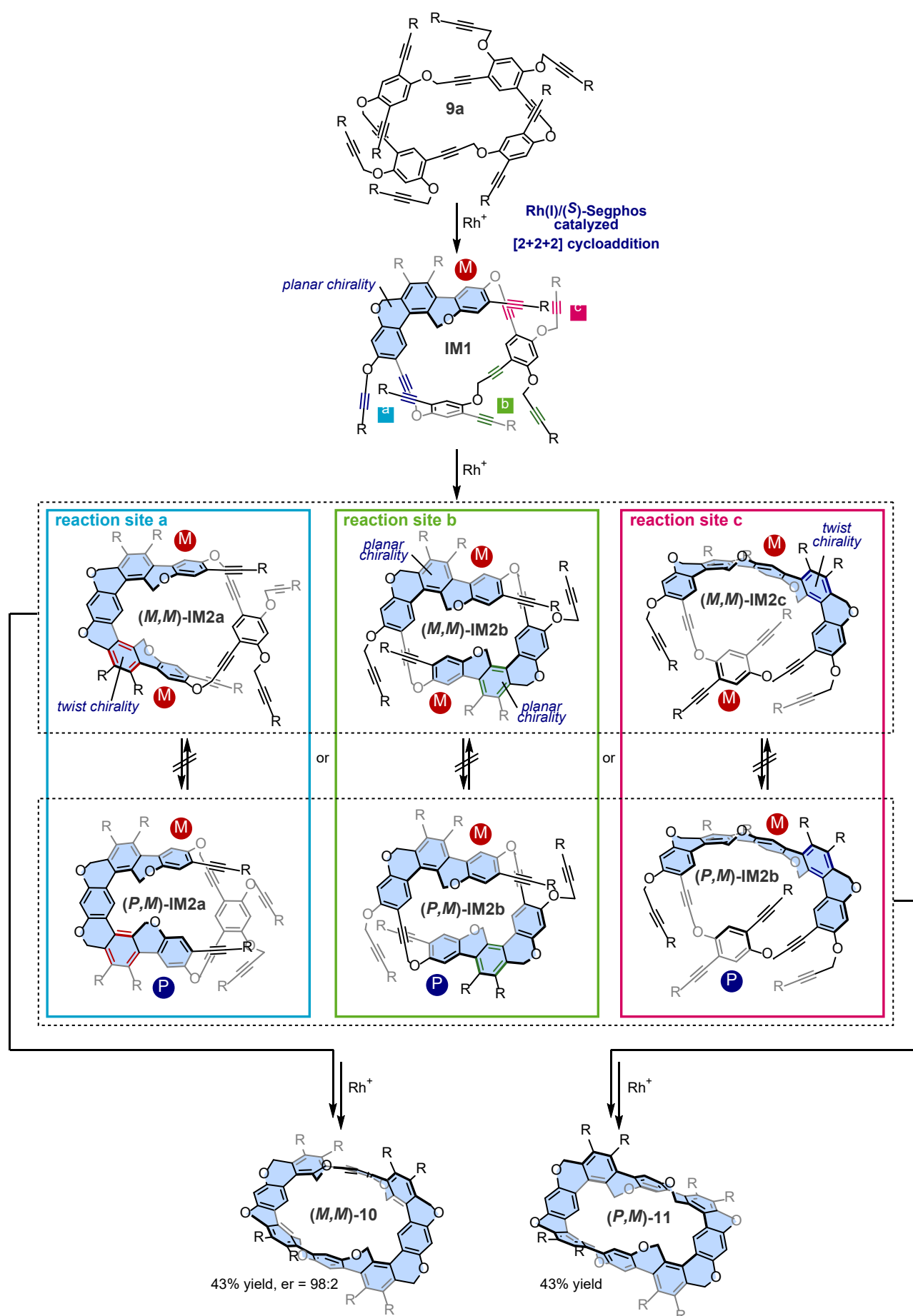


Figure S4. Plausible reaction pathways of rhodium-catalyzed [2+2+2] cycloaddition of **9a** affording doubly twisted belt **10** and **11**.

5. Photophysical and chiroptical properties

Table S6. Photophysical Data of **10**, **11**, **12**, **13**, and **14** in CH₂Cl₂ at 25 °C.

compound	absorption λ_{max} (nm)	emission λ_{max} (nm) (excitation wavelength, nm)	Φ_{F} (excitation wavelength, nm)
(<i>M,M</i>)- 10 ^a	326, 280	382 (330)	0.036 (330)
(<i>P,M</i>)- 11 ^b	328, 288	404 (330)	0.022 (330)
(<i>M,M,M</i>)- 12 ^c	342, 285, 271	404 (340)	0.14 (340)
(<i>P,M,M</i>)- 13 ^d	342, 284, 272	411 (340)	0.098 (340)
(<i>P,M,P,M</i>)- 14 ^e	342, 286, 273	405 (340)	0.21 (340)

^a 1.0×10^{-5} M. ^b 5.0×10^{-6} M. ^c 5.0×10^{-6} M. ^d 7.0×10^{-6} M. ^e 5.0×10^{-6} M.

Table S7. Chiroptical Data of (*M,M*)-**10**, (*M,M,M*)-**12**, and (*P,M,M*)-**13** in CH₂Cl₂ at 25 °C.

compound	$[\alpha]^{25}_{\text{D}}$	$g_{\text{abs}} / 10^{-3}$
(<i>M,M</i>)- 10 ^a	-775°	0.14
(<i>M,M,M</i>)- 12 ^b	-664°	5.0
(<i>P,M,M</i>)- 13 ^c	-34.4°	1.9

^a 1.0×10^{-5} M. ^b 5.0×10^{-6} M. ^c 7.0×10^{-6} M.

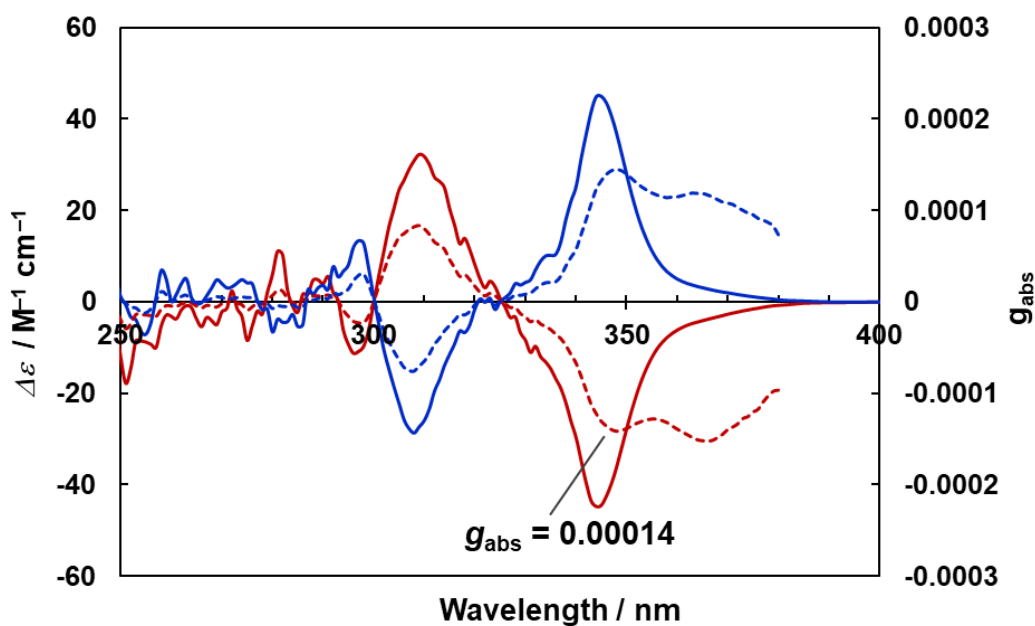


Figure S5. Experimental ECD spectra of (*M,M*)-(-)-**10** (in CH₂Cl₂; red solid line) and (*P,P*)-(+)-**10** (in CH₂Cl₂; blue solid line), and anisotropy dissymmetry factor g_{abs} of (*M,M*)-(-)-**10** (red broken line) and (*P,P*)-(+)-**10** (blue broken line).

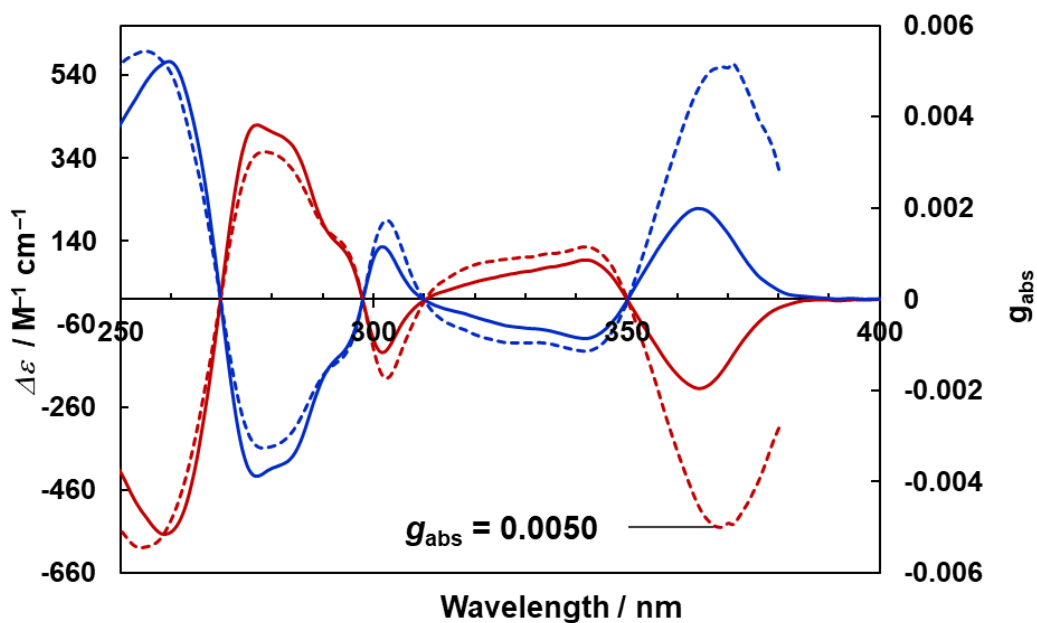


Figure S6. Experimental ECD spectra of (M,M,M)-(-)-**12** (in CH₂Cl₂; red solid line) and (P,P,P)-(+)-**12** (in CH₂Cl₂; blue solid line), and anisotropy dissymmetry factor g_{abs} of (M,M,M)-(-)-**12** (red broken line) and (P,P,P)-(+)-**12** (blue broken line).

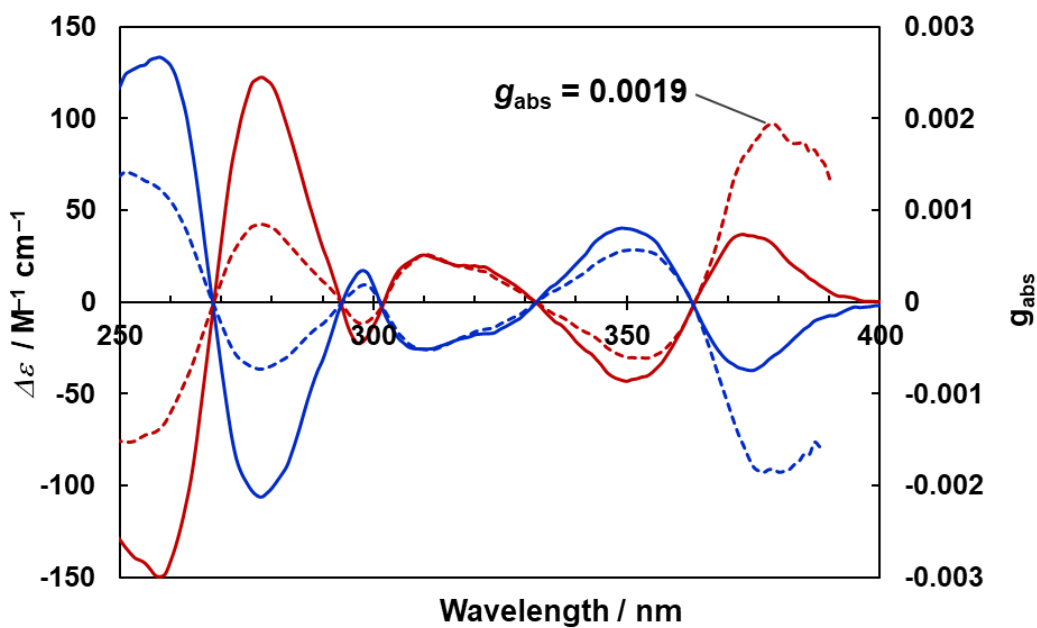


Figure S7. Experimental ECD spectra of (P,M,M)-(-)-**13** (in CH₂Cl₂; red solid line) and (P,P,M)-(+)-**13** (in CH₂Cl₂; blue solid line), and anisotropy dissymmetry factor g_{abs} of (P,M,M)-(-)-**13** (red broken line) and (P,P,M)-(+)-**13** (blue broken line).

6. DFT calculations

All calculations were carried out using the Gaussian 16 program¹⁰. The hybrid density functional method based on B3LYP^{11,12} with a 6-31g(d) basis set or M062X-D3¹³ with a 6-31g(d) basis set was used for geometry optimizations. Compounds **10**, **11**, **12**, **13**, and **14** were optimized with D_2 , D_2 , D_3 , C_2 , and D_2 symmetry assumptions, respectively. Harmonic vibration frequency calculations at the same level were performed to verify all stationary points as local minima (with no imaginary frequency). Optimized structures and frontier molecular orbitals of **10**, **11**, **12**, **13**, and **14** are shown in Figs. S8–S12, S26. Cartesian coordinates of optimized **10–14** and **S1–S8** are listed in Tables S20–S35. Strain energies were calculated according to the reported procedure¹⁴. Zero-point energy, enthalpy, and Gibbs free energy at 298.15 K and 1 atm were calculated by B3LYP/6-31G(d) level of theory for estimation of strain energy, and estimated from the gas-phase studies. The results are shown in Tables S8, S9, S36, and Fig. S13.

Time-dependent (TD) DFT calculations were carried out at the B3LYP/6-31G(d) level of theory based on the optimized structure. TDDFT vertical one-electron excitations calculated for **10**, **11**, **12**, **13**, and **14** are summarized in Tables S11–S19 and Figs. S27–S29. The vectors of transition electric/magnetic dipole moments were generated with Multiwfn¹⁵ in Figs. S27–S29. The nucleus-independent chemical shift^{16,17} (NICS) values were calculated using NMR/GIAO keyword at B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d) (Figs. S19 and 20). The anisotropy of the induced current density^{18,19} (ACID) plot based on the optimized structures was performed by using the AICD program provided by Herges at B3LYP/6-31+g(d,p) level (Figs. S14–S18). The electron density of delocalized bonds^{20–22} (EDDB) analysis was carried out at CAM-B3LYP/6-311G(d,p)//M062X-D3/6-31G(d) level and the VMD²³ was used to visualize cube files (Table S10 and Figs. S21–S25).

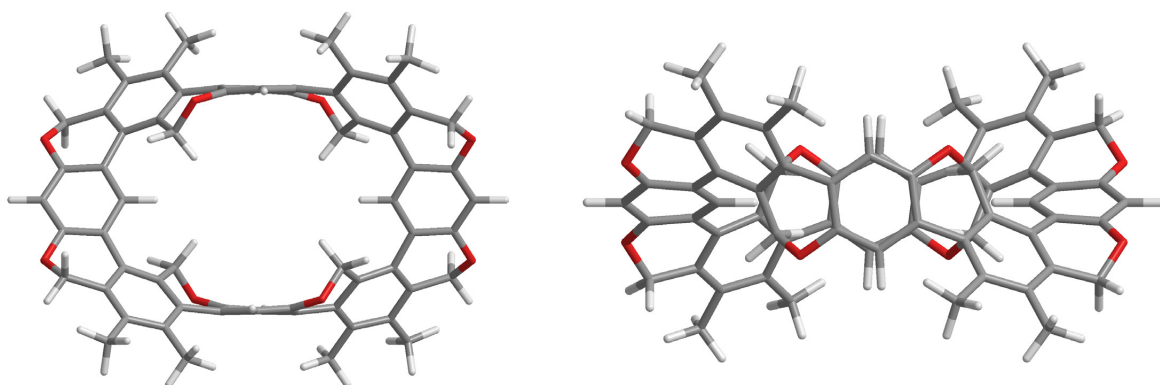


Figure S8. DFT optimized structures of (*M,M*)-**10** constrained to D_2 symmetry. (left: topview, right: sideview).

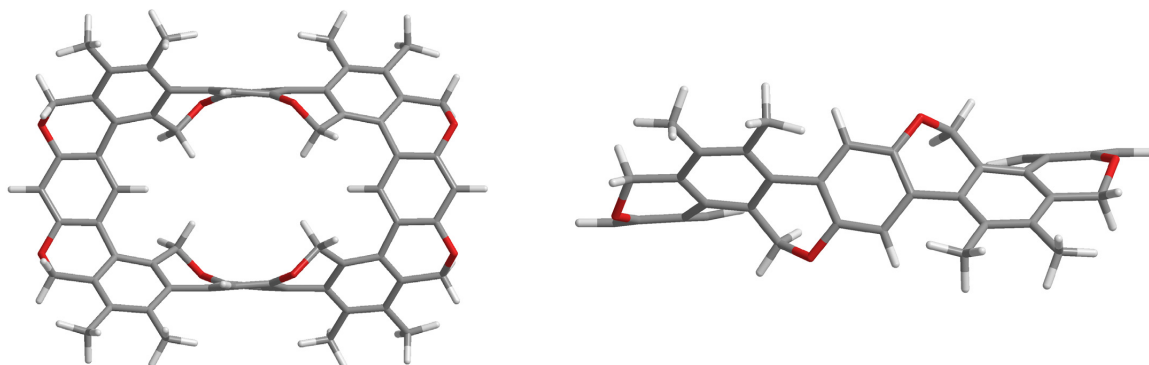


Figure S9. DFT optimized structures of (*P,M*)-**11** constrained to D_2 symmetry. (left: topview, right: sideview).

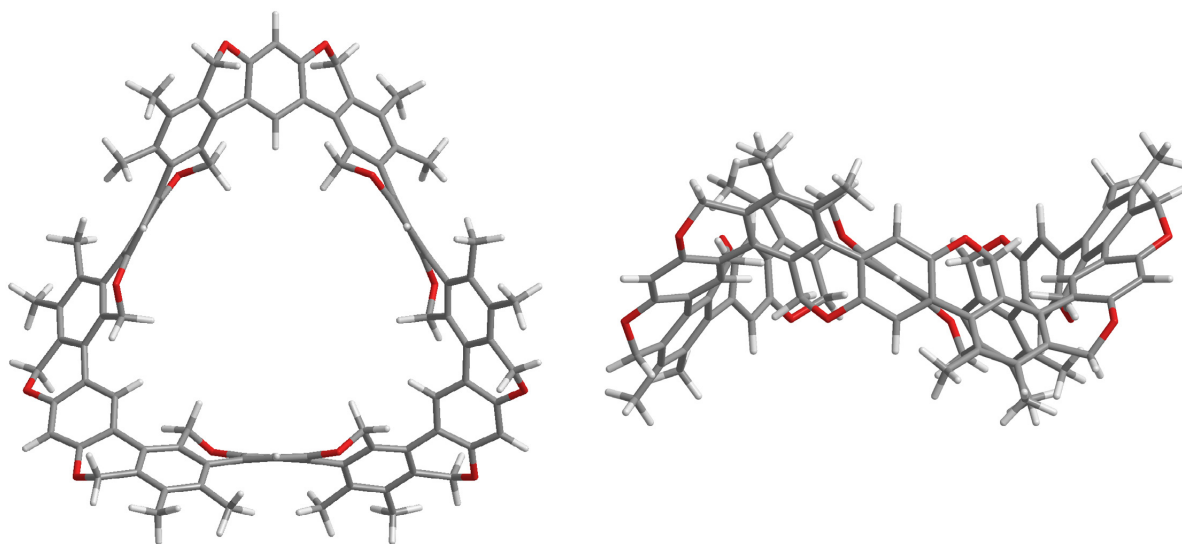


Figure S10. DFT optimized structures of (*M,M,M*)-**12** constrained to D_3 symmetry. (left: topview, right: sideview).

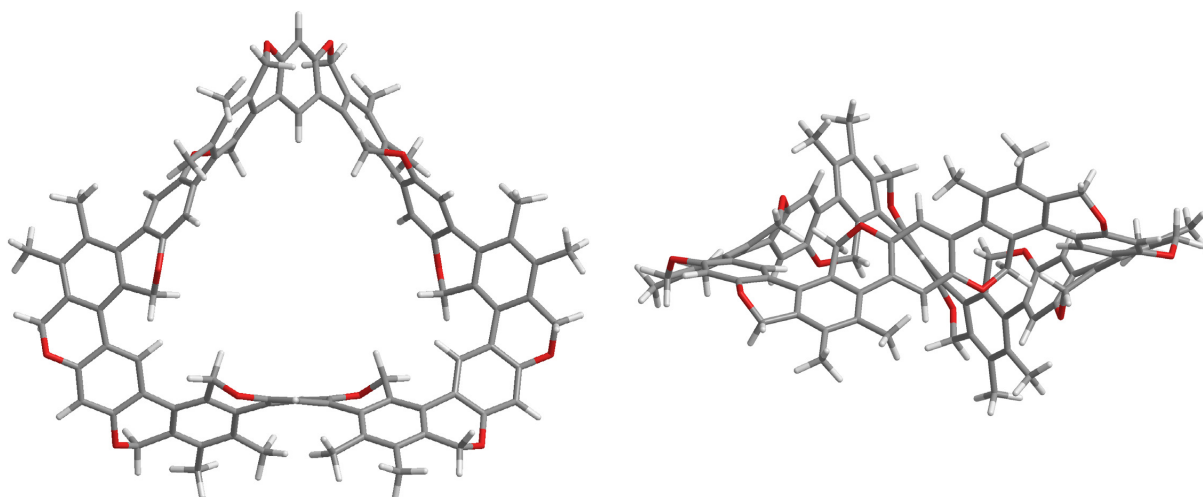


Figure S11. DFT optimized structures of (*P,M,M*)-**13** constrained to C_2 symmetry. (left: topview, right: sideview).

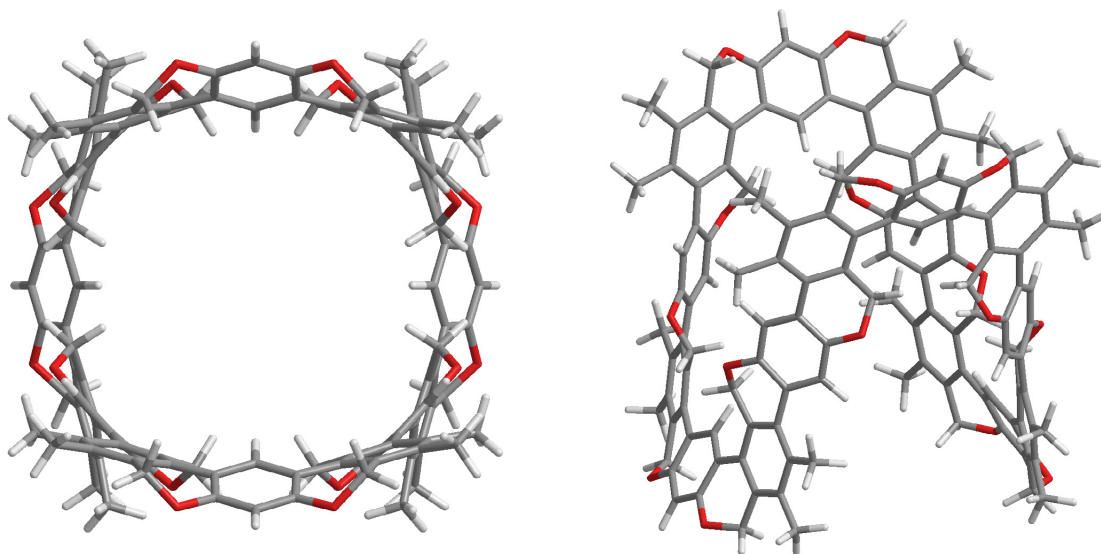
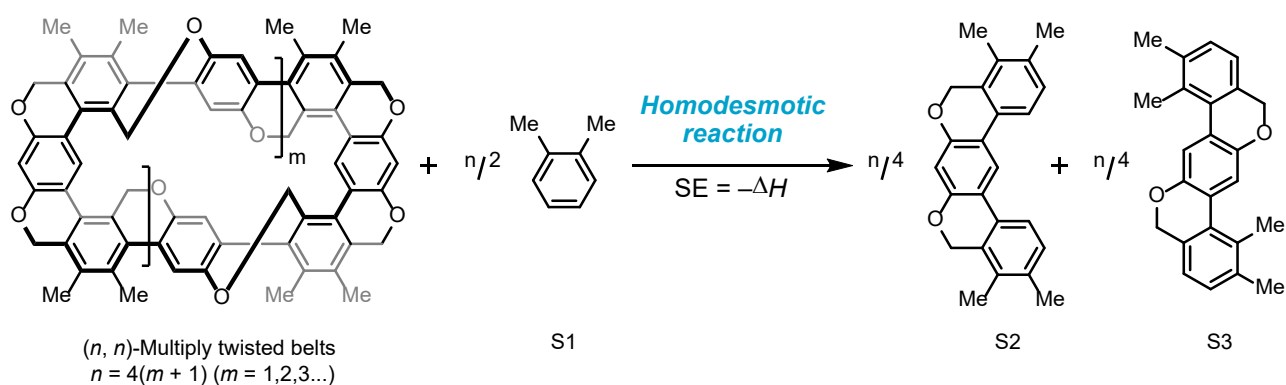


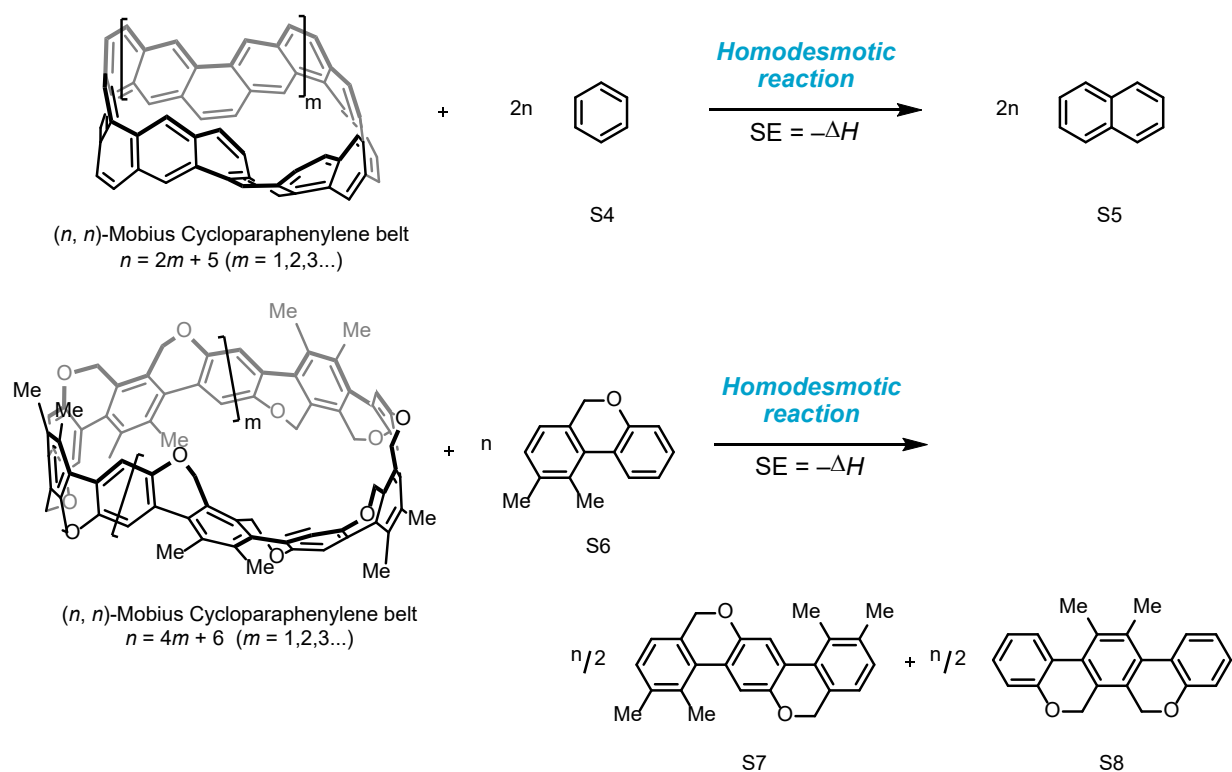
Figure S12. DFT optimized structures of (*P,M,P,M*)-**14** constrained to D_2 symmetry. (left: topview, right: sideview).

Table S8. Homodesmotic reactions for calculating strain energies of multiply twisted belts at the B3LYP/6-31G(d) level.



$n = 2$		$n = 3$		$n = 4$	
(<i>M, M</i>) (= 10)	35.9 kcal/mol	(<i>M, M, M</i>) (= 12)	26.6 kcal/mol	(<i>M, M, M, M</i>)	44.4 kcal/mol
(<i>P, M</i>) (= 11)	51.4 kcal/mol	(<i>P, M, M</i>) (= 13)	43.8 kcal/mol	(<i>P, M, M, M</i>)	47.8 kcal/mol
				(<i>P, P, M, M</i>)	61.8 kcal/mol
				(<i>P, M, P, M</i>) (= 14)	34.5 kcal/mol

Table S9. Ring-size dependent strain energies of multiply twisted belts (This work), Möbius $[n]$ carbon nanobelt²⁴, and Möbius $[n]$ cycloparaphenylene belt⁴ by using Homodesmotic reaction method at the B3LYP/6-31G(d) level.



n	(n,n) -Multiply twisted belt (kcal/mol)	$[n]$ Möbius Carbon Nanotube (MCNB) (kcal/mol)	$[n]$ Möbius Cycloparaphenylene Belt (MCPP) (kcal/mol)
7		191.5	
8	35.9 [= (M,M)-10], 51.4 [= (P,M)-11]		
9		146.9	
10			80.1
11		118.3	
12	26.6 [= (M,M,M)-12], 43.8 [= (P,M,M)-13]		
13		98.2	
14			42.6
15		83.4	
16	34.5 [= (P,M,P,M)-14]		
17		72.2	
18			27.1
19		63.4	
20			
21		56.4	
22			18.2
23		50.6	
24			
25		45.7	
26			
27		41.5	
28			
29		38.0	

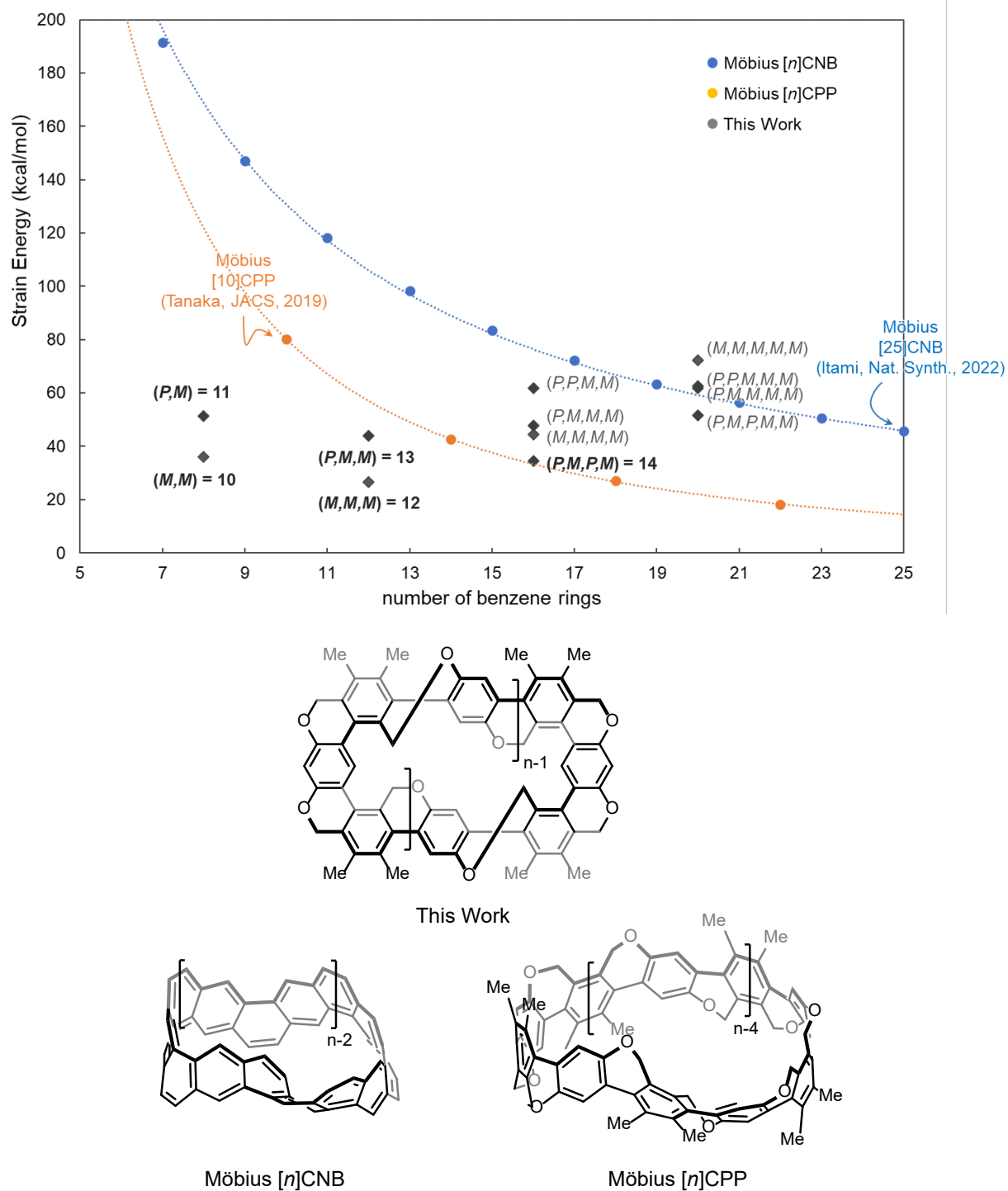


Figure S13. The relationship between the strain energy and the ring size (the number of the benzene rings) of this work (gray), Möbius $[n]$ carbon nanobelts²⁴ (blue), and Möbius $[n]$ cycloparaphenylene belts⁴ (orange) estimated by the homodesmotic reaction method [B3LYP/6-31g(d) level of theory].

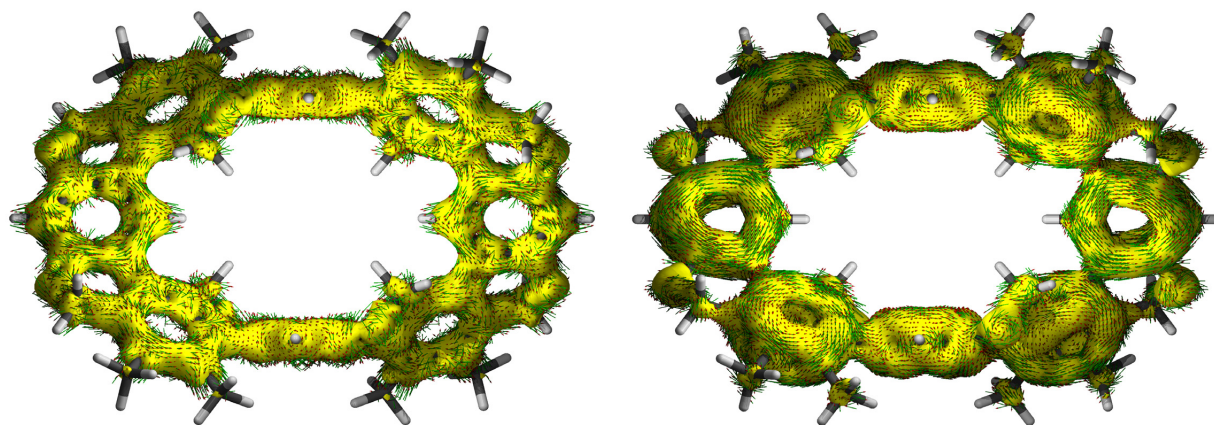


Figure S14. Anisotropy of the induced current density (ACID) plot of (*M,M*)-**10** based on all electrons with isovalue of 0.05 (left) and π -electrons only with isovalue of 0.02 (right), respectively. The external magnetic field vector is perpendicular to the paper. [B3LYP/6-31+g(d,p) level of theory]

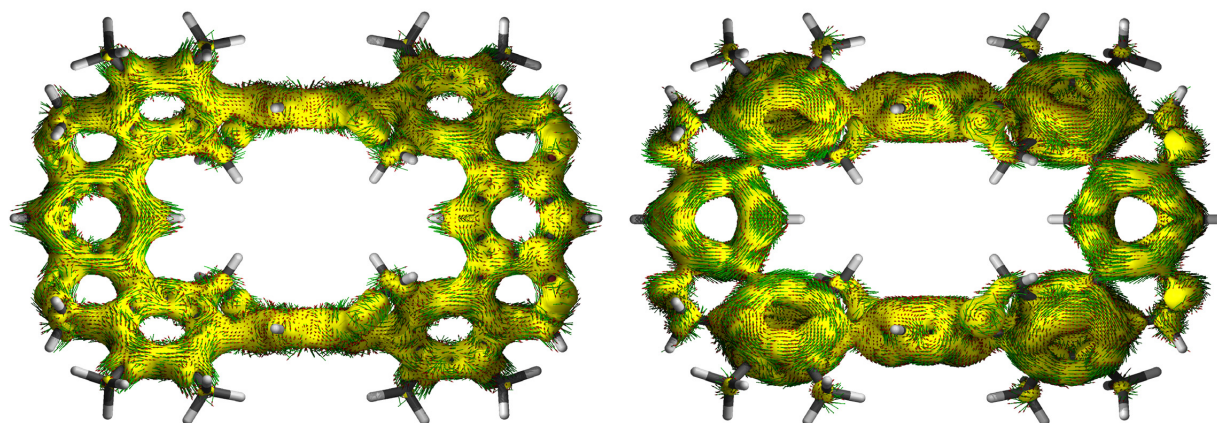


Figure S15. Anisotropy of the induced current density (ACID) plot of (*P,M*)-**11** based on all electrons with isovalue of 0.05 (left) and π -electrons only with isovalue of 0.02 (right), respectively. The external magnetic field vector is perpendicular to the paper. [B3LYP/6-31+g(d,p) level of theory]

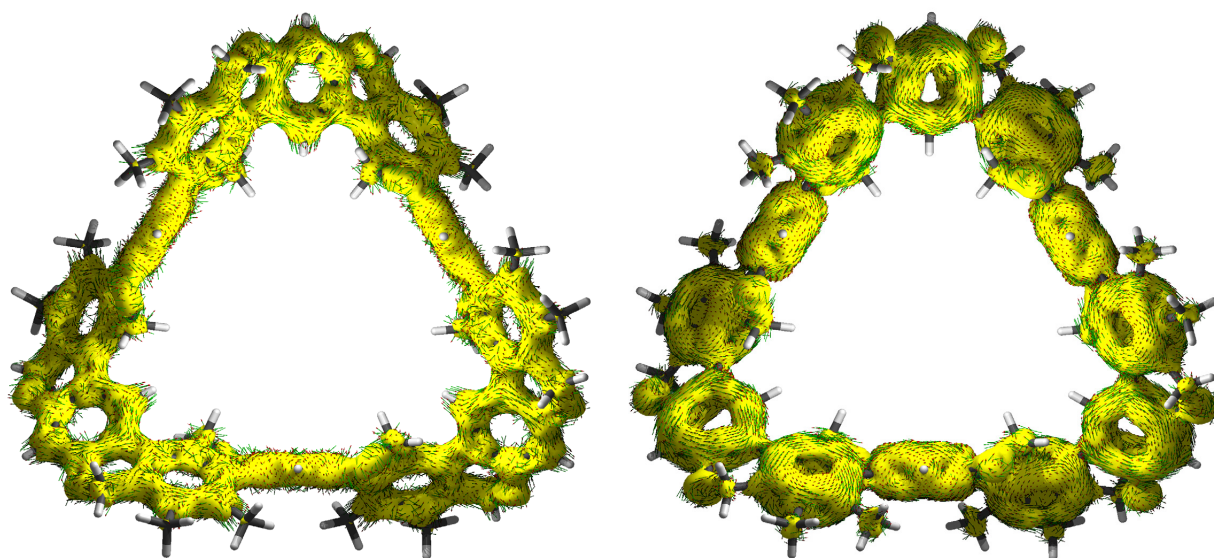


Figure S16. Anisotropy of the induced current density (ACID) plot of (*M,M,M*)-**12** based on all electrons with isovalue of 0.05 (left) and π -electrons only with isovalue of 0.02 (right), respectively. The external magnetic field vector is perpendicular to the paper. [B3LYP/6-31+g(d,p) level of theory]

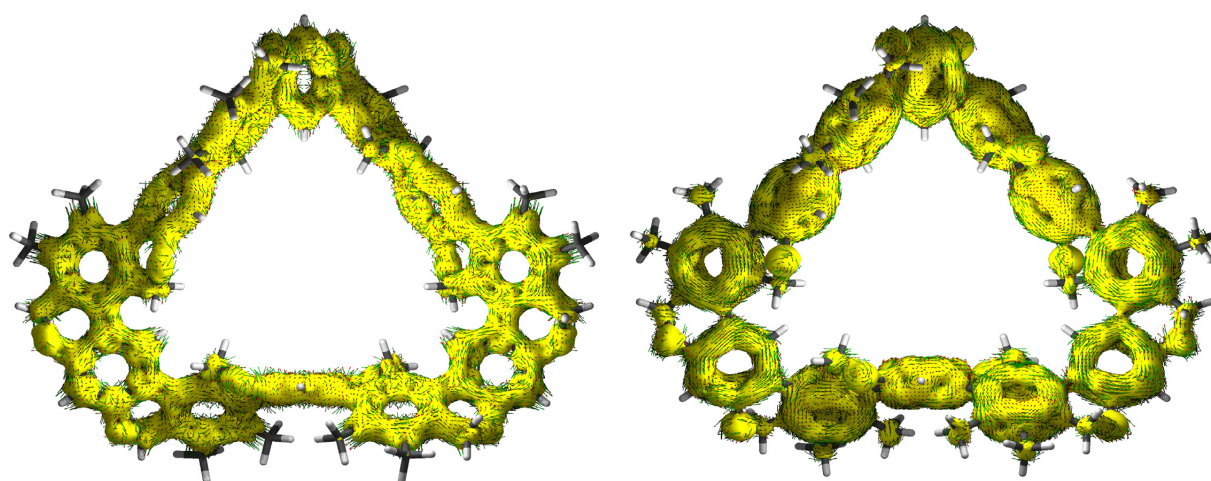


Figure S17. Anisotropy of the induced current density (ACID) plot of (*P,M,M*)-**13** based on all electrons with isovalue of 0.05 (left) and π -electrons only with isovalue of 0.02 (right), respectively. The external magnetic field vector is perpendicular to the paper. [B3LYP/6-31+g(d,p) level of theory]

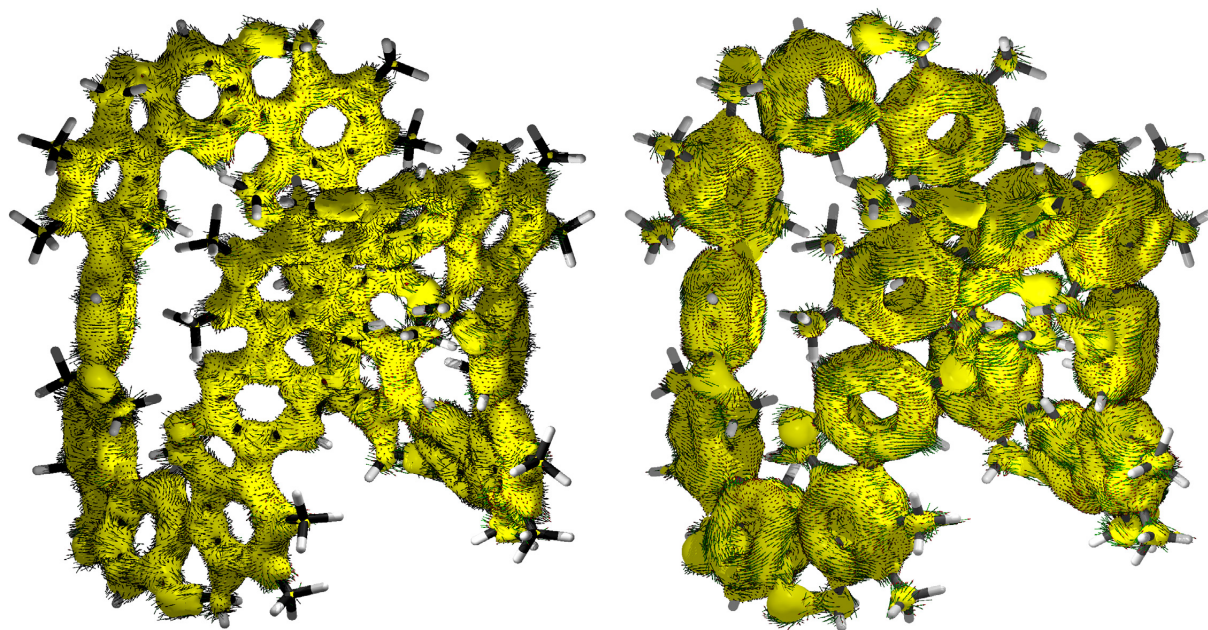


Figure S18. Anisotropy of the induced current density (ACID) plot of *(P,M,P,M)*-**14** based on all electrons with isovalue of 0.05 (left) and π -electrons only with isovalue of 0.02 (right), respectively. The external magnetic field vector is parallel to the D_2 -axis.

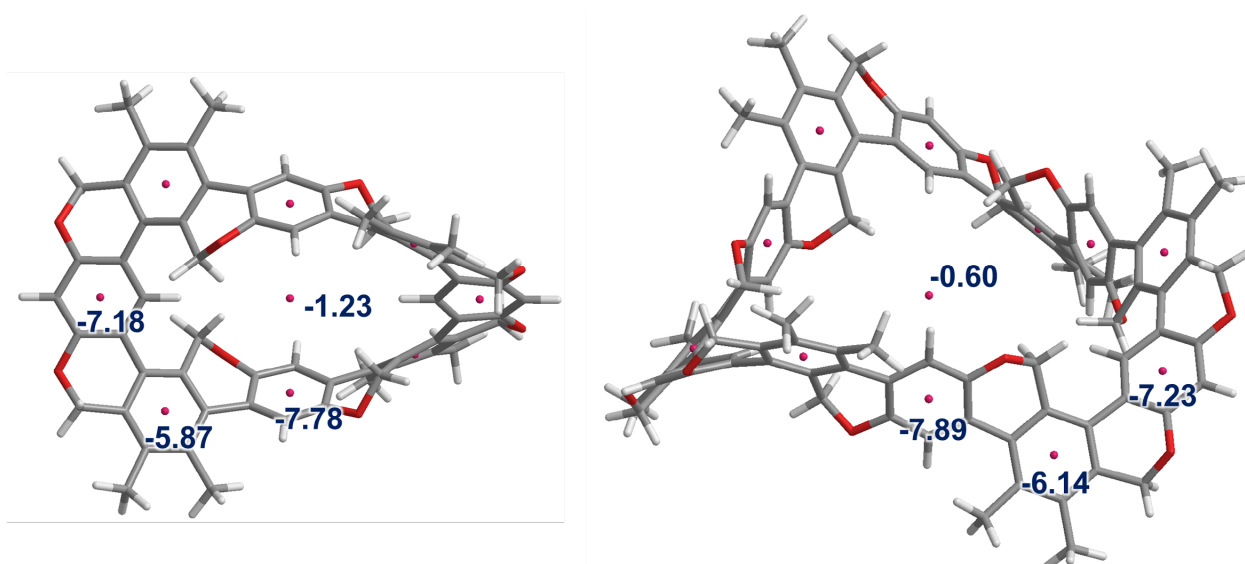


Figure S19. NICS(0) values (ppm, B3LYP/6-311+G(2d,p)) of (*M,M*)-**10** (left) and (*M,M,M*)-**12** (right). Dummy atoms are placed at the center of the benzene rings and the molecular center.

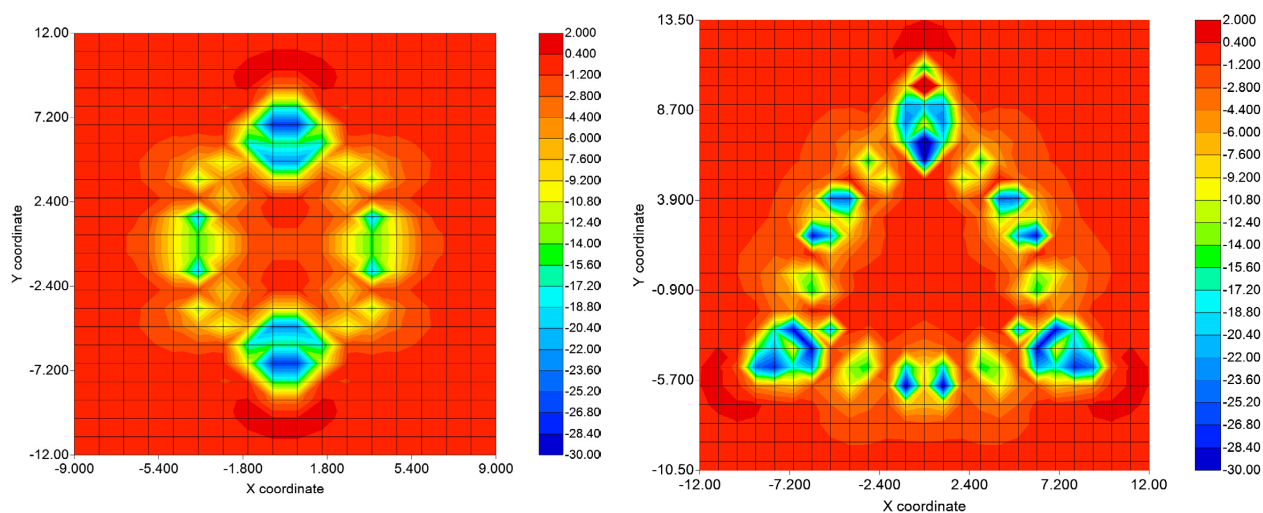


Figure S20. Contour plots of nucleus-independent chemical shift (NICS) at the median plane of **10** (left) and **12** (right) calculated at the B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d) level of theory.

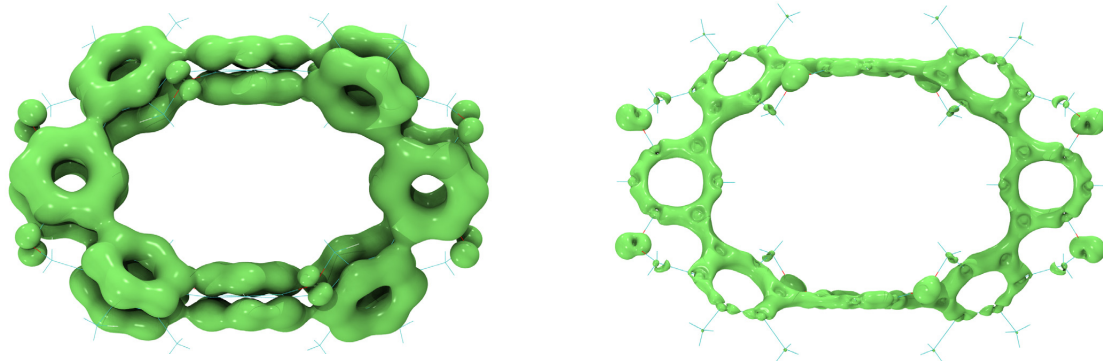


Figure S21. The electron density of delocalized bonds (EDDB) analysis for **10**. π -EDDB with isovalue of 0.015 (left) and σ -EDDB with isovalue of 0.01 (right) calculated at CAM-B3LYP/6-311G(d,p)//M062X-D3/6-31G(d).

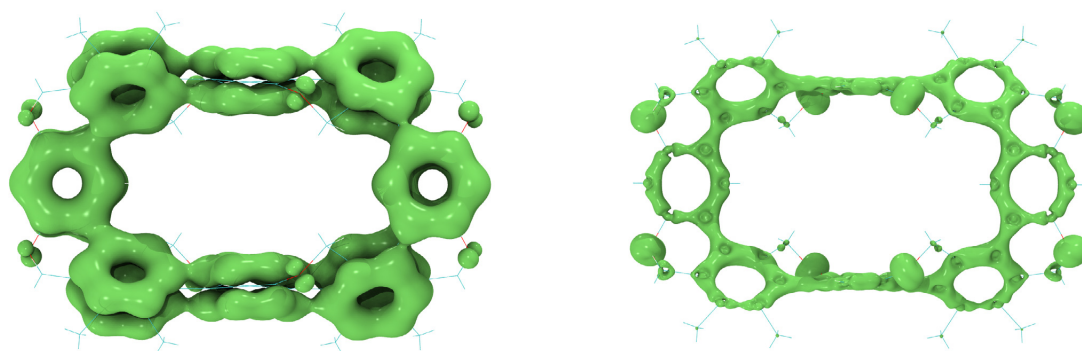


Figure S22. The electron density of delocalized bonds (EDDB) analysis for **11**. π -EDDB with isovalue of 0.015 (left) and σ -EDDB with isovalue of 0.01 (right) calculated at CAM-B3LYP/6-311G(d,p)//M062X-D3/6-31G(d).

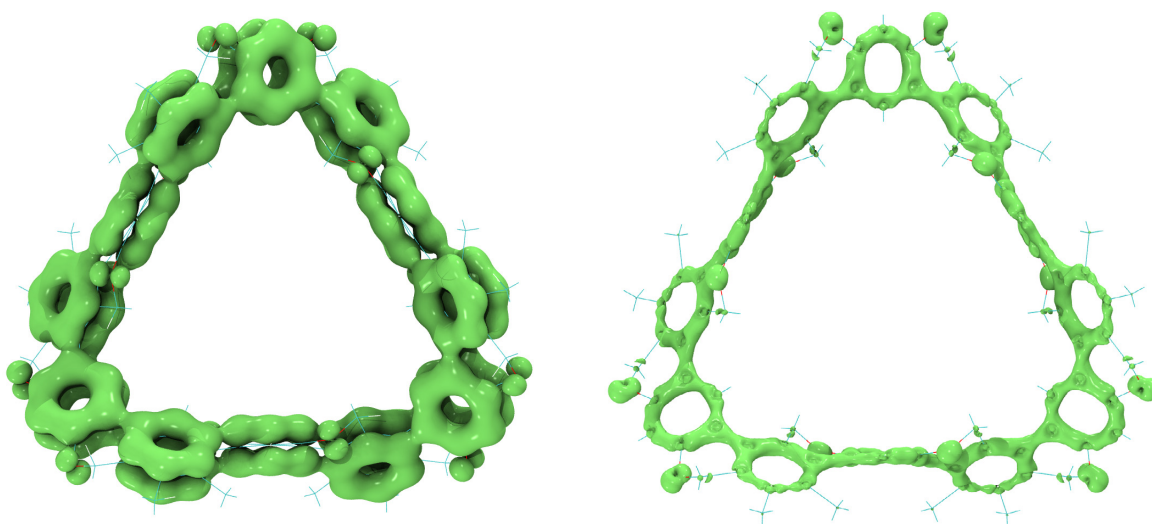


Figure S23. The electron density of delocalized bonds (EDDB) analysis for **12**. π -EDDB with isovalue of 0.015 (left) and σ -EDDB with isovalue of 0.01 (right) calculated at CAM-B3LYP/6-311G(d,p)//M062X-D3/6-31G(d).

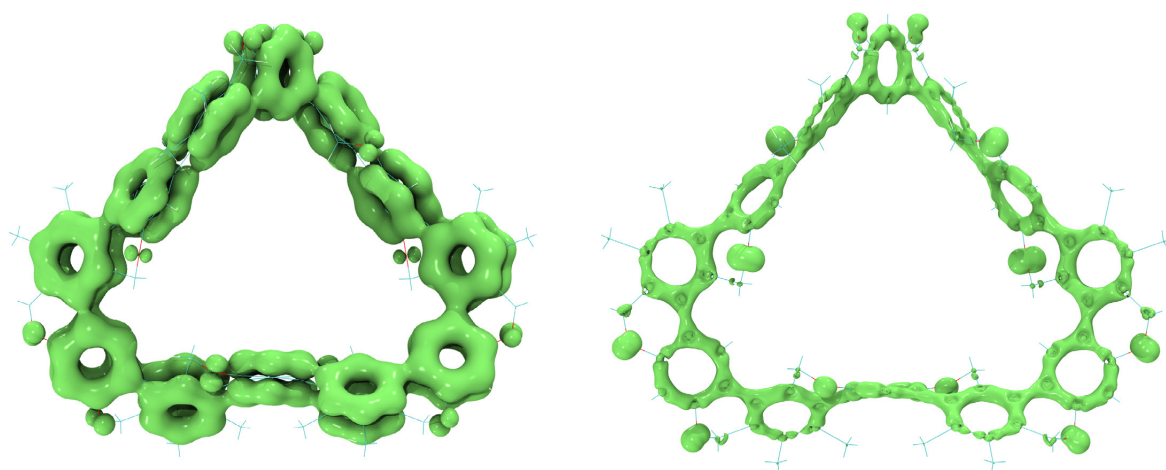


Figure S24. The electron density of delocalized bonds (EDDB) analysis for **13**. π -EDDB with isovalue of 0.015 (left) and σ -EDDB with isovalue of 0.01 (right) calculated at CAM-B3LYP/6-311G(d,p)//M062X-D3/6-31G(d).

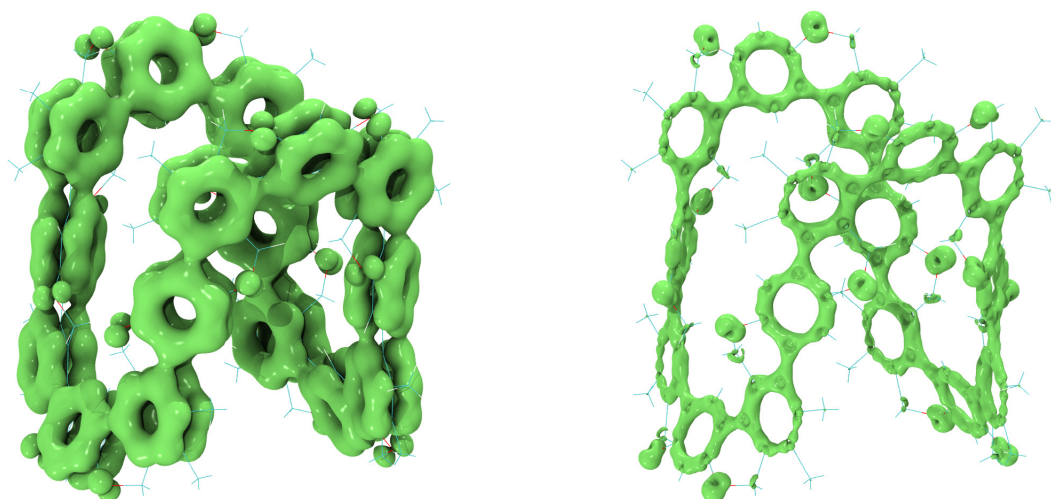


Figure S25. The electron density of delocalized bonds (EDDB) analysis for **14**. π -EDDB with isovalue of 0.015 (left) and σ -EDDB with isovalue of 0.01 (right) calculated at CAM-B3LYP/6-311G(d,p)//M062X-D3/6-31G(d).

Table S10. EDDB results¹⁵ of **10-14**.

	EDDB _{total} = σ -EDDB + π -EDDB	σ - EDDB	π - EDDB	Formal π - electrons of phenylene	π - delocalization efficiency ^a	Local EDDB of phenylene	Sum of local EDDB	Δ EDDB per C _{ipso} - C _{ipso} ^b
10	43.79	4.13	39.66	48.00	0.826	4.83	37.43	0.79
11	44.11	4.16	39.95	48.00	0.832	4.79	37.68	0.80
12	65.45	6.05	59.40	72.00	0.825	4.72	55.57	0.82
13	65.69	6.28	59.40	72.00	0.825	4.73	55.84	0.82
14	87.43	7.81	79.62	96.00	0.829	4.73	74.24	0.82

^a π -EDDB/Formal π -electrons. ^b (EDDB_{total} - Sum of local EDDB)/(The number of C_{ipso}-C_{ipso} bonds).

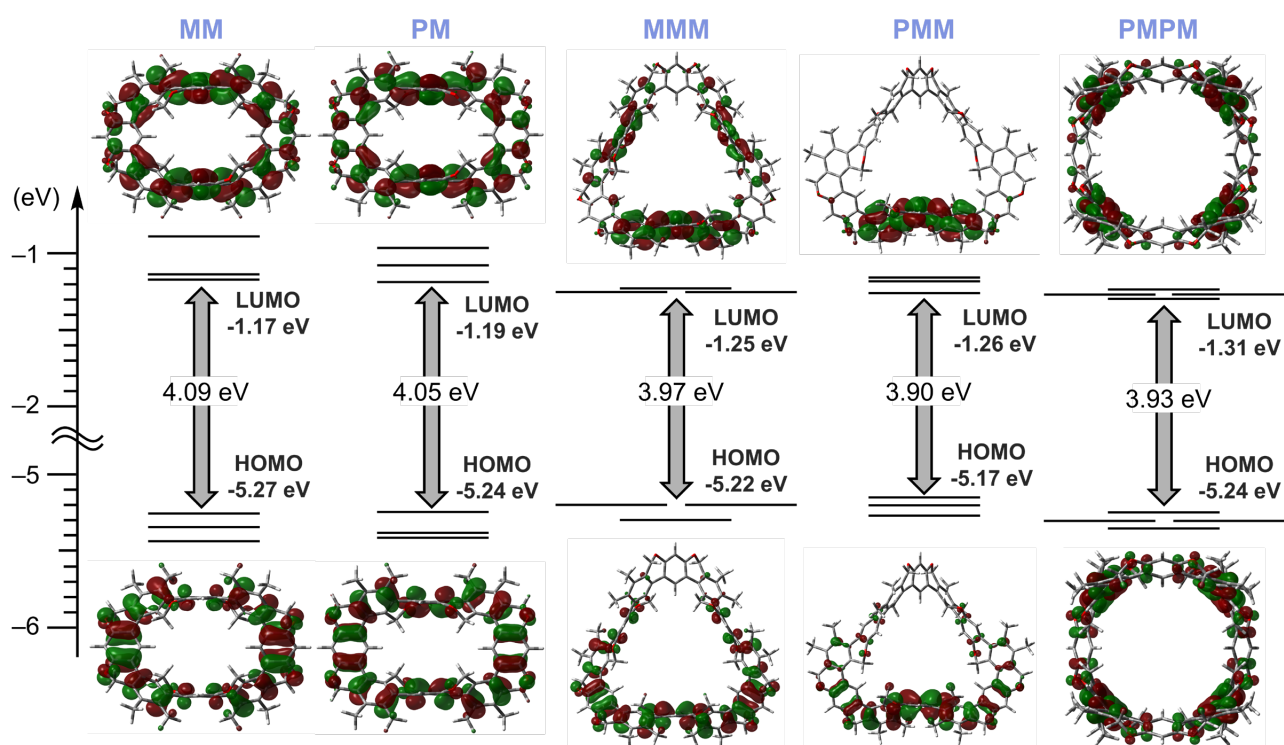


Figure S26. The energy diagram and the pictorial representation of frontier molecular orbitals of **10-14** calculated by the DFT method at the B3LYP/6-31G(d) level of theory.

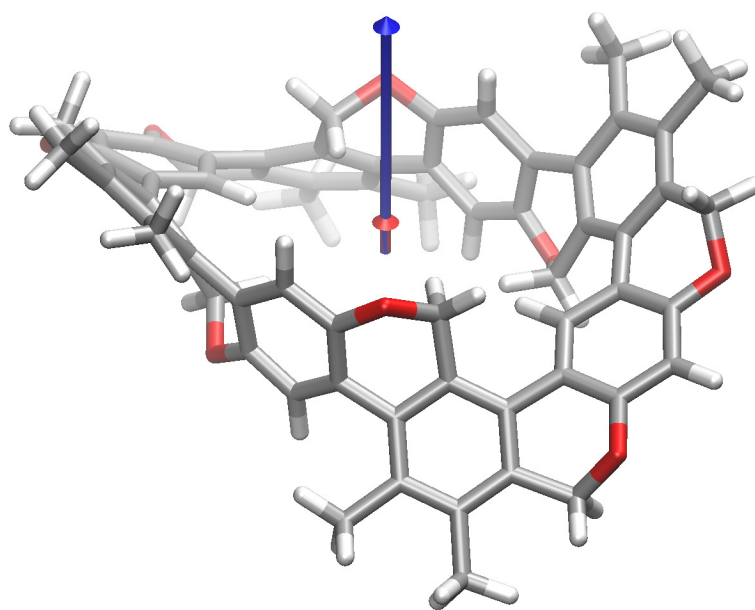


Figure S27. The transition electric dipole moment μ (red arrow) and the transition magnetic dipole moment m (blue arrow) of (*M,M*)-**10** from $S_0 \rightarrow S_1$ transition calculated by the TD-DFT method at B3LYP/6-31G(d).

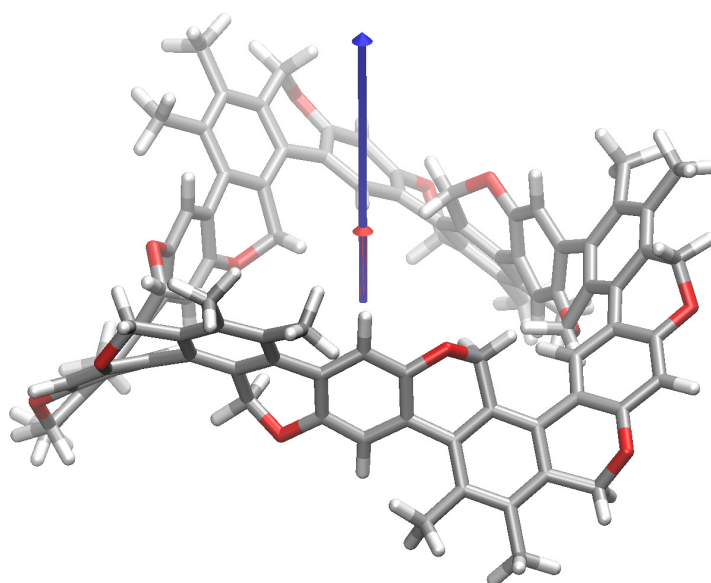


Figure S28. The transition electric dipole moment μ (red arrow) and the transition magnetic dipole moment m (blue arrow) of (M,M,M) -**12** from $S_0 \rightarrow S_1$ transition calculated by the TD-DFT method at B3LYP/6-31G(d).

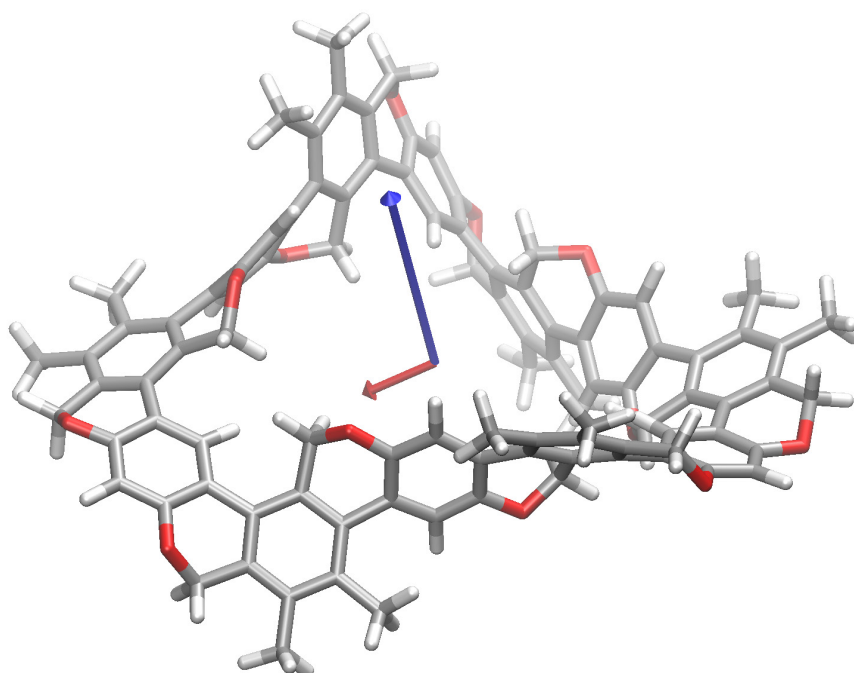


Figure S29. The transition electric dipole moment μ (red arrow) and the transition magnetic dipole moment m (blue arrow) of (P,M,M) -**13** from $S_0 \rightarrow S_1$ transition calculated by the TD-DFT method at B3LYP/6-31G(d).

Table S11. Calculated chiroptical properties of (M,M) -**10**, (M,M,M) -**12**, and (P,M,M) -**13**.

compound	state	$ \mu $ / 10^{-20} esu·cm ^a	$ m $ / 10^{-20} erg·G ⁻¹ ^b	$\cos\theta$ (E-M Angle) ^c	g (4R/D) ^d
(M,M) - 10	1	114.23	5.967	1.00	0.2084
(M,M,M) - 12	1	326.39	8.258	1.00	0.1011
(P,M,M) - 13	1	444.54	5.78	-0.26	-0.01364

^a μ : Transition electric dipole moment. ^b m : Transition magnetic dipole moment. ^c θ : Angle between μ and m . ^d g : dissymmetry factor [$g = 4R/D = 4(|\mu||m|\cos\theta)/(|\mu|^2 + |m|^2)$].

Table S12. TD-DFT vertical one-electron excitations calculated for (*M,M*)-**10**.

excited state	energy (eV)	wavelength (nm)	oscillator strength (<i>f</i>) ^a	description ^b
1	3.6923	335.79	0.0183	HOMO-3 → LUMO+1 (0.40536) (33.0%) HOMO-2 → LUMO (0.47703) (45.7%) HOMO-2 → LUMO+3 (-0.0751) (1.13%) HOMO-1 → LUMO+4 (0.22995) (10.6%) HOMO → LUMO+5 (0.18941) (7.21%)
2	3.7054	334.61	0.0458	HOMO → LUMO (0.68729) (94.8%) HOMO → LUMO+3 (-0.0857) (1.47%)
3	3.7317	332.24	0.0737	HOMO-3 → LUMO+1 (-0.0754) (1.14%) HOMO-2 → LUMO+3 (-0.0868) (1.51%) HOMO → LUMO+1 (0.67423) (91.1%) HOMO → LUMO+5 (0.12172) (2.97%)
5	3.7499	330.63	0.0871	HOMO-3 → LUMO+4 (0.10617) (2.26%) HOMO-2 → LUMO+2 (-0.11840) (2.81%) HOMO-1 → LUMO+1 (0.67347) (91.0)
6	3.7969	326.54	0.3214	HOMO-4 → LUMO+1 (0.09756) (1.91%) HOMO-3 → LUMO (0.46961) (44.2%) HOMO-2 → LUMO+1 (0.47451) (45.2%) HOMO → LUMO+3 (0.13815) (3.83%)
7	3.8851	319.12	0.0752	HOMO-5 → LUMO+2 (-0.0905) (1.64%) HOMO-4 → LUMO (-0.1508) (4.56%) HOMO-3 → LUMO+1 (-0.0957) (1.84%) HOMO-2 → LUMO (-0.2645) (14.0%) HOMO-2 → LUMO+3 (-0.1712) (5.88%) HOMO-1 → LUMO+4 (0.33912) (23.0%) HOMO → LUMO+1 (-0.1151) (2.65%) HOMO → LUMO+5 (0.45309) (41.1%)
8	3.9061	317.41	0.2845	HOMO-5 → LUMO (-0.1574) (4.96%) HOMO-4 → LUMO+2 (-0.0946) (1.79%) HOMO-2 → LUMO+2 (-0.2142) (9.20%) HOMO-1 → LUMO+5 (0.34944) (24.5%) HOMO → LUMO+4 (0.51614) (53.4%)
10	3.9303	315.46	0.1818	HOMO-3 → LUMO (-0.3052) (18.7%) HOMO-3 → LUMO+3 (-0.1028) (2.12%) HOMO-2 → LUMO+1 (0.44034) (38.9%) HOMO-2 → LUMO+5 (0.13671) (3.75%) HOMO-1 → LUMO+2 (-0.1162) (2.71%) HOMO → LUMO (-0.1075) (2.32%) HOMO → LUMO+3 (-0.3718) (27.7%)

^a Excitation energies with oscillator strength larger than 0.01 are listed. ^b Relative contribution larger than 1% is listed.

Table S13. TD-DFT vertical one-electron excitations calculated for (*P,M*)-11.

excited state	energy (eV)	wavelength (nm)	oscillator strength (<i>f</i>) ^a	description ^b
2	3.6684	337.98	0.2241	HOMO-2 → LUMO+1 (-0.09037) (1.64%) HOMO → LUMO (0.6878) (94.8%)
5	3.7871	327.38	0.0471	HOMO-5 → LUMO (-0.11685) (38.5%) HOMO-2 → LUMO+2 (-0.28115) (16.4%) HOMO-1 → LUMO+1 (0.44004) (16.4%) HOMO-1 → LUMO+4 (-0.207) (16.4%) HOMO → LUMO+5 (-0.37637) (31.2%)
6	3.7973	326.51	0.0241	HOMO-4 → LUMO+1 (-0.09894) (1.96%) HOMO-3 → LUMO (0.49827) (49.8%) HOMO-2 → LUMO+1 (0.19281) (7.45%) HOMO-2 → LUMO+4 (0.18441) (6.82%) HOMO-1 → LUMO+6 (0.08413) (1.42%) HOMO → LUMO+3 (0.38124) (29.1%)
9	3.8553	321.60	0.6573	HOMO-7 → LUMO (0.07479) (1.12%) HOMO-6 → LUMO+1 (0.07638) (1.17%) HOMO-3 → LUMO (0.1692) (5.74%) HOMO-3 → LUMO+3 (0.12874) (3.33%) HOMO-2 → LUMO+1 (0.47687) (45.6%) HOMO-2 → LUMO+4 (-0.13623) (3.72%) HOMO-1 → LUMO+2 (-0.12608) (3.19%) HOMO → LUMO (0.10738) (2.31%) HOMO → LUMO+3 (-0.39384) (31.1%)
10	3.8621	321.03	0.2809	HOMO-5 → LUMO (0.0913) (1.67%) HOMO-4 → LUMO+2 (-0.10117) (2.05%) HOMO-3 → LUMO+5 (0.13388) (3.60%) HOMO-1 → LUMO+1 (0.45596) (41.7%) HOMO-1 → LUMO+4 (0.28859) (16.7%) HOMO → LUMO+5 (0.38666) (30.0%)

^a Excitation energies with oscillator strength larger than 0.01 are listed. ^b Relative contribution larger than 1% is listed.

Table S14. TD-DFT vertical one-electron excitations calculated for (*M,M,M*)-12.

excited state	energy (eV)	wavelength (nm)	oscillator strength (<i>f</i>) ^a	description ^b
1	3.4730	356.99	0.1403	HOMO-5 → LUMO+1 (0.21716) (9.48%) HOMO-4 → LUMO (0.21716) (9.48%) HOMO-2 → LUMO+2 (0.37591) (28.4%) HOMO-1 → LUMO+1 (0.32543) (21.3%) HOMO-1 → LUMO+7 (-0.10535) (2.23%) HOMO → LUMO (0.32543) (21.3%) HOMO → LUMO+8 (-0.10535) (2.23%)
2	3.5339	350.84	0.5452	HOMO-5 → LUMO (-0.11356) (2.59%) HOMO-5 → LUMO+2 (0.12631) (3.20%) HOMO-4 → LUMO+1 (-0.11356) (2.59%) HOMO-2 → LUMO+1 (0.35258) (25.0%) HOMO-1 → LUMO (-0.26557) (14.2%) HOMO-1 → LUMO+2 (0.40915) (33.6%) HOMO → LUMO+1 (-0.26557) (14.2%)
3	3.5339	350.84	0.5452	HOMO-5 → LUMO+1 (-0.11356) (2.59%) HOMO-4 → LUMO (0.11356) (2.59%) HOMO-4 → LUMO+2 (0.12631) (3.20%) HOMO-2 → LUMO (0.35258) (25.0%) HOMO-1 → LUMO+1 (-0.26557) (14.2%) HOMO → LUMO (0.26557) (14.2%) HOMO → LUMO+2 (0.40915) (33.6%)
4	3.6358	341.01	0.0285	HOMO-5 → LUMO+1 (0.12321) (3.05%) HOMO-4 → LUMO (-0.12312) (3.05%) HOMO-3 → LUMO+1 (0.42374) (36.1%) HOMO-2 → LUMO+4 (0.08356) (1.40%) HOMO-1 → LUMO+1 (-0.31474) (19.9%) HOMO → LUMO (0.31474) (19.9%) HOMO → LUMO+2 (-0.24021) (11.6%)
5	3.6358	341.01	0.0285	HOMO-5 → LUMO (-0.12321) (3.05%) HOMO-4 → LUMO+1 (-0.12312) (3.05%) HOMO-3 → LUMO (0.42374) (36.1%) HOMO-2 → LUMO+3 (-0.08356) (1.40%) HOMO-1 → LUMO (0.31474) (19.9%) HOMO-1 → LUMO+2 (0.24021) (11.6%) HOMO → LUMO+1 (0.31474) (19.9%)
7	3.6428	340.36	0.0547	HOMO-5 → LUMO+1 (-0.29452) (17.1%) HOMO-4 → LUMO (-0.29152) (17.1%) HOMO-2 → LUMO+2 (-0.25948) (13.5%) HOMO-1 → LUMO+1 (0.34283) (23.6%) HOMO → LUMO (0.34283) (23.6%)

8	3.6529	339.41	0.0318	HOMO-5 → LUMO+1 (0.20307) (8.30%)
				HOMO-4 → LUMO (-0.20307) (8.30%)
				HOMO-4 → LUMO+2 (-0.32902) (21.8%)
				HOMO-3 → LUMO+1 (-0.11929) (2.86%)
				HOMO-2 → LUMO (-0.34701) (24.2%)
				HOMO-1 → LUMO+1 (-0.1087) (23.8%)
				HOMO → LUMO (0.1087) (23.8%)
				HOMO → LUMO+2 (0.353) (25.1%)
9	3.6529	339.41	0.0318	HOMO-5 → LUMO (0.20307) (8.30%)
				HOMO-5 → LUMO+2 (-0.32902) (21.8%)
				HOMO-4 → LUMO+1 (0.20307) (8.30%)
				HOMO-3 → LUMO (0.11929) (2.86%)
				HOMO-2 → LUMO+1 (-0.34701) (24.2%)
				HOMO-1 → LUMO (-0.1087) (23.8%)
				HOMO-1 → LUMO+2 (0.353) (25.1%)
				HOMO → LUMO+1 (-0.1087) (23.8%)
10	3.7607	329.68	0.0019	HOMO-5 → LUMO+1 (0.13944) (3.90%)
				HOMO-4 → LUMO (-0.13944) (3.90%)
				HOMO-4 → LUMO+2 (0.1733) (6.03%)
				HOMO-3 → LUMO+1 (0.41953) (35.3%)
				HOMO-1 → LUMO+1 (-0.23822) (11.4%)
				HOMO → LUMO (-0.23822) (11.4%)
				HOMO → LUMO+2 (0.34512) (23.9%)

^a Excitation energies with oscillator strength larger than 0.01 are listed. ^b Relative contribution larger than 1% is listed.

Table S15. TD-DFT vertical one-electron excitations calculated for (*P,M,M*)-**13**.

excited state	energy (eV)	wavelength (nm)	oscillator strength (<i>f</i>) ^a	description ^b
1	3.4125	363.32	0.2557	HOMO-5 → LUMO (0.11473) (2.64%) HOMO-2 → LUMO (0.21102) (8.94%) HOMO-1 → LUMO+1 (-0.10455) (21.9%) HOMO → LUMO (0.60578) (7.37%) HOMO → LUMO+2 (0.10953) (2.41%) HOMO → LUMO+7 (0.1064) (22.7%)
2	3.5513	349.12	0.6353	HOMO-5 → LUMO+2 (-0.08546) (1.47%) HOMO-4 → LUMO+1 (-0.16578) (5.53%) HOMO-3 → LUMO+1 (-0.1196) (2.88%) HOMO-2 → LUMO+2 (0.35698) (25.7%) HOMO-1 → LUMO+1 (0.42783) (36.9%) HOMO-1 → LUMO+8 (-0.11733) (2.77%) HOMO → LUMO (0.22815) (10.5%) HOMO → LUMO+2 (-0.2032) (8.31%)
3	3.5755	346.76	0.3730	HOMO-5 → LUMO+1 (-0.08742) (1.54%) HOMO-4 → LUMO+2 (-0.11944) (2.87%) HOMO-2 → LUMO+1 (0.35992) (26.1%) HOMO-1 → LUMO (-0.12897) (3.35%) HOMO-1 → LUMO+2 (0.48803) (47.9%) HOMO → LUMO+1 (-0.24998) (12.6%)
5	3.6679	338.03	0.0115	HOMO-5 → LUMO (0.35102) (24.8%) HOMO-2 → LUMO (0.51682) (53.7%) HOMO → LUMO (-0.1898) (7.24%) HOMO → LUMO+2 (-0.18458) (6.85%) HOMO → LUMO+4 (-0.07161) (1.03%) HOMO → LUMO+7 (-0.10728) (2.31%)
6	3.6706	337.78	0.0290	HOMO-4 → LUMO+1 (0.10887) (2.38%) HOMO-3 → LUMO+1 (0.36927) (27.4%) HOMO-2 → LUMO (0.0784) (1.24%) HOMO-2 → LUMO+2 (-0.09842) (1.95%) HOMO-2 → LUMO+4 (0.07371) (1.09%) HOMO-1 → LUMO+1 (0.43295) (37.7%) HOMO → LUMO+2 (0.33268) (22.2%)
7	3.6731	337.55	0.0025	HOMO-3 → LUMO (-0.09083) (1.66%) HOMO-3 → LUMO+2 (0.26481) (14.1%) HOMO-1 → LUMO+2 (0.29714) (17.8%) HOMO → LUMO+1 (0.55057) (61.0%)

8	3.6973	335.33	0.0454	HOMO-5 → LUMO (0.10245) (2.11%)
				HOMO-5 → LUMO+2 (-0.1332) (3.57%)
				HOMO-4 → LUMO+1 (-0.2881) (16.7%)
				HOMO-3 → LUMO+1 (-0.10245) (2.11%)
				HOMO-2 → LUMO (0.08323) (1.39%)
				HOMO-2 → LUMO+2 (0.30787) (19.1%)
				HOMO-1 → LUMO+1 (0.1567) (4.94%)
				HOMO → LUMO (0.0818) (1.35%)
				HOMO → LUMO+2 (0.47296) (45.0%)
9	3.7036	334.76	0.0401	HOMO-5 → LUMO+1 (-0.12882) (3.34%)
				HOMO-4 → LUMO+2 (-0.29708) (17.8%)
				HOMO-3 → LUMO (0.07299) (1.07%)
				HOMO-3 → LUMO+2 (-0.24781) (12.4%)
				HOMO-2 → LUMO+1 (0.40274) (32.7%)
				HOMO-1 → LUMO (0.09561) (1.84%)
				HOMO-1 → LUMO+2 (-0.26474) (14.1%)
				HOMO → LUMO+1 (0.23791) (11.4%)

^a Excitation energies with oscillator strength larger than 0.01 are listed. ^b Relative contribution larger than 1% is listed.

Table S16. TD-DFT vertical one-electron excitations calculated for (*P,M,P,M*)-**14**.

excited state	energy (eV)	wavelength (nm)	oscillator strength (<i>f</i>) ^a	description ^b
2	3.4971	354.54	0.1165	HOMO-7 → LUMO+1 (-0.16062) (5.19%) HOMO-6 → LUMO+3 (0.17229) (5.97%) HOMO-5 → LUMO (-0.12302) (3.04%) HOMO-3 → LUMO+2 (-0.28787) (16.7%) HOMO-2 → LUMO (0.34087) (23.4%) HOMO-1 → LUMO+3 (-0.26296) (13.9%) HOMO → LUMO+1 (0.3594) (26.0%)
3	3.4971	354.54	0.1164	HOMO-7 → LUMO+2 (-0.16062) (5.19%) HOMO-6 → LUMO (0.12302) (3.04%) HOMO-5 → LUMO+3 (-0.17229) (5.97%) HOMO-3 → LUMO+1 (-0.28787) (16.7%) HOMO-2 → LUMO+3 (0.26296) (13.9%) HOMO-1 → LUMO (-0.34087) (23.4%) HOMO → LUMO+2 (0.3594) (26.0%)
4	3.5548	348.78	1.2320	HOMO-7 → LUMO (-0.11088) (2.47%) HOMO-6 → LUMO+2 (0.09827) (1.94%) HOMO-5 → LUMO+1 (-0.09827) (1.94%) HOMO-3 → LUMO+3 (-0.22417) (10.1%) HOMO-2 → LUMO+1 (0.31047) (19.4%) HOMO-1 → LUMO+2 (-0.31047) (19.4%) HOMO → LUMO (0.45118) (40.9%)
7	3.6370	340.90	0.0164	HOMO-6 → LUMO+3 (0.12344) (3.06%) HOMO-5 → LUMO (0.13181) (3.49%) HOMO-3 → LUMO+6 (0.07097) (1.01%) HOMO-2 → LUMO (0.37449) (28.2%) HOMO-1 → LUMO+3 (0.42346) (36.1%) HOMO → LUMO+1 (-0.09469) (1.80%)
8	3.6370	340.90	0.0164	HOMO-5 → LUMO+3 (0.12348) (3.06%) HOMO-4 → LUMO+2 (0.33225) (22.2%) HOMO-3 → LUMO+5 (0.07099) (1.01%) HOMO-2 → LUMO+3 (0.42347) (36.1%) HOMO-1 → LUMO (0.37447) (28.2%) HOMO → LUMO+2 (0.09478) (1.81%)
10	3.6399	340.62	0.0435	HOMO-7 → LUMO+1 (0.25116) (12.7%) HOMO-5 → LUMO+3 (-0.22367) (10.1%) HOMO-5 → LUMO (0.2485) (12.4%) HOMO-3 → LUMO+2 (0.28902) (16.8%) HOMO → LUMO+1 (0.46257) (43.0%)

^a Excitation energies with oscillator strength larger than 0.01 are listed. ^b Relative contribution larger than 1% is listed.

Table S17. Transition moments of (*M,M*)-10.

Ground to excited state transition electric dipole moments (Au):						
state	X	Y	Z	Dip. S.	Osc.	
1	0.4494	0	0	0.202	0.0183	
Ground to excited state transition velocity dipole moments (Au):						
state	X	Y	Z	Dip. S.	Osc.	
1	-0.0642	0	0	0.0041	0.0202	
Ground to excited state transition magnetic dipole moments (Au):						
state	X	Y	Z			
1	6.4342	0	0			
Ground to excited state transition velocity quadrupole moments (Au):						
state	XX	YY	ZZ	XY	XZ	YZ
1	0	0	0	0	0	0.4226
$\langle 0 \text{del} b\rangle * \langle b \text{rxdel} 0\rangle + \langle 0 \text{del} b\rangle * \langle b \text{delr+rdel} 0\rangle$						
Rotatory Strengths (R) in cgs (10^{*-40} erg-esu-cm/Gauss)						
state	XX	YY	ZZ	R(velocity)	E-M Angle	
1	0	-1146.9255	-1005.5563	-717.494	90	
$1/2[\langle 0 r b\rangle * \langle b \text{rxdel} 0\rangle + (\langle 0 \text{rxdel} b\rangle * \langle b r 0\rangle)^*]$						
Rotatory Strengths (R) in cgs (10^{*-40} erg-esu-cm/Gauss)						
state	XX	YY	ZZ	R(length)		
1	-2045.0074	0	0	-681.6691		
$1/2[\langle 0 \text{del} b\rangle * \langle b r 0\rangle + (\langle 0 r b\rangle * \langle b \text{del} 0\rangle)^*]$ (Au)						
state	X	Y	Z	Dip. S.	Osc.(frdel)	
1	-0.0288	0	0	0.0288	0.0192	

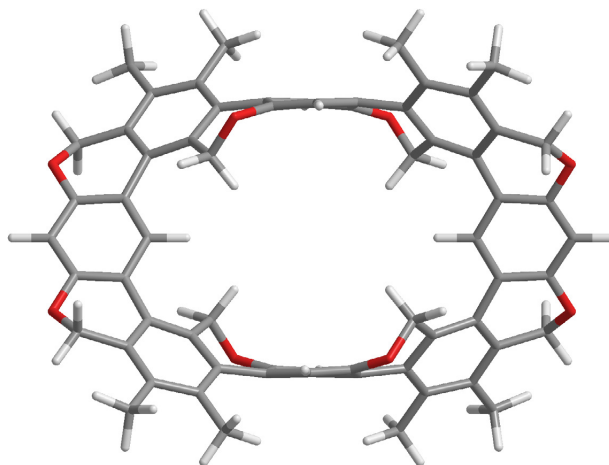
Table S18. Transition moments of (M,M,M)-12.

Ground to excited state transition electric dipole moments (Au):						
state	X	Y	Z	Dip. S.	Osc.	
1	0	0	-1.2841	1.6488	0.1403	
Ground to excited state transition velocity dipole moments (Au):						
state	X	Y	Z	Dip. S.	Osc.	
1	0	0	0.1652	0.0273	0.1425	
Ground to excited state transition magnetic dipole moments (Au):						
state	X	Y	Z			
1	0	0	-8.9042			
Ground to excited state transition velocity quadrupole moments (Au):						
state	XX	YY	ZZ	XY	XZ	YZ
1	0	0	0	0	0	0
$\langle 0 \text{del} b\rangle * \langle b \text{rxdel} 0\rangle + \langle 0 \text{del} b\rangle * \langle b \text{delr+rdel} 0\rangle$						
Rotatory Strengths (R) in cgs (10^{*-40} erg-esu-cm/Gauss)						
state	XX	YY	ZZ	R(velocity)	E-M Angle	
1	-4074.8698	-4074.8405	0	-2716.5701	90	
$1/2[\langle 0 r b\rangle * \langle b \text{rxdel} 0\rangle + (\langle 0 \text{rxdel} b\rangle * \langle b r 0\rangle)^*]$						
Rotatory Strengths (R) in cgs (10^{*-40} erg-esu-cm/Gauss)						
state	XX	YY	ZZ	R(length)		
1	0	0	-8085.4005	-2695.1335		
$1/2[\langle 0 \text{del} b\rangle * \langle b r 0\rangle + (\langle 0 r b\rangle * \langle b \text{del} 0\rangle)^*]$ (Au)						
state	X	Y	Z	Dip. S.	Osc.(frdel)	
1	0	0	-0.2121	0.2121	0.1414	

Table S19. Transition moments of (*P,M,M*)-13.

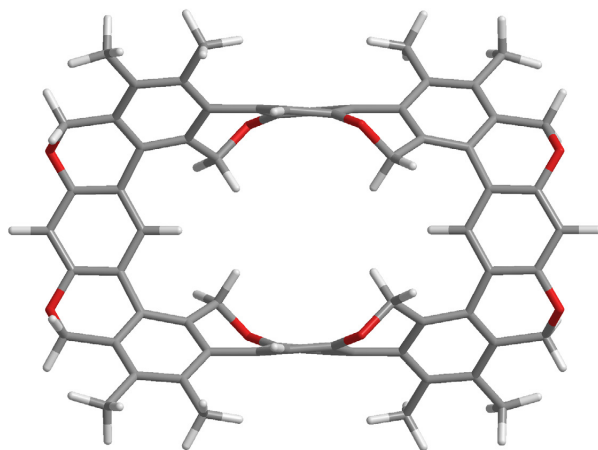
Ground to excited state transition electric dipole moments (Au):						
state	X	Y	Z	Dip. S.	Osc.	
1	0.7402	1.5846	0	3.0587	0.2557	
Ground to excited state transition velocity dipole moments (Au):						
state	X	Y	Z	Dip. S.	Osc.	
1	-0.093	-0.1952	0	0.0467	0.2484	
Ground to excited state transition magnetic dipole moments (Au):						
state	X	Y	Z			
1	-6.1388	1.0624	0			
Ground to excited state transition velocity quadrupole moments (Au):						
state	XX	YY	ZZ	XY	XZ	YZ
1	0	0	0	0	1.7957	1.7248
$\langle 0 \text{del} b\rangle * \langle b \text{rxdel} 0\rangle + \langle 0 \text{del} b\rangle * \langle b \text{delr+rdel} 0\rangle$						
Rotatory Strengths (R) in cgs (10^{*-40} erg-esu-cm/Gauss)						
state	XX	YY	ZZ	R(velocity)	E-M Angle	
1	403.4902	1157.2382	488.9879	683.2387	74.34	
$1/2[\langle 0 r b\rangle * \langle b \text{rxdel} 0\rangle + (\langle 0 \text{rxdel} b\rangle * \langle b r 0\rangle)^*]$						
Rotatory Strengths (R) in cgs (10^{*-40} erg-esu-cm/Gauss)						
state	XX	YY	ZZ	R(length)		
1	3213.1625	-1190.4834	0	674.2264		
$1/2[\langle 0 \text{del} b\rangle * \langle b r 0\rangle + (\langle 0 r b\rangle * \langle b \text{del} 0\rangle)^*]$ (Au)						
state	X	Y	Z	Dip. S.	Osc.(frdel)	
1	-0.0688	-0.3092	0	0.3781	0.252	

Table S20. Cartesian coordinates of optimized (*M,M*)-**10** [B3LYP/6-31g(d) level of theory].



C	-0.90719	2.345465	4.681628	C	2.928698	5.47344	-2.47721
C	-0.39233	2.766371	3.450523	C	-0.56005	-1.06333	-6.76854
C	0.960912	2.340806	2.914633	C	-0.45243	-1.13131	-5.36747
O	1.572851	3.439606	2.212055	C	-0.90719	-2.34547	-4.68163
O	-1.17876	2.091261	7.423865	C	-0.39233	-2.76637	-3.45052
C	-2.29778	2.651934	6.699641	C	0.960912	-2.34081	-2.91463
C	-1.94432	3.078665	5.283653	O	1.572851	-3.43961	-2.21206
C	-2.589	4.10504	4.577958	O	-1.17876	-2.09126	-7.42387
C	-3.72967	4.887966	5.195481	C	-2.29778	-2.65193	-6.69964
C	0.799965	3.751553	1.115273	C	-1.94432	-3.07867	-5.28365
C	1.394383	3.831664	-0.14054	C	-2.589	-4.10504	-4.57796
C	0.594201	3.856786	-1.29307	C	-3.72967	-4.88797	-5.19548
C	-0.79997	3.751553	-1.11527	C	0.799965	-3.75155	-1.11527
C	-1.39438	3.831664	0.140537	C	1.394383	-3.83166	0.140537
C	-0.5942	3.856786	1.293073	C	0.594201	-3.85679	1.293073
C	-1.10221	3.709505	2.682174	C	-0.79997	-3.75155	1.115273
C	1.102208	3.709505	-2.68217	C	-1.39438	-3.83166	-0.14054
C	-2.20065	4.391377	3.243981	C	-0.5942	-3.85679	-1.29307
C	2.200648	4.391377	-3.24398	C	-1.10221	-3.70951	-2.68217
C	0.907194	2.345465	-4.68163	C	1.102208	-3.70951	2.682174
C	0.392327	2.766371	-3.45052	C	-2.20065	-4.39138	-3.24398
C	-0.96091	2.340806	-2.91463	C	2.200648	-4.39138	3.243981
O	-1.57285	3.439606	-2.21206	C	0.560046	-1.06333	6.768543
O	1.178758	2.091261	-7.42387	C	0.452428	-1.13131	5.367473
C	2.297784	2.651934	-6.69964	C	0.907194	-2.34547	4.681628
C	1.944315	3.078665	-5.28365	C	0.392327	-2.76637	3.450523
C	2.588997	4.10504	-4.57796	C	-0.96091	-2.34081	2.914633
C	3.729672	4.887966	-5.19548	O	-1.57285	-3.43961	2.212055
C	-2.9287	5.47344	2.477205	O	1.178758	-2.09126	7.423865

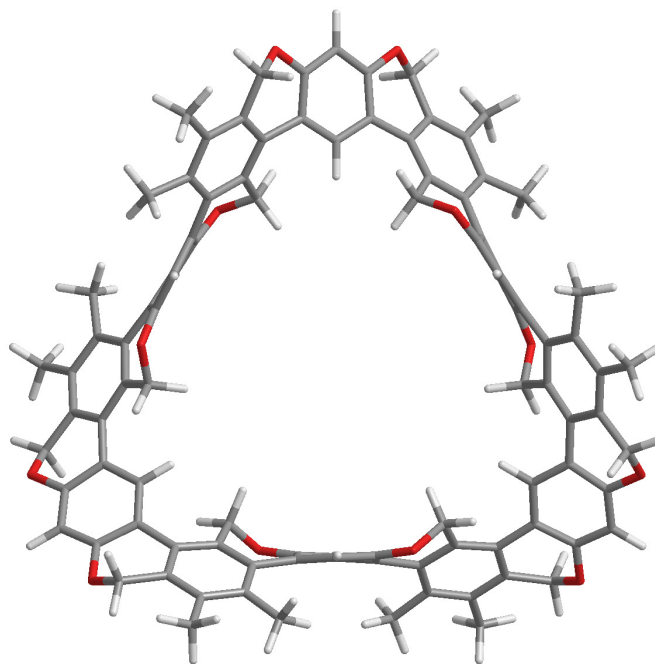
C	2.297784	-2.65193	6.699641	H	-3.93111	5.151624	2.161288
C	1.944315	-3.07867	5.283653	H	-2.38069	5.770625	1.581824
C	2.588997	-4.10504	4.577958	H	3.067756	6.369145	-3.09305
C	3.729672	-4.88797	5.195481	H	3.93111	5.151624	-2.16129
C	-2.9287	-5.47344	-2.47721	H	2.380692	5.770625	-1.58182
C	2.928698	-5.47344	2.477205	H	1.640553	-2.08859	-3.7307
C	0	0	-7.48366	H	0.912035	-1.48293	-2.22602
C	0.560046	1.063333	-6.76854	H	-2.61124	-3.49697	-7.31321
C	0.452428	1.131305	-5.36747	H	-3.11035	-1.90759	-6.69959
C	0	0	-4.68866	H	-4.61552	-4.8757	-4.54979
C	0	0	4.688661	H	-3.46255	-5.94279	-5.3432
C	-0.45243	1.131305	5.367473	H	-4.03656	-4.4913	-6.16519
C	-0.56005	1.063333	6.768543	H	2.47434	-3.75312	0.208912
C	0	0	7.483662	H	-2.47434	-3.75312	-0.20891
H	1.640553	2.088588	3.730699	H	-1.64055	-2.08859	3.730699
H	0.912035	1.482926	2.226024	H	-0.91204	-1.48293	2.226024
H	-2.61124	3.49697	7.313211	H	2.611241	-3.49697	7.313211
H	-3.11035	1.907587	6.699586	H	3.110347	-1.90759	6.699586
H	-4.03656	4.491301	6.165187	H	4.615524	-4.8757	4.549787
H	-3.46255	5.942794	5.343195	H	4.036563	-4.4913	6.165187
H	-4.61552	4.875704	4.549787	H	3.462545	-5.94279	5.343195
H	2.47434	3.753124	-0.20891	H	-3.06776	-6.36915	-3.09305
H	-2.47434	3.753124	0.208912	H	-3.93111	-5.15162	-2.16129
H	-1.64055	2.088588	-3.7307	H	-2.38069	-5.77063	-1.58182
H	-0.91204	1.482926	-2.22602	H	3.067756	-6.36915	3.093054
H	2.611241	3.49697	-7.31321	H	2.380692	-5.77063	1.581824
H	3.110347	1.907587	-6.69959	H	3.93111	-5.15162	2.161288
H	4.615524	4.875704	-4.54979	H	0	0	-8.56813
H	3.462545	5.942794	-5.3432	H	0	0	-3.60548
H	4.036563	4.491301	-6.16519	H	0	0	3.605481
H	-3.06776	6.369145	3.093054	H	0	0	8.568131

Table S21. Cartesian coordinates of optimized (*P,M*)-**11** [B3LYP/6-31g(d) level of theory].

C	-0.47881	4.876892	2.487021	C	-2.00641	-3.01151	5.51721
C	-0.6043	3.506006	2.744908	C	0.983206	-6.92547	-1.19921
C	-1.69243	2.626205	2.165539	C	0.90461	-5.52176	-1.22691
O	-2.12907	1.679598	3.164152	C	0.478805	-4.87689	-2.48702
O	-0.8622	7.610951	2.380903	C	0.604301	-3.50601	-2.74491
C	0.259511	7.165749	3.163053	C	1.692428	-2.62621	-2.16554
C	0.293349	5.660448	3.367826	O	2.129068	-1.6796	-3.16415
C	1.08184	5.059691	4.359765	O	0.862204	-7.61095	-2.3809
C	1.938095	5.89894	5.287	C	-0.25951	-7.16575	-3.16305
C	-1.08727	0.840964	3.490928	C	-0.29335	-5.66045	-3.36783
C	-1.2988	-0.53054	3.591181	C	-1.08184	-5.05969	-4.35977
C	-0.1973	-1.39917	3.645677	C	-1.9381	-5.89894	-5.287
C	1.087266	-0.84096	3.490928	C	1.087266	-0.84096	-3.49093
C	1.298796	0.53054	3.591181	C	1.298796	0.53054	-3.59118
C	0.197304	1.399168	3.645677	C	0.197304	1.399168	-3.64568
C	0.273071	2.878959	3.649523	C	-1.08727	0.840964	-3.49093
C	-0.27307	-2.87896	3.649523	C	-1.2988	-0.53054	-3.59118
C	1.119492	3.65034	4.471372	C	-0.1973	-1.39917	-3.64568
C	-1.11949	-3.65034	4.471372	C	-0.27307	-2.87896	-3.64952
C	0.478805	-4.87689	2.487021	C	0.273071	2.878959	-3.64952
C	0.604301	-3.50601	2.744908	C	-1.11949	-3.65034	-4.47137
C	1.692428	-2.62621	2.165539	C	1.119492	3.65034	-4.47137
O	2.129068	-1.6796	3.164152	C	-0.98321	6.92547	-1.19921
O	0.862204	-7.61095	2.380903	C	-0.90461	5.521755	-1.22691
C	-0.25951	-7.16575	3.163053	C	-0.47881	4.876892	-2.48702
C	-0.29335	-5.66045	3.367826	C	-0.6043	3.506006	-2.74491
C	-1.08184	-5.05969	4.359765	C	-1.69243	2.626205	-2.16554
C	-1.9381	-5.89894	5.287	O	-2.12907	1.679598	-3.16415
C	2.006409	3.011513	5.51721	O	-0.8622	7.610951	-2.3809

C	0.259511	7.165749	-3.16305	H	1.742019	1.967008	5.687902
C	0.293349	5.660448	-3.36783	H	1.925858	3.535776	6.475995
C	1.08184	5.059691	-4.35977	H	-3.0673	-3.04107	5.23118
C	1.938095	5.89894	-5.287	H	-1.74202	-1.96701	5.687902
C	-2.00641	-3.01151	-5.51721	H	-1.92586	-3.53578	6.475995
C	2.006409	3.011513	-5.51721	H	2.574364	-3.213	-1.90189
C	1.06469	-7.63142	0	H	1.371311	-2.05744	-1.27845
C	0.983206	-6.92547	1.199214	H	-0.14871	-7.68905	-4.11513
C	0.90461	-5.52176	1.226912	H	-1.18612	-7.52541	-2.68492
C	0.877033	-4.84558	0	H	-2.96853	-5.52794	-5.32093
C	-0.87703	4.845578	0	H	-1.55998	-5.87494	-6.31812
C	-0.90461	5.521755	1.226912	H	-1.98646	-6.94672	-4.98373
C	-0.98321	6.92547	1.199214	H	2.312194	0.913369	-3.52915
C	-1.06469	7.631424	0	H	-2.31219	-0.91337	-3.52915
H	-2.57436	3.212999	1.901891	H	-2.57436	3.212999	-1.90189
H	-1.37131	2.05744	1.278447	H	-1.37131	2.05744	-1.27845
H	1.186122	7.525409	2.684918	H	0.14871	7.689053	-4.11513
H	0.14871	7.689053	4.115126	H	1.186122	7.525409	-2.68492
H	1.559982	5.874941	6.31812	H	2.968533	5.527942	-5.32093
H	1.986457	6.946715	4.983725	H	1.559982	5.874941	-6.31812
H	2.968533	5.527942	5.32093	H	1.986457	6.946715	-4.98373
H	-2.31219	-0.91337	3.529147	H	-3.0673	-3.04107	-5.23118
H	2.312194	0.913369	3.529147	H	-1.74202	-1.96701	-5.6879
H	2.574364	-3.213	1.901891	H	-1.92586	-3.53578	-6.476
H	1.371311	-2.05744	1.278447	H	3.067299	3.041067	-5.23118
H	-0.14871	-7.68905	4.115126	H	1.742019	1.967008	-5.6879
H	-1.18612	-7.52541	2.684918	H	1.925858	3.535776	-6.476
H	-2.96853	-5.52794	5.32093	H	1.071649	-8.71571	0
H	-1.55998	-5.87494	6.31812	H	0.668807	-3.78214	0
H	-1.98646	-6.94672	4.983725	H	-0.66881	3.782136	0
H	3.067299	3.041067	5.23118	H	-1.07165	8.715706	0

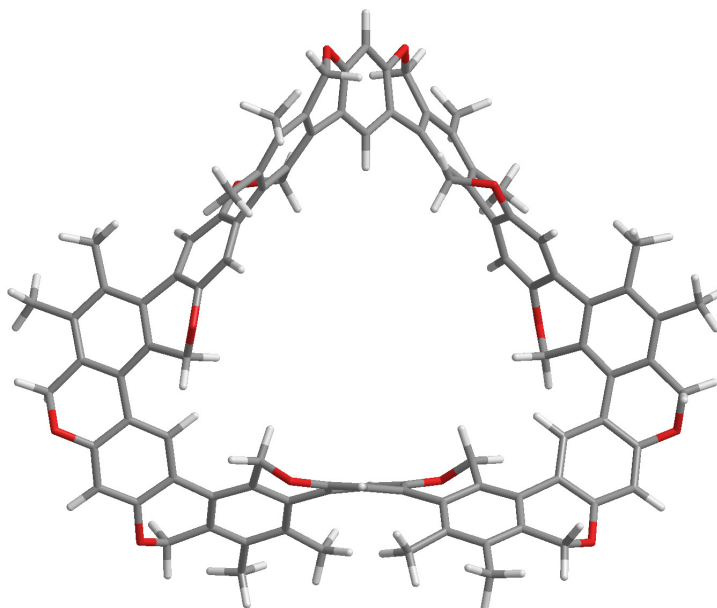
Table S22. Cartesian coordinates of optimized (*M,M,M*)-**12** [B3LYP/6-31g(d) level of theory].



C	-2.25671	-7.00543	-1.18612	C	-8.06528	1.33838	2.2741
C	-2.84076	-5.83757	-0.67478	C	-8.11442	0.104236	2.93289
C	-2.45913	-5.23203	0.658534	C	-9.00408	-0.08892	4.146973
O	-3.63284	-4.82714	1.380574	C	-5.7455	-5.30754	-3.14383
O	-1.87077	-9.73638	-1.46727	C	-7.46922	-2.32198	3.143833
C	-2.2958	-9.00678	-2.63528	C	-7.35759	5.360867	-0.7123
C	-2.87357	-7.65393	-2.2741	C	-6.09441	4.738052	-0.62037
C	-3.96694	-7.07941	-2.93289	C	-8.4553	4.88167	0
C	-4.57905	-7.7533	-4.14697	C	-8.32144	3.691423	0.712298
C	-4.35595	-3.89252	0.686046	C	-7.15048	2.908891	0.620372
C	-4.99716	-2.882	1.395652	C	-6.03487	3.484234	0
C	-5.67509	-1.85611	0.719304	C	-4.93852	5.457081	-1.18612
C	-5.54899	-1.8261	-0.68605	C	-3.63511	5.378955	-0.67478
C	-4.99446	-2.88667	-1.39565	C	-3.30151	4.745681	0.658534
C	-4.44499	-3.98671	-0.7193	O	-2.36401	5.559702	1.380574
C	-3.92363	-5.22643	-1.34462	O	-7.49657	6.488322	-1.46727
C	-6.48804	-0.78475	1.344623	C	-6.6522	6.491606	-2.63528
C	-4.50378	-5.85454	-2.47092	C	-5.19171	6.31555	-2.2741
C	-7.32208	-0.97312	2.470922	C	-4.14748	6.975171	-2.93289
C	-7.19523	1.548344	1.186124	C	-4.42503	7.842221	-4.14697
C	-6.47586	0.458616	0.674775	C	-1.19304	5.718621	0.686046
C	-5.76063	0.486347	-0.65853	C	0.002696	5.768667	1.395652
O	-5.99685	-0.73256	-1.38057	C	1.230102	5.842829	0.719304
O	-9.36734	3.248061	1.467269	C	1.193044	5.718621	-0.68605
C	-8.948	2.515172	2.635278	C	-0.0027	5.768667	-1.39565

C	-1.2301	5.842829	-0.7193	C	2.840759	-5.83757	0.674775
C	-2.56441	6.011179	-1.34462	C	2.459127	-5.23203	-0.65853
C	2.564408	6.011179	1.344623	O	3.632839	-4.82714	-1.38057
C	-2.81829	6.827663	-2.47092	O	1.870765	-9.73638	1.467269
C	2.818291	6.827663	2.470922	C	2.295795	-9.00678	2.635278
C	4.938522	5.457081	1.186124	C	2.87357	-7.65393	2.2741
C	3.635105	5.378955	0.674775	C	3.966936	-7.07941	2.93289
C	3.301506	4.745681	-0.65853	C	4.579048	-7.7533	4.146973
O	2.364008	5.559702	-1.38057	C	7.469216	-2.32198	-3.14383
O	7.496573	6.488322	1.467269	C	5.745503	-5.30754	3.143833
C	6.652202	6.491606	2.635278	C	-0.96385	-9.05229	-0.7123
C	5.191713	6.31555	2.2741	C	-1.05607	-7.64694	-0.62037
C	4.147479	6.975171	2.93289	C	0	-9.76334	0
C	4.425029	7.842221	4.146973	C	0.963853	-9.05229	0.712298
C	-1.72371	7.629522	-3.14383	C	1.056067	-7.64694	0.620372
C	1.723713	7.629522	3.143833	C	0	-6.96847	0
C	8.32144	3.691423	-0.7123	H	-1.96426	-5.96038	1.300693
C	7.150479	2.908891	-0.62037	H	-1.80005	-4.3548	0.550556
C	8.4553	4.88167	0	H	-3.03289	-9.65762	-3.10419
C	7.357586	5.360867	0.712298	H	-1.43294	-8.91271	-3.31462
C	6.094413	4.738052	0.620372	H	-4.79957	-7.02539	-4.93397
C	6.03487	3.484234	0	H	-3.91455	-8.49936	-4.58751
C	7.195232	1.548344	-1.18612	H	-5.5244	-8.25822	-3.90484
C	6.475864	0.458616	-0.67478	H	-4.92772	-2.89572	2.477091
C	5.760633	0.486347	0.658534	H	-4.97162	-2.81967	-2.47709
O	5.996847	-0.73256	1.380574	H	-6.14397	1.279091	-1.30069
O	9.367338	3.248061	-1.46727	H	-4.6714	0.618511	-0.55056
C	8.947997	2.515172	-2.63528	H	-9.88019	2.202249	3.104194
C	8.065283	1.33838	-2.2741	H	-8.4351	3.215394	3.31462
C	8.114415	0.104236	-2.93289	H	-8.48396	-0.64386	4.933973
C	9.004077	-0.08892	-4.14697	H	-9.31794	0.859577	4.587509
C	5.548993	-1.8261	0.686046	H	-9.91403	-0.65516	3.904837
C	4.994464	-2.88667	1.395652	H	-6.32671	-4.68035	-2.46648
C	4.444987	-3.98671	0.719304	H	-5.50934	-4.69992	-4.02905
C	4.355949	-3.89252	-0.68605	H	-6.3979	-6.11757	-3.48187
C	4.99716	-2.882	-1.39565	H	-7.21666	-3.13891	2.466475
C	5.675089	-1.85611	-0.7193	H	-6.82493	-2.42127	4.029052
C	6.488038	-0.78475	-1.34462	H	-8.49693	-2.48196	3.481872
C	3.92363	-5.22643	1.344623	H	-9.39431	5.42381	0
C	7.322075	-0.97312	-2.47092	H	-5.09558	2.941936	0
C	4.503784	-5.85454	2.470922	H	-4.17971	4.68129	1.300693
C	2.25671	-7.00543	1.186124	H	-2.87134	3.736293	0.550556

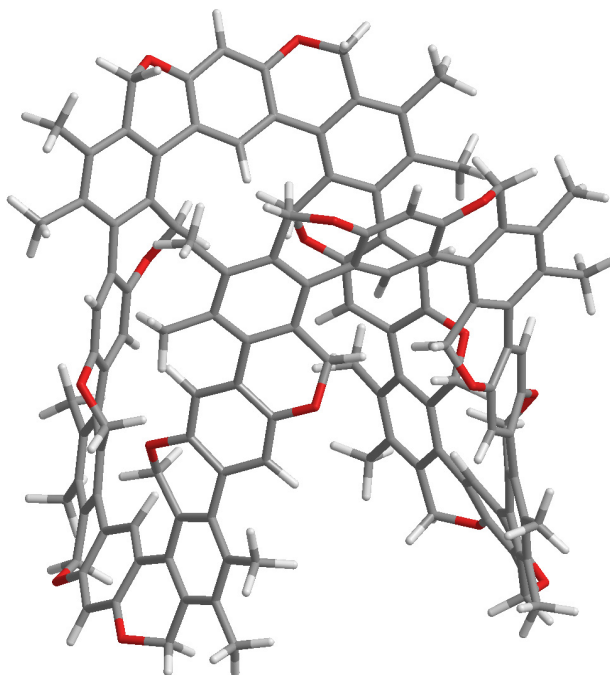
H	-6.8473	7.455373	-3.10419	H	4.671397	0.618511	0.550556
H	-7.00216	5.697313	-3.31462	H	9.880192	2.202249	-3.10419
H	-3.68438	7.669249	-4.93397	H	8.435099	3.215394	-3.31462
H	-5.40338	7.639781	-4.58751	H	8.483955	-0.64386	-4.93397
H	-4.38963	8.913383	-3.90484	H	9.317936	0.859577	-4.58751
H	-0.0439	5.715389	2.477091	H	9.914032	-0.65516	-3.90484
H	0.043905	5.715389	-2.47709	H	4.971624	-2.81967	2.477091
H	4.179712	4.68129	-1.30069	H	4.927719	-2.89572	-2.47709
H	2.871345	3.736293	-0.55056	H	1.96426	-5.96038	-1.30069
H	6.847299	7.455373	3.104194	H	1.800052	-4.3548	-0.55056
H	7.002163	5.697313	3.31462	H	3.032893	-9.65762	3.104194
H	5.403384	7.639781	4.587509	H	1.432936	-8.91271	3.31462
H	3.684381	7.669249	4.933973	H	3.914552	-8.49936	4.587509
H	4.389631	8.913383	3.904837	H	4.799575	-7.02539	4.933973
H	-0.88995	7.819267	-2.46648	H	5.524401	-8.25822	3.904837
H	-1.31558	7.121194	-4.02905	H	7.216659	-3.13891	-2.46648
H	-2.09902	8.599533	-3.48187	H	6.824926	-2.42127	-4.02905
H	0.889951	7.819267	2.466475	H	8.496925	-2.48196	-3.48187
H	1.315582	7.121194	4.029052	H	6.326709	-4.68035	2.466475
H	2.099022	8.599533	3.481872	H	5.509344	-4.69992	4.029052
H	9.394315	5.42381	0	H	6.397903	-6.11757	3.481872
H	5.095583	2.941936	0	H	0	-10.8476	0
H	6.143972	1.279091	1.300693	H	0	-5.88387	0

Table S23. Cartesian coordinates of optimized (*P,M,M*)-13 [B3LYP/6-31g(d) level of theory].

C	0.016571	7.893052	1.353191	C	5.425425	2.918351	-6.99245
C	0.484911	6.965948	0.410093	C	-0.4088	8.714378	-2.90172
C	1.321692	5.748878	0.74842	C	4.732583	4.328665	-4.55959
O	2.365826	5.567928	-0.23065	C	-1.00186	-0.66037	-8.52155
O	-0.06025	9.998331	3.148883	C	-0.92289	-0.79214	-7.12109
C	-0.77846	10.19452	1.923778	C	0	0	-9.23894
C	-0.45449	9.139513	0.885317	C	1.001859	0.660371	-8.52155
C	-0.61578	9.393	-0.4821	C	0.92289	0.792141	-7.12109
C	-1.17711	10.72021	-0.95696	C	0	0	-6.43669
C	1.841803	5.365485	-1.48494	C	-1.81579	-1.75903	-6.47389
C	2.455581	4.478711	-2.36879	C	-1.43776	-2.5273	-5.36789
C	1.830649	4.151101	-3.5859	C	0.00159	-2.7124	-4.95097
C	0.5178	4.638005	-3.78435	O	0.258722	-4.11815	-4.78493
C	-0.01374	5.642623	-2.98631	O	-2.04617	-1.25162	-9.17345
C	0.682748	6.077457	-1.85289	C	-3.26777	-1.27567	-8.39521
C	0.258935	7.178889	-0.96449	C	-3.07862	-1.96026	-7.05332
C	2.382411	3.332623	-4.69855	C	-4.03146	-2.76582	-6.41501
C	-0.27632	8.400629	-1.42628	C	-5.42542	-2.91835	-6.99245
C	3.696853	3.438424	-5.21152	C	-0.5178	-4.63801	-3.78435
C	1.815788	1.759026	-6.47389	C	0.013741	-5.64262	-2.98631
C	1.437757	2.527302	-5.36789	C	-0.68275	-6.07746	-1.85289
C	-0.00159	2.712397	-4.95097	C	-1.8418	-5.36549	-1.48494
O	-0.25872	4.118154	-4.78493	C	-2.45558	-4.47871	-2.36879
O	2.046171	1.251618	-9.17345	C	-1.83065	-4.1511	-3.5859
C	3.267771	1.275671	-8.39521	C	-2.38241	-3.33262	-4.69855
C	3.078618	1.960256	-7.05332	C	-0.25893	-7.17889	-0.96449
C	4.031459	2.765825	-6.41501	C	-3.69685	-3.43842	-5.21152

C	0.276318	-8.40063	-1.42628	C	-2.59208	6.395834	6.787201
C	-0.01657	-7.89305	1.353191	C	-2.2696	5.008564	6.27327
C	-0.48491	-6.96595	0.410093	C	-2.90444	3.866929	6.774289
C	-1.32169	-5.74888	0.74842	C	-4.0546	4.007611	7.755631
O	-2.36583	-5.56793	-0.23065	C	3.103171	-1.3711	7.02343
O	0.060247	-9.99833	3.148883	C	-3.10317	1.371103	7.02343
C	0.778461	-10.1945	1.923778	C	-0.23912	8.740507	3.658269
C	0.454492	-9.13951	0.885317	C	-0.14289	7.625969	2.800916
C	0.615777	-9.393	-0.4821	C	-0.60076	8.612714	4.994128
C	1.177115	-10.7202	-0.95696	C	-0.9253	7.35204	5.482466
C	-4.73258	-4.32867	-4.55959	C	-0.81104	6.193211	4.687493
C	0.408801	-8.71438	-2.90172	C	-0.43081	6.363473	3.345984
C	0.9253	-7.35204	5.482466	H	1.835941	5.874536	1.702653
C	0.811041	-6.19321	4.687493	H	0.727953	4.821141	0.787101
C	0.600756	-8.61271	4.994128	H	-0.47519	11.1869	1.586397
C	0.239124	-8.74051	3.658269	H	-1.85865	10.22644	2.147736
C	0.142892	-7.62597	2.800916	H	-1.71928	11.24967	-0.17036
C	0.430811	-6.36347	3.345984	H	-0.38695	11.39276	-1.31937
C	1.265719	-4.91705	5.286414	H	-1.87961	10.58035	-1.78399
C	0.794521	-3.64412	4.933823	H	3.393784	4.019088	-2.07683
C	-0.46494	-3.41494	4.131231	H	-0.99315	6.037152	-3.2331
O	-1.28403	-2.42109	4.770939	H	-0.24863	2.201229	-4.00708
O	1.44289	-7.25633	6.744998	H	-0.69309	2.377435	-5.72304
C	2.592081	-6.39583	6.787201	H	3.97714	1.804082	-9.03171
C	2.269604	-5.00856	6.27327	H	3.613094	0.236419	-8.27629
C	2.904435	-3.86693	6.774289	H	6.191541	2.754913	-6.22673
C	4.054602	-4.00761	7.755631	H	5.622967	2.204356	-7.79471
C	-0.63631	-1.22358	4.914011	H	5.593063	3.924285	-7.40025
C	-1.39318	-0.05704	4.969037	H	0.226512	8.070099	-3.51059
C	-0.76651	1.195007	5.0784	H	-1.43962	8.592452	-3.26346
C	0.636305	1.223578	4.914011	H	-0.12268	9.75061	-3.10754
C	1.393185	0.057039	4.969037	H	5.358977	4.826328	-5.30553
C	0.766515	-1.19501	5.0784	H	5.409279	3.760034	-3.90561
C	1.414415	-2.47816	5.437274	H	4.269015	5.104906	-3.94897
C	-1.41441	2.478158	5.437274	H	0	0	-10.3234
C	2.477356	-2.58386	6.36655	H	0	0	-5.35054
C	-2.47736	2.583858	6.36655	H	0.248627	-2.20123	-4.00708
C	-1.26572	4.917047	5.286414	H	0.693092	-2.37744	-5.72304
C	-0.79452	3.644124	4.933823	H	-3.97714	-1.80408	-9.03171
C	0.464936	3.414938	4.131231	H	-3.61309	-0.23642	-8.27629
O	1.284031	2.421086	4.770939	H	-6.19154	-2.75491	-6.22673
O	-1.44289	7.256334	6.744998	H	-5.62297	-2.20436	-7.79471

H	-5.59306	-3.92428	-7.40025	H	3.408081	-6.87012	6.216015
H	0.99315	-6.03715	-3.2331	H	4.853544	-3.29407	7.533842
H	-3.39378	-4.01909	-2.07683	H	4.506166	-5.00162	7.72154
H	-1.83594	-5.87454	1.702653	H	3.740031	-3.82591	8.792789
H	-0.72795	-4.82114	0.787101	H	-2.47228	-0.147	4.93101
H	0.475194	-11.1869	1.586397	H	2.472277	0.146997	4.93101
H	1.858649	-10.2264	2.147736	H	1.083966	4.310937	4.086462
H	1.879614	-10.5803	-1.78399	H	0.252149	3.077217	3.103671
H	0.386949	-11.3928	-1.31937	H	-2.87919	6.37656	7.838864
H	1.719281	-11.2497	-0.17036	H	-3.40808	6.870124	6.216015
H	-5.35898	-4.82633	-5.30553	H	-4.50617	5.00162	7.72154
H	-5.40928	-3.76003	-3.90561	H	-4.85354	3.294067	7.533842
H	-4.26901	-5.10491	-3.94897	H	-3.74003	3.825914	8.792789
H	-0.22651	-8.0701	-3.51059	H	2.393509	-0.54584	7.099681
H	1.439619	-8.59245	-3.26346	H	3.975776	-0.99703	6.469563
H	0.122677	-9.75061	-3.10754	H	3.444537	-1.60282	8.035151
H	0.724104	-9.49188	5.616159	H	-2.39351	0.545839	7.099681
H	0.463726	-5.50376	2.684812	H	-3.97578	0.997028	6.469563
H	-1.08397	-4.31094	4.086462	H	-3.44454	1.60282	8.035151
H	-0.25215	-3.07722	3.103671	H	-0.7241	9.491882	5.616159
H	2.879187	-6.37656	7.838864	H	-0.46373	5.503758	2.684812

Table S24. Cartesian coordinates of optimized (*P,M,P,M*)-**14** [B3LYP/6-31g(d) level of theory].

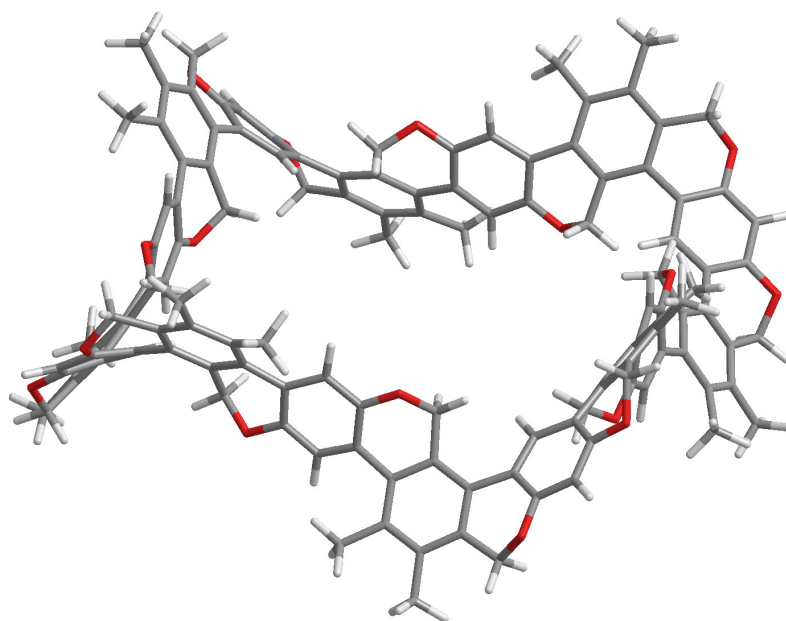
C	-5.19265	4.694952	3.798951	C	-1.85072	5.514149	2.201282
C	-2.5714	5.393764	4.659465	O	-2.48623	6.073603	1.046569
O	-2.35758	6.683847	7.117462	C	-3.44952	5.242341	0.535848
C	-3.33108	5.63489	7.01718	C	3.576196	5.142974	-0.84546
C	-3.64081	5.293385	5.576773	C	4.132931	4.789423	2.869099
C	-4.92837	4.930708	5.165554	C	2.850386	5.206422	3.294906
C	5.192654	4.694952	3.798951	C	1.850719	5.514149	2.201282
C	2.5714	5.393764	4.659465	O	2.486226	6.073603	1.046569
O	2.357579	6.683847	7.117462	C	3.449515	5.242341	0.535848
C	3.331082	5.63489	7.01718	C	4.694952	5.192654	-3.79895
C	3.640814	5.293385	5.576773	C	5.393764	2.5714	-4.65947
C	4.928372	4.930708	5.165554	O	6.683847	2.357579	-7.11746
C	-1.19892	6.394933	6.456437	C	5.63489	3.331082	-7.01718
C	-1.23571	5.714491	5.219655	C	5.293385	3.640814	-5.57677
C	0	6.750664	7.063107	C	4.930708	4.928372	-5.16555
C	1.198921	6.394933	6.456437	C	4.694952	-5.19265	-3.79895
C	1.235711	5.714491	5.219655	C	4.930708	-4.92837	-5.16555
C	0	5.360205	4.650127	C	4.525337	4.281797	-1.41803
C	-5.24234	3.449515	-0.53585	C	4.789423	4.132931	-2.8691
C	-5.14297	3.576196	0.845459	C	5.206422	2.850386	-3.29491
C	-4.2818	4.525337	1.418025	C	5.514149	1.850719	-2.20128
C	-3.5762	5.142974	-0.84546	O	6.073603	2.486226	-1.04657
C	-4.52534	4.281797	-1.41803	C	5.242341	3.449515	-0.53585
C	-4.13293	4.789423	2.869099	C	4.789423	-4.13293	-2.8691
C	-2.85039	5.206422	3.294906	C	5.206422	-2.85039	-3.29491

C	5.514149	-1.85072	-2.20128	C	-4.93071	-4.92837	-5.16555
O	6.073603	-2.48623	-1.04657	C	-4.69495	5.192654	-3.79895
C	5.192654	-4.69495	3.798951	C	-5.39376	2.5714	-4.65947
C	2.5714	-5.39376	4.659465	O	-6.68385	2.357579	-7.11746
O	2.357579	-6.68385	7.117462	C	-5.63489	3.331082	-7.01718
C	3.331082	-5.63489	7.01718	C	-5.29339	3.640814	-5.57677
C	3.640814	-5.29339	5.576773	C	-4.93071	4.928372	-5.16555
C	4.928372	-4.93071	5.165554	C	-6.39493	-1.19892	-6.45644
C	-5.19265	-4.69495	3.798951	C	-5.71449	-1.23571	-5.21966
C	-2.5714	-5.39376	4.659465	C	-6.75066	0	-7.06311
O	-2.35758	-6.68385	7.117462	C	-6.39493	1.198921	-6.45644
C	-3.33108	-5.63489	7.01718	C	-5.71449	1.235711	-5.21966
C	-3.64081	-5.29339	5.576773	C	-5.36021	0	-4.65013
C	-4.92837	-4.93071	5.165554	C	-4.52534	-4.2818	-1.41803
C	1.198921	-6.39493	6.456437	C	-4.78942	-4.13293	-2.8691
C	1.235711	-5.71449	5.219655	C	-5.20642	-2.85039	-3.29491
C	0	-6.75066	7.063107	C	-5.51415	-1.85072	-2.20128
C	-1.19892	-6.39493	6.456437	O	-6.0736	-2.48623	-1.04657
C	-1.23571	-5.71449	5.219655	C	-5.24234	-3.44952	-0.53585
C	0	-5.36021	4.650127	C	-5.20642	2.850386	-3.29491
C	5.142974	-3.5762	0.845459	C	-5.51415	1.850719	-2.20128
C	4.281797	-4.52534	1.418025	O	-6.0736	2.486226	-1.04657
C	3.576196	-5.14297	-0.84546	C	5.242341	-3.44952	-0.53585
C	4.525337	-4.2818	-1.41803	C	-4.78942	4.132931	-2.8691
C	4.132931	-4.78942	2.869099	C	5.142974	3.576196	0.845459
C	2.850386	-5.20642	3.294906	C	4.281797	4.525337	1.418025
C	1.850719	-5.51415	2.201282	C	5.393764	-2.5714	-4.65947
O	2.486226	-6.0736	1.046569	C	6.394933	1.198921	-6.45644
C	3.449515	-5.24234	0.535848	C	5.714491	1.235711	-5.21966
C	-5.14297	-3.5762	0.845459	C	6.750664	0	-7.06311
C	-4.2818	-4.52534	1.418025	C	6.394933	-1.19892	-6.45644
C	-3.5762	-5.14297	-0.84546	C	5.714491	-1.23571	-5.21966
C	-4.13293	-4.78942	2.869099	C	5.360205	0	-4.65013
C	-2.85039	-5.20642	3.294906	C	5.63489	-3.33108	-7.01718
C	-1.85072	-5.51415	2.201282	C	5.293385	-3.64081	-5.57677
O	-2.48623	-6.0736	1.046569	O	6.683847	-2.35758	-7.11746
C	-3.44952	-5.24234	0.535848	H	-5.03788	7.31736	-3.97594
C	-4.69495	-5.19265	-3.79895	H	-3.96687	-6.72242	-5.91297
C	-5.39376	-2.5714	-4.65947	C	-4.44783	6.624485	-3.36885
O	-6.68385	-2.35758	-7.11746	H	-5.66684	4.55424	7.182112
C	-5.63489	-3.33108	-7.01718	H	6.722415	3.96687	5.912973
C	-5.29339	-3.64081	-5.57677	H	5.666835	-4.55424	7.182112

C	-6.04548	4.781823	6.183002	H	6.274429	1.141484	-2.52725
H	-6.92561	3.396095	3.475148	H	4.619717	-1.28699	-1.88696
H	-4.55424	5.666835	-7.18211	H	6.274429	-1.14148	-2.52725
H	4.55424	5.666835	-7.18211	H	4.203677	-6.02432	7.540682
C	-6.62449	4.447828	3.36885	H	2.958922	-4.75731	7.572599
H	-5.66684	-4.55424	7.182112	H	-4.20368	-6.02432	7.540682
H	3.396095	6.925606	-3.47515	H	-2.95892	-4.75731	7.572599
H	6.784251	4.727653	2.326782	H	0	-7.24254	8.02899
C	6.045478	4.781823	6.183002	H	0	-4.73393	3.766919
H	4.55424	-5.66684	-7.18211	H	5.727825	-2.90038	1.457182
C	6.624485	4.447828	3.36885	H	2.900377	-5.72783	-1.45718
C	4.781823	6.045478	-6.183	H	1.286989	-4.61972	1.886958
C	4.447828	6.624485	-3.36885	H	1.141484	-6.27443	2.527246
H	6.784251	-4.72765	2.326782	H	-5.72783	-2.90038	1.457182
H	4.727653	-6.78425	-2.32678	H	-2.90038	-5.72783	-1.45718
C	4.447828	-6.62449	-3.36885	H	-1.28699	-4.61972	1.886958
C	6.045478	-4.78182	6.183002	H	-1.14148	-6.27443	2.527246
C	6.624485	-4.44783	3.36885	H	-6.02432	-4.20368	-7.54068
C	-6.04548	-4.78182	6.183002	H	-4.75731	-2.95892	-7.5726
H	-4.72765	-6.78425	-2.32678	H	-6.02432	4.203677	-7.54068
H	-7.31736	-5.03788	3.97594	H	-4.75731	2.958922	-7.5726
C	-6.62449	-4.44783	3.36885	H	-7.24254	0	-8.02899
C	-4.78182	-6.04548	-6.183	H	-4.73393	0	-3.76692
C	-4.44783	-6.62449	-3.36885	H	-4.61972	-1.28699	-1.88696
C	-4.78182	6.045478	-6.183	H	-6.27443	-1.14148	-2.52725
C	4.781823	-6.04548	-6.183	H	-4.61972	1.286989	-1.88696
H	-4.20368	6.024316	7.540682	H	-6.27443	1.141484	-2.52725
H	-2.95892	4.757309	7.572599	H	5.727825	2.900377	1.457182
H	4.203677	6.024316	7.540682	H	7.24254	0	-8.02899
H	2.958922	4.757309	7.572599	H	4.733929	0	-3.76692
H	0	7.24254	8.02899	H	6.024316	-4.20368	-7.54068
H	0	4.733929	3.766919	H	4.757309	-2.95892	-7.5726
H	-5.72783	2.900377	1.457182	H	-3.3961	6.925606	-3.47515
H	-2.90038	5.727825	-1.45718	H	-4.72765	6.784251	-2.32678
H	-1.28699	4.619717	1.886958	H	-6.72242	3.96687	5.912973
H	-1.14148	6.274429	2.527246	H	-6.65522	5.692887	6.263125
H	2.900377	5.727825	-1.45718	H	-6.78425	4.727653	2.326782
H	1.286989	4.619717	1.886958	H	-7.31736	5.037878	3.97594
H	1.141484	6.274429	2.527246	H	6.655224	5.692887	6.263125
H	6.024316	4.203677	-7.54068	H	5.666835	4.55424	7.182112
H	4.757309	2.958922	-7.5726	H	6.925606	3.396095	3.475148
H	4.619717	1.286989	-1.88696	H	7.31736	5.037878	3.97594

H	5.692887	6.655224	-6.26313	H	-6.72242	-3.96687	5.912973
H	3.96687	6.722415	-5.91297	H	-6.78425	-4.72765	2.326782
H	4.727653	6.784251	-2.32678	H	-6.92561	-3.3961	3.475148
H	5.037878	7.31736	-3.97594	H	-5.69289	-6.65522	-6.26313
H	5.037878	-7.31736	-3.97594	H	-4.55424	-5.66684	-7.18211
H	3.396095	-6.92561	-3.47515	H	-3.3961	-6.92561	-3.47515
H	6.655224	-5.69289	6.263125	H	-5.03788	-7.31736	-3.97594
H	6.722415	-3.96687	5.912973	H	-5.69289	6.655224	-6.26313
H	6.925606	-3.3961	3.475148	H	-3.96687	6.722415	-5.91297
H	7.31736	-5.03788	3.97594	H	5.692887	-6.65522	-6.26313
H	-6.65522	-5.69289	6.263125	H	3.96687	-6.72242	-5.91297

Table S25. Cartesian coordinates of optimized (*M,M,M,M*)-isomer of **14** [B3LYP/6-31g(d) level of theory].



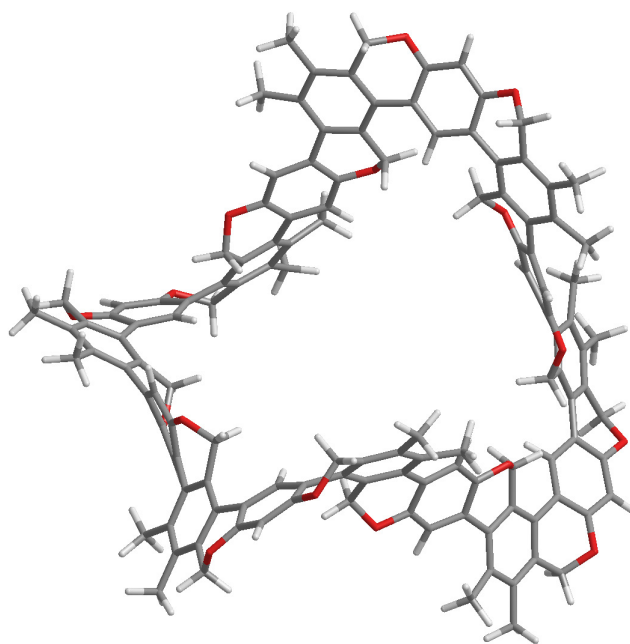
C	9.163323	2.200993	1.32756	C	2.730564	9.826392	-2.45403
C	8.057432	2.896126	0.811936	C	3.859883	9.342666	-3.12207
C	7.409454	2.555661	-0.51125	C	4.352516	10.02511	-4.38593
O	7.166161	3.739168	-1.28343	C	7.831631	5.862489	3.266432
O	11.8733	1.704739	1.642313	C	5.862489	7.831631	-3.26643
C	11.12179	2.044671	2.822926	C	-0.89071	11.179	0.799055
C	9.826392	2.730564	2.454028	C	-1.00488	9.772457	0.705895
C	9.342666	3.859883	3.122067	C	0	11.88875	0
C	10.02511	4.352516	4.385926	C	0.890705	11.179	-0.79906
C	6.383581	4.648976	-0.62638	C	1.004883	9.772457	-0.7059
C	5.579284	5.48969	-1.38953	C	0	9.093698	0
C	4.757964	6.451558	-0.77978	C	-2.20099	9.163323	1.32756
C	4.648976	6.383581	0.626378	C	-2.89613	8.057432	0.811936
C	5.48969	5.579284	1.389529	C	-2.55566	7.409454	-0.51125
C	6.451558	4.757964	0.779783	O	-3.73917	7.166161	-1.28343
C	7.562201	4.050777	1.463455	O	-1.70474	11.8733	1.642313
C	4.050777	7.562201	-1.46346	C	-2.04467	11.12179	2.822926
C	8.218796	4.550468	2.614718	C	-2.73056	9.826392	2.454028
C	4.550468	8.218796	-2.61472	C	-3.85988	9.342666	3.122067
C	2.200993	9.163323	-1.32756	C	-4.35252	10.02511	4.385926
C	2.896126	8.057432	-0.81194	C	-4.64898	6.383581	-0.62638
C	2.555661	7.409454	0.511247	C	-5.48969	5.579284	-1.38953
O	3.739168	7.166161	1.283427	C	-6.45156	4.757964	-0.77978
O	1.704739	11.8733	-1.64231	C	-6.38358	4.648976	0.626378
C	2.044671	11.12179	-2.82293	C	-5.57928	5.48969	1.389529

C	-4.75796	6.451558	0.779783	C	-2.89613	-8.05743	-0.81194
C	-4.05078	7.562201	1.463455	C	-2.55566	-7.40945	0.511247
C	-7.5622	4.050777	-1.46346	O	-3.73917	-7.16616	1.283427
C	-4.55047	8.218796	2.614718	O	-1.70474	-11.8733	-1.64231
C	-8.2188	4.550468	-2.61472	C	-2.04467	-11.1218	-2.82293
C	-9.16332	2.200993	-1.32756	C	-2.73056	-9.82639	-2.45403
C	-8.05743	2.896126	-0.81194	C	-3.85988	-9.34267	-3.12207
C	-7.40945	2.555661	0.511247	C	-4.35252	-10.0251	-4.38593
O	-7.16616	3.739168	1.283427	C	-7.83163	-5.86249	3.266432
O	-11.8733	1.704739	-1.64231	C	-5.86249	-7.83163	-3.26643
C	-11.1218	2.044671	-2.82293	C	0.890705	-11.179	0.799055
C	-9.82639	2.730564	-2.45403	C	1.004883	-9.77246	0.705895
C	-9.34267	3.859883	-3.12207	C	0	-11.8888	0
C	-10.0251	4.352516	-4.38593	C	-0.89071	-11.179	-0.79906
C	-5.86249	7.831631	3.266432	C	-1.00488	-9.77246	-0.7059
C	-7.83163	5.862489	-3.26643	C	0	-9.0937	0
C	-11.179	-0.89071	0.799055	C	2.200993	-9.16332	1.32756
C	-9.77246	-1.00488	0.705895	C	2.896126	-8.05743	0.811936
C	-11.8888	0	0	C	2.555661	-7.40945	-0.51125
C	-11.179	0.890705	-0.79906	O	3.739168	-7.16616	-1.28343
C	-9.77246	1.004883	-0.7059	O	1.704739	-11.8733	1.642313
C	-9.0937	0	0	C	2.044671	-11.1218	2.822926
C	-9.16332	-2.20099	1.32756	C	2.730564	-9.82639	2.454028
C	-8.05743	-2.89613	0.811936	C	3.859883	-9.34267	3.122067
C	-7.40945	-2.55566	-0.51125	C	4.352516	-10.0251	4.385926
O	-7.16616	-3.73917	-1.28343	C	4.648976	-6.38358	-0.62638
O	-11.8733	-1.70474	1.642313	C	5.48969	-5.57928	-1.38953
C	-11.1218	-2.04467	2.822926	C	6.451558	-4.75796	-0.77978
C	-9.82639	-2.73056	2.454028	C	6.383581	-4.64898	0.626378
C	-9.34267	-3.85988	3.122067	C	5.579284	-5.48969	1.389529
C	-10.0251	-4.35252	4.385926	C	4.757964	-6.45156	0.779783
C	-6.38358	-4.64898	-0.62638	C	4.050777	-7.5622	1.463455
C	-5.57928	-5.48969	-1.38953	C	7.562201	-4.05078	-1.46346
C	-4.75796	-6.45156	-0.77978	C	4.550468	-8.2188	2.614718
C	-4.64898	-6.38358	0.626378	C	8.218796	-4.55047	-2.61472
C	-5.48969	-5.57928	1.389529	C	9.163323	-2.20099	-1.32756
C	-6.45156	-4.75796	0.779783	C	8.057432	-2.89613	-0.81194
C	-7.5622	-4.05078	1.463455	C	7.409454	-2.55566	0.511247
C	-4.05078	-7.5622	-1.46346	O	7.166161	-3.73917	1.283427
C	-8.2188	-4.55047	2.614718	O	11.8733	-1.70474	-1.64231
C	-4.55047	-8.2188	-2.61472	C	11.12179	-2.04467	-2.82293
C	-2.20099	-9.16332	-1.32756	C	9.826392	-2.73056	-2.45403

C	9.342666	-3.85988	-3.12207	H	-5.61536	5.376316	2.465659
C	10.02511	-4.35252	-4.38593	H	-8.06131	1.944896	1.133971
C	5.862489	-7.83163	3.266432	H	-6.45249	2.024132	0.376764
C	7.831631	-5.86249	-3.26643	H	-11.7883	2.690918	-3.39193
C	11.179	0.890705	0.799055	H	-10.9509	1.121576	-3.40008
C	9.772457	1.004883	0.705895	H	-9.29257	4.68844	-5.12553
C	11.88875	0	0	H	-10.6157	3.569426	-4.86625
C	11.179	-0.89071	-0.79906	H	-10.6982	5.199265	-4.19226
C	9.772457	-1.00488	-0.7059	H	-6.5571	7.402711	2.542595
C	9.093698	0	0	H	-5.73533	7.093839	4.071154
H	6.452494	2.024132	-0.37676	H	-6.35133	8.70262	3.709411
H	8.061314	1.944896	-1.13397	H	-7.40271	6.5571	-2.5426
H	11.78833	2.690918	3.391931	H	-7.09384	5.735331	-4.07115
H	10.95092	1.121576	3.400079	H	-8.70262	6.351333	-3.70941
H	9.292573	4.68844	5.125526	H	-12.973	0	0
H	10.61566	3.569426	4.866251	H	-8.00872	0	0
H	10.69819	5.199265	4.192256	H	-8.06131	-1.9449	-1.13397
H	5.61536	5.376316	-2.46566	H	-6.45249	-2.02413	-0.37676
H	5.376316	5.61536	2.465659	H	-11.7883	-2.69092	3.391931
H	1.944896	8.061314	1.133971	H	-10.9509	-1.12158	3.400079
H	2.024132	6.452494	0.376764	H	-10.6157	-3.56943	4.866251
H	2.690918	11.78833	-3.39193	H	-9.29257	-4.68844	5.125526
H	1.121576	10.95092	-3.40008	H	-10.6982	-5.19927	4.192256
H	3.569426	10.61566	-4.86625	H	-5.61536	-5.37632	-2.46566
H	4.68844	9.292573	-5.12553	H	-5.37632	-5.61536	2.465659
H	5.199265	10.69819	-4.19226	H	-1.9449	-8.06131	1.133971
H	7.402711	6.5571	2.542595	H	-2.02413	-6.45249	0.376764
H	7.093839	5.735331	4.071154	H	-2.69092	-11.7883	-3.39193
H	8.70262	6.351333	3.709411	H	-1.12158	-10.9509	-3.40008
H	6.5571	7.402711	-2.5426	H	-4.68844	-9.29257	-5.12553
H	5.735331	7.093839	-4.07115	H	-3.56943	-10.6157	-4.86625
H	6.351333	8.70262	-3.70941	H	-5.19927	-10.6982	-4.19226
H	0	12.97298	0	H	-7.40271	-6.5571	2.542595
H	0	8.008719	0	H	-7.09384	-5.73533	4.071154
H	-1.9449	8.061314	-1.13397	H	-8.70262	-6.35133	3.709411
H	-2.02413	6.452494	-0.37676	H	-6.5571	-7.40271	-2.5426
H	-2.69092	11.78833	3.391931	H	-5.73533	-7.09384	-4.07115
H	-1.12158	10.95092	3.400079	H	-6.35133	-8.70262	-3.70941
H	-4.68844	9.292573	5.125526	H	0	-12.973	0
H	-3.56943	10.61566	4.866251	H	0	-8.00872	0
H	-5.19927	10.69819	4.192256	H	1.944896	-8.06131	-1.13397
H	-5.37632	5.61536	-2.46566	H	2.024132	-6.45249	-0.37676

H	2.690918	-11.7883	3.391931	H	10.61566	-3.56943	-4.86625
H	1.121576	-10.9509	3.400079	H	9.292573	-4.68844	-5.12553
H	5.199265	-10.6982	4.192256	H	10.69819	-5.19927	-4.19226
H	4.68844	-9.29257	5.125526	H	5.735331	-7.09384	4.071154
H	3.569426	-10.6157	4.866251	H	6.351333	-8.70262	3.709411
H	5.376316	-5.61536	-2.46566	H	6.5571	-7.40271	2.542595
H	5.61536	-5.37632	2.465659	H	7.402711	-6.5571	-2.5426
H	8.061314	-1.9449	1.133971	H	7.093839	-5.73533	-4.07115
H	6.452494	-2.02413	0.376764	H	8.70262	-6.35133	-3.70941
H	11.78833	-2.69092	-3.39193	H	12.97298	0	0
H	10.95092	-1.12158	-3.40008	H	8.008719	0	0

Table S26. Cartesian coordinates of optimized (*P,M,M,M*)-isomer of **14** [B3LYP/6-31g(d) level of theory].



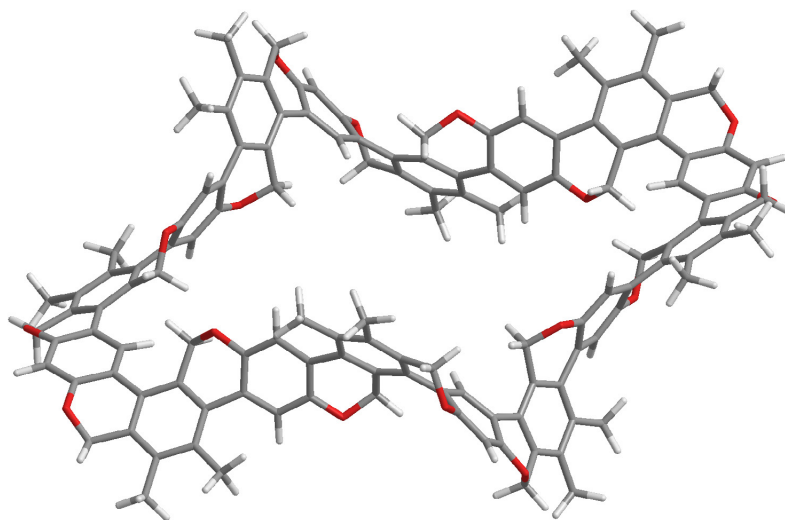
C	4.990551	-6.55972	2.389707	C	-4.09529	-4.8807	-5.13649
C	5.060352	-6.80003	1.012978	C	-3.94752	-6.9684	-3.62306
C	1.797655	-4.73737	7.454912	C	-2.74632	-6.73312	-2.92663
C	1.444759	-3.39593	7.27164	C	-1.67902	-5.76829	-3.40354
C	2.288441	-2.40879	6.499184	O	-0.3537	-6.23151	-3.11185
O	2.445121	-1.20517	7.277465	O	-5.7811	-8.1241	-5.38231
O	3.202911	-6.8618	8.507021	C	-6.00882	-8.33192	-3.98499
C	1.786477	-6.82801	8.778803	C	-4.77616	-8.02102	-3.16867
C	1.179213	-5.4691	8.485588	C	-4.4616	-8.77557	-2.03365
C	0.089253	-4.93863	9.187207	C	-0.15987	-6.49243	-1.7794
C	2.445121	7.451192	-1.74644	C	1.086838	-6.23141	-1.21471
C	3.269142	8.520661	-1.32764	C	1.332477	-6.48815	0.147794
C	3.947518	6.968397	-3.62306	C	-1.01881	-7.15881	0.350767
C	2.746319	6.733122	-2.92663	C	-1.21279	-7.05312	-1.03176
C	1.679021	5.768285	-3.40354	C	-2.44512	-7.45119	-1.74644
O	0.353697	6.23151	-3.11185	C	-3.26914	-8.52066	-1.32764
O	5.781103	8.124098	-5.38231	C	2.647419	-6.43859	0.843662
C	6.00882	8.331918	-3.98499	C	3.8817	-6.76567	0.230295
C	4.776161	8.021022	-3.16867	C	3.778068	-6.19655	3.008275
C	4.4616	8.775566	-2.03365	C	2.603774	-6.18238	2.236527
C	-5.35237	-6.85831	-5.65893	C	1.227303	-6.04113	2.844575
C	-4.4294	-6.20816	-4.80696	O	0.320815	-6.99167	2.278462
C	-5.90437	-6.23179	-6.76829	O	5.721029	-7.48519	4.516391
C	-5.55611	-4.91734	-7.04681	C	6.146171	-6.75664	3.344554
C	-4.60129	-4.22155	-6.27254	C	3.498221	-6.50664	7.220819

C	2.771242	-5.45933	6.619819	C	-3.8817	6.765673	0.230295
C	4.52309	-7.15615	6.538687	C	-1.23411	0.608677	7.516224
C	4.704428	-6.87344	5.183586	C	0.213364	-6.86643	0.921728
C	3.803965	-6.04115	4.478596	C	0.159867	6.492431	-1.7794
C	2.916218	-5.26967	5.240789	C	3.734511	0.25674	-7.77814
C	1.234109	-0.60868	7.516224	C	4.238485	2.857948	-6.73516
C	1.162637	0.778449	7.605493	O	6.202726	4.292923	-8.07264
C	-0.08588	1.413133	7.692224	C	6.490362	2.917815	-7.77527
C	-1.16264	-0.77845	7.605493	C	5.22026	2.158791	-7.47201
C	0.085882	-1.41313	7.692224	C	4.995533	0.865867	-7.95457
C	0.33422	-2.85171	7.947774	C	5.352374	6.858309	-5.65893
C	-0.36012	-3.62606	8.905864	C	4.429402	6.208164	-4.80696
C	-0.33422	2.85171	7.947774	C	5.904367	6.23179	-6.76829
C	0.360121	3.626063	8.905864	C	5.556106	4.917341	-7.04681
C	-1.79766	4.737365	7.454912	C	4.60129	4.221553	-6.27254
C	-1.44476	3.395934	7.27164	C	4.095289	4.880703	-5.13649
C	-2.28844	2.408787	6.499184	C	1.018812	-0.94614	-6.74009
O	-2.44512	1.205172	7.277465	C	1.369926	0.410307	-6.82939
O	-3.20291	6.861795	8.507021	C	-1.01881	0.946136	-6.74009
C	-1.78648	6.828009	8.778803	C	2.737215	0.941251	-7.04359
C	-1.17921	5.469104	8.485588	C	2.982247	2.251364	-6.56618
C	-0.08925	4.938627	9.187207	C	1.796937	2.977608	-5.97148
C	-4.70443	6.873444	5.183586	O	0.58659	2.680917	-6.67496
C	-3.80397	6.04115	4.478596	C	0.314816	1.340648	-6.73084
C	-4.52309	7.156151	6.538687	C	-3.73451	-0.25674	-7.77814
C	-3.49822	6.506641	7.220819	C	-4.23849	-2.85795	-6.73516
C	-2.77124	5.459333	6.619819	O	-6.20273	-4.29292	-8.07264
C	-2.91622	5.269665	5.240789	C	-6.49036	-2.91782	-7.77527
C	-3.77807	6.196551	3.008275	C	-5.22026	-2.15879	-7.47201
C	-2.60377	6.182376	2.236527	C	-4.99553	-0.86587	-7.95457
C	-1.2273	6.041129	2.844575	C	-1.36993	-0.41031	-6.82939
O	-0.32082	6.991674	2.278462	C	-2.73722	-0.94125	-7.04359
O	-5.72103	7.485189	4.516391	C	-2.98225	-2.25136	-6.56618
C	-6.14617	6.756638	3.344554	C	-1.79694	-2.97761	-5.97148
C	-4.99055	6.559719	2.389707	O	-0.58659	-2.68092	-6.67496
C	-5.06035	6.80003	1.012978	C	-0.31482	-1.34065	-6.73084
C	-0.21336	6.866434	0.921728	C	6.392645	-7.10811	0.353491
C	1.018812	7.158805	0.350767	C	5.405614	9.865894	-1.55759
C	1.212789	7.053119	-1.03176	C	2.868798	9.471077	-0.21633
C	-1.08684	6.231409	-1.21471	C	-5.40561	-9.86589	-1.55759
C	-1.33248	6.488153	0.147794	C	-2.8688	-9.47108	-0.21633
C	-2.64742	6.438591	0.843662	C	3.973281	-7.18455	-1.22278

C	-0.62639	-5.76633	10.23793	H	-6.94512	7.364668	2.923822
C	-1.51082	-3.05968	9.709773	H	-6.57051	5.796208	3.677289
C	0.626392	5.766331	10.23793	H	1.820067	7.457329	1.01489
C	1.510816	3.059682	9.709773	H	-1.85218	5.817827	-1.85929
C	-6.39265	7.108112	0.353491	H	7.203829	2.884058	-6.9351
C	-3.97328	7.184551	-1.22278	H	6.991358	2.544481	-8.66731
C	6.102259	0.116626	-8.67598	H	6.65104	6.740913	-7.36659
C	3.471091	-1.05917	-8.48261	H	3.469141	4.316428	-4.45619
C	-6.10226	-0.11663	-8.67598	H	1.76961	-1.72326	-6.67822
C	-3.47109	1.059168	-8.48261	H	-1.76961	1.723264	-6.67822
H	3.298122	-2.78528	6.333281	H	1.652324	2.73024	-4.90613
H	1.847787	-2.13396	5.527676	H	1.913029	4.056268	-6.06517
H	1.710503	-7.08466	9.835691	H	-7.20383	-2.88406	-6.9351
H	1.303633	-7.62764	8.19363	H	-6.99136	-2.54448	-8.66731
H	1.801215	4.766165	-2.95825	H	-1.65232	-2.73024	-4.90613
H	1.702887	5.670295	-4.48837	H	-1.91303	-4.05627	-6.06517
H	6.293227	9.380856	-3.90769	H	6.490383	-6.58597	-0.60313
H	6.87092	7.71805	-3.67184	H	7.238742	-6.79422	0.968145
H	-6.65104	-6.74091	-7.36659	H	6.516142	-8.18033	0.148168
H	-3.46914	-4.31643	-4.45619	H	5.357871	9.989632	-0.47324
H	-1.70289	-5.6703	-4.48837	H	5.170344	10.84211	-2.00506
H	-1.80122	-4.76617	-2.95825	H	6.447356	9.639801	-1.799
H	-6.29323	-9.38086	-3.90769	H	3.339657	9.229086	0.746676
H	-6.87092	-7.71805	-3.67184	H	3.164113	10.49489	-0.46456
H	1.852179	-5.81783	-1.85929	H	1.789699	9.472328	-0.05855
H	-1.82007	-7.45733	1.01489	H	-5.17034	-10.8421	-2.00506
H	0.812522	-5.02927	2.700055	H	-5.35787	-9.98963	-0.47324
H	1.231404	-6.26451	3.909128	H	-6.44736	-9.6398	-1.799
H	6.945115	-7.36467	2.923822	H	-3.16411	-10.4949	-0.46456
H	6.57051	-5.79621	3.677289	H	-3.33966	-9.22909	0.746676
H	5.145316	-7.89168	7.0363	H	-1.7897	-9.47233	-0.05855
H	2.286879	-4.53724	4.745354	H	3.053846	-7.66787	-1.55712
H	2.083885	1.349607	7.568102	H	4.158318	-6.33602	-1.89658
H	-2.08389	-1.34961	7.568102	H	4.788553	-7.89524	-1.37713
H	-1.84779	2.133962	5.527676	H	-0.36071	-6.8243	10.18617
H	-3.29812	2.785278	6.333281	H	-1.71289	-5.70728	10.1156
H	-1.7105	7.084663	9.835691	H	-0.40119	-5.42122	11.25634
H	-1.30363	7.627635	8.19363	H	-1.49325	-3.42604	10.74029
H	-5.14532	7.891681	7.0363	H	-2.48668	-3.34184	9.289204
H	-2.28688	4.537239	4.745354	H	-1.47838	-1.96993	9.747609
H	-1.2314	6.264509	3.909128	H	1.712893	5.707275	10.1156
H	-0.81252	5.029272	2.700055	H	0.36071	6.8243	10.18617

H	0.401189	5.421219	11.25634	H	7.094137	0.470085	-8.38506
H	1.493247	3.426035	10.74029	H	6.072816	-0.95171	-8.44565
H	2.486682	3.341843	9.289204	H	3.752376	-1.93244	-7.87749
H	1.478375	1.96993	9.747609	H	4.042268	-1.1211	-9.41256
H	-6.49038	6.585965	-0.60313	H	2.4172	-1.17052	-8.74114
H	-6.51614	8.18033	0.148168	H	-6.02665	-0.213	-9.76825
H	-7.23874	6.794218	0.968145	H	-6.07282	0.951708	-8.44565
H	-4.78855	7.895237	-1.37713	H	-7.09414	-0.47009	-8.38506
H	-4.15832	6.336022	-1.89658	H	-4.04227	1.121096	-9.41256
H	-3.05385	7.667872	-1.55712	H	-3.75238	1.932435	-7.87749
H	6.026653	0.212996	-9.76825	H	-2.4172	1.170518	-8.74114

Table S27. Cartesian coordinates of optimized (*P,P,M,M*)-isomer of **14** [B3LYP/6-31g(d) level of theory].

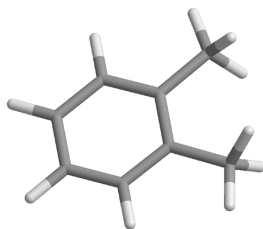


C	2.917414	2.214652	8.207238	C	-0.5532	8.55295	4.112118
C	3.761171	3.215817	7.711239	C	-1.26724	9.318906	5.063692
C	-1.67899	-1.93951	7.598595	C	2.017015	3.869544	6.128031
C	-1.2144	-2.80256	6.595379	C	3.31479	4.061058	6.667557
C	0.210284	-2.80106	6.101042	C	1.678988	1.939505	7.598595
O	0.761936	-4.12055	6.232021	C	1.214395	2.80256	6.595379
O	-1.98777	-1.30911	10.26425	C	-0.21028	2.801058	6.101042
C	-3.18772	-1.42032	9.466217	O	-0.76194	4.120552	6.232021
C	-2.91741	-2.21465	8.207238	O	1.987765	1.309113	10.26425
C	-3.76117	-3.21582	7.711239	C	3.18772	1.420316	9.466217
C	-0.29264	12.48415	1.19595	C	-0.96994	-0.70033	9.59314
C	-0.34212	11.07502	1.231464	C	-0.87884	-0.84933	8.190448
C	-0.23359	13.1886	0	C	0	0	10.30804
C	-0.37462	10.39876	0	C	0.969941	0.70033	9.59314
C	-0.52767	10.43924	2.556729	C	0.878835	0.849325	8.190448
C	-0.14254	9.131963	2.891582	C	0	0	7.505778
C	0.810784	8.295889	2.065527	C	0.055024	-5.0505	5.52521
O	1.782217	7.651948	2.909693	C	0.719315	-6.20852	5.136836
O	-0.38618	13.19549	2.3604	C	0.064019	-7.18234	4.373265
C	-1.40775	12.67645	3.223053	C	-1.90631	-5.73795	4.326829
C	-1.18619	11.21243	3.537519	C	-1.32502	-4.86668	5.267937
C	-1.58792	10.65864	4.757523	C	-2.01702	-3.86954	6.128031
C	1.202092	6.841783	3.851224	C	-3.31479	-4.06106	6.667557
C	1.906311	5.737947	4.326829	C	0.553197	-8.55295	4.112118
C	1.325018	4.866676	5.267937	C	1.267243	-9.31891	5.063692
C	-0.71932	6.208516	5.136836	C	0.527672	-10.4392	2.556729
C	-0.06402	7.182335	4.373265	C	0.142537	-9.13196	2.891582

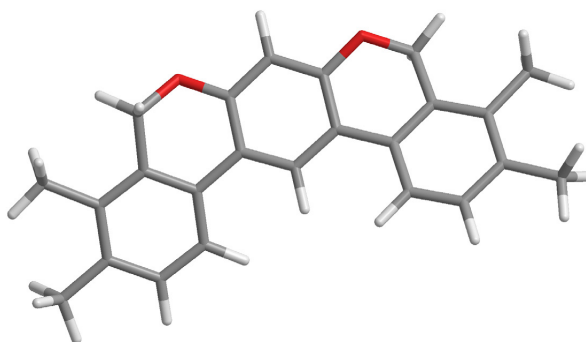
C	-0.81078	-8.29589	2.065527	O	-0.76194	4.120552	-6.23202
O	-1.78222	-7.65195	2.909693	O	1.987765	1.309113	-10.2642
O	0.386183	-13.1955	2.3604	C	3.18772	1.420316	-9.46622
C	1.407749	-12.6764	3.223053	C	-0.96994	-0.70033	-9.59314
C	1.186188	-11.2124	3.537519	C	-0.87884	-0.84933	-8.19045
C	1.587919	-10.6586	4.757523	C	0	0	-10.308
C	0.292641	-12.4841	1.19595	C	0.969941	0.70033	-9.59314
C	0.342116	-11.075	1.231464	C	0.878835	0.849325	-8.19045
C	-1.20209	-6.84178	3.851224	C	0	0	-7.50578
C	-0.05502	5.050497	5.52521	C	0.055024	-5.0505	-5.52521
C	2.917414	2.214652	-8.20724	C	0.719315	-6.20852	-5.13684
C	3.761171	3.215817	-7.71124	C	0.064019	-7.18234	-4.37327
C	-1.67899	-1.93951	-7.5986	C	-1.90631	-5.73795	-4.32683
C	-1.2144	-2.80256	-6.59538	C	-1.32502	-4.86668	-5.26794
C	0.210284	-2.80106	-6.10104	C	-2.01702	-3.86954	-6.12803
O	0.761936	-4.12055	-6.23202	C	-3.31479	-4.06106	-6.66756
O	-1.98777	-1.30911	-10.2642	C	0.553197	-8.55295	-4.11212
C	-3.18772	-1.42032	-9.46622	C	1.267243	-9.31891	-5.06369
C	-2.91741	-2.21465	-8.20724	C	0.527672	-10.4392	-2.55673
C	-3.76117	-3.21582	-7.71124	C	0.142537	-9.13196	-2.89158
C	-0.29264	12.48415	-1.19595	C	-0.81078	-8.29589	-2.06553
C	-0.34212	11.07502	-1.23146	O	-1.78222	-7.65195	-2.90969
C	-0.52767	10.43924	-2.55673	O	0.386183	-13.1955	-2.3604
C	-0.14254	9.131963	-2.89158	C	1.407749	-12.6764	-3.22305
C	0.810784	8.295889	-2.06553	C	1.186188	-11.2124	-3.53752
O	1.782217	7.651948	-2.90969	C	1.587919	-10.6586	-4.75752
O	-0.38618	13.19549	-2.3604	C	0.292641	-12.4841	-1.19595
C	-1.40775	12.67645	-3.22305	C	0.342116	-11.075	-1.23146
C	-1.18619	11.21243	-3.53752	C	-1.20209	-6.84178	-3.85122
C	-1.58792	10.65864	-4.75752	C	-0.05502	5.050497	-5.52521
C	1.202092	6.841783	-3.85122	C	0.233588	-13.1886	0
C	1.906311	5.737947	-4.32683	C	0.374619	-10.3988	0
C	1.325018	4.866676	-5.26794	C	5.147663	3.402229	8.301846
C	-0.71932	6.208516	-5.13684	C	-2.37413	11.49568	5.750697
C	-0.06402	7.182335	-4.37327	C	-1.60695	8.791871	6.442696
C	-0.5532	8.55295	-4.11212	C	4.198795	5.212211	6.23647
C	-1.26724	9.318906	-5.06369	C	-5.14766	-3.40223	8.301846
C	2.017015	3.869544	-6.12803	C	-4.1988	-5.21221	6.23647
C	3.31479	4.061058	-6.66756	C	2.374131	-11.4957	5.750697
C	1.678988	1.939505	-7.5986	C	1.606952	-8.79187	6.442696
C	1.214395	2.80256	-6.59538	C	5.147663	3.402229	-8.30185
C	-0.21028	2.801058	-6.10104	C	-2.37413	11.49568	-5.7507

C	-1.60695	8.791871	-6.4427	H	3.904669	1.90958	-10.1239
C	4.198795	5.212211	-6.23647	H	3.546557	0.402178	-9.24768
C	-5.14766	-3.40223	-8.30185	H	0	0	-11.3924
C	-4.1988	-5.21221	-6.23647	H	0	0	-6.41913
C	2.374131	-11.4957	-5.7507	H	1.750668	-6.33054	-5.4458
C	1.606952	-8.79187	-6.4427	H	-2.91074	-5.5779	-3.95437
H	0.856561	-2.16171	6.698899	H	-0.28911	-7.51678	-1.48561
H	0.283852	-2.49652	5.044699	H	-1.39273	-8.91266	-1.38014
H	-3.90467	-1.90958	10.12392	H	1.344876	-13.2916	-4.1212
H	-3.54656	-0.40218	9.247679	H	2.390548	-12.8537	-2.75364
H	-0.23978	14.27252	0	H	0.239778	-14.2725	0
H	-0.52787	9.32456	0	H	0.527873	-9.32456	0
H	0.289107	7.516783	1.485614	H	5.899251	3.521196	7.515055
H	1.392725	8.912659	1.380137	H	5.457687	2.543409	8.900652
H	-1.34488	13.2916	4.121204	H	5.211125	4.29062	8.944563
H	-2.39055	12.85371	2.75364	H	-1.73497	11.90308	6.546649
H	2.910737	5.577904	3.954365	H	-3.15375	10.90351	6.238171
H	-1.75067	6.330539	5.445795	H	-2.87662	12.3396	5.272476
H	-0.28385	2.496515	5.044699	H	-1.56524	9.591094	7.18745
H	-0.85656	2.161711	6.698899	H	-2.61744	8.36218	6.492559
H	3.904669	1.90958	10.12392	H	-0.91059	8.014122	6.758809
H	3.546557	0.402178	9.247679	H	3.610381	6.108865	6.029856
H	0	0	11.39241	H	4.7654	4.982712	5.323308
H	0	0	6.419133	H	4.927128	5.471256	7.006665
H	1.750668	-6.33054	5.445795	H	-5.45769	-2.54341	8.900652
H	-2.91074	-5.5779	3.954365	H	-5.89925	-3.5212	7.515055
H	-0.28911	-7.51678	1.485614	H	-5.21113	-4.29062	8.944563
H	-1.39273	-8.91266	1.380137	H	-4.92713	-5.47126	7.006665
H	1.344876	-13.2916	4.121204	H	-4.7654	-4.98271	5.323308
H	2.390548	-12.8537	2.75364	H	-3.61038	-6.10887	6.029856
H	0.856561	-2.16171	-6.6989	H	2.876621	-12.3396	5.272476
H	0.283852	-2.49652	-5.0447	H	3.153753	-10.9035	6.238171
H	-3.90467	-1.90958	-10.1239	H	1.734972	-11.9031	6.546649
H	-3.54656	-0.40218	-9.24768	H	1.565244	-9.59109	7.18745
H	0.289107	7.516783	-1.48561	H	2.617437	-8.36218	6.492559
H	1.392725	8.912659	-1.38014	H	0.910592	-8.01412	6.758809
H	-1.34488	13.2916	-4.1212	H	5.899251	3.521196	-7.51506
H	-2.39055	12.85371	-2.75364	H	5.457687	2.543409	-8.90065
H	2.910737	5.577904	-3.95437	H	5.211125	4.29062	-8.94456
H	-1.75067	6.330539	-5.4458	H	-1.73497	11.90308	-6.54665
H	-0.28385	2.496515	-5.0447	H	-3.15375	10.90351	-6.23817
H	-0.85656	2.161711	-6.6989	H	-2.87662	12.3396	-5.27248

H	-1.56524	9.591094	-7.18745	H	-4.92713	-5.47126	-7.00667
H	-2.61744	8.36218	-6.49256	H	-4.7654	-4.98271	-5.32331
H	-0.91059	8.014122	-6.75881	H	-3.61038	-6.10887	-6.02986
H	3.610381	6.108865	-6.02986	H	2.876621	-12.3396	-5.27248
H	4.7654	4.982712	-5.32331	H	3.153753	-10.9035	-6.23817
H	4.927128	5.471256	-7.00667	H	1.734972	-11.9031	-6.54665
H	-5.45769	-2.54341	-8.90065	H	0.910592	-8.01412	-6.75881
H	-5.89925	-3.5212	-7.51506	H	2.617437	-8.36218	-6.49256
H	-5.21113	-4.29062	-8.94456	H	1.565244	-9.59109	-7.18745

Table S28. Cartesian coordinates of optimized unit **S1** [B3LYP/6-31g(d) level of theory].

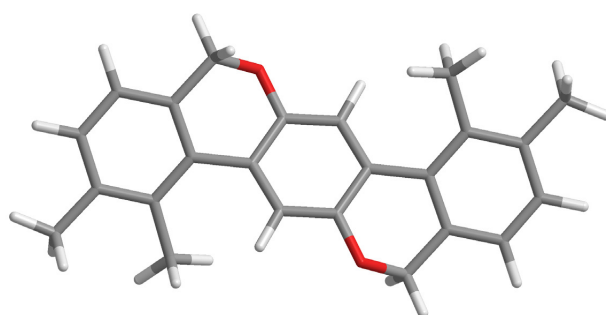
C	0	0.69675	1.960829	H	0	-1.24776	2.897616
C	0	-0.69675	1.960829	H	0	2.472229	0.745076
C	0	1.384328	0.746337	H	0	-2.47223	0.745076
C	0	0.705755	-0.47765	H	0	2.558642	-1.59057
C	0	-1.38433	0.746337	H	-0.88022	1.246944	-2.38872
C	0	-0.70576	-0.47765	H	0.880217	1.246944	-2.38872
C	0	1.480045	-1.7753	H	0	-2.55864	-1.59057
C	0	-1.48005	-1.7753	H	-0.88022	-1.24694	-2.38872
H	0	1.247758	2.897616	H	0.880217	-1.24694	-2.38872

Table S29. Cartesian coordinates of optimized unit **S2** [B3LYP/6-31g(d) level of theory].

C	0.460098	3.990557	-2.25267	C	0	0	-0.37977
C	0.076549	5.125962	-1.52823	C	0	-2.54036	-0.37298
C	0	2.54036	-0.37298	C	-0.43159	-2.71909	-1.69288
C	0.431585	2.719093	-1.69288	O	0.152285	-2.35388	2.426191
O	-0.15229	2.35388	2.426191	C	0.842946	-3.43545	1.785086
C	-0.84295	3.435452	1.785086	C	0.367916	-3.67813	0.370651
C	-0.36792	3.678128	0.370651	C	0.343524	-4.96563	-0.1904
C	-0.34352	4.965632	-0.1904	C	-0.4601	-3.99056	-2.25267
C	0.092107	-1.19746	1.703071	C	-0.07655	-5.12596	-1.52823
C	0.05147	-1.22637	0.292365	C	-0.77588	6.156066	0.643183
C	0	0	2.40714	C	0.13186	6.481928	-2.19816
C	-0.09211	1.197456	1.703071	C	0.775882	-6.15607	0.643183
C	-0.05147	1.226367	0.292365	C	-0.13186	-6.48193	-2.19816

H	0.797308	4.110773	-3.27964	H	-0.79662	7.078298	0.060549
H	0.764709	1.868991	-2.28042	H	-1.78016	6.016158	1.061736
H	-0.66809	4.2956	2.432695	H	-0.8554	6.958494	-2.2512
H	-1.92436	3.215826	1.800478	H	0.795902	7.178	-1.67052
H	0	0	3.491248	H	0.504033	6.388544	-3.22296
H	0	0	-1.46508	H	1.78016	-6.01616	1.061736
H	-0.76471	-1.86899	-2.28042	H	0.097176	-6.32363	1.490248
H	0.668092	-4.2956	2.432695	H	0.79662	-7.0783	0.060549
H	1.924359	-3.21583	1.800478	H	-0.7959	-7.178	-1.67052
H	-0.79731	-4.11077	-3.27964	H	-0.50403	-6.38854	-3.22296
H	-0.09718	6.323628	1.490248	H	0.855402	-6.95849	-2.2512

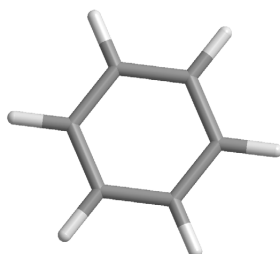
Table S30. Cartesian coordinates of optimized unit **S3** [B3LYP/6-31g(d) level of theory].



C	-4.73944	1.82118	0.204489	C	5.657559	-0.7758	-0.17782
C	-3.37964	1.545381	0.151979	C	5.23294	0.546913	-0.02768
C	-2.35554	2.649554	0.185197	C	-6.27555	-1.64176	-0.05044
O	-1.25336	2.355335	-0.67994	C	-3.44134	-2.26593	-0.36466
C	-5.65756	0.775796	0.177822	C	6.275549	1.64176	0.050441
C	-5.23294	-0.54691	0.027677	C	3.441335	2.265926	0.364658
C	-0.65529	1.163037	-0.3473	H	-5.08258	2.851193	0.272035
C	0.730644	1.094916	-0.44123	H	-1.9698	2.810177	1.20624
C	1.43595	-0.06084	-0.06944	H	-2.77628	3.591726	-0.17466
C	0.655287	-1.16304	0.347301	H	-6.72167	0.988911	0.24446
C	-0.73064	-1.09492	0.441229	H	1.239395	1.972824	-0.81474
C	-1.43595	0.060835	0.069443	H	-1.2394	-1.97282	0.81474
C	-2.91174	0.214283	0.065086	H	5.082577	-2.85119	-0.27204
C	-3.85246	-0.83894	-0.06645	H	1.969801	-2.81018	-1.20624
C	2.911735	-0.21428	-0.06509	H	2.776276	-3.59173	0.174659
C	3.852464	0.838939	0.066454	H	6.721669	-0.98891	-0.24446
C	4.739435	-1.82118	-0.20449	H	-7.26955	-1.24215	0.172351
C	3.379636	-1.54538	-0.15198	H	-6.32339	-2.09653	-1.04886
C	2.355537	-2.64955	-0.1852	H	-6.07613	-2.4533	0.659384
O	1.253358	-2.35534	0.679938	H	-2.50678	-2.30655	-0.92778

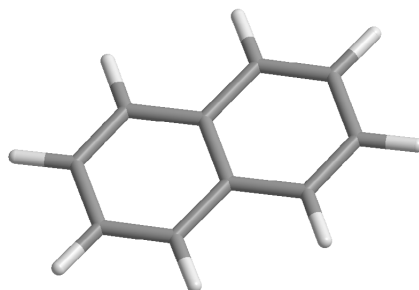
H	-3.30326	-2.86534	0.546181	H	6.323394	2.096533	1.048859
H	-4.20563	-2.77272	-0.95985	H	2.50678	2.306553	0.927775
H	7.269547	1.242147	-0.17235	H	4.205625	2.772717	0.95985
H	6.076133	2.453295	-0.65938	H	3.303263	2.86534	-0.54618

Table S31. Cartesian coordinates of optimized unit **S4** [B3LYP/6-31g(d) level of theory].

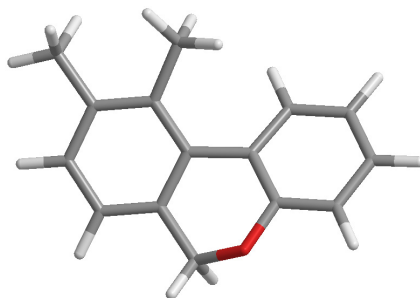


C	-9.62236	1.07015	-0.28387	H	-8.96065	1.90476	-0.50537
C	-9.08795	-0.17377	0.04845	H	-8.00929	-0.30974	0.08632
C	-9.93561	-1.24339	0.33215	H	-9.51847	-2.21414	0.59129
C	-11.31783	-1.06912	0.28373	H	-11.97946	-1.90380	0.50512
C	-11.85231	0.17466	-0.04862	H	-12.93097	0.31062	-0.08653
C	-11.00458	1.24431	-0.33248	H	-11.42187	2.21485	-0.59198

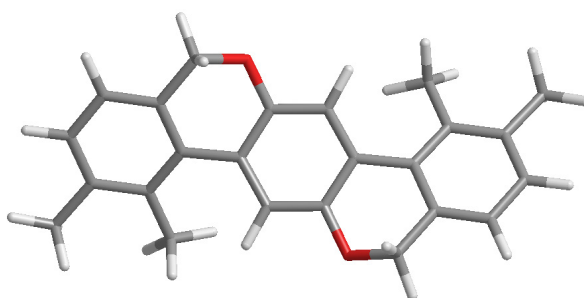
Table S32. Cartesian coordinates of optimized unit **S5** [B3LYP/6-31g(d) level of theory].



C	2.43368	0.70849	0.00000	C	-1.24485	1.40250	0.00000
C	2.43368	-0.70849	0.00000	H	3.37838	1.24558	0.00003
C	1.24485	-1.40250	0.00000	H	3.37838	-1.24558	-0.00001
C	0.00000	-0.71695	0.00000	H	1.242028	-2.49018	-0.000007
C	0.00000	0.71695	-0.00001	H	1.242029	2.49018	-0.000006
C	1.24485	1.40250	0.00000	H	-1.242029	-2.490181	0.000007
C	-1.24485	-1.40250	0.00000	H	-3.378381	-1.245573	-0.000001
C	-2.43368	-0.70849	0.00000	H	-3.378382	1.245572	0.000013
C	-2.43368	0.70849	0.00000	H	-1.242029	2.490181	-0.000009

Table S33. Cartesian coordinates of optimized unit **S6** [B3LYP/6-31g(d) level of theory].

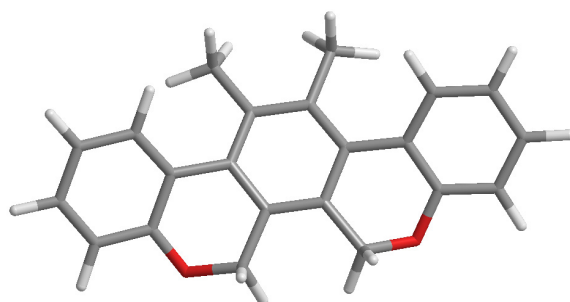
C	1.98108	1.92837	-0.22600	C	4.002026	-1.264155	0.153253
C	3.04245	1.03128	-0.15060	H	2.169946	2.996368	-0.309218
C	2.81345	-0.33640	0.02034	H	4.064921	1.398403	-0.194878
C	1.48884	-0.82782	0.08598	H	-0.239558	3.392851	0.050216
C	0.40796	0.07119	-0.09520	H	-0.884982	2.459032	-1.320359
C	0.67626	1.45391	-0.20235	H	-0.872034	-2.29893	-0.926107
C	-1.02868	-0.30351	-0.12127	H	-3.263899	-2.815932	-0.757981
C	-1.97041	0.67497	0.27603	H	-4.85453	-1.110344	0.12747
O	-1.56937	1.95325	0.56323	H	-4.000275	1.166269	0.728309
C	-0.50133	2.38777	-0.28889	H	2.078901	-2.659277	1.065282
C	-1.54236	-1.55000	-0.52261	H	0.333243	-2.465377	0.91777
C	-2.90286	-1.84199	-0.44006	H	1.298818	-2.930139	-0.486604
C	-3.794635	-0.884511	0.047724	H	4.93348	-0.728063	-0.052541
C	-3.328864	0.382061	0.392704	H	4.085191	-1.686523	1.16356
C	1.283965	-2.293397	0.409332	H	3.944418	-2.110958	-0.541011

Table S34 Cartesian coordinates of optimized unit **S7** [B3LYP/6-31g(d) level of theory].

C	-4.80860	-1.59078	-0.61104	O	-1.27832	-2.43439	-0.37232
C	-5.67068	-0.62236	-0.10415	C	-2.47073	-2.37399	-1.16355
C	-5.17425	0.55283	0.46607	C	-0.72461	1.18528	-0.24954
C	-3.77954	0.78264	0.50688	C	0.66560	1.20879	-0.27215
C	-2.90697	-0.15846	-0.09462	C	1.43369	0.025029	-0.186894
C	-3.43925	-1.36126	-0.61093	C	0.724575	-1.18533	-0.24962
C	-1.43371	-0.02508	-0.18691	O	1.278279	2.43434	-0.372237
C	-0.66563	-1.20884	-0.27222	C	2.470642	2.373952	-1.163534

C	3.439195	1.36123	-0.610965	H	2.893785	3.381255	-1.144298
C	2.906954	0.158426	-0.094605	H	2.191078	2.135722	-2.203679
C	4.808538	1.590768	-0.61115	H	5.203926	2.521362	-1.012275
C	5.670661	0.622378	-0.104284	H	6.744647	0.790722	-0.125899
C	5.174283	-0.552785	0.466011	H	3.92975	-2.250999	2.08303
C	3.779577	-0.782624	0.506912	H	2.270064	-1.847304	1.646176
C	3.272766	-2.004443	1.244215	H	3.233296	-2.896471	0.60319
C	6.151175	-1.551276	1.048692	H	7.180791	-1.264493	0.814124
C	-3.272609	2.004523	1.243999	H	6.071478	-1.616805	2.141982
C	-6.151108	1.551372	1.048715	H	5.989402	-2.562854	0.657619
H	-5.20402	-2.521377	-1.01212	H	-3.92946	2.251168	2.082891
H	-6.744667	-0.79068	-0.125716	H	-2.269843	1.8474	1.645814
H	-2.893874	-3.381294	-1.144289	H	-3.233211	2.896491	0.602886
H	-2.19122	-2.135764	-2.203707	H	-7.180734	1.264611	0.814163
H	-1.237894	2.135678	-0.317456	H	-6.071405	1.616939	2.142002
H	1.237852	-2.135723	-0.317626	H	-5.989308	2.562929	0.657602

Table S35. Cartesian coordinates of optimized unit **S8** [B3LYP/6-31g(d) level of theory].



C	5.68077	-0.11156	-0.32778	C	-3.502163	-0.998556	0.187509
C	5.08456	1.07534	-0.76064	C	-2.878702	0.222016	-0.149482
C	4.88586	-1.15884	0.13358	C	1.440498	2.779572	0.723181
C	3.50215	-0.99851	0.18758	C	-1.440613	2.779405	0.723552
C	2.87871	0.22205	-0.14954	C	-4.885865	-1.158873	0.133401
C	3.70253	1.23438	-0.67392	C	-5.680734	-0.111534	-0.327917
O	2.74135	-2.06704	0.58322	C	-5.08449	1.075415	-0.760609
C	1.51515	-2.16023	-0.15098	C	-3.702464	1.234428	-0.673788
C	0.69580	-0.89564	-0.03392	H	6.758922	-0.235373	-0.381331
C	1.41138	0.32012	0.03690	H	5.693738	1.87692	-1.168407
C	-0.69579	-0.89566	-0.03390	H	5.311355	-2.11203	0.431345
C	-1.41138	0.32007	0.03699	H	3.254464	2.152342	-1.037271
C	-0.707795	1.510605	0.335245	H	1.002032	-3.025634	0.27127
C	0.707748	1.510648	0.33516	H	1.752077	-2.38682	-1.20409
C	-1.515116	-2.160274	-0.150929	H	-1.751952	-2.386954	-1.204046
O	-2.74138	-2.06709	0.583167	H	-1.001997	-3.025634	0.271416

H	0.979852	3.243726	1.60045	H	-1.423042	3.536867	-0.072364
H	2.482161	2.584146	0.975992	H	-5.311399	-2.112078	0.431058
H	1.423907	3.536364	-0.073401	H	-6.758886	-0.23533	-0.381544
H	-2.482555	2.58405	0.975234	H	-5.693641	1.877043	-1.16832
H	-0.98068	3.242663	1.60169	H	-3.254336	2.152426	-1.036995

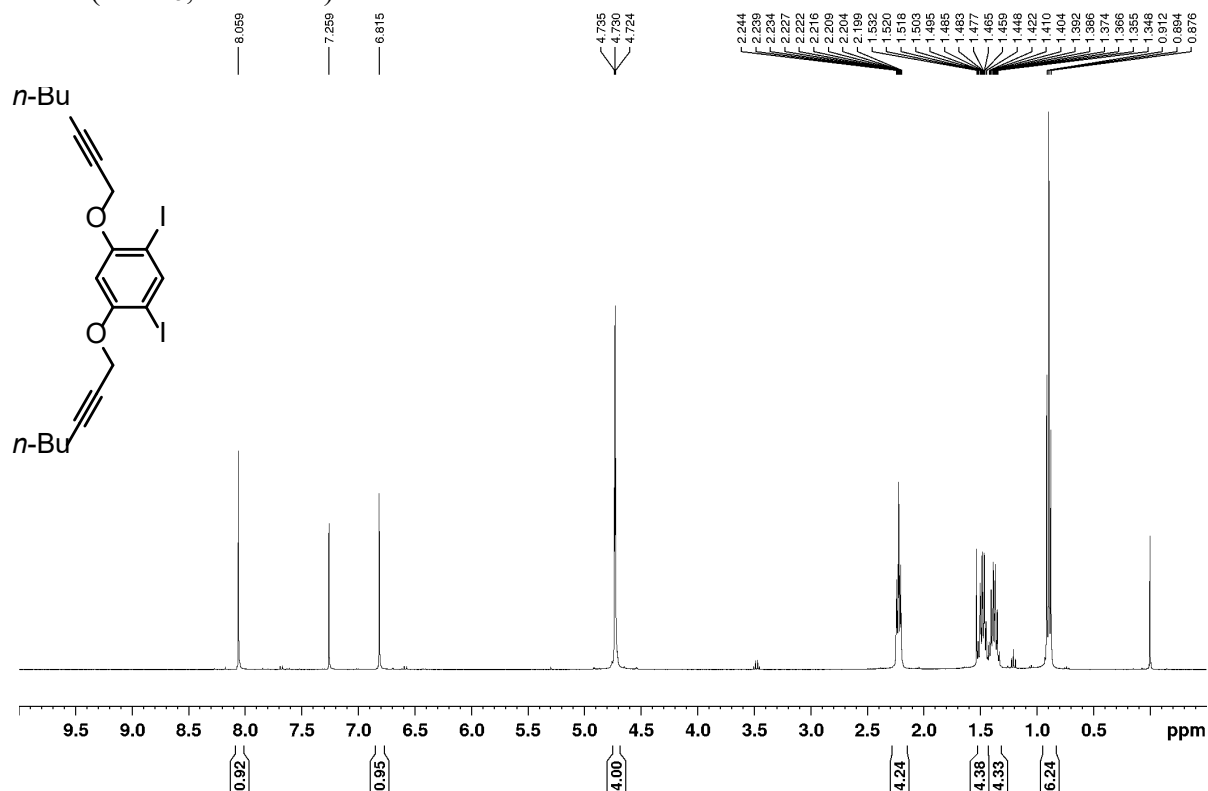
Table S36. Uncorrected and thermally-corrected (298K) energies of stationary points (Hartree) calculated by the B3LYP/6-31G(d) level of theory.

compound	Sum of electronic and zero-point Energies	Sum of electronic and thermal Energies	Sum of electronic and thermal Enthalpies	Sum of electronic and thermal Free Energies
(M,M)-10	-3068.543109	-3068.487067	-3068.486122	-3068.625937
(P,M)-11	-3068.518576	-3068.462443	-3068.461499	-3068.602307
(M,M,M)-12	-4602.858031	-4602.773607	-4602.772663	-4602.971728
(P,M,M)-13	-4602.830950	-4602.746134	-4602.745189	-4602.947272
(P,M,P,M)-14	-6137.146099	-6137.032703	-6137.031758	-6137.294352
(P,P,M,M)-14	-6137.102494	-6136.989227	-6136.988283	-6137.251927
(P,M,M,M)-14	-6137.124725	-6137.011412	-6137.010468	-6137.273728
(M,M,M,M)-14	-6137.129848	-6137.016946	-6137.016002	-6137.276892
[10]Möbius-CPP	-3835.579541	-3835.509774	-3835.508830	-3835.679474
[14]Möbius-CPP	-5369.922040	-5369.823988	-5369.823044	-5370.052221
[18]Möbius-CPP	-6904.230380	-6904.103264	-6904.102320	-6904.393978
[22]Möbius-CPP	-8438.528375	-8438.372132	-8438.371188	-8438.726174
S1	-310.727626	-310.720071	-310.719126	-310.758478
S2	-1077.884404	-1077.862177	-1077.861233	-1077.934468
S3	-1077.871033	-1077.849643	-1077.848699	-1077.919923
S4	-232.147936	-232.143551	-232.142607	-232.175398
S5	-385.744913	-385.738111	-385.737167	-385.776111
S6	-655.010261	-654.997562	-654.996618	-655.048630
S7	-1077.872872	-1077.851431	-1077.850487	-1077.921795
S8	-999.289369	-999.270980	-999.270036	-999.335093

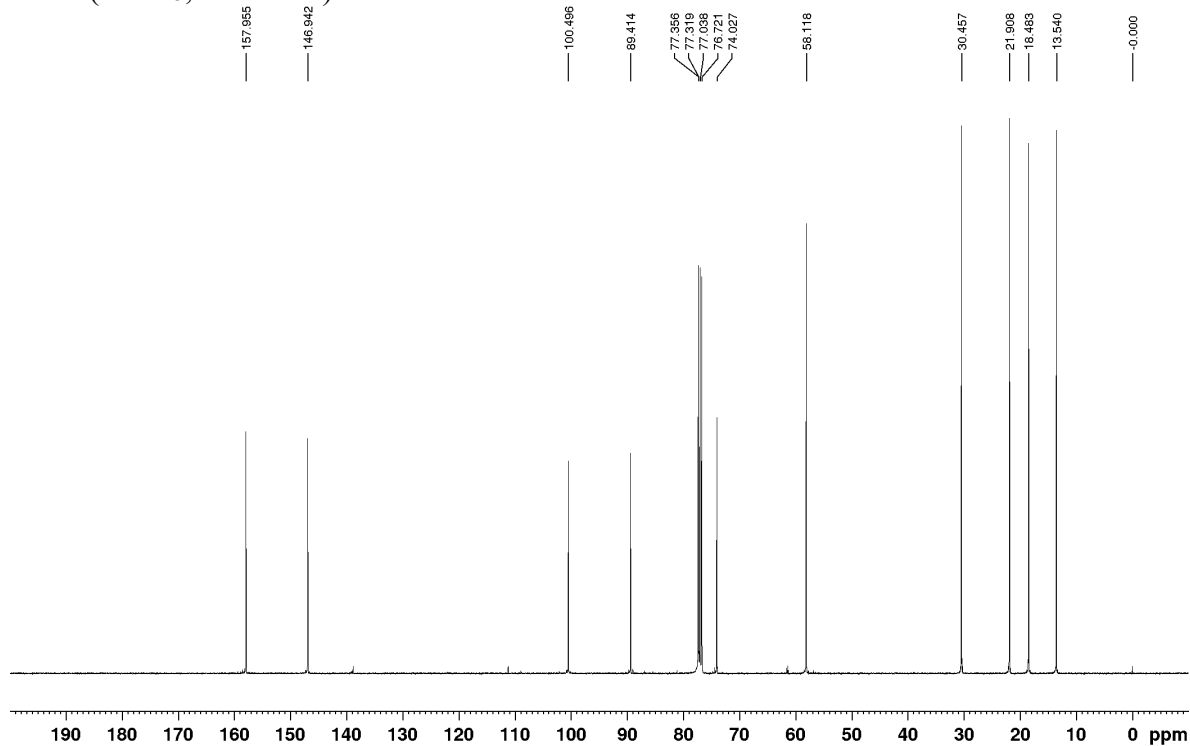
7. ^1H , ^{13}C , and 2D NMR Spectra of New Compounds

1,5-Bis(hept-2-yn-1-yloxy)-2,4-diiodobenzene (**3**)

^1H NMR (CDCl_3 , 400 MHz)

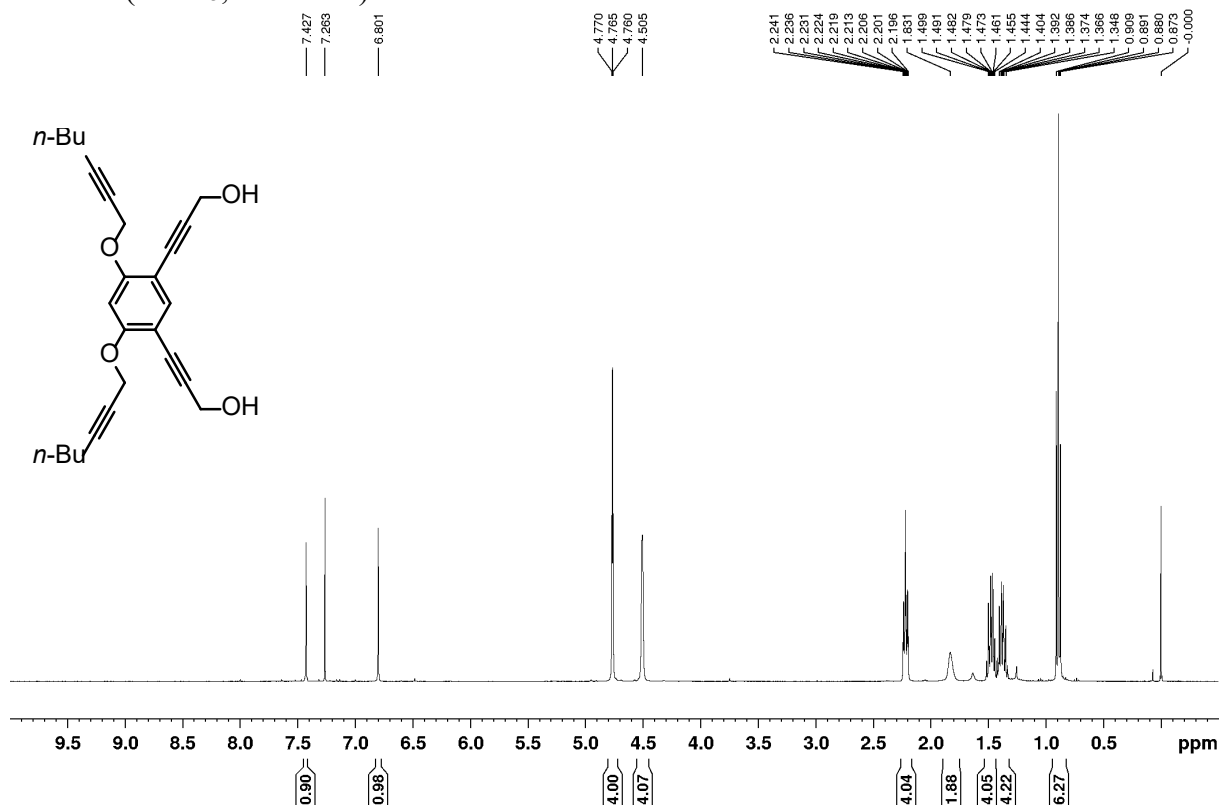


^{13}C NMR (CDCl_3 , 100 MHz)

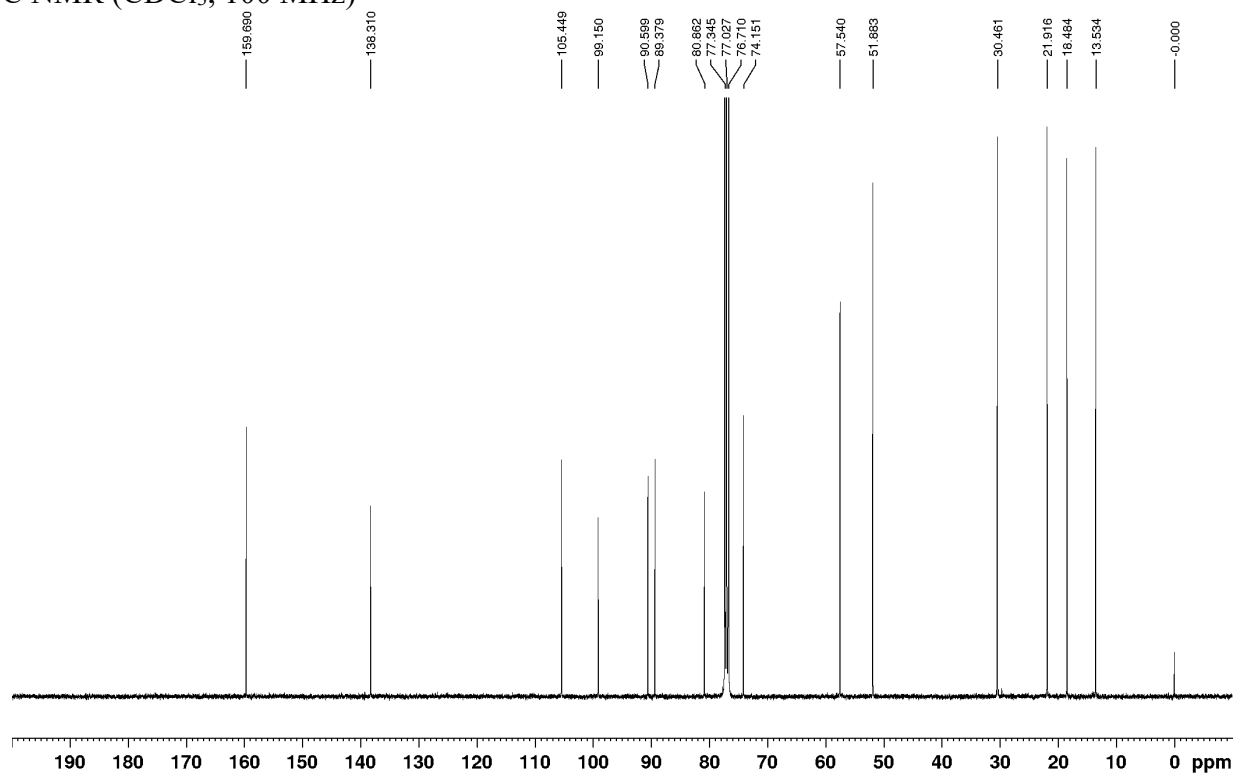


3,3'-(4,6-Bis(hept-2-yn-1-yloxy)-1,3-phenylene)bis(prop-2-yn-1-ol) (6)

^1H NMR (CDCl_3 , 400 MHz)

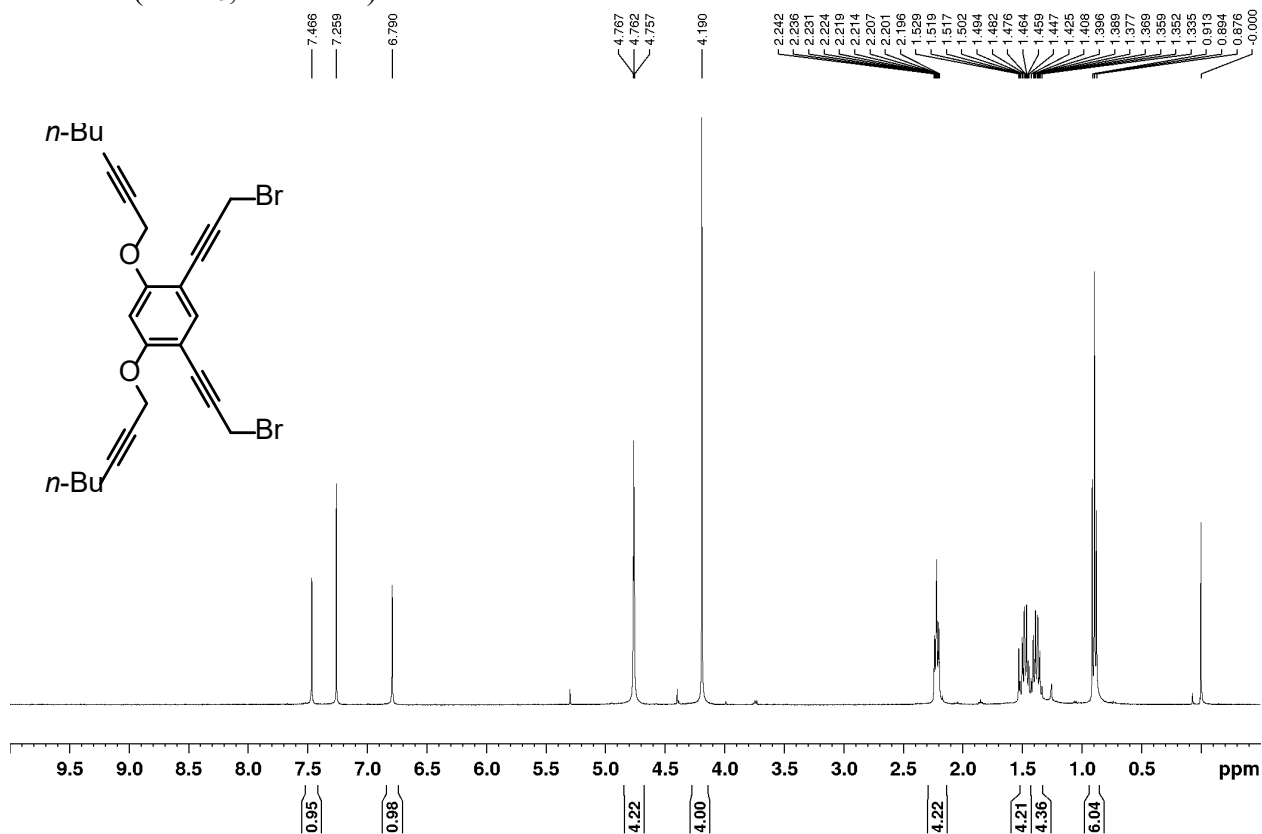


^{13}C NMR (CDCl_3 , 100 MHz)

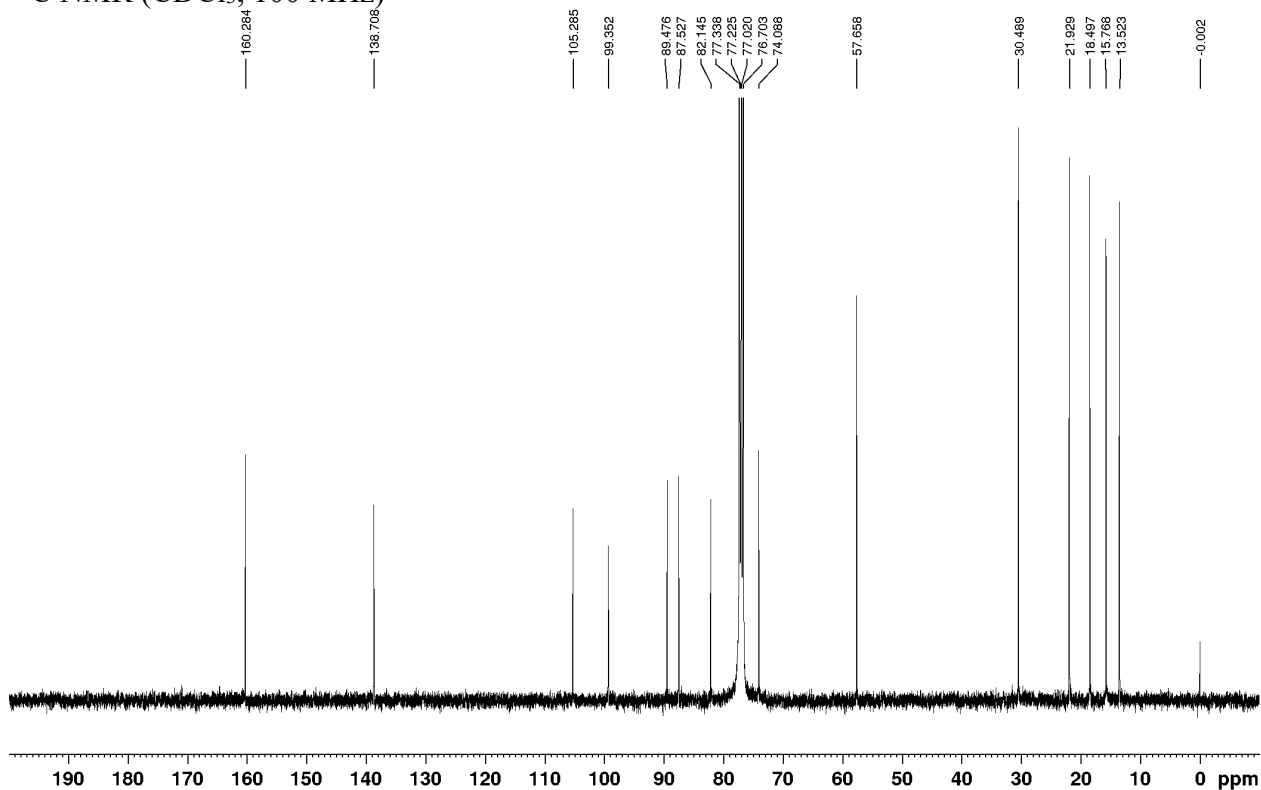


1,5-Bis(3-bromoprop-1-yn-1-yl)-2,4-bis(hept-2-yn-1-yloxy)benzene (7)

^1H NMR (CDCl_3 , 400 MHz)

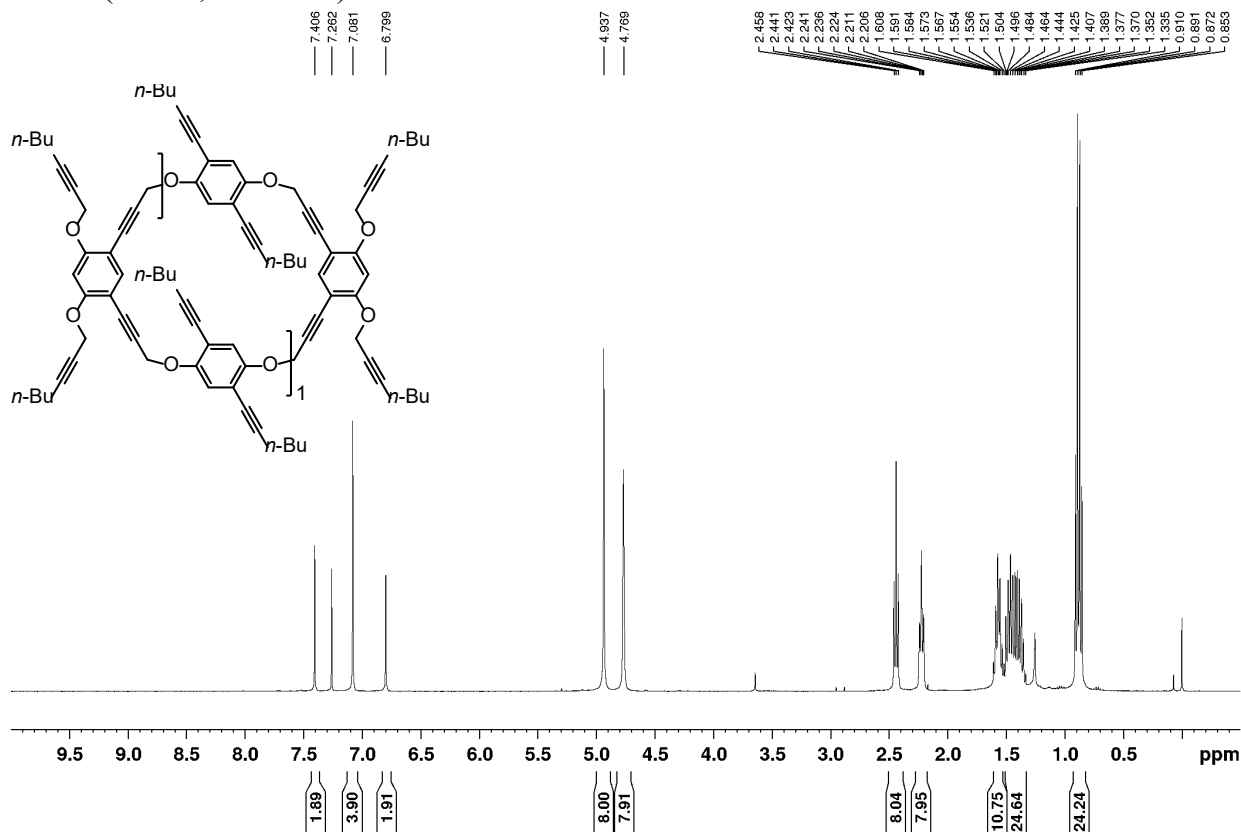


^{13}C NMR (CDCl_3 , 100 MHz)

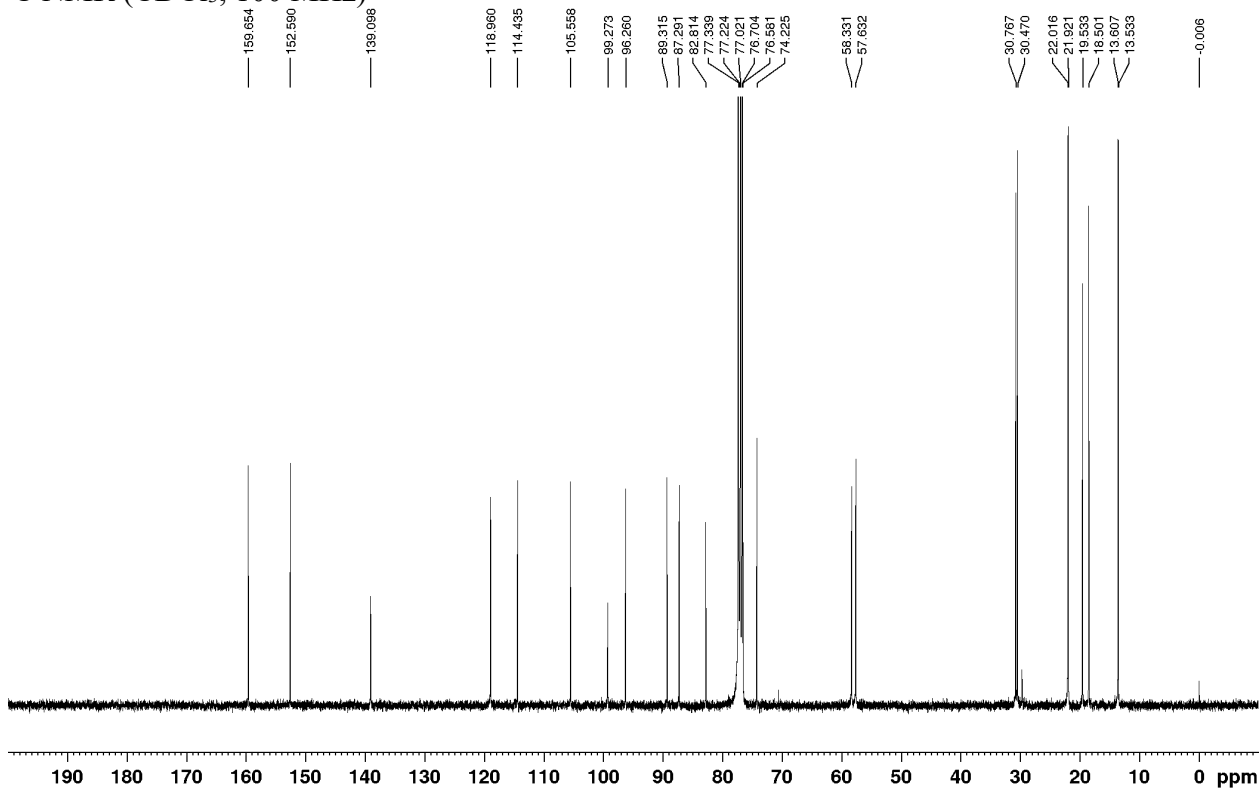


Macrocycle 9a

^1H NMR (CDCl_3 , 400 MHz)

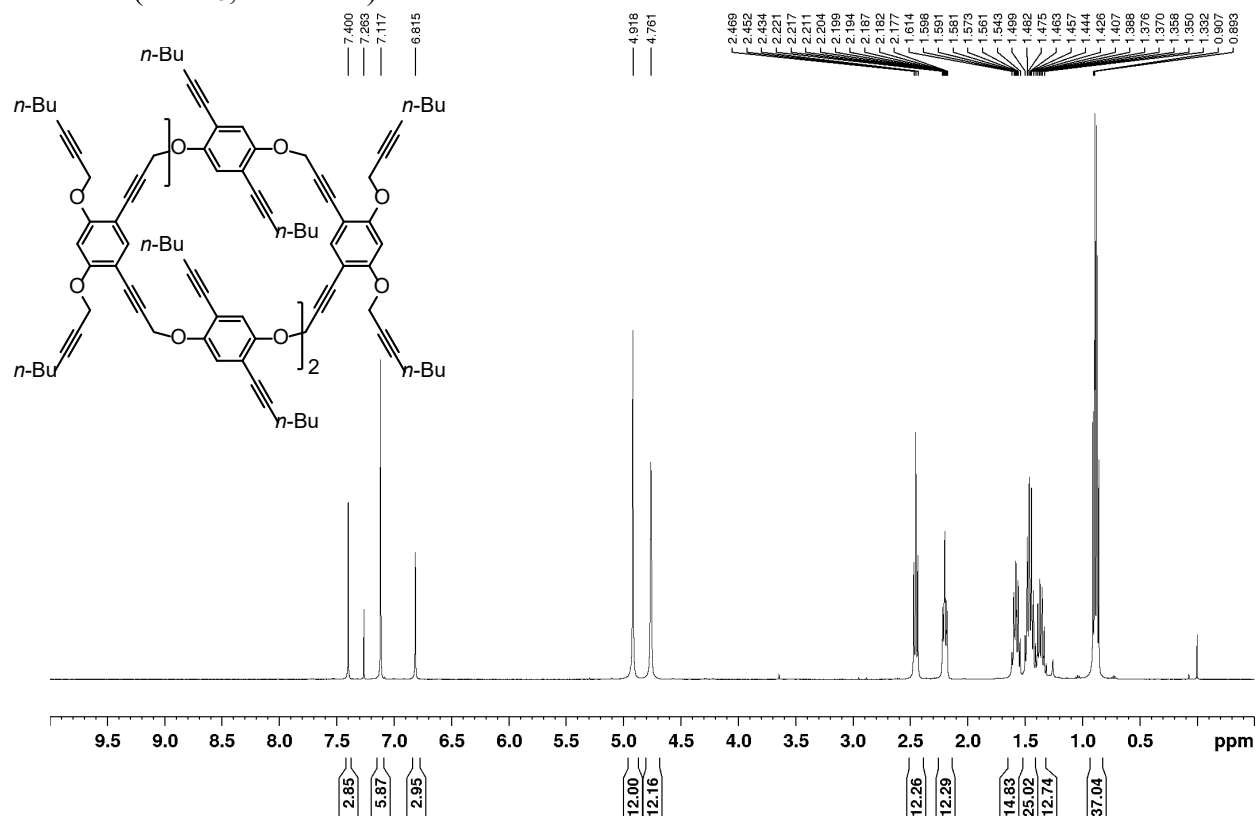


^{13}C NMR (CDCl_3 , 100 MHz)

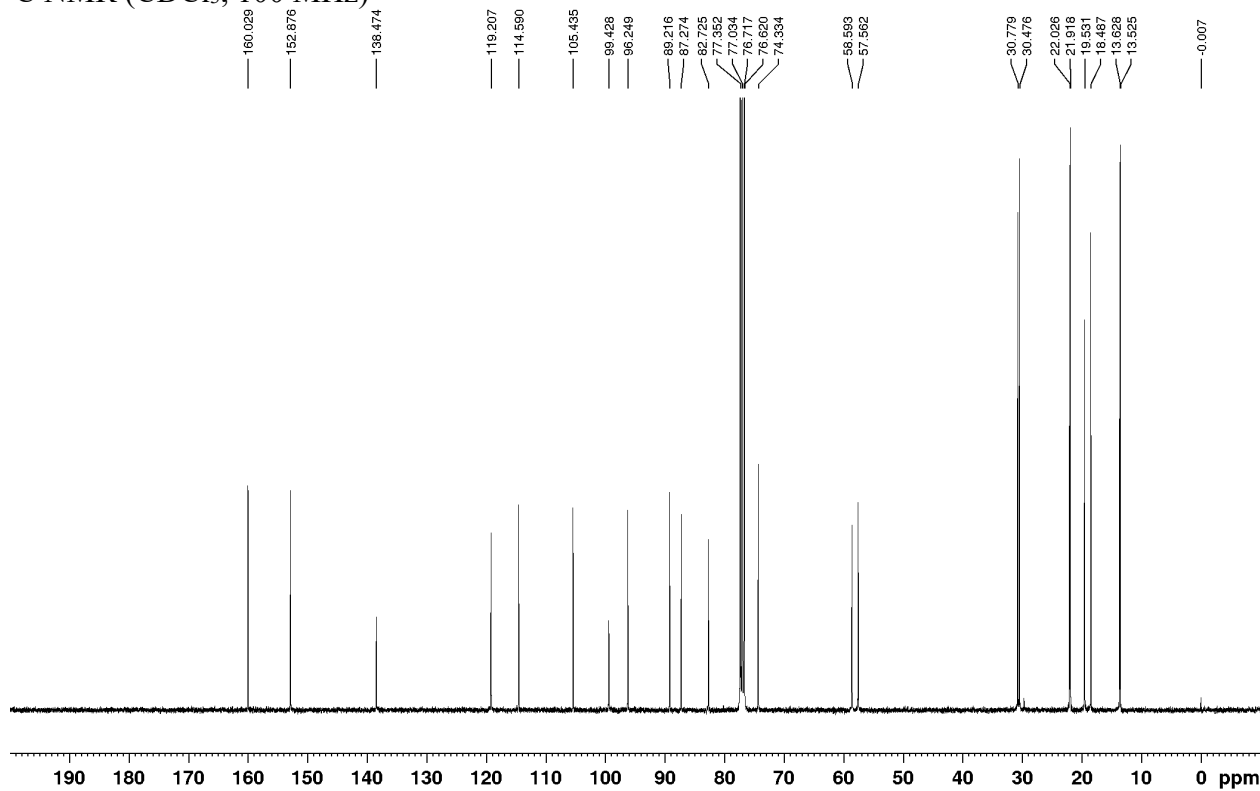


Macrocycle 9b

^1H NMR (CDCl_3 , 400 MHz)

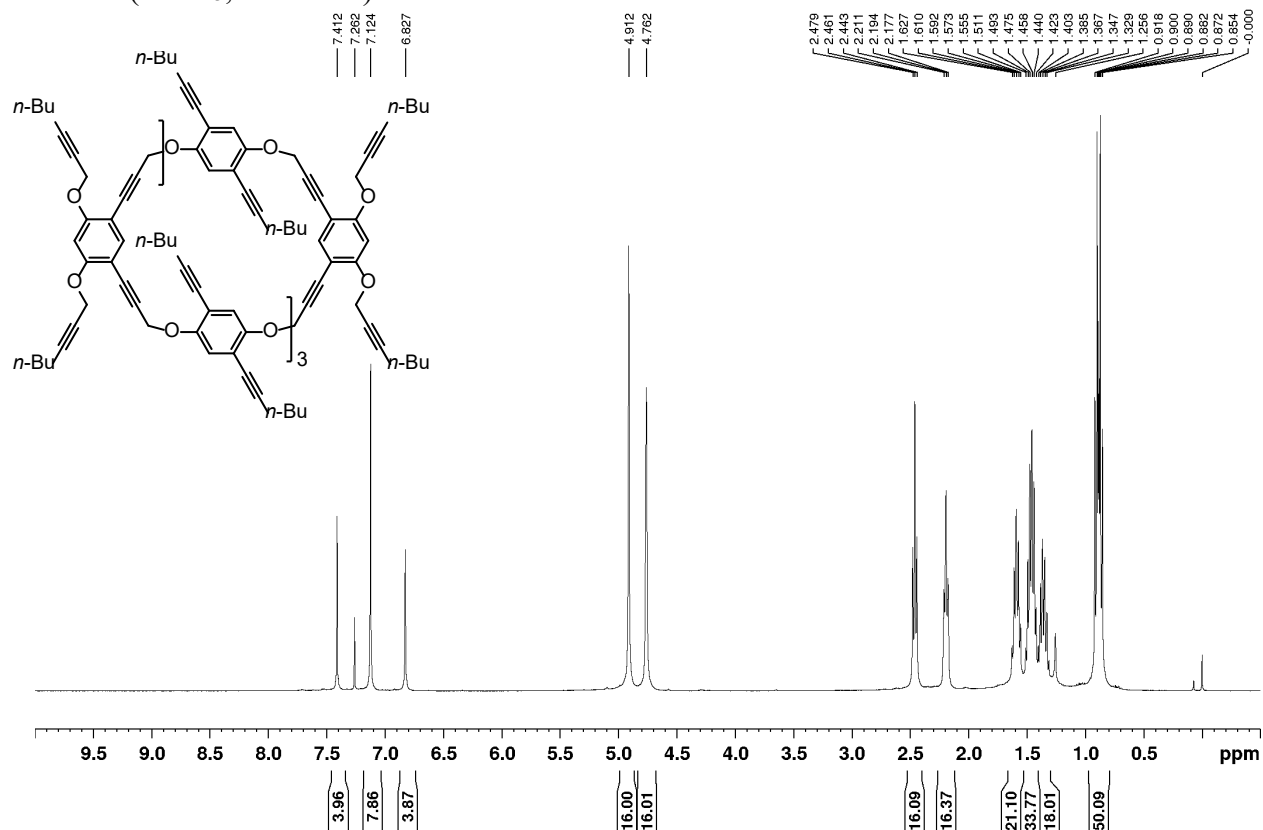


^{13}C NMR (CDCl_3 , 100 MHz)

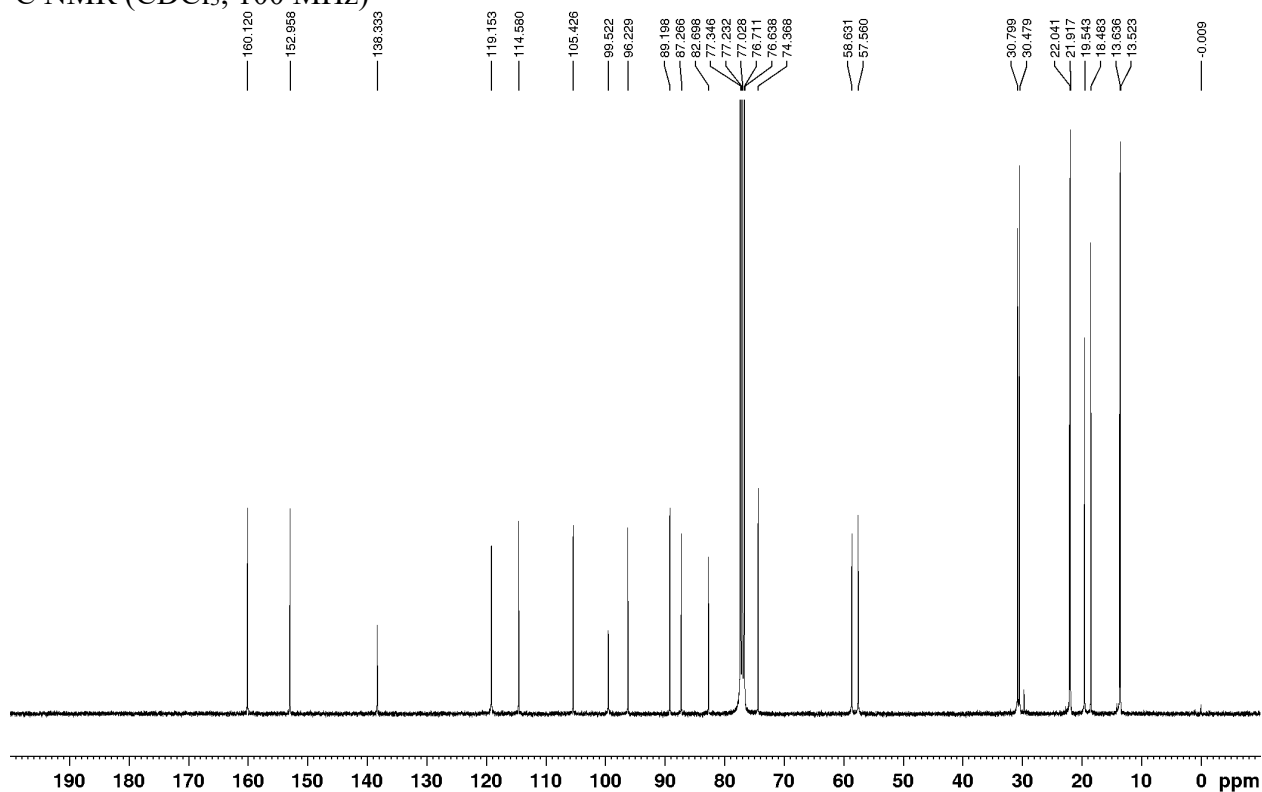


Macrocycle 9c

^1H NMR (CDCl_3 , 400 MHz)

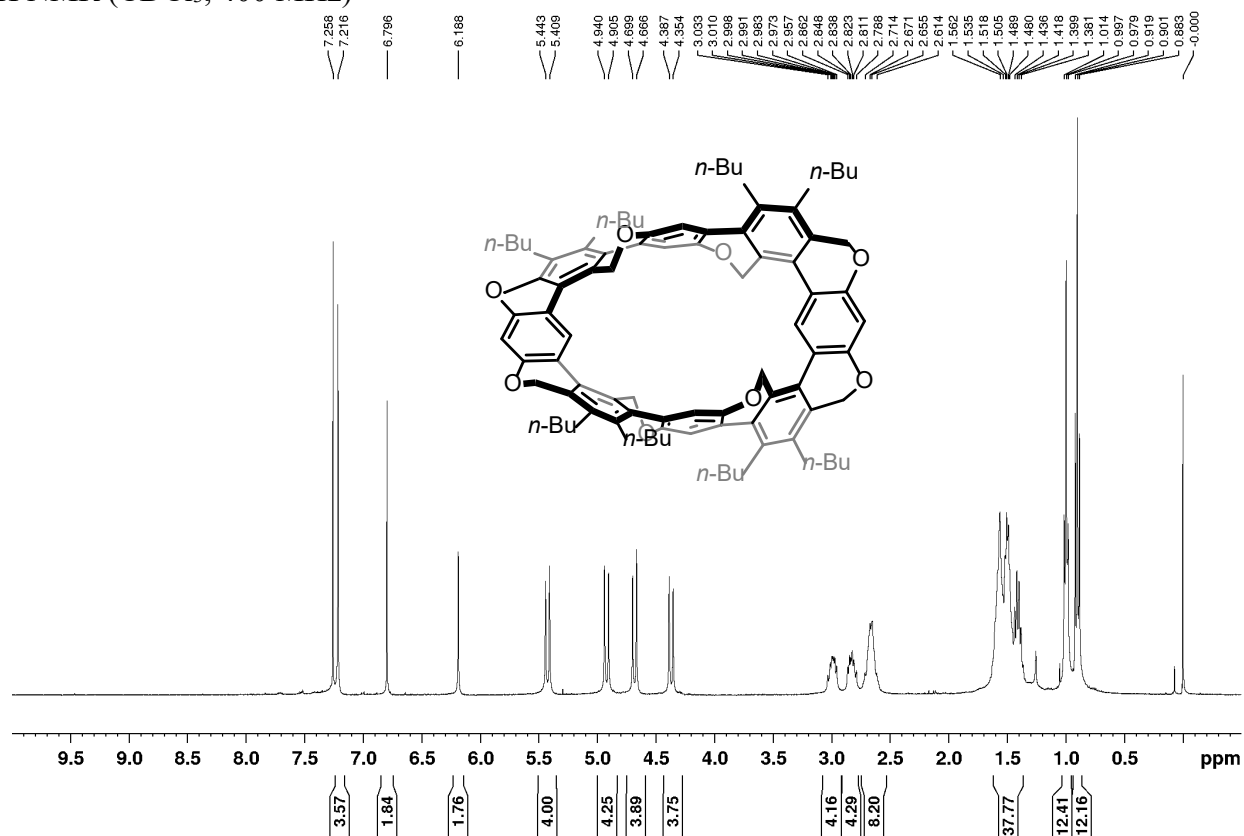


^{13}C NMR (CDCl_3 , 100 MHz)

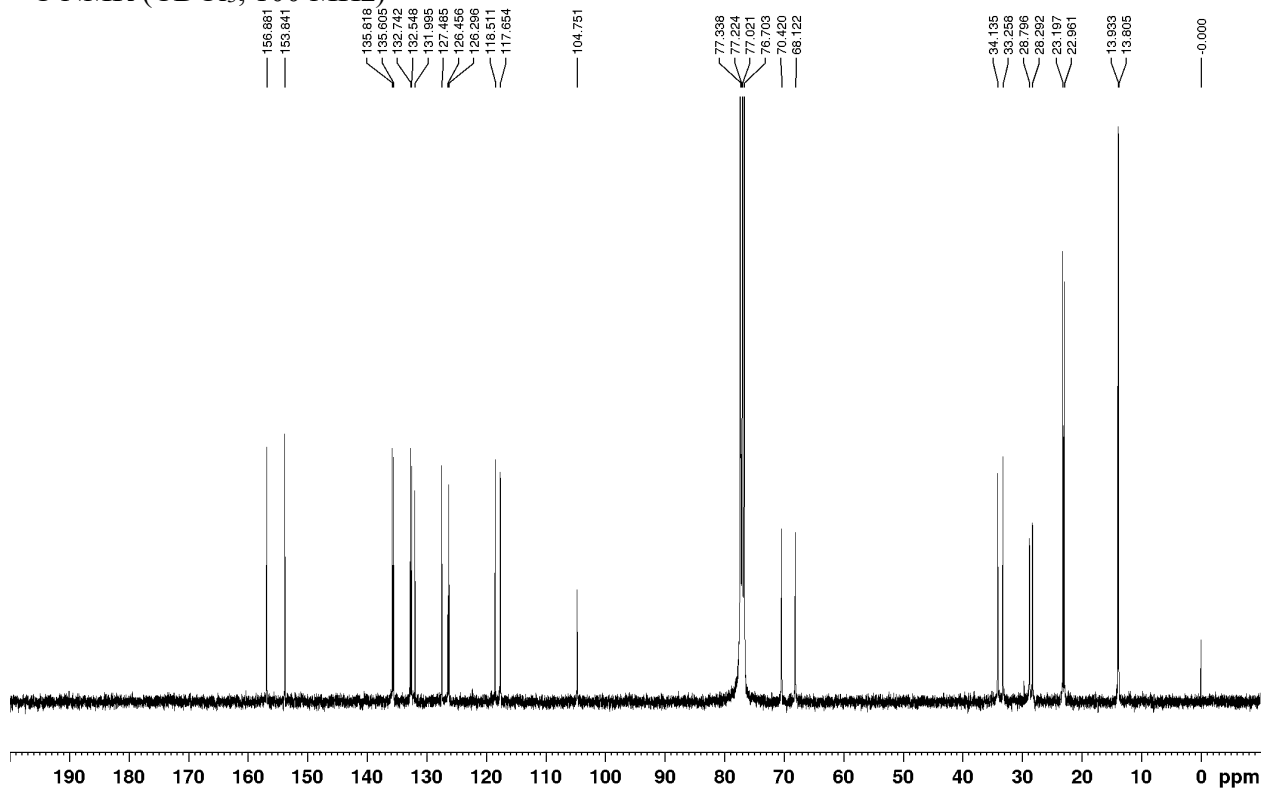


(*M,M*)-(-)-10

¹H NMR (CDCl₃, 400 MHz)



¹³C NMR (CDCl₃, 100 MHz)



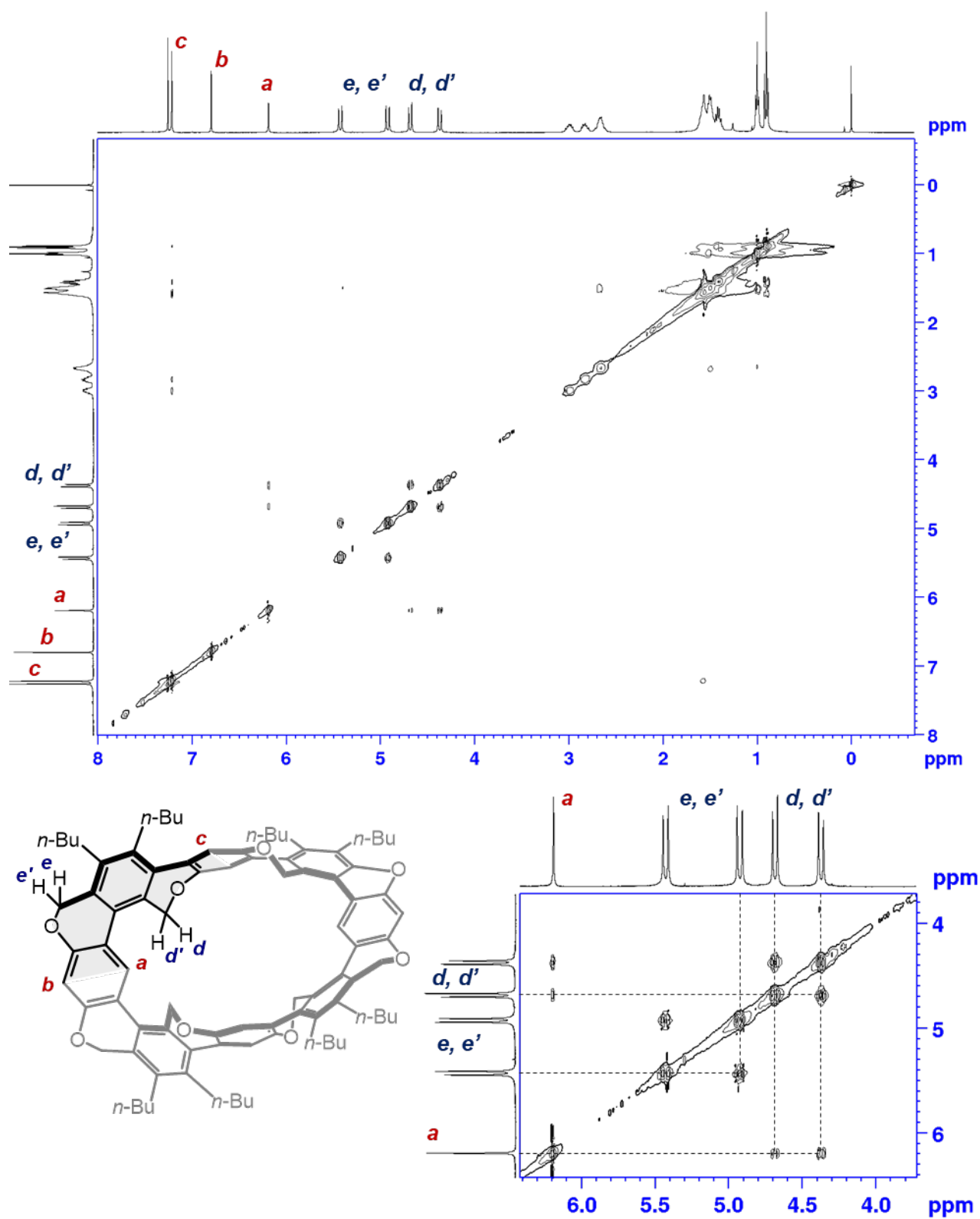
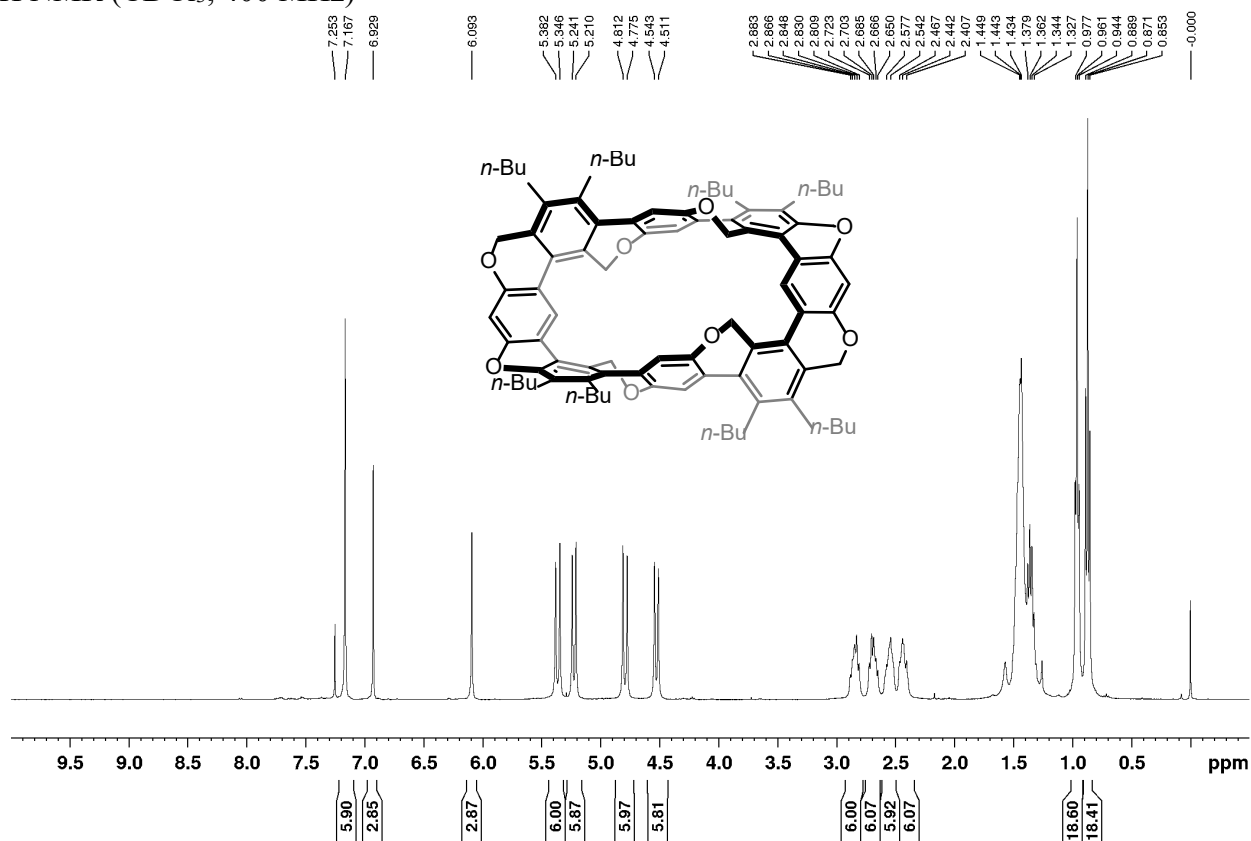


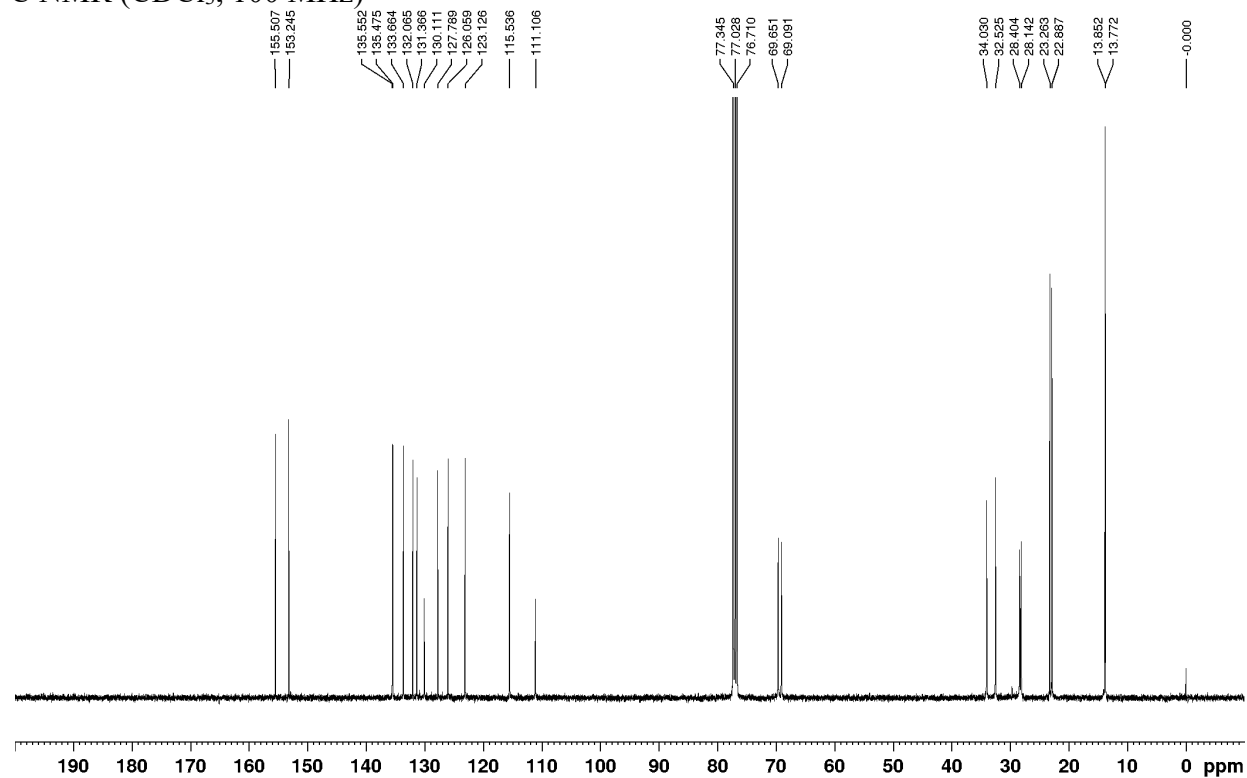
Figure S30. NOESY spectrum of *(M,M)*-(-)-**10** (CDCl_3 , 400 MHz).

(*P,M*)-**11**

¹H NMR (CDCl₃, 400 MHz)



¹³C NMR (CDCl₃, 100 MHz)



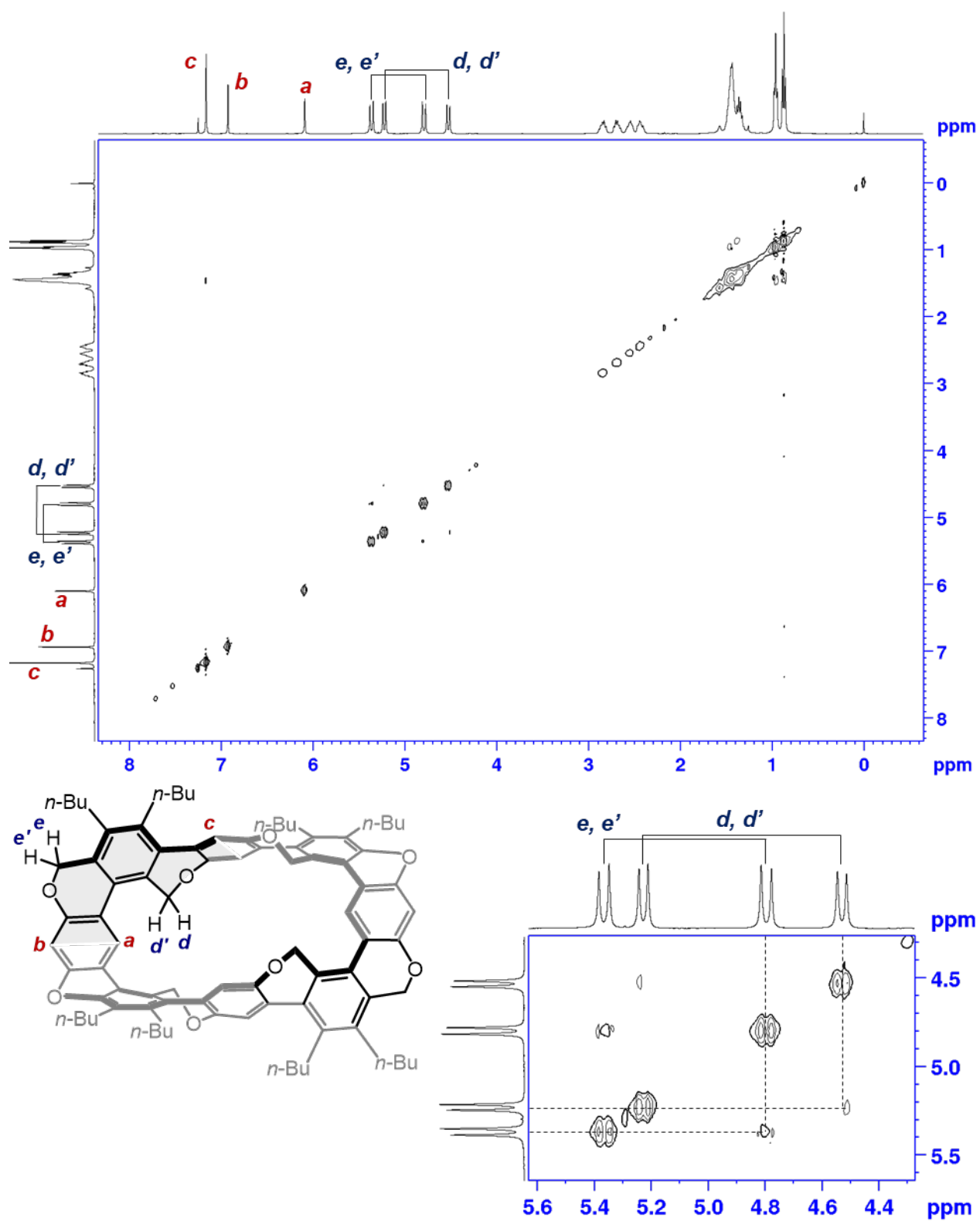


Figure S31. NOESY spectrum of *(P,M)*-11 (CDCl_3 , 400 MHz).

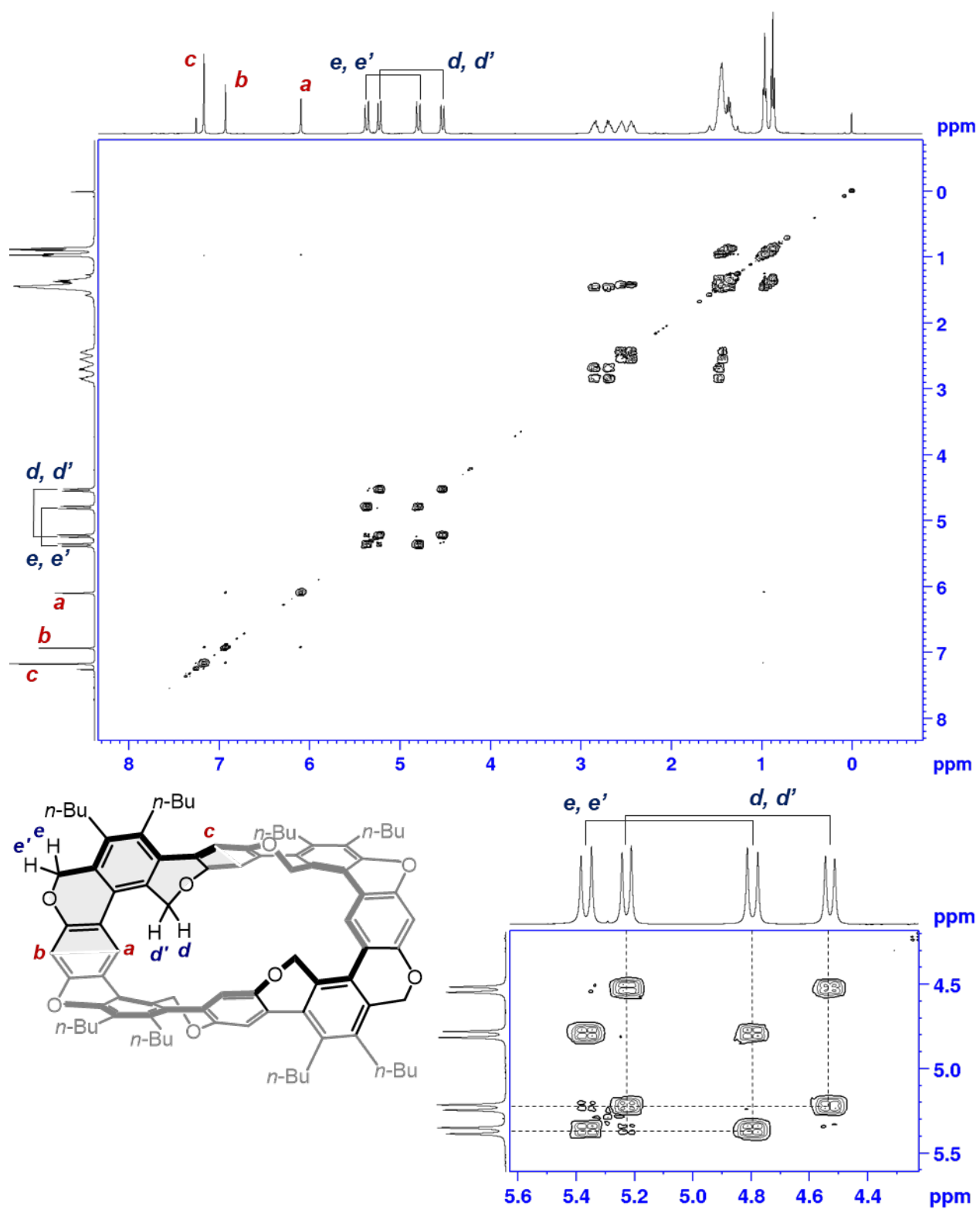


Figure S32. COSY spectrum of **(P,M)-11** (CDCl_3 , 400 MHz).

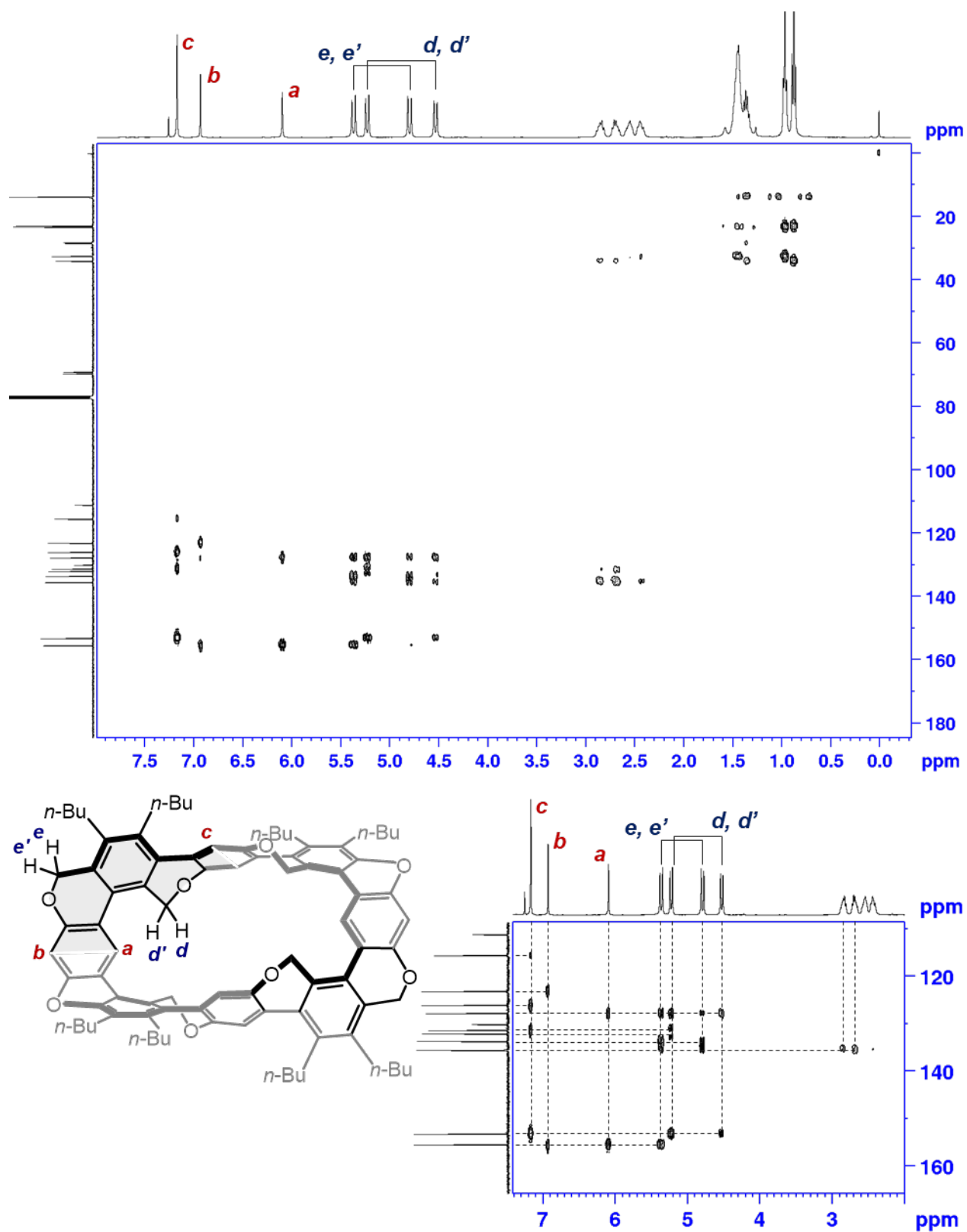


Figure S33. HMBC spectrum of *(P,M)*-11 (CDCl₃, 400 MHz).

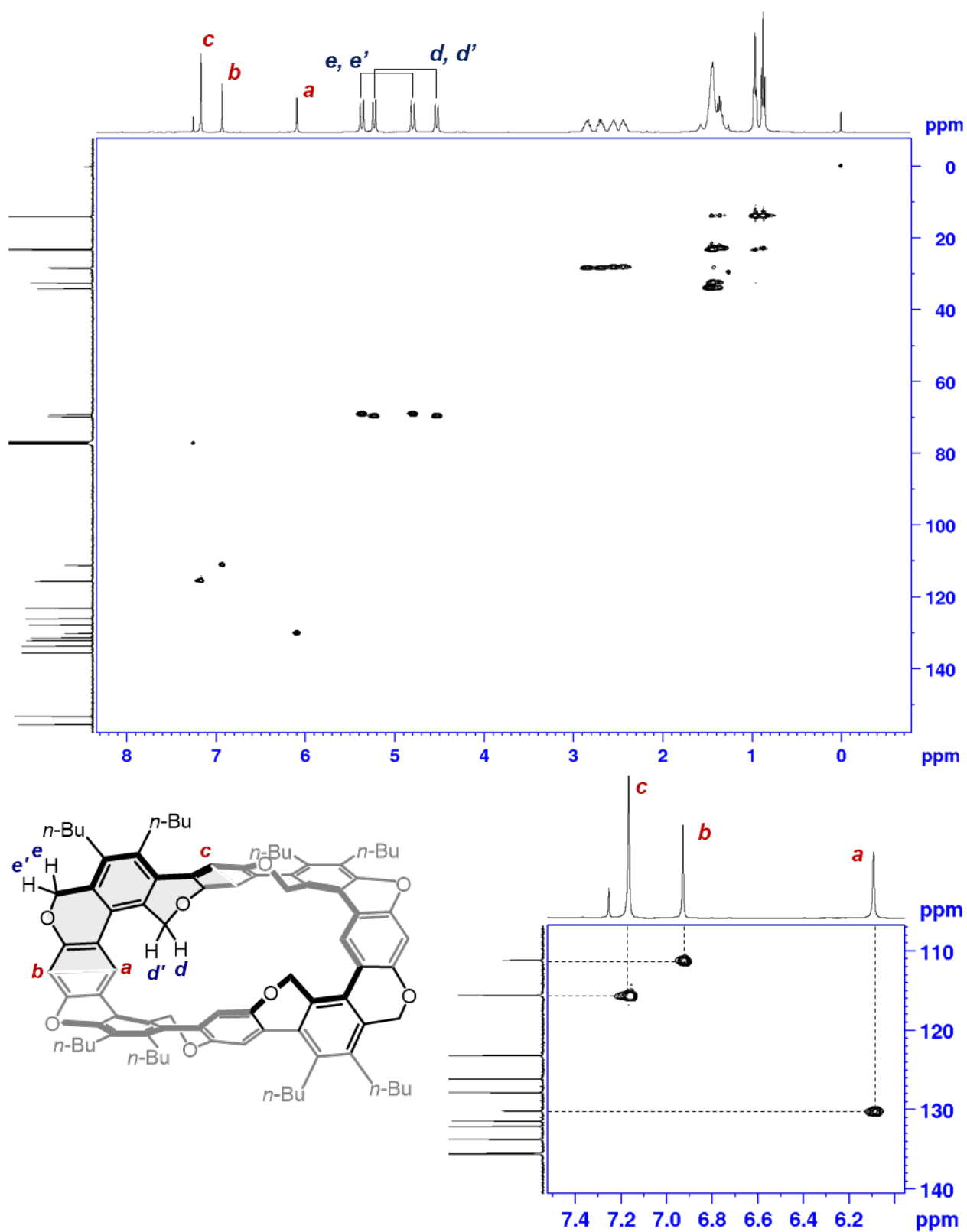
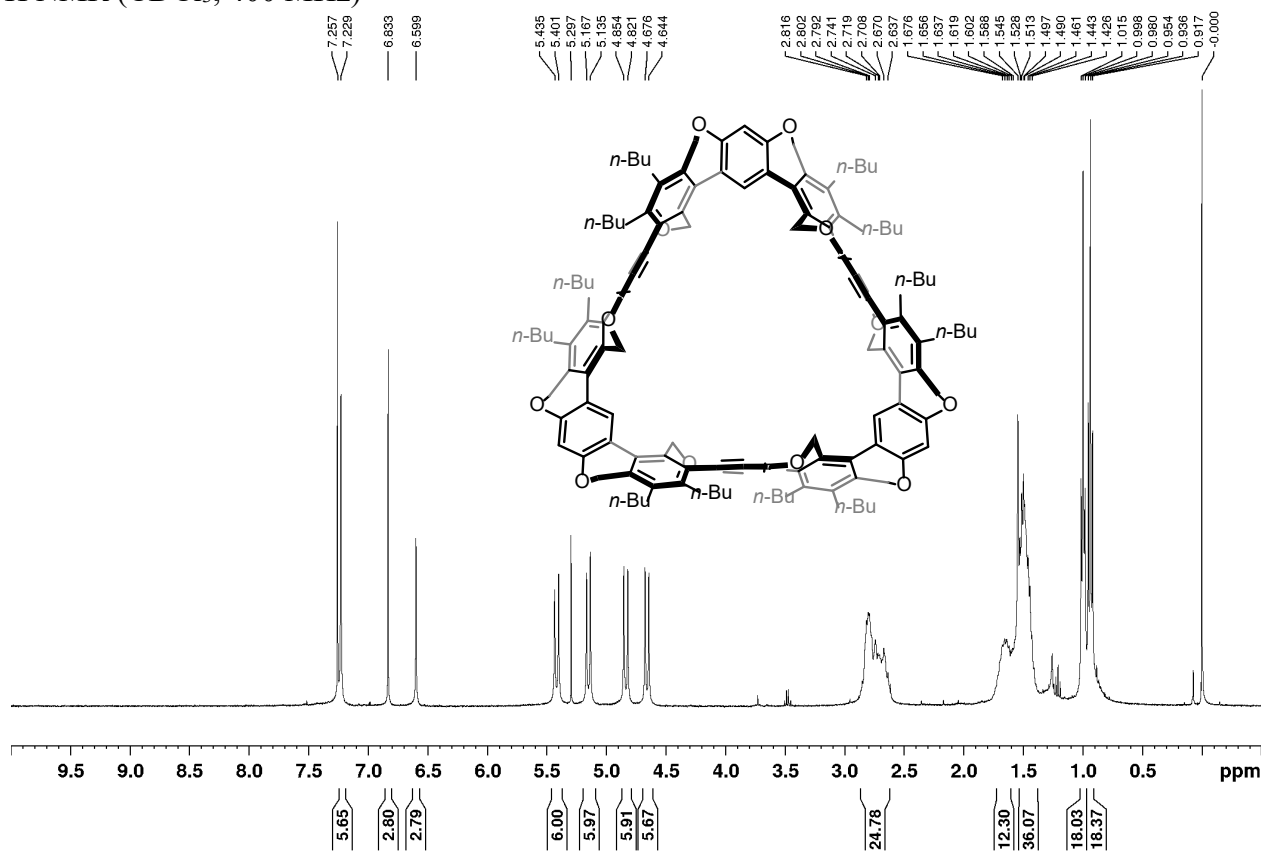


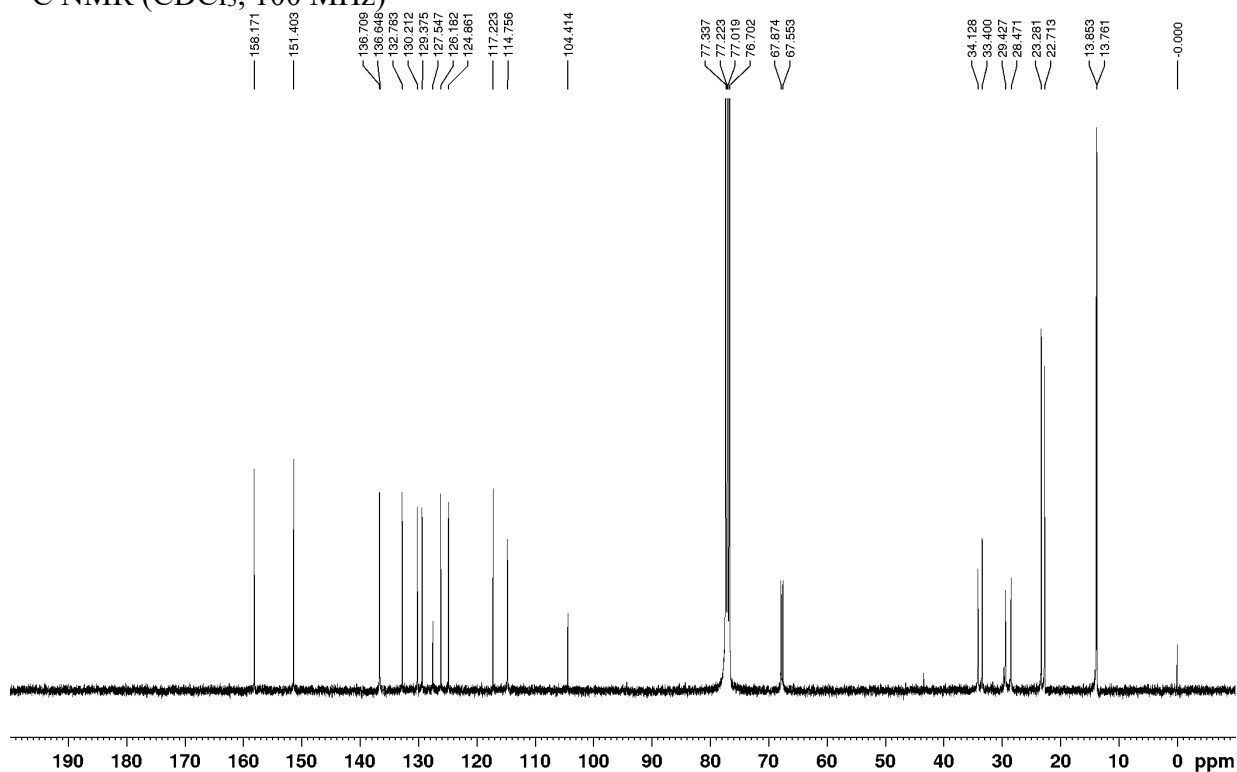
Figure S34. HSQC spectrum of *(P,M)*-11 (CDCl₃, 400 MHz).

(*M,M,M*)-(-)-12

¹H NMR (CDCl₃, 400 MHz)



¹³C NMR (CDCl₃, 100 MHz)



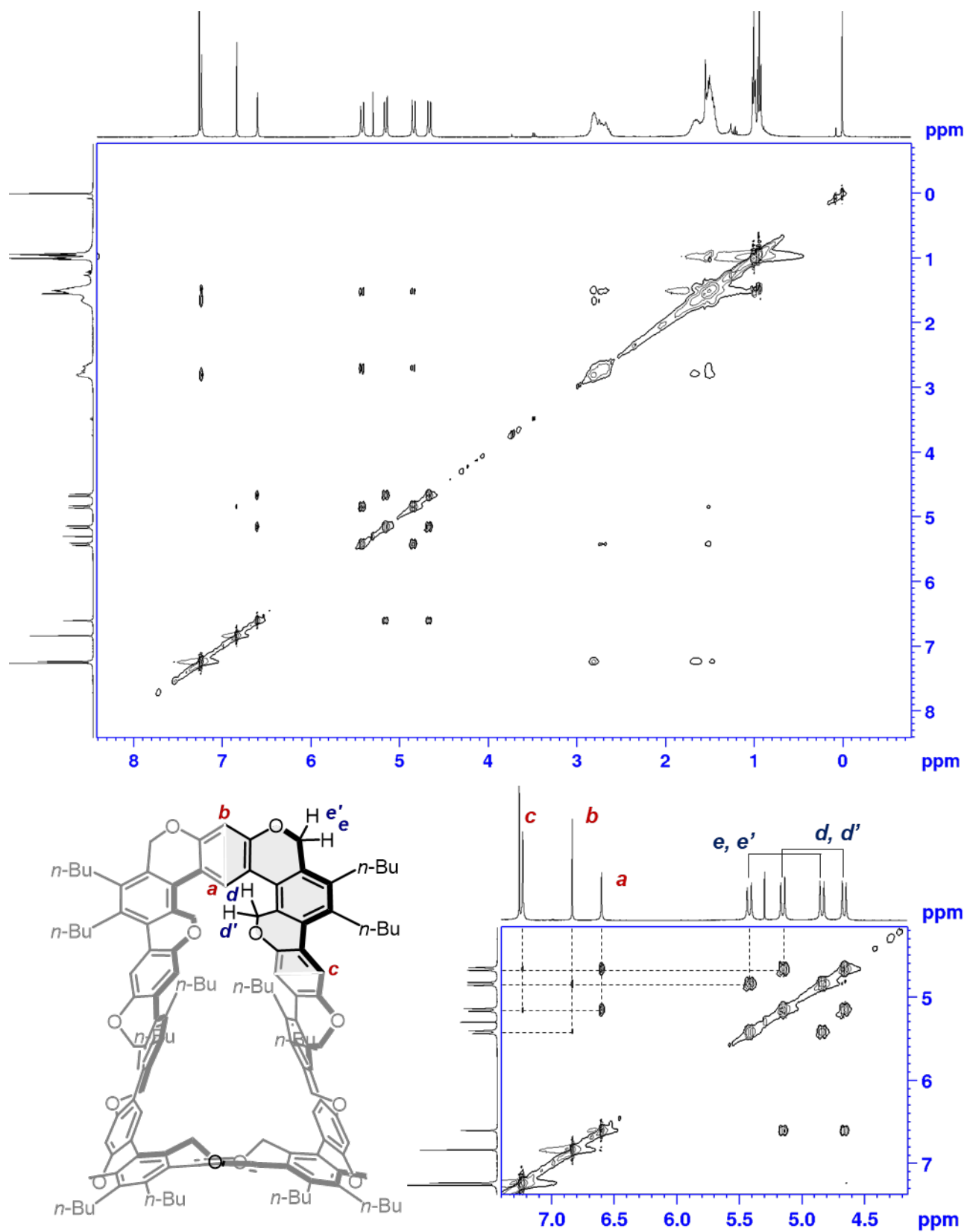
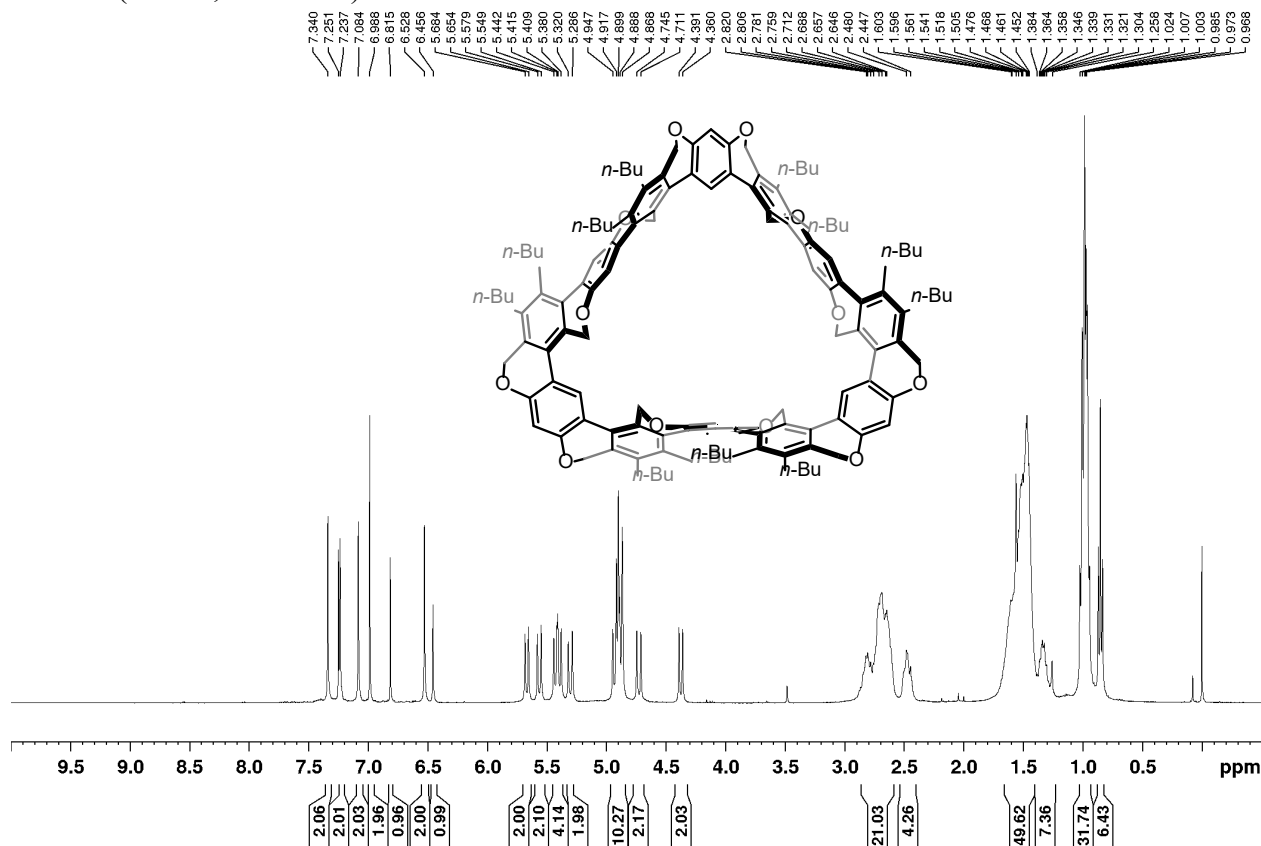


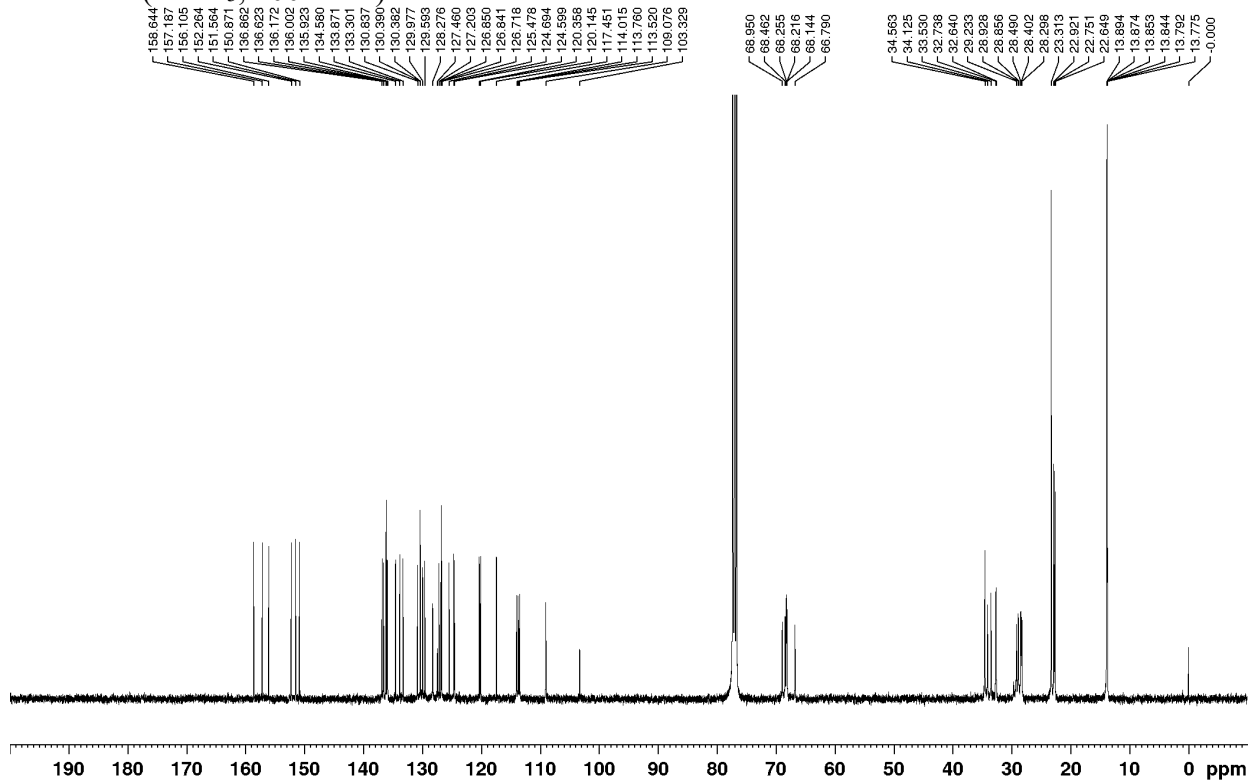
Figure S35. NOESY spectrum of (M,M,M) -(-)-12 (CDCl_3 , 400 MHz).

(*P,M,M*)-(-)-13

¹H NMR (CDCl₃, 400 MHz)



¹³C NMR (CDCl₃, 100 MHz)



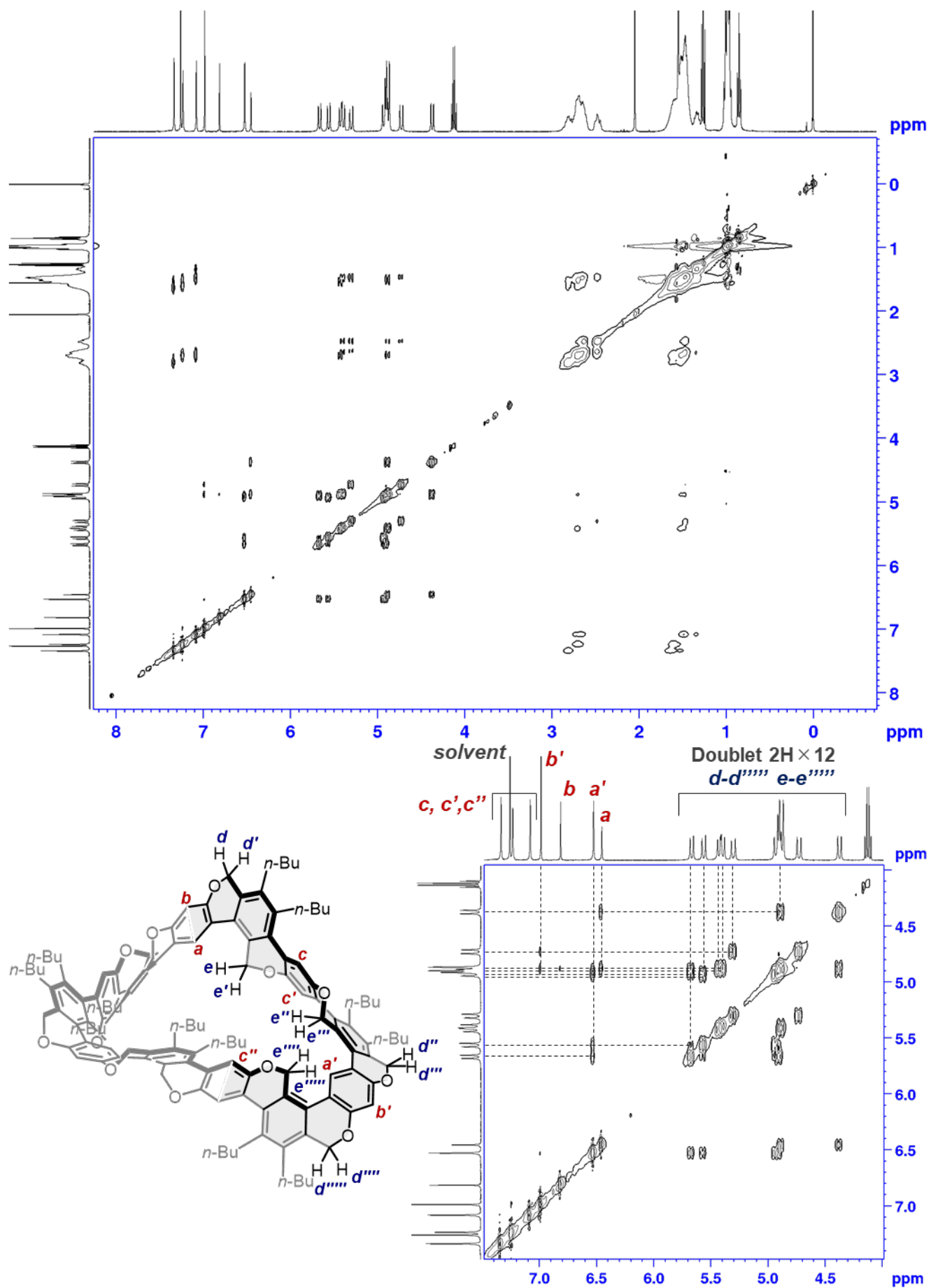


Figure S36. NOESY spectrum of (P,M,M) -(-)-**13** (CDCl_3 , 400 MHz).

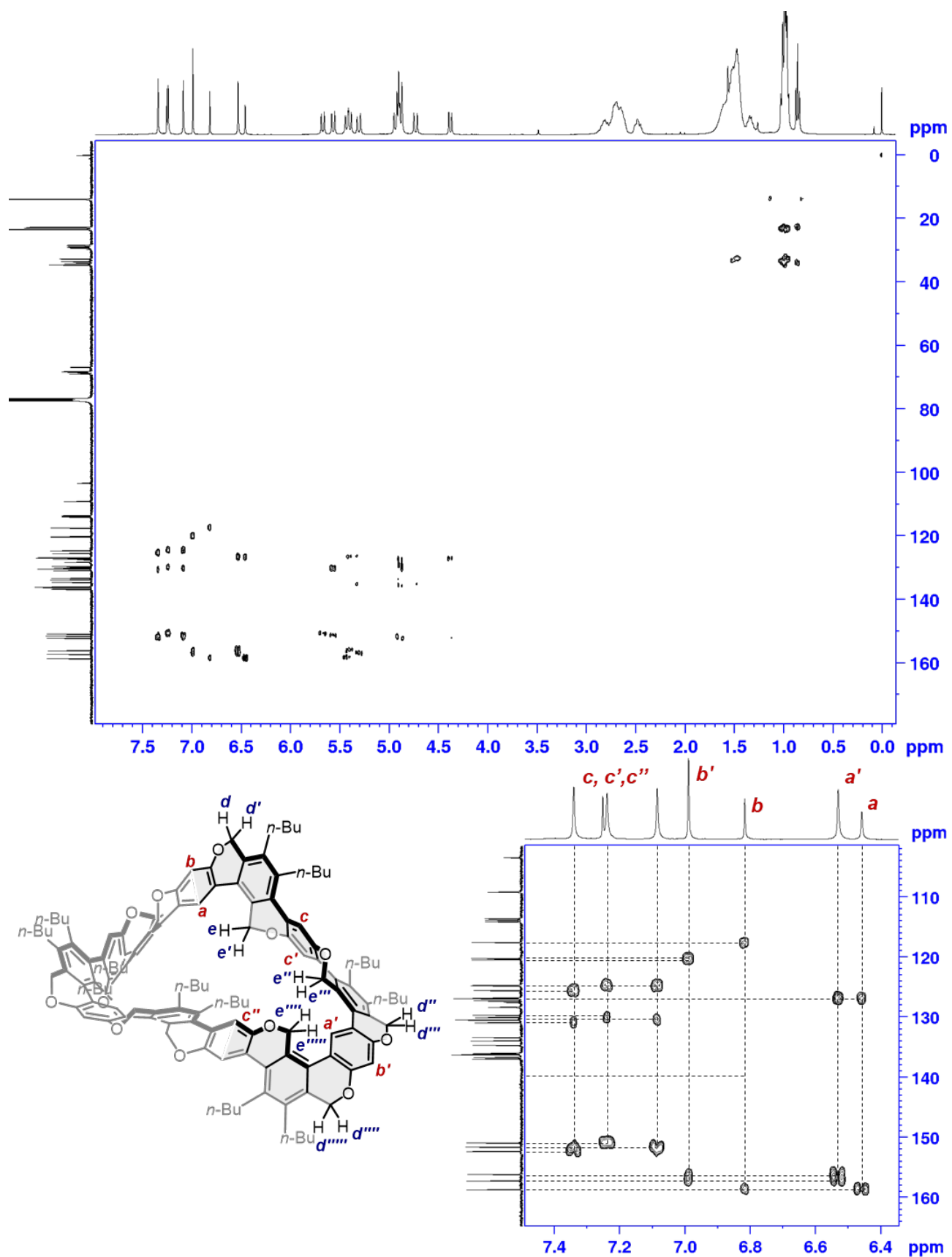


Figure S38. HMBC spectrum of *(P,M,M)*-(-)-13 (CDCl₃, 400 MHz).

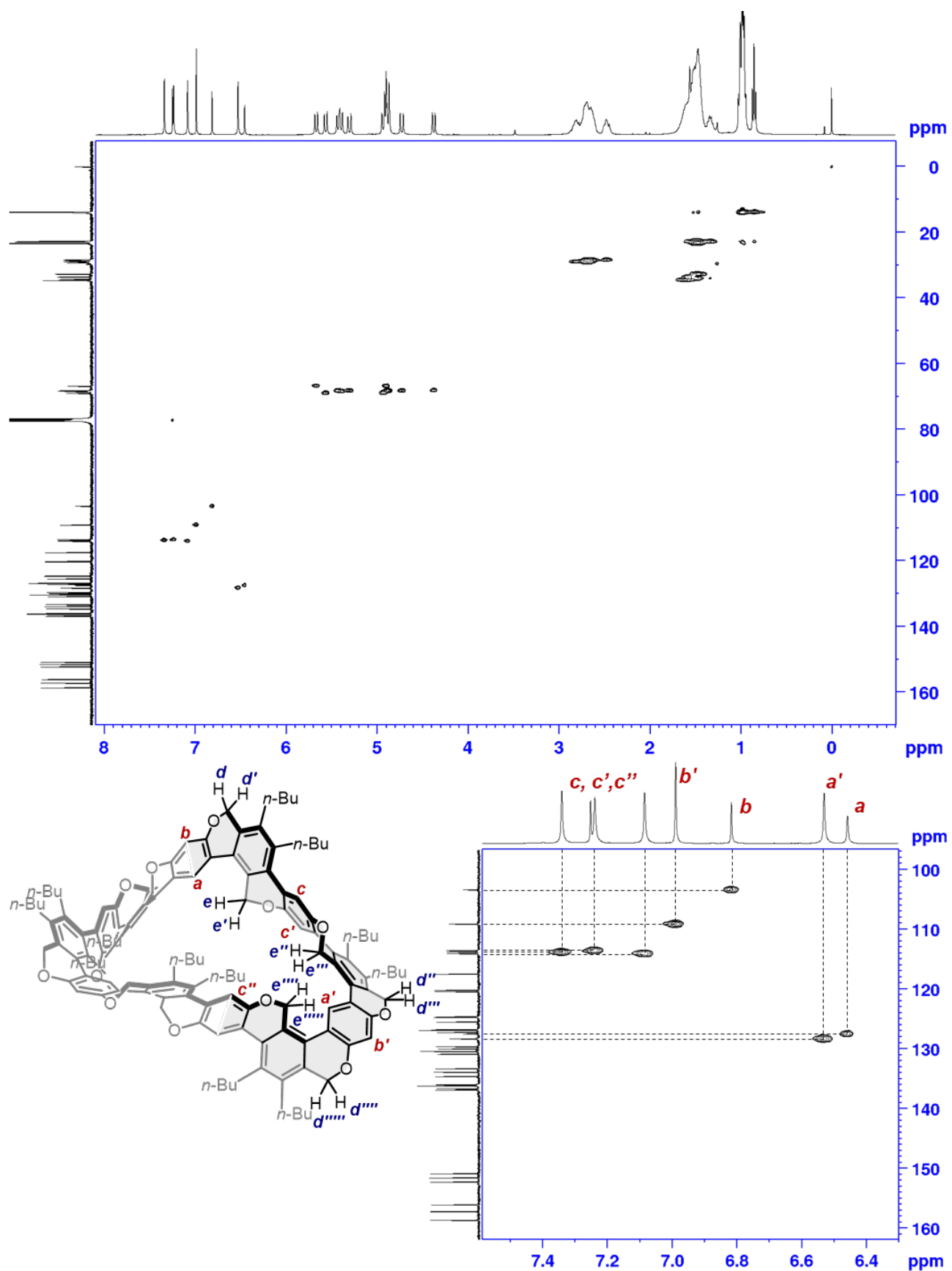
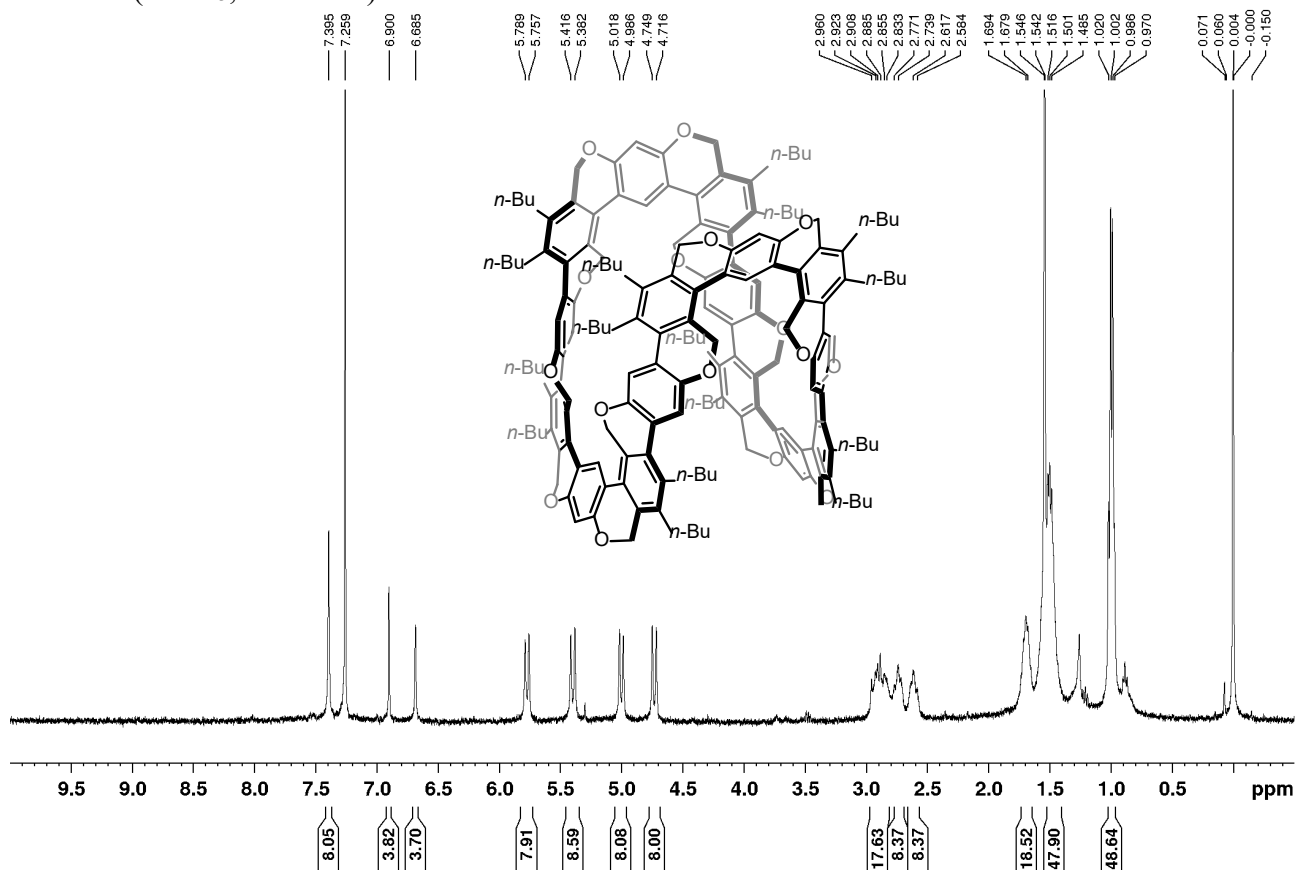


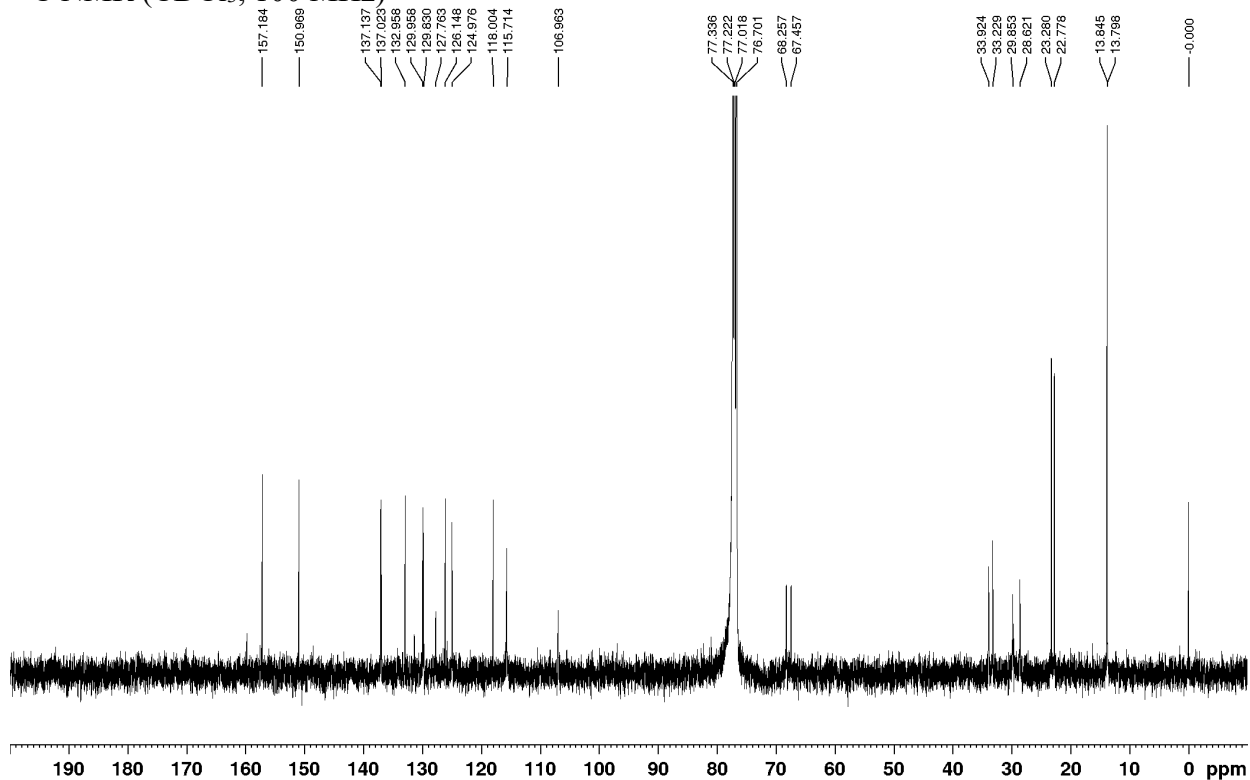
Figure S39. HSQC spectrum of (P,M,M) -(-)-13 (CDCl_3 , 400 MHz).

(*P,M,P,M*)-14

¹H NMR (CDCl₃, 400 MHz)



¹³C NMR (CDCl₃, 100 MHz)



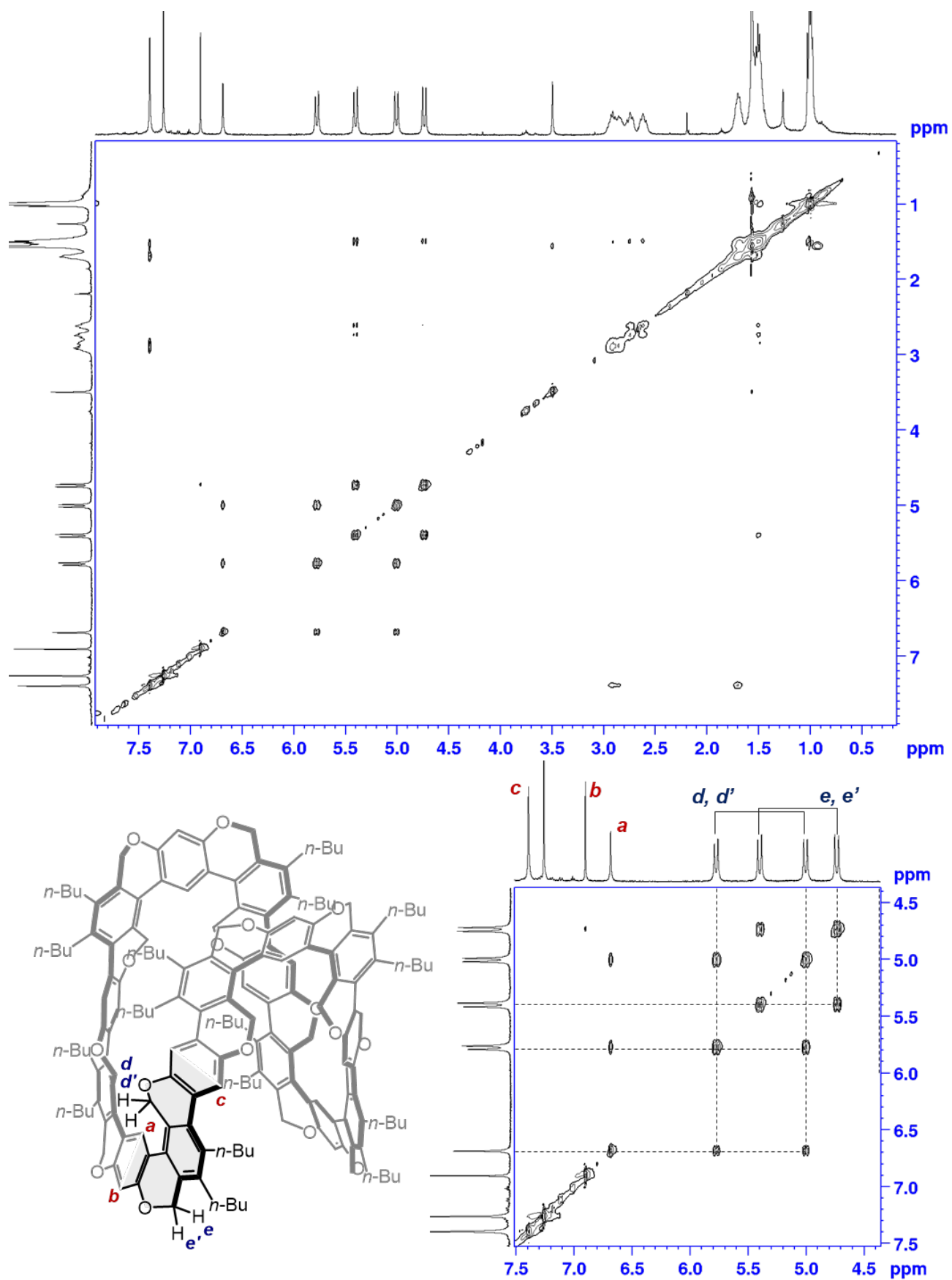


Figure S40. NOESY spectrum of *(P,M,P,M)*-14 (CDCl_3 , 400 MHz).

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