Supporting Information

Asymmetric Synthesis, Structures, and Chiroptical Properties of Helical Cycloparaphenylenes

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1. Synthetic Experiments

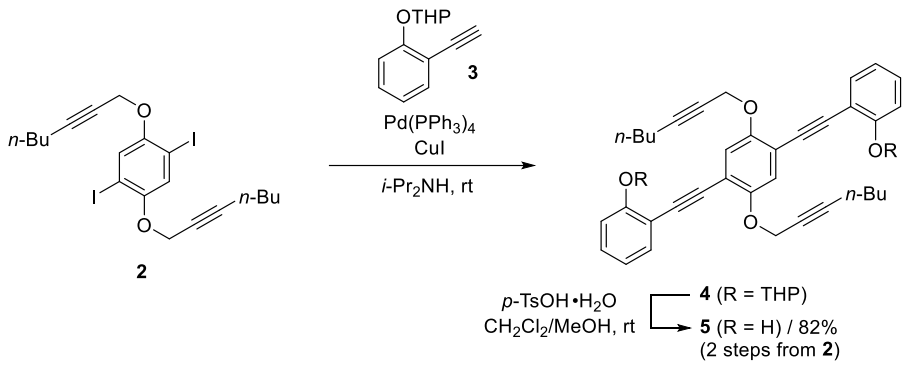
1.1. General Experimental Information

Dry degassed *i*-Pr_2NH (*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 **7a** and **7b**, anhydrous $(CH_2Cl)_2$ (No. 284505, Aldrich) for the synthesis of **1a** and **1b** were used as received. Solvents for the synthesis of substrates were dried over Molecular Sieves 4Å (Wako) prior to use. H_8-BINAP and Segphos were obtained from Takasago International Corporation. $[Rh(cod)_2]BF_4$ was obtained from Umicore AG. 1,4-Bis(hept-2-yn-1-yloxy)-2,5-diiodobenzene (**2**),[1] 2-(2-ethynylphenoxy) tetrahydro-2*H*-pyran (**3**),[2] and 1,4-bis(3-bromoprop-1-yn-1-yl)benzene (**6**)[3] 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 ^{13}C NMR spectroscopy. Copies of the ^1H and ^{13}C NMR spectra for all new compounds can be found at the section 3 "^1H NMR and ^{13}C NMR Spectra of New Compounds" of the Supplementary Materials. All previously unreported compounds were additionally characterized by high-resolution mass spectrometry (HRMS). ^1H, ^{13}C, 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 ^{13}C NMR spectra are reported in ppm relative to deuterochloroform (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 $\Delta\varepsilon/M^{-1}$ cm^{-1}. The CPL spectra were obtained on a JASCO CPL-300 circularly polarized luminescence spectrophotometer using a 10 mm quartz cell. The magnitude of the CPL signal is expressed in terms of θ / mdeg (normalized).

1.3. Synthesis of 2,2'-((2,5-bis(hept-2-yn-1-yloxy)-1,4-phenylene)bis(ethyne-2,1-diyl)) diphenol (5)

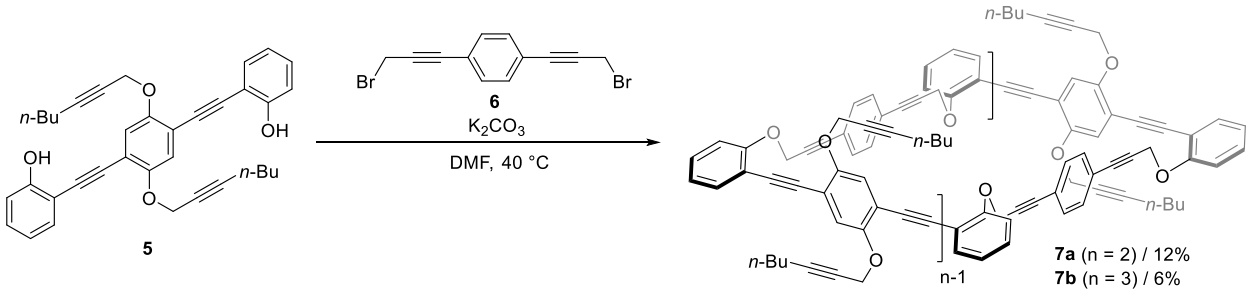


To a solution of 1,4-bis(hept-2-yn-1-yloxy)-2,5-diiodobenzene[1] (**2**, 1.54 g, 2.80 mmol), $Pd(PPh_3)_4$ (0.162 g, 0.140 mmol), and CuI (53.3 mg, 0.280 mmol) in dry degassed *i*-Pr_2NH (100 mL) was added a solution of THP-protected 2-ethynylphenol[2] (**3**, 1.47 g, 7.28 mmol) in dry degassed *i*-Pr_2NH (10 mL). The mixture was stirred at room temperature for 1.5 h. The resulting mixture was filtered and concentrated. The residue was roughly purified by silica gel column chromatography (eluent: *n*-hexane/EtOAc = 4:1) to give impure **4**, which was used in the next step without further purification.

p-Toluenesulfonic acid monohydrate (53.3 mg, 0.280 mmol) was added to a solution of the above impure **4** in CH_2Cl_2 (18 mL) and MeOH (18 ml) at room temperature. After stirring at room temperature for 45 min, the reaction mixture was concentrated *in vacuo*. The residue was purified by silica gel column chromatography (eluent: *n*-hexane/EtOAc = 8:1) to give **5** (1.22 g, 2.30 mmol, 82% yield from **2**).

Yellow solid; mp 119.3–120.0 °C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.39 (dd, J = 1.5, 7.6 Hz, 2H), 7.28 (m, 2H), 7.00 (d, J = 8.2 Hz, 2H), 6.90 (t, J = 7.5 Hz, 2H), 6.72 (s, 2H), 4.80 (t, J = 2.0 Hz, 4H), 2.25 (tt, J = 2.0, 10.3 Hz, 4H), 1.51 (m, 4H), 1.42 (m, 4H), 0.89 (t, J = 7.3 Hz, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 157.6, 152.3, 130.7, 130.2, 120.1, 115.3, 114.7, 113.5, 109.5, 93.1, 90.8, 89.9, 74.0, 58.0, 30.4, 21.9, 18.5, 13.6; HRMS (ESI) calcd for $C_{36}H_{34}O_4Na$ $[M+Na]^+$ 553.2349, found 553.2349.

1.4. Synthesis of macrocycle 7a and 7b



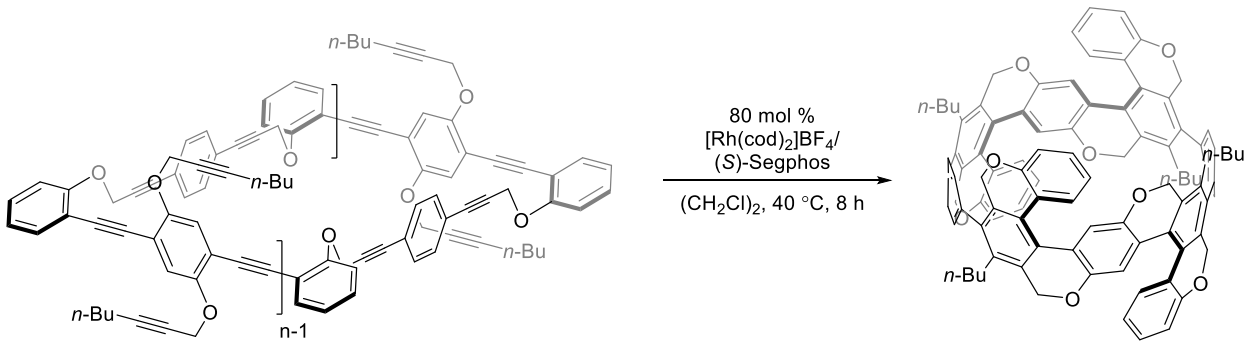
To a Schlenk tube was added a solution of **5** (0.265 g, 0.500 mmol), 1,4-bis(3-bromoprop-1-yn-1-yl)benzene[3] (**6**, 0.156 g, 0.500 mmol), and K_2CO_3 (0.346 g, 2.50 mmol) in DMF (20 mL) at room temperature. The mixture was stirred at 40 °C for 16 h. The reaction was quenched with water and extracted 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 crude product was purified by silica gel PTLC (eluent: *n*-hexane/CH_2Cl_2 = 2:3) to give **7a** (39.2 mg, 0.0288 mmol, 12% yield) and **7b** (21.5 mg, 0.0105 mmol, 6% yield).

Data for **7a**; colorless solid; mp 193.1–194.9 °C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.54 (dd, *J* = 1.4, 7.6 Hz, 4H), 7.39 (s, 8H), 7.31 (m, 4H), 7.21 (s, 4H), 7.05 (d, *J* = 8.3 Hz, 4H), 7.00 (t, *J* = 7.5 Hz, 4H), 5.03 (s, 8H), 4.73 (s, 8H), 2.17 (tt, *J* = 2.0, 7.0 Hz, 8H), 1.44 (m, 8H), 1.34 (m, 8H), 0.84 (t, *J* = 7.2 Hz, 12H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 158.5, 152.9, 133.6, 131.7, 129.7, 122.6, 121.7, 119.3, 114.9, 114.0, 113.8, 91.3, 90.2, 88.8, 86.7, 85.8, 75.0, 58.5, 58.0, 30.5, 21.9, 18.5, 13.6; HRMS (ESI) calcd for $C_{96}H_{80}O_8Na$ $[M+Na]^+$ 1383.5745, found 1383.5664.

Data for **7b**: colorless solid; mp 97.9–98.2 °C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.54 (dd, *J* = 1.6, 7.6 Hz, 6H), 7.35 (s, 12H), 7.31 (ddd, *J* = 1.8, 8.4, 7.4 Hz, 6H), 7.20 (s, 6H), 7.08 (d, *J* = 7.8 Hz, 6H), 6.99 (ddd, *J* = 0.9, 7.5, 7.5 Hz, 6H), 5.06 (s, 12H), 4.75 (t, *J* = 2.1 Hz, 12H), 2.18 (tt, *J* = 2.0, 7.0 Hz, 12H), 1.45 (m,12H), 1.36 (m, 12H), 0.84 (t, *J* = 7.2 Hz, 18H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 158.3, 152.9, 133.7, 131.7, 129.7, 122.6, 121.6, 119.2, 114.8, 113.82, 113.78, 91.4, 90.2, 88.8, 86.9, 85.9, 75.0, 58.5, 57.8, 30.5, 21.9, 18.5, 13.6; HRMS (ESI) calcd for $C_{144}H_{120}O_{12}Na$ $[M+Na]^+$ 2063.8672, found 2063.8450.

1.5. Synthesis of (*Sp*,*Sp*)-(*M*,*M*,*M*,*M*)-(–)-1a



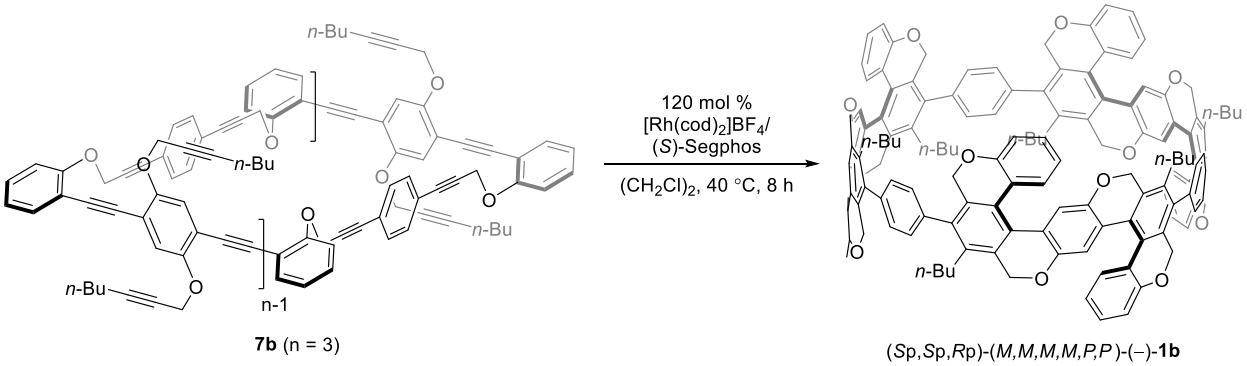
7a (n = 2) (*Sp*,*Sp*)-(*M*,*M*,*M*,*M*)-(–)-**1a**

(*S*)-Segphos (3.13 mg, 0.00513 mmol) and $[Rh(cod)_2]BF_4$ (2.08 mg, 0.00513 mmol) 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 $(CH_2Cl)_2$ (2.1 mL). To this solution was added a solution of **7a** (8.73 mg, 0.00641 mmol) in $(CH_2Cl)_2$ (4.3 mL). The mixture was stirred at 40 °C for 8 h. The resulting mixture was concentrated and purified by silica gel PTLC (eluent: *n*-hexane/CH_2Cl_2 = 2:3) to give (*Sp*,*Sp*)-(*M*,*M*,*M*,*M*)-(–)-**1a** (3.47 mg, 0.00255 mmol, 40% yield, >99% ee).

Yellow solid; mp 164 °C (decomposition); $[\alpha]^{25}_D$ –3357° [*c* 13.6 μg/cm^3, CH_2Cl_2, 99% ee]; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.91 (dd, *J* = 1.5, 7.7 Hz, 4H), 7.42 (s, 4H), 7.29 (ddd, *J* = 1.6, 7.9, 7.5 Hz, 4H), 7.07 (ddd, *J* = 1.4, 7.7, 7.5 Hz, 4H), 7.03 (dd, *J* = 0.9, 8.1 Hz, 4H), 6.86 (s, 4H), 6.32 (s, 4H), 5.03 (d, *J* = 13.9 Hz, 4H), 4.98 (d, *J* = 13.2 Hz, 4H), 4.87 (d, *J* = 13.2 Hz, 4H), 4.76 (d, *J* = 13.9 Hz, 4H), 2.28 (m, 4H), 2.19 (m, 4H), 1.25 (m, 16H), 0.83 (t, *J* = 6.9 Hz, 12H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 154.9, 148.0, 138.1, 137.7, 136.7, 133.6, 132.8, 130.1, 130.05, 130.00, 129.8, 128.8, 127.0, 124.9, 124.3, 122.2, 117.5, 114.9, 67.0, 65.9, 34.0, 29.3,

22.6, 13.8; HRMS (ESI) calcd for $C_{96}H_{80}O_8Na$ $[M+Na]^+$ 1383.5745, found 1383.5626; CHIRALPAK IG-3, *n*-hexane/CH_2Cl_2 = 60:40, 1.0 mL min^{-1}, retention times: 4.39 min (major isomer) and 6.64 min (minor isomer).

1.6. Synthesis of (*S*p,*S*p,*R*p)-(*M*,*M*,*M*,*M*,*P*,*P*)-(–)-1b

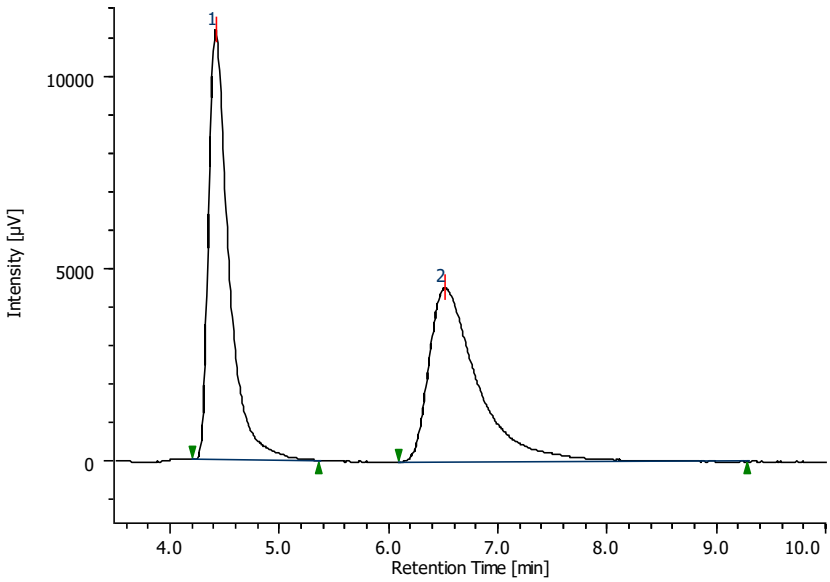


(*S*)-Segphos (1.23 mg, 0.00304 mmol) and $[Rh(cod)_2]BF_4$ (1.86 mg, 0.00304 mmol) were dissolved in CH_2Cl_2 (2.0 mL), and the mixture was stirred at room temperature for 10 min. H_2 was introduced to the resulting solution in a Schlenk tube. After stirring at room temperature for 30 min, the resulting mixture was concentrated to dryness. The residue was dissolved in $(CH_2Cl)_2$ (1.2 mL). To this solution was added a solution of **7b** (5.17 mg, 0.00253 mmol) in $(CH_2Cl)_2$ (1.3 mL). The mixture was stirred at 40 °C for 8 h. The resulting mixture was concentrated and purified by silica gel PTLC (eluent: *n*-hexane/CH_2Cl_2 = 2:3) to give (*S*p,*S*p,*R*p)-(*M*,*M*,*M*,*M*,*P*,*P*)-(–)-**1b** (3.06 mg, 0.00150 mmol, 59% yield, 62% ee).

Yellow solid; mp 279 °C (decomposition); $[\alpha]^{25}_D$ –466° [*c* 0.151 mg/cm^3, CH_2Cl_2, 62% ee]; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.94 (dd, *J* = 1.4, 7.9 Hz, 4H), 7.92 (dd, *J* = 1.5, 7.7 Hz, 2H), 7.46 (s, 4H), 7.37 (s, 2H), 7.29 (m, 6H), 7.12 (dd, *J* = 1.0, 8.1 Hz, 2H), 7.11 (dd, *J* = 1.0, 8.1 Hz, 2H), 7.06 (m, 4H), 7.02 (m, 4H), 6.85 (s, 4H), 6.84 (s, 2H), 6.78 (d, *J* = 0.9 Hz, 4H), 6.63 (s, 2H), 5.17 (d, *J* = 14.1 Hz, 2H), 5.16 (d, *J* = 14.3 Hz, 2H), 5.14 (d, *J* = 14.3 Hz, 2H), 5.11 (d, *J* = 14.4 Hz, 2H), 5.09 (d, *J* = 14.2 Hz, 2H), 4.93 (d, *J* = 13.8 Hz, 2H), 4.83 (d, *J* = 14.1 Hz, 2H), 4.79 (d, *J* = 14.2 Hz, 2H), 4.75 (d, *J* = 14.1 Hz, 2H), 4.61 (d, *J* = 14.2 Hz, 2H), 4.58 (d, *J* = 14.2 Hz, 2H), 2.25 (m, 2H), 2.09 (m, 2H), 1.93 (m, 4H), 1.75 (m, 4H), 1.18 (m, 24H), 0.74 (t, *J* = 7.1 Hz, 6H), 0.73 (t, *J* = 7.1 Hz, 12H) ; ^{13}C NMR ($CDCl_3$, 100 MHz) δ 155.4, 155.0, 149.3, 149.1, 148.9, 138.00, 137.99, 137.7, 137.0, 136.6, 136.0, 135.89, 135.86, 135.8, 135.7, 135.1, 133.4, 133.3, 133.2, 132.1, 131.2, 131.1, 129.79, 129.77, 129.73, 129.72, 129.71, 129.6, 128.2, 128.11, 128.10, 128.06, 128.0, 127.9, 127.7, 125.5, 125.4, 125.0, 124.1, 124.0, 123.6, 123.5, 122.2, 122.06, 122.05, 118.3, 118.1, 117.9, 117.74, 117.73, 117.6, 68.02, 68.01, 67.7, 67.64, 67.60, 67.1, 33.0, 32.9, 32.6, 29.7, 28.73, 28.69, 23.10, 23.08, 22.5, 13.8, 13.6, 1.0; HRMS (ESI) calcd for $C_{144}H_{120}O_{12}$ $[M]^+$ 2040.8774, found 2040.8703; CHIRALPAK IG-3, *n*-hexane/CH_2Cl_2 = 60:40, 1.0 mL min^{-1}, retention times: 4.53 min (major isomer) and 5.96 min (minor isomer).

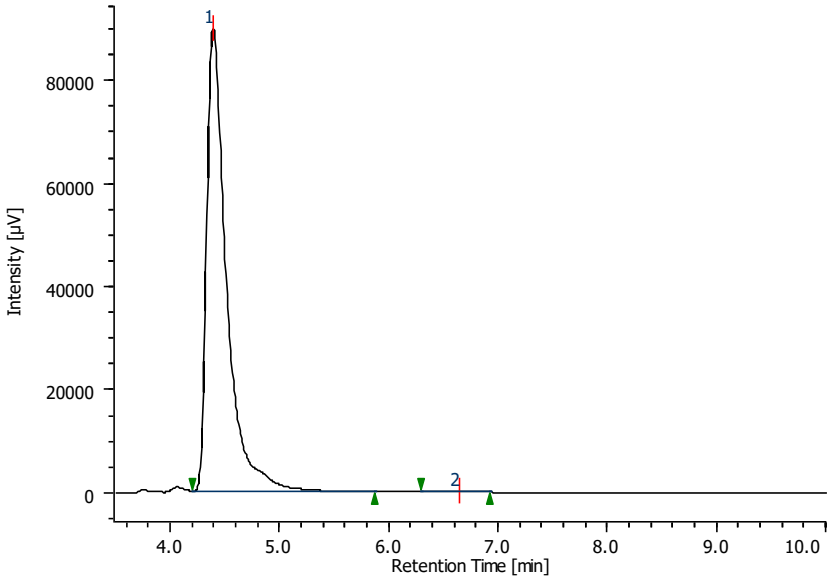
2. Chiral HPLC Charts of 1a and 1b

(±)-1a



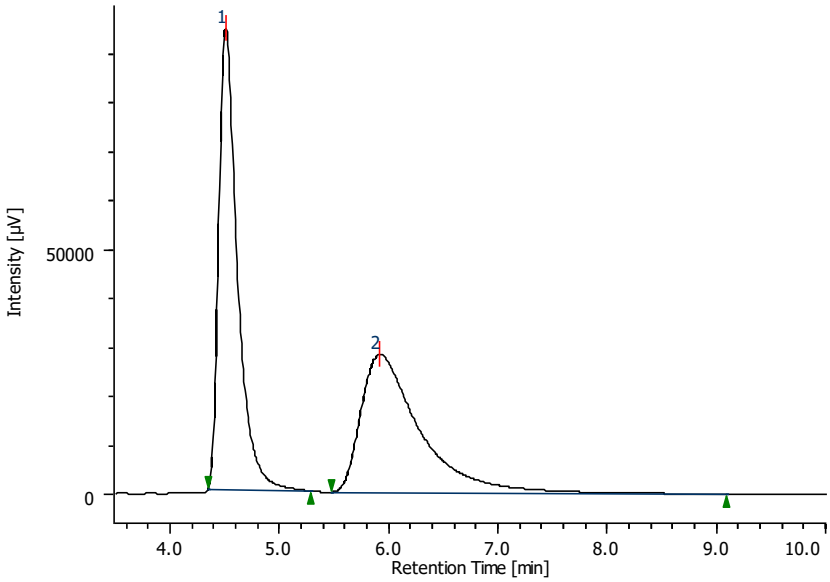
Peak No.	Retention time (min)	Area (%)
1	4.417	50.622
2	6.508	49.378

(*Sp*,*Sp*)-(*M*,*M*,*M*,*M*)-(–)-1a (>99% ee)



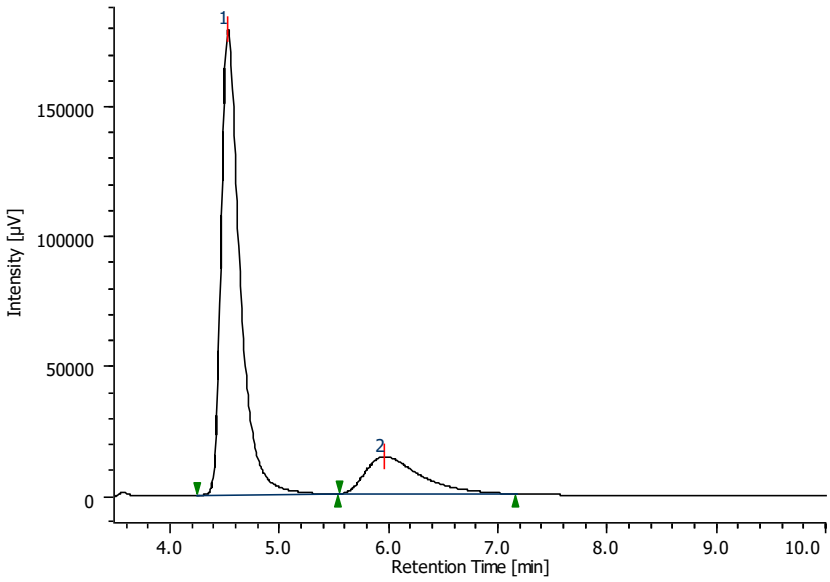
Peak No.	Retention time (min)	Area (%)
1	4.392	99.537
2	6.642	0.463

(±)-1b



Peak No.	Retention time (min)	Area (%)
1	4.508	51.422
2	5.917	48.578

(*S*p,*S*p,*R*p)-(*M*,*M*,*M*,*M*,*P*,*P*)-(–)-1b (62% ee)

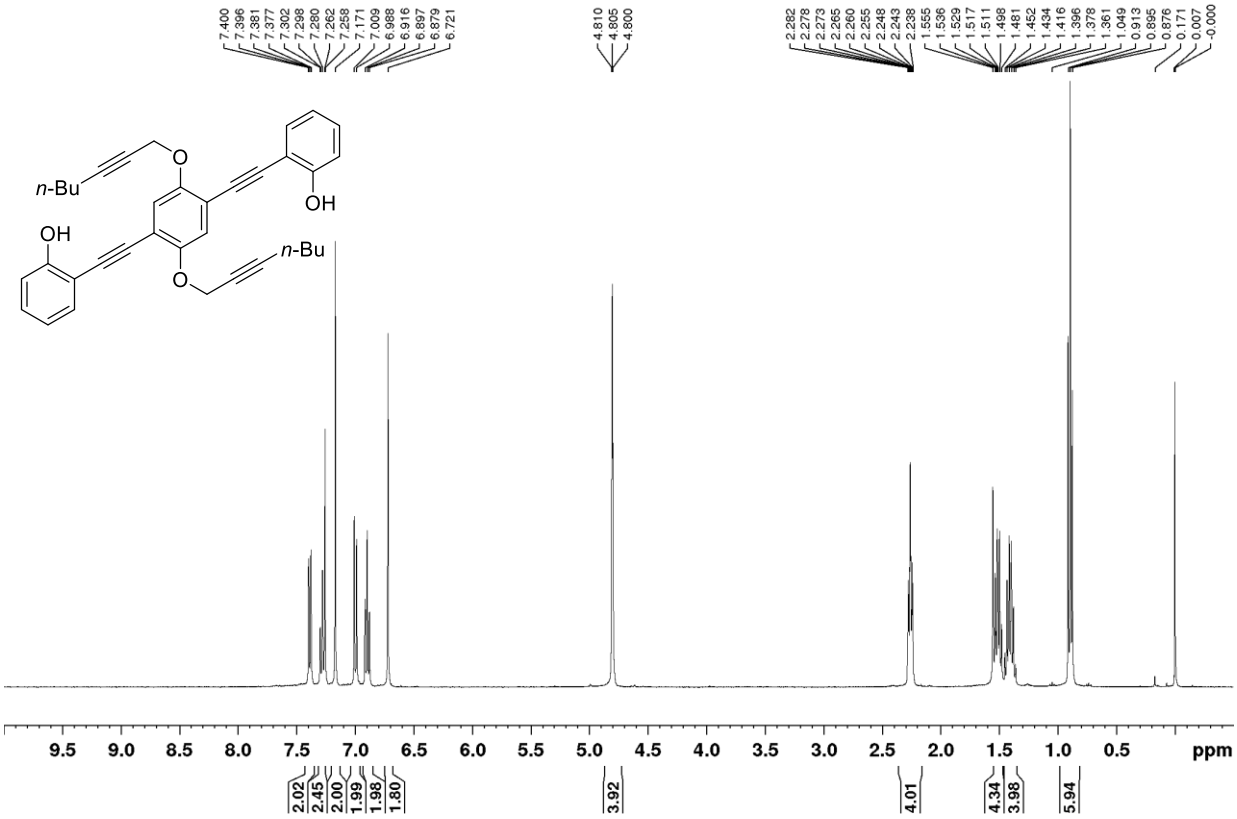


Peak No.	Retention time (min)	Area (%)
1	4.525	81.041
2	5.958	18.959

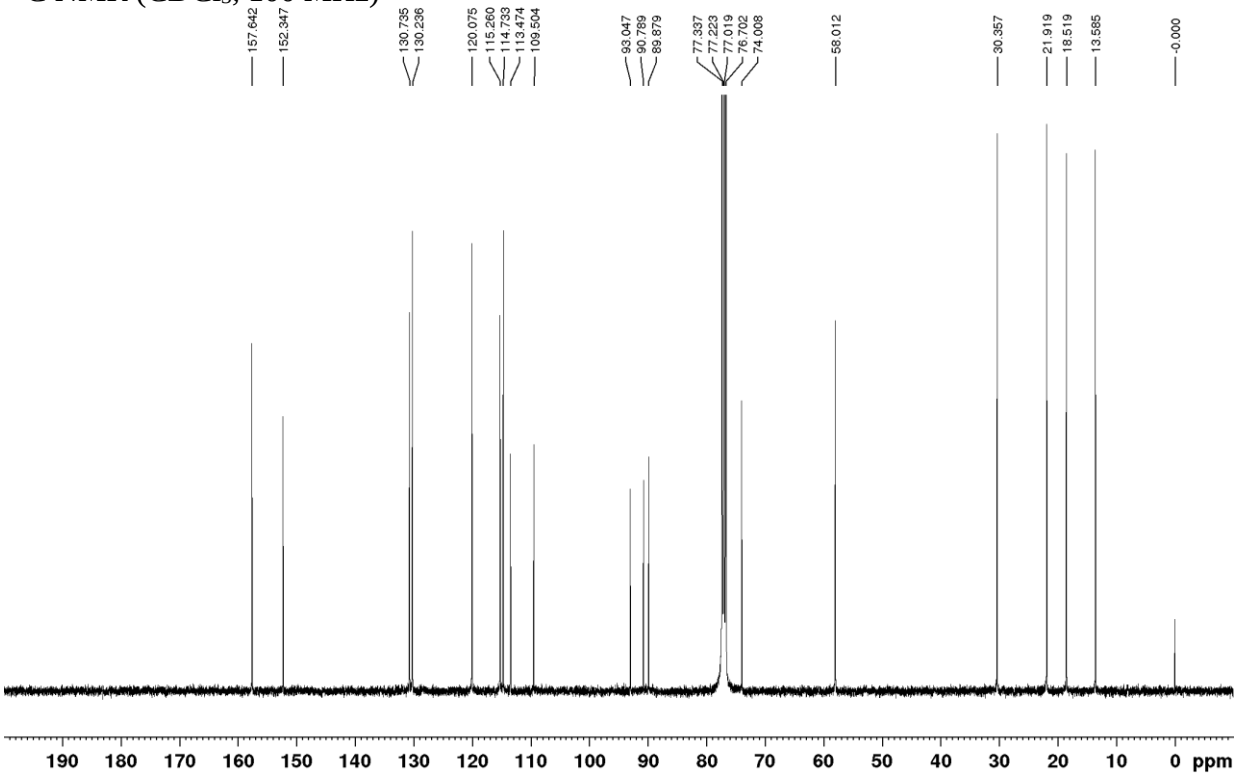
3. ^{1}H, ^{13}C, and 2D NMR Spectra of New Compounds

2,2'-((2,5-Bis(hept-2-yn-1-yloxy)-1,4-phenylene)bis(ethyne-2,1-diyl))diphenol (5)

^{1}H NMR ($CDCl_3$, 400 MHz)

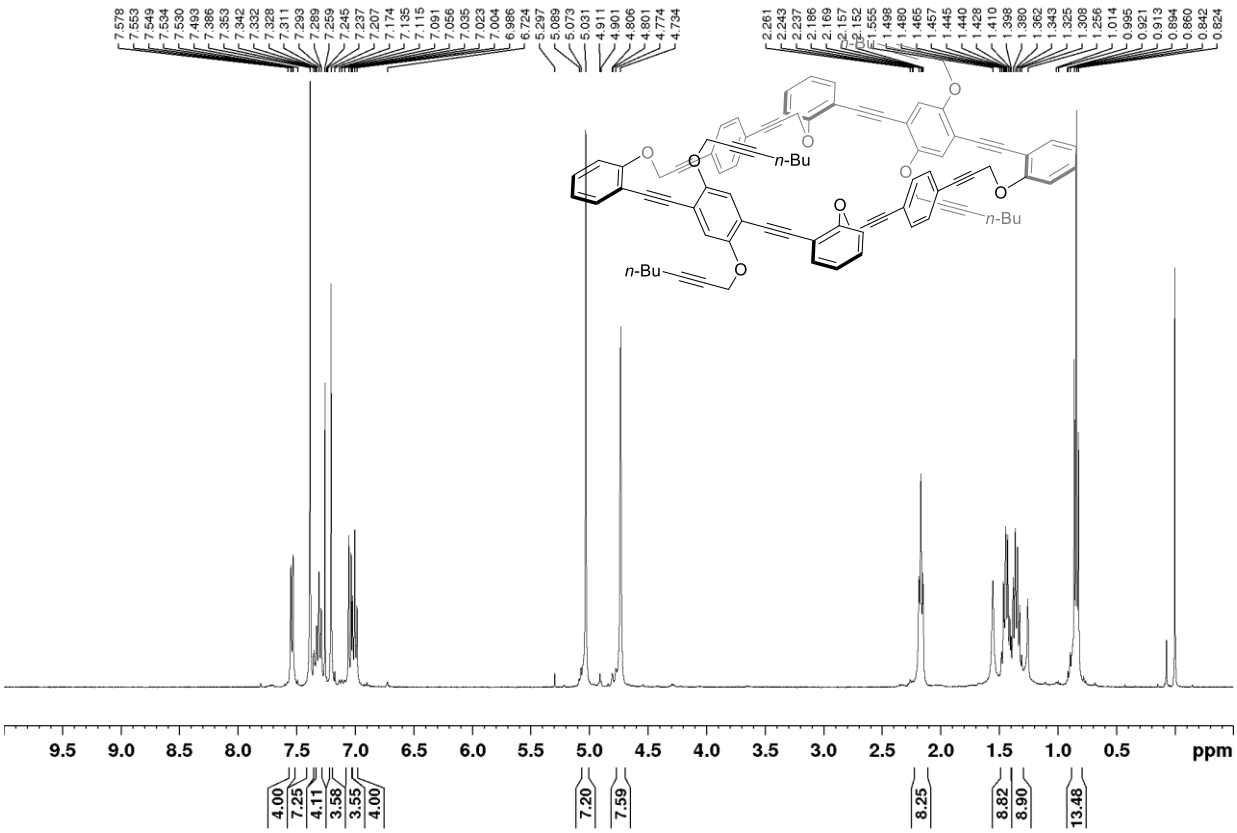


^{13}C NMR ($CDCl_3$, 100 MHz)

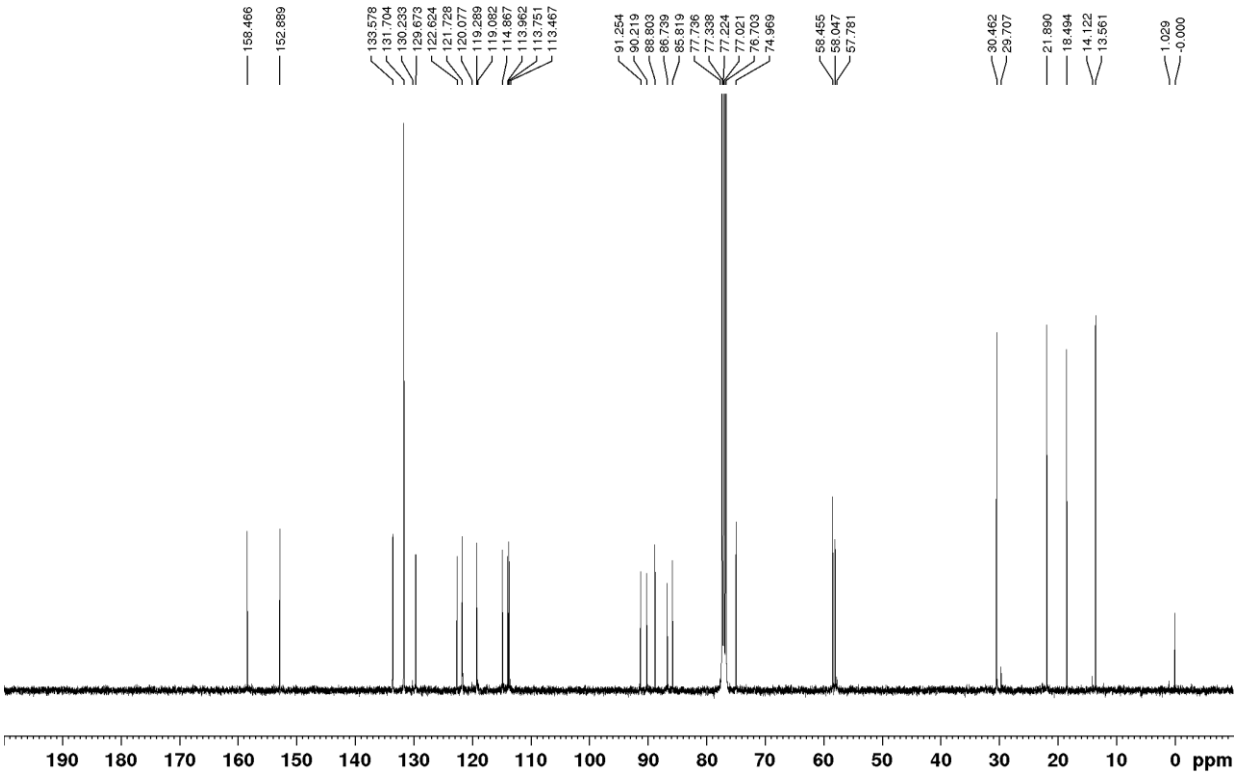


Macrocycle 7a

^{1}H NMR ($CDCl_3$, 400 MHz)

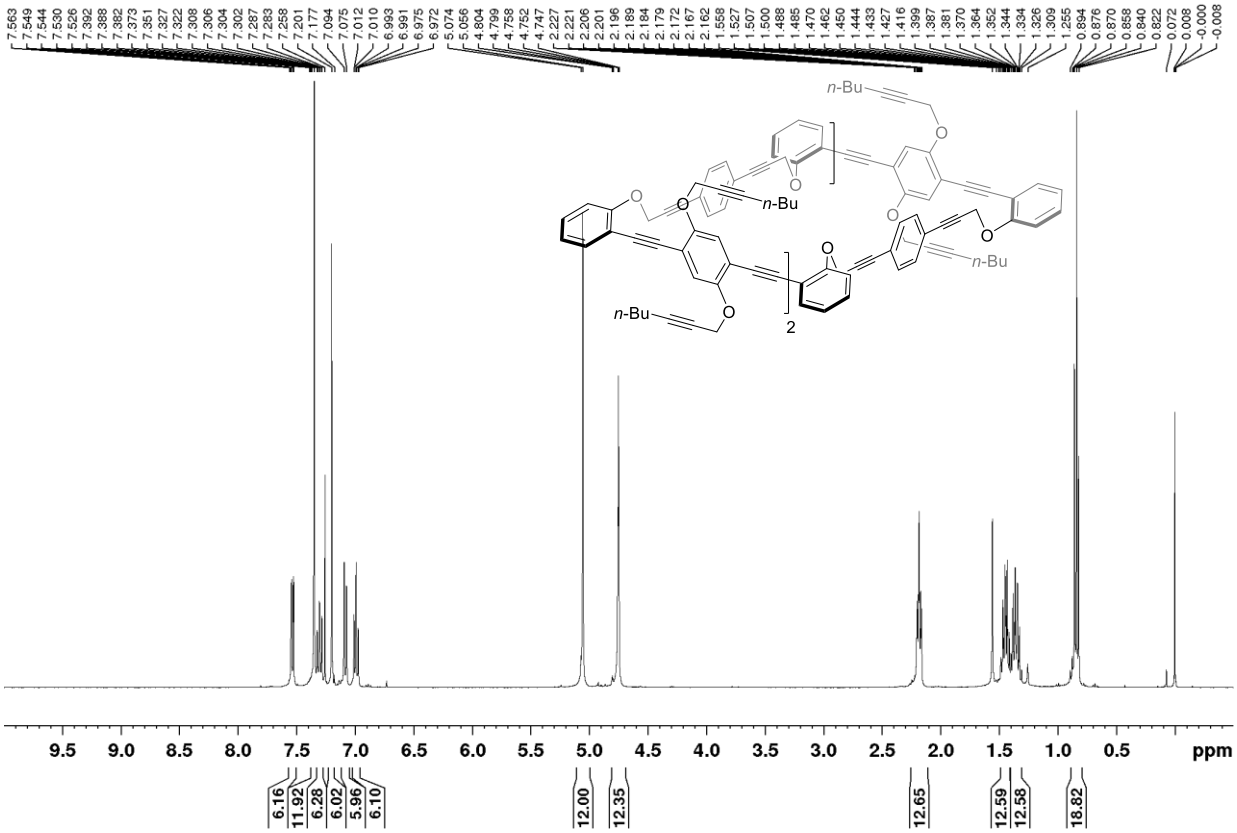


^{13}C NMR ($CDCl_3$, 100 MHz)

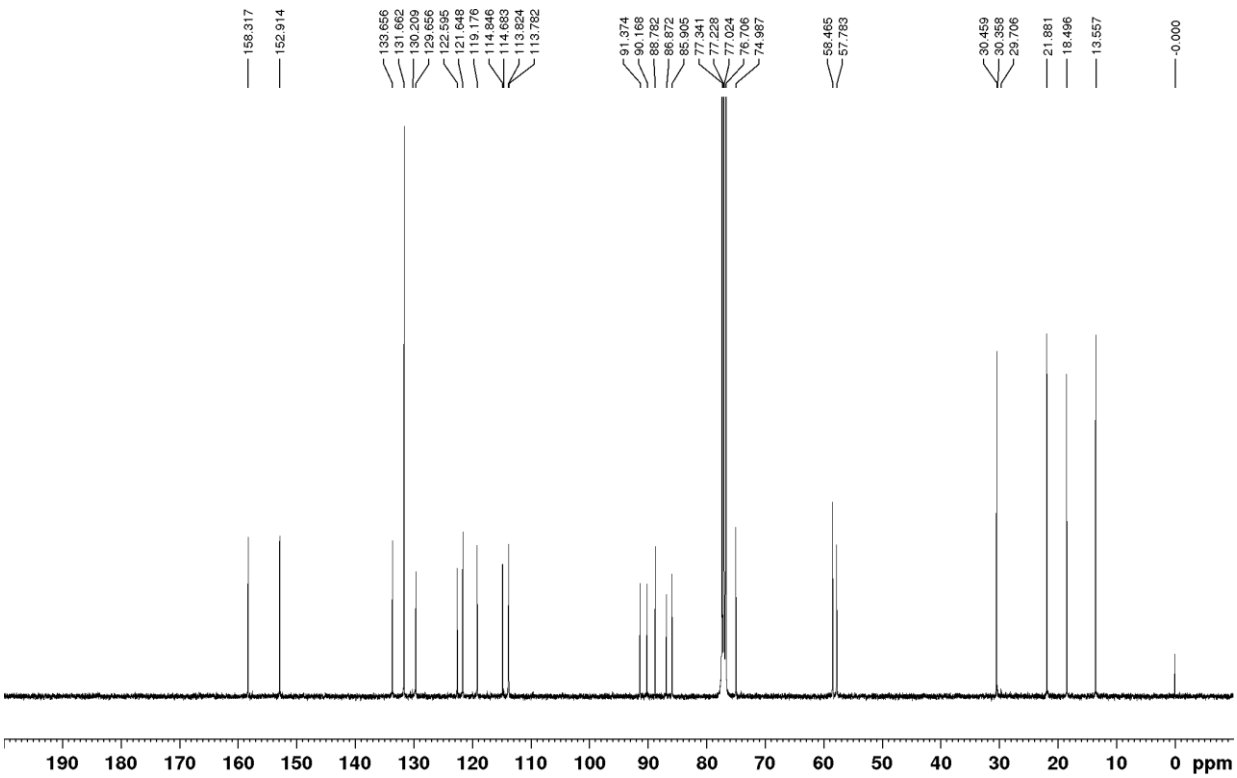


Macrocycle 7b

^{1}H NMR ($CDCl_3$, 400 MHz)

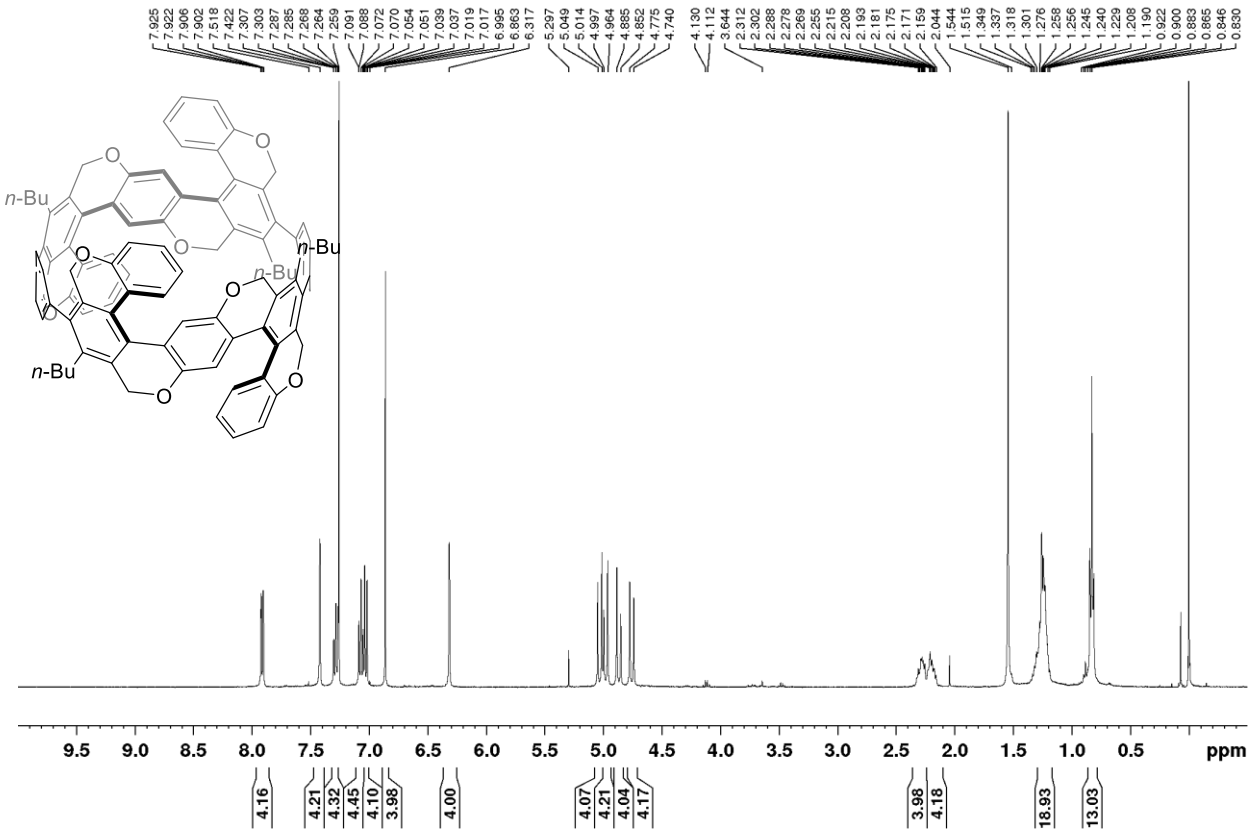


^{13}C NMR ($CDCl_3$, 100 MHz)

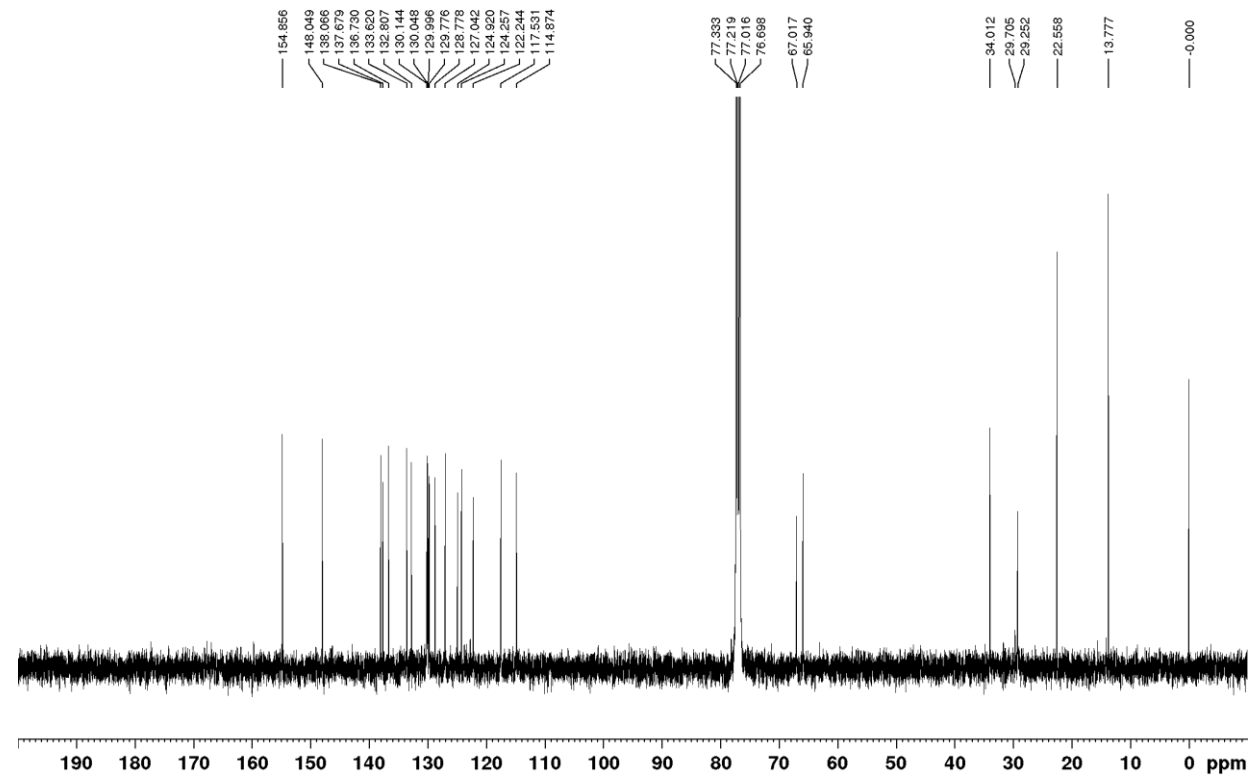


(*Sp*,*Sp*)-(*M*,*M*,*M*,*M*)-(–)-1a

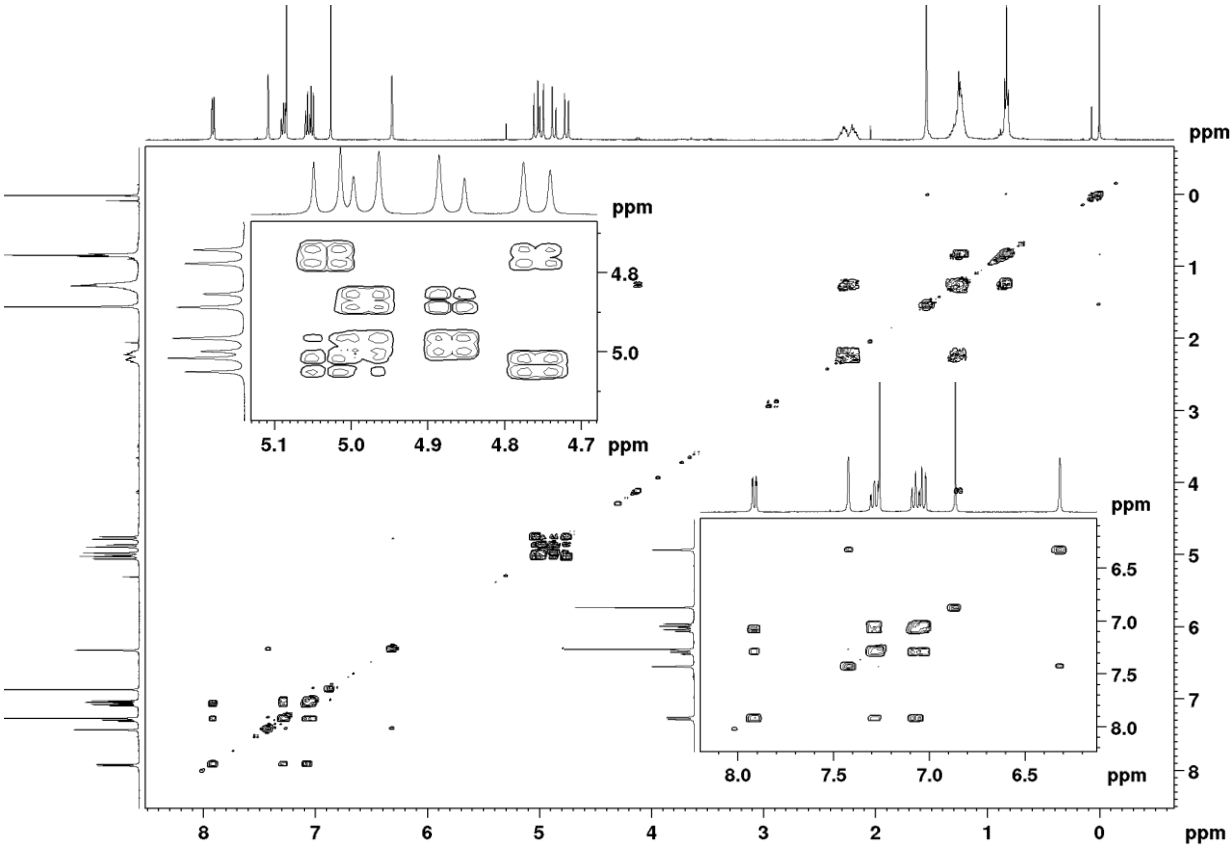
^{1}H NMR ($CDCl_3$, 400 MHz)



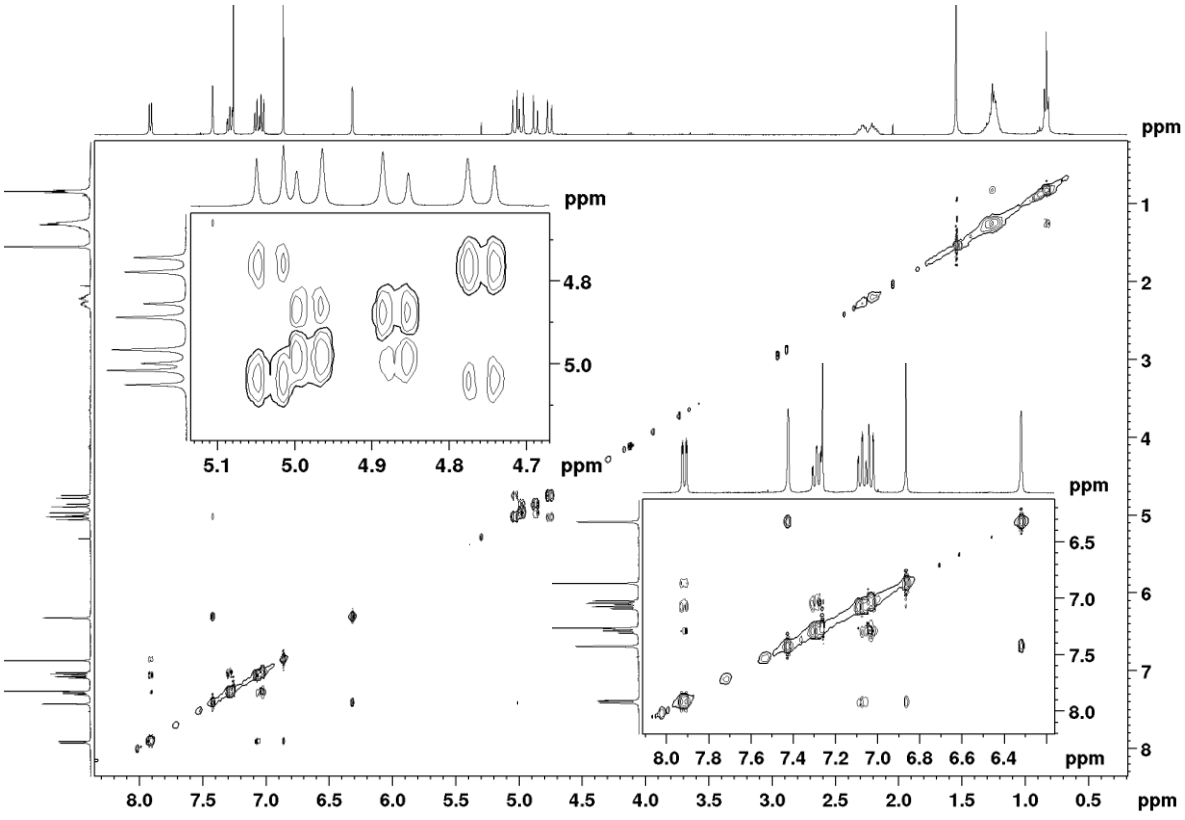
^{13}C NMR ($CDCl_3$, 100 MHz)



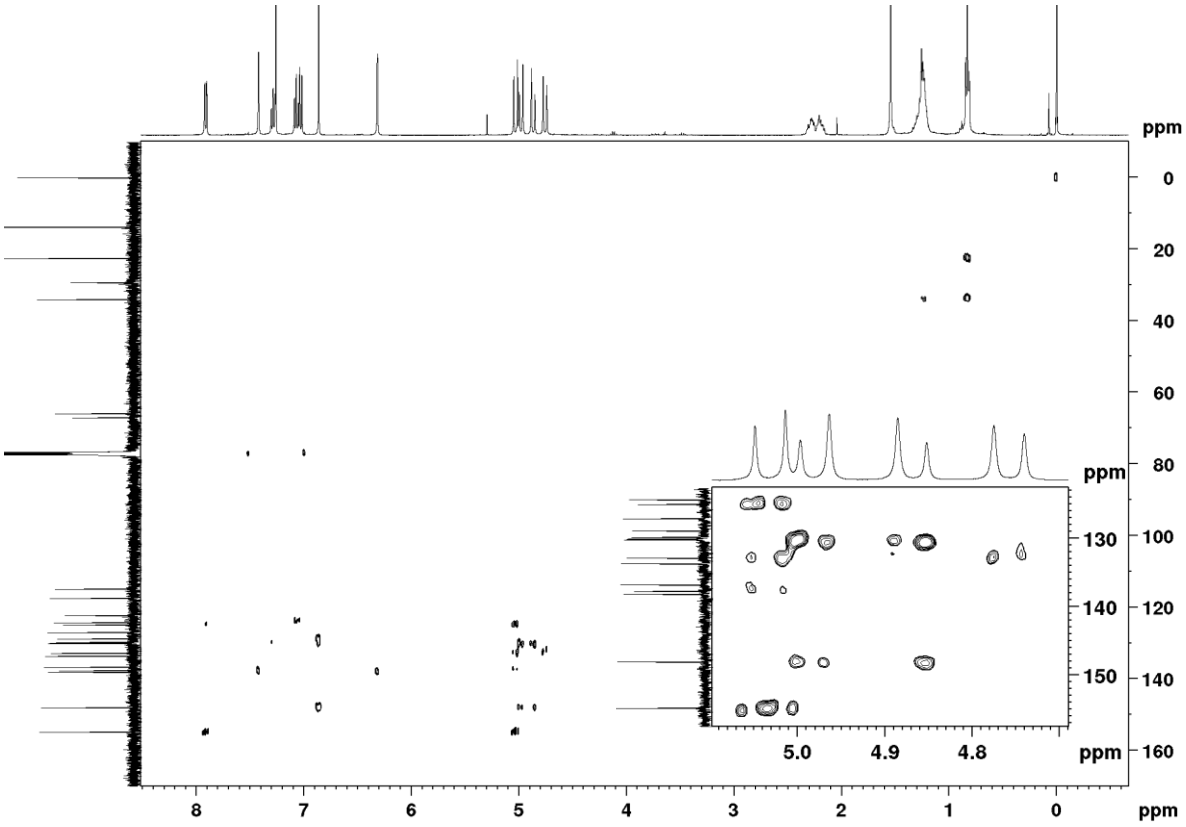
COSY


ppm
0
1
2
3
4
5
6
7
8
ppm
8 7 6 5 4 3 2 1 0 ppm
ppm
4.8
5.0
5.1 5.0 4.9 4.8 4.7 ppm
ppm
6.5
7.0
7.5
8.0
8.0 7.5 7.0 6.5 ppm

NOESY


ppm
1
2
3
4
5
6
7
8
ppm
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
ppm
4.8
5.0
5.1 5.0 4.9 4.8 4.7 ppm
ppm
6.5
7.0
7.5
8.0
8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 ppm

HMBC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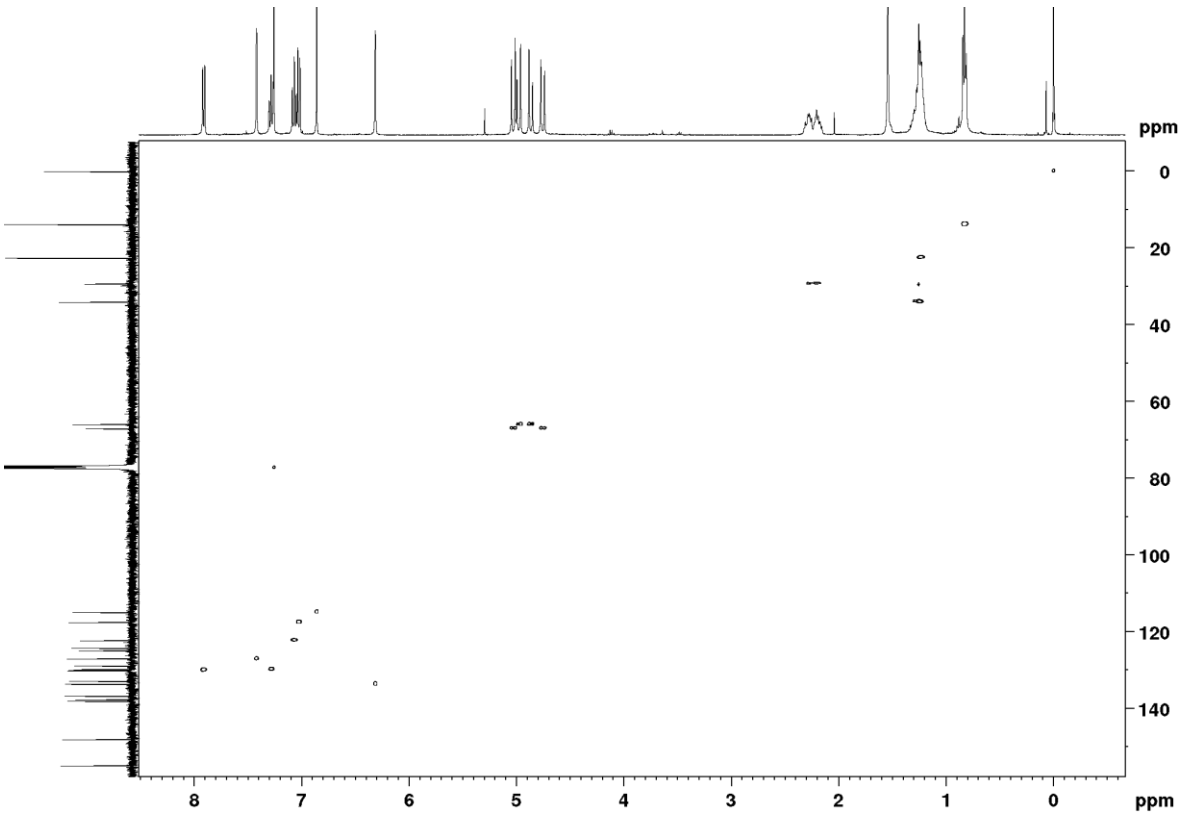
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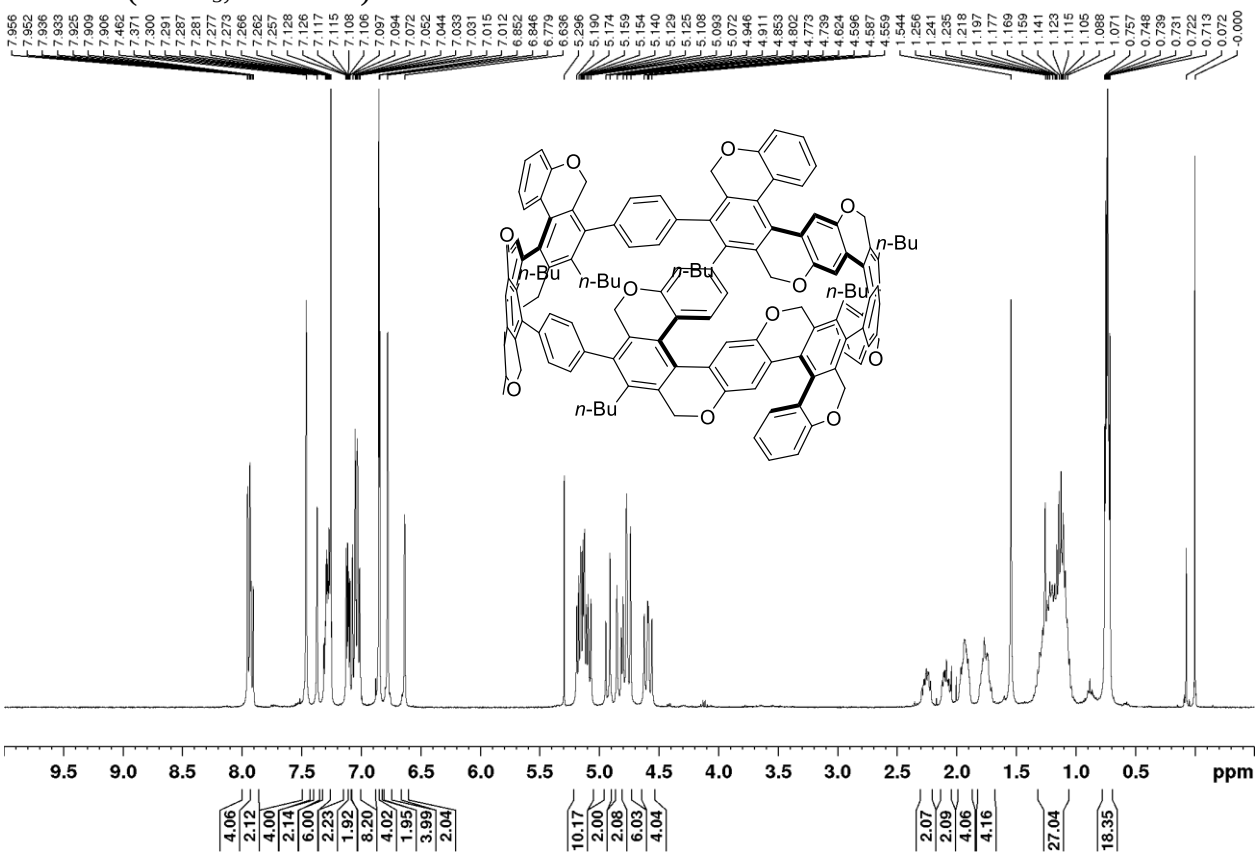
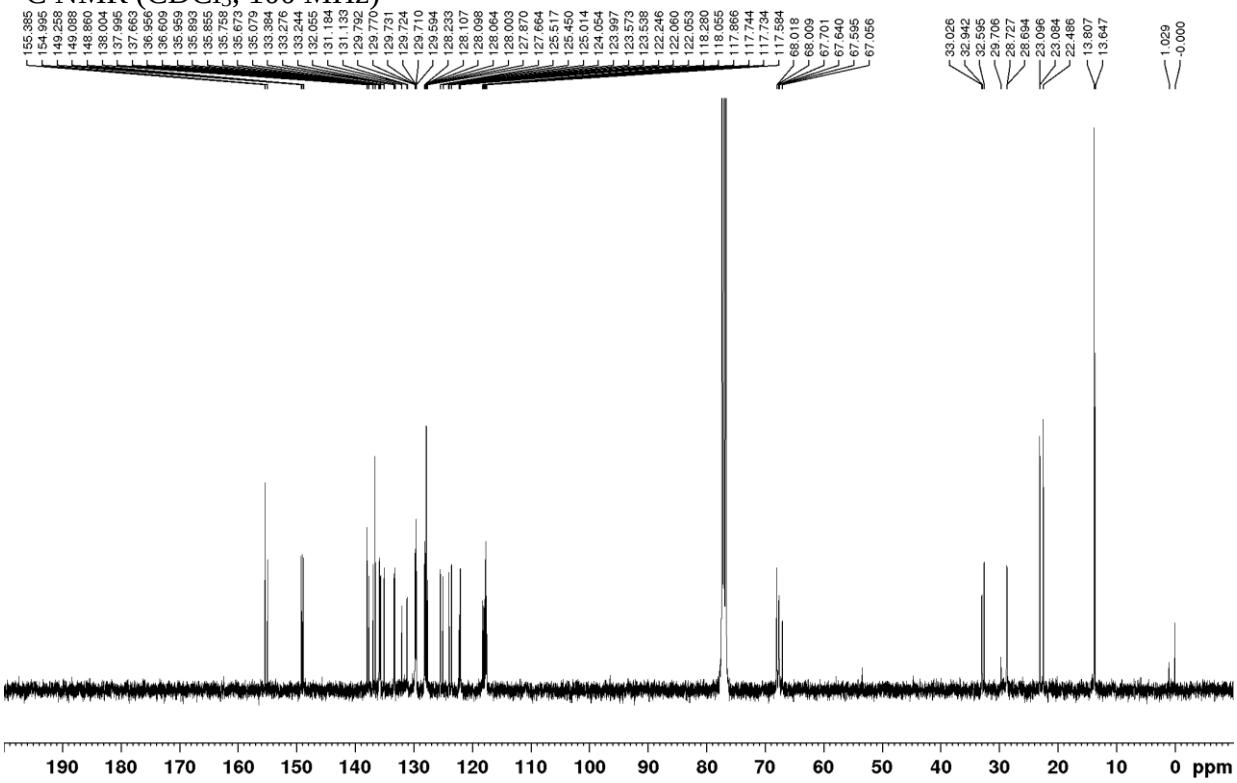
(*S*p,*S*p,*R*p)-(*M,M,M,M,P,P*)-**(–)-1b**

^{1}H NMR ($CDCl_3$, 400 MHz)



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



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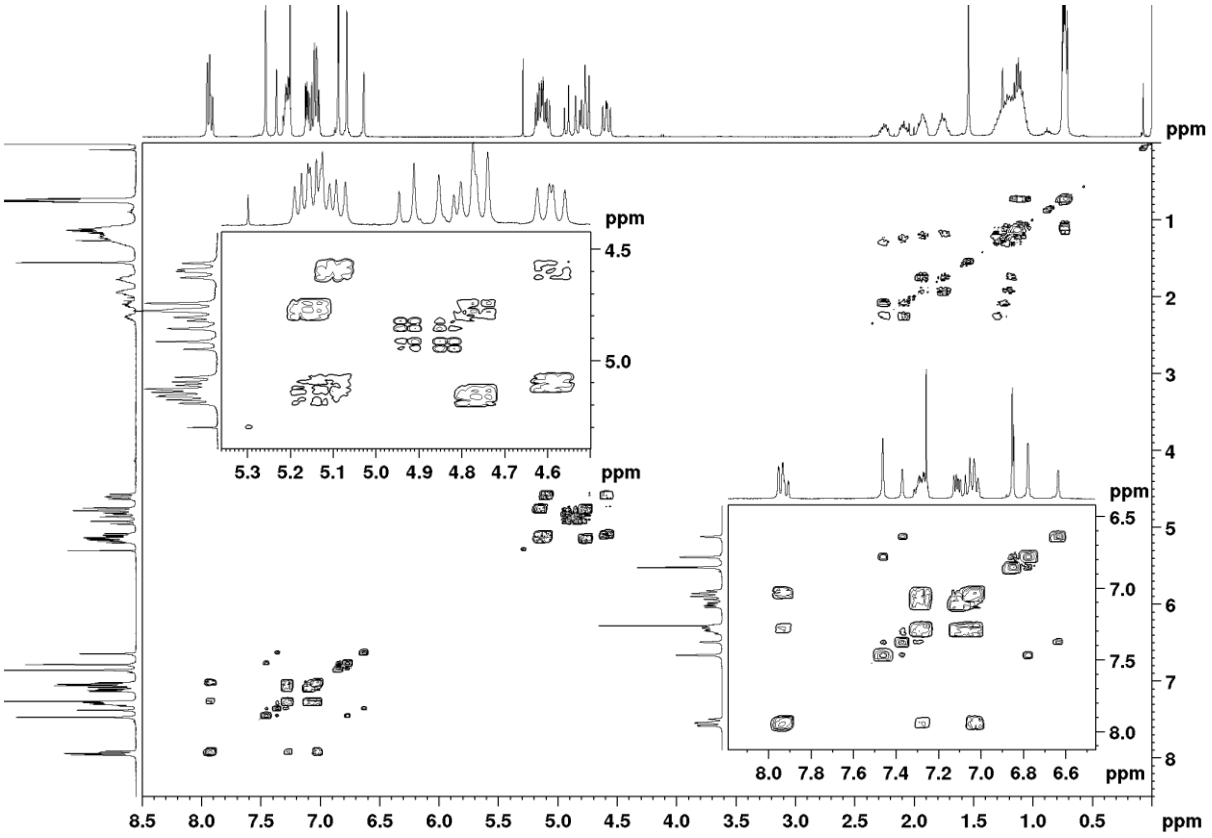
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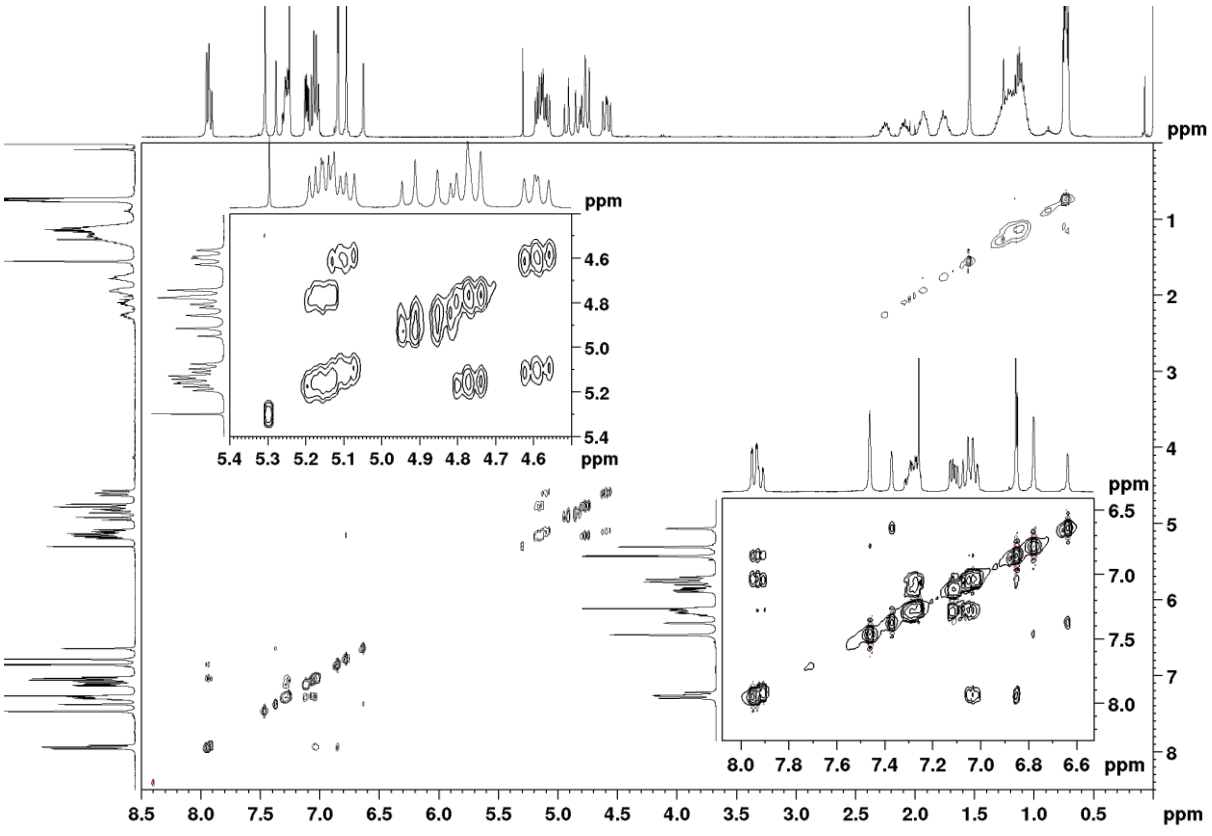
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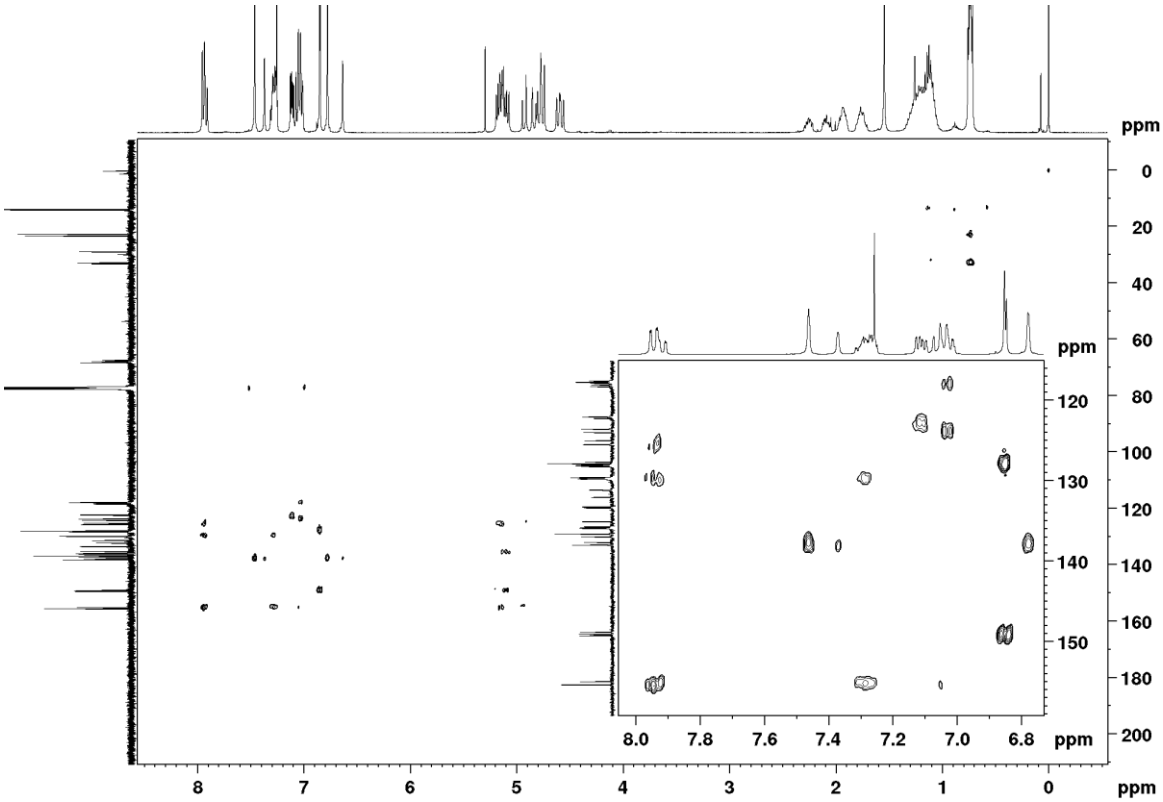
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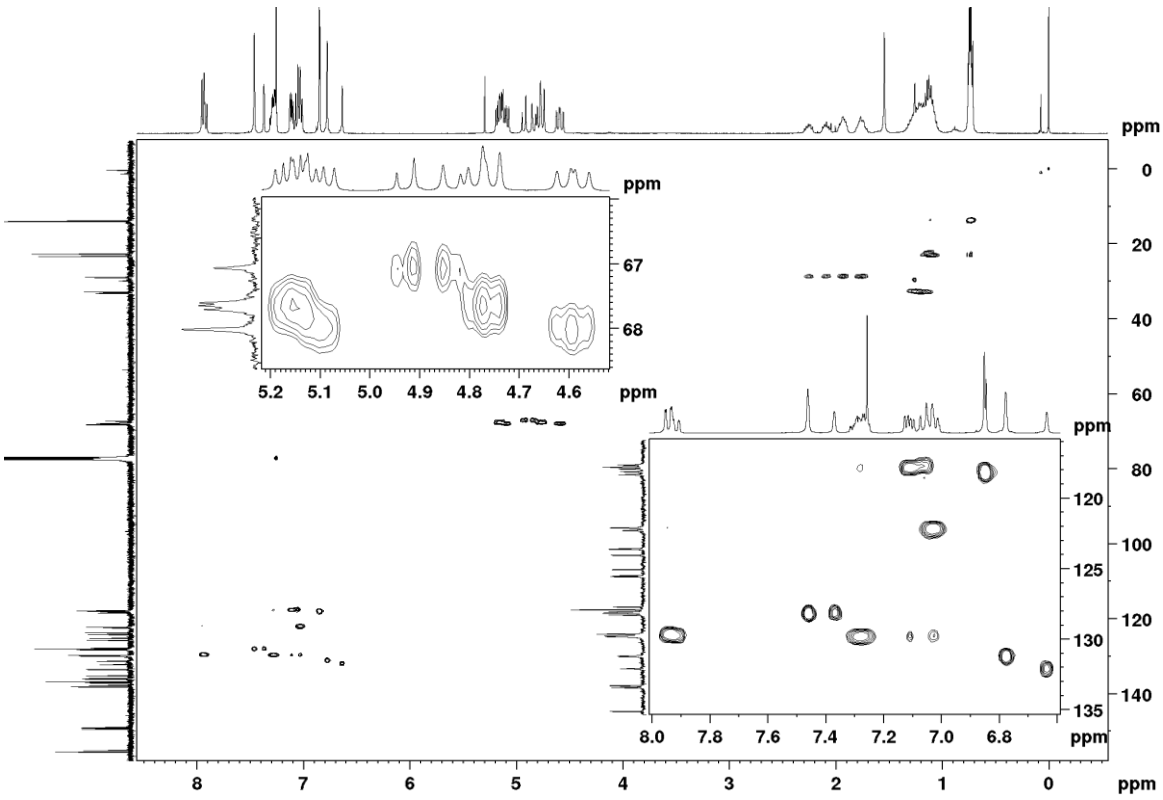
HSQC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ppm
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ppm
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68
8.0
7.8
7.6
7.4
7.2
7.0
6.8
ppm

4. Single-Crystal X-Ray Diffraction Analysis of (±)-1a

Single crystal X-ray diffraction data were collected using a Rigaku XtaLAB Synergy, Single source at home/near, HyPix diffractometer equipped with a Cu-Kα radiation source. Details of the crystal data and the summaries of the intensity data collection parameters for (±)-**1a** are listed in Table S1 (CCDC Deposition Number: 2050855).

Table S1. Crystallographic data and structure refinement details for (±)-**1a**.

formula	$C_{96}H_{80}O_8 \cdot CH_2Cl_2$
formula weight	1444.51
crystal color, shape	colorless plate
crystal system	Triclinic
space group	*P*-1
a (Å)	12.9562(5)
b (Å)	14.7057(5)
c (Å)	21.8040(3)
α (deg)	96.529(2)
β (deg)	97.374(3)
γ (deg)	110.822(3)
V (Å^3)	3793.6(2)
Z	2
d_{calc} (g/cm^3)	1.265
μ (Cu Kα) (mm^{-1})	1.249
F_{000}	1520
crystal size (mm)	0.18×0.13×0.07
temperature (K)	93(2)
θ range (deg)	2.074–68.244
number of independent reflections	13862
number of parameters	968
R_1, wR_2 [$I>2\sigma(I)$]	0.1189, 0.3223
R_1, wR_2 (all data)	0.1335, 0.3345
S	1.067
largest difference peak and hole (eÅ^{-3})	0.943, -1.514

5. Computational Studies

All calculations were carried out using the Gaussian 16 program.[4] Full optimizations were performed with B3LYP,[5] the 6-31G(d) basis set.[6] 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 (*S*p,*S*p)-(*M*,*M*,*M*,*M*)-Me$_4$-**1a** and (*S*p,*S*p,*R*p)-(*M*,*M*,*M*,*M*,*P*,*P*)-Me$_6$-**1b** are shown in Figs. S1–S6. Cartesian coordinates of optimized (*S*p,*S*p)-(*M*,*M*,*M*,*M*)-Me$_4$-**1a**, (*S*p,*R*p)-(*M*,*M*,*P*,*P*)-Me$_4$-**1a**, (*S*p,*S*p,*R*p)-(*M*,*M*,*M*,*M*,*P*,*P*)-Me$_6$-**1b**, (*S*p,*S*p,*S*p)-(*M*,*M*,*M*,*M*,*M*,*M*)-Me$_6$-**1b**, (*M*,*M*)-**8**, (*R*,*R*,*R*,*R*)-**9**, **S1**, and **S2** are listed in Tables S2–S12.

Time-dependent (TD) DFT calculations were carried out at the B3LYP/6-31G(d) level of theory[6] with PCM model as solvation of dichloromethane based on the optimized structure. TDDFT vertical one-electron excitations calculated for (*S*p,*S*p)-(*M*,*M*,*M*,*M*)-Me$_4$-**1a**, (*S*p,*R*p)-(*M*,*M*,*P*,*P*)-Me$_4$-**1a**, (*S*p,*S*p,*R*p)-(*M*,*M*,*M*,*M*,*P*,*P*)-Me$_6$-**1b**, (*S*p,*S*p,*S*p)-(*M*,*M*,*M*,*M*,*M*,*M*)-Me$_6$-**1b**, (*M*,*M*)-**8**, and (*R*,*R*,*R*,*R*)-**9** are summarized in Tables S13–S22 and Figs. S10–S13.

Strain energies of (*S*p,*S*p)-(*M*,*M*,*M*,*M*)-Me$_4$-**1a** and (*S*p,*S*p,*S*p)-(*M*,*M*,*M*,*M*,*M*,*M*)-Me$_6$-**1b** were calculated according to the reported procedure.[7,8] 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[6] for estimation of strain energy and estimated from the gas-phase studies. The results are shown in Table S23 and Figs. S7–S9 The ring strain of (*S*p,*S*p)-(*M*,*M*,*M*,*M*)-Me$_4$-**1a** (63 kcal/mol) is larger than that of (*S*p,*S*p,*S*p)-(*M*,*M*,*M*,*M*,*M*,*M*)-Me$_6$-**1b** (44 kcal/mol). This small ring strain of **1b** would result in facile racemization. The relative Gibbs energies of diastereomers revealed that (*S*p,*S*p)-(*M*,*M*,*M*,*M*)-Me$_4$-**1a** and (*S*p,*S*p,*R*p)-(*M*,*M*,*M*,*M*,*P*,*P*)-Me$_6$-**1b** are more stable than (*S*p,*R*p)-(*M*,*M*,*P*,*P*)-Me$_4$-**1a** and (*S*p,*S*p,*S*p)-(*M*,*M*,*M*,*M*,*M*,*M*)-Me$_6$-**1b** (2.47 and 0.55 kcal/mol), respectively. These theoretically stable diastereomers are the same as the experimentally obtained diastereomers (Figure. 1).

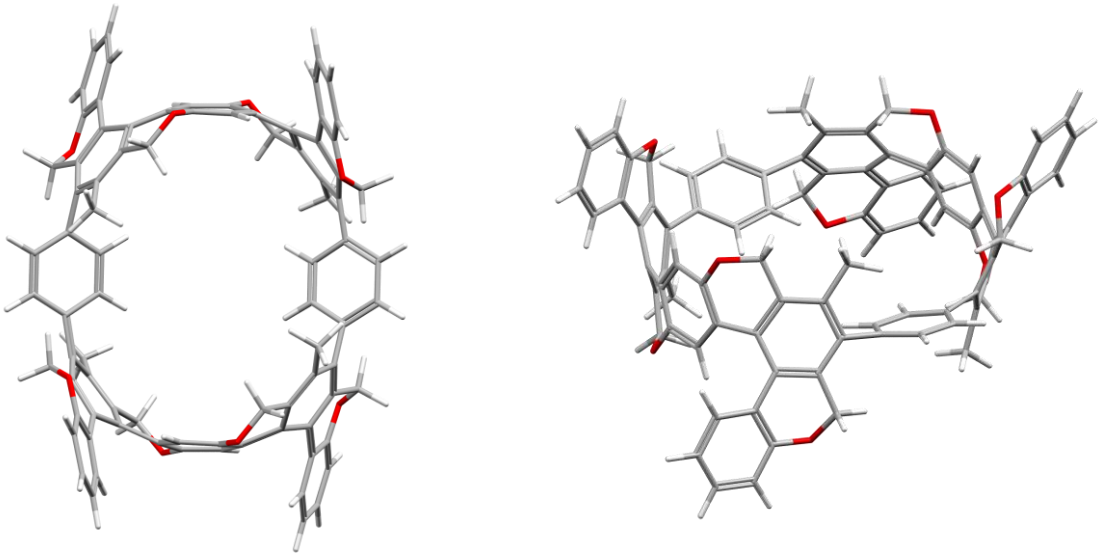


Fig. S1. Optimized structures of (*S*p,*S*p)-(*M*,*M*,*M*,*M*)-Me$_4$-**1a** constrained to C_2 symmetry. (left: top view, right: side view).

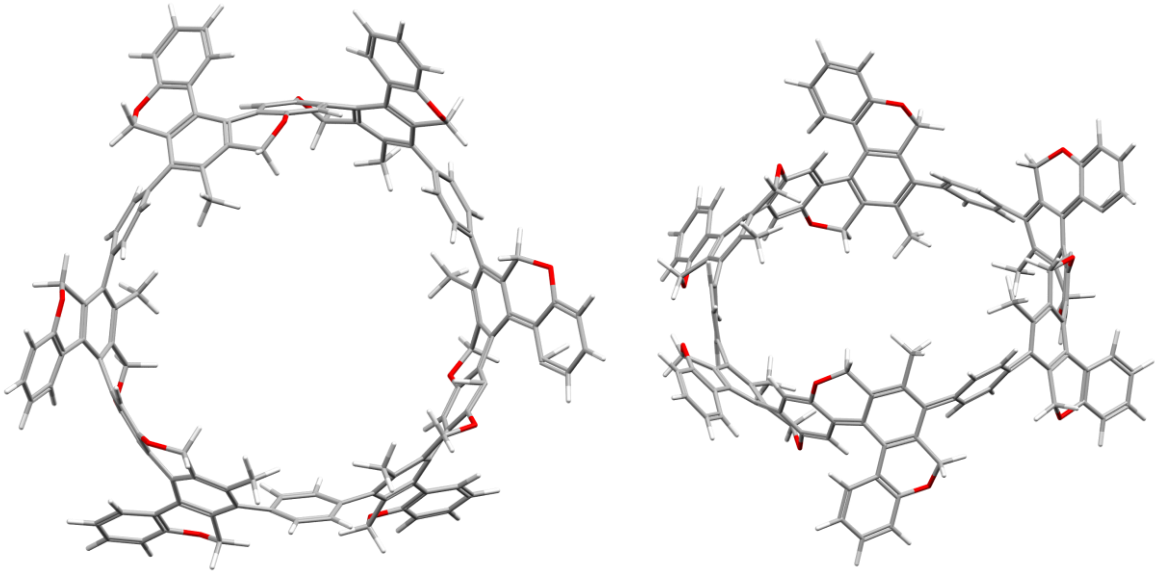


Fig. S2. Optimized structures of (*S*p,*S*p,*R*p)-(*M*,*M*,*M*,*M*,*P*,*P*)-Me$_6$-**1b** constrained to C_2 symmetry. (left: top view, right: side view)**.**

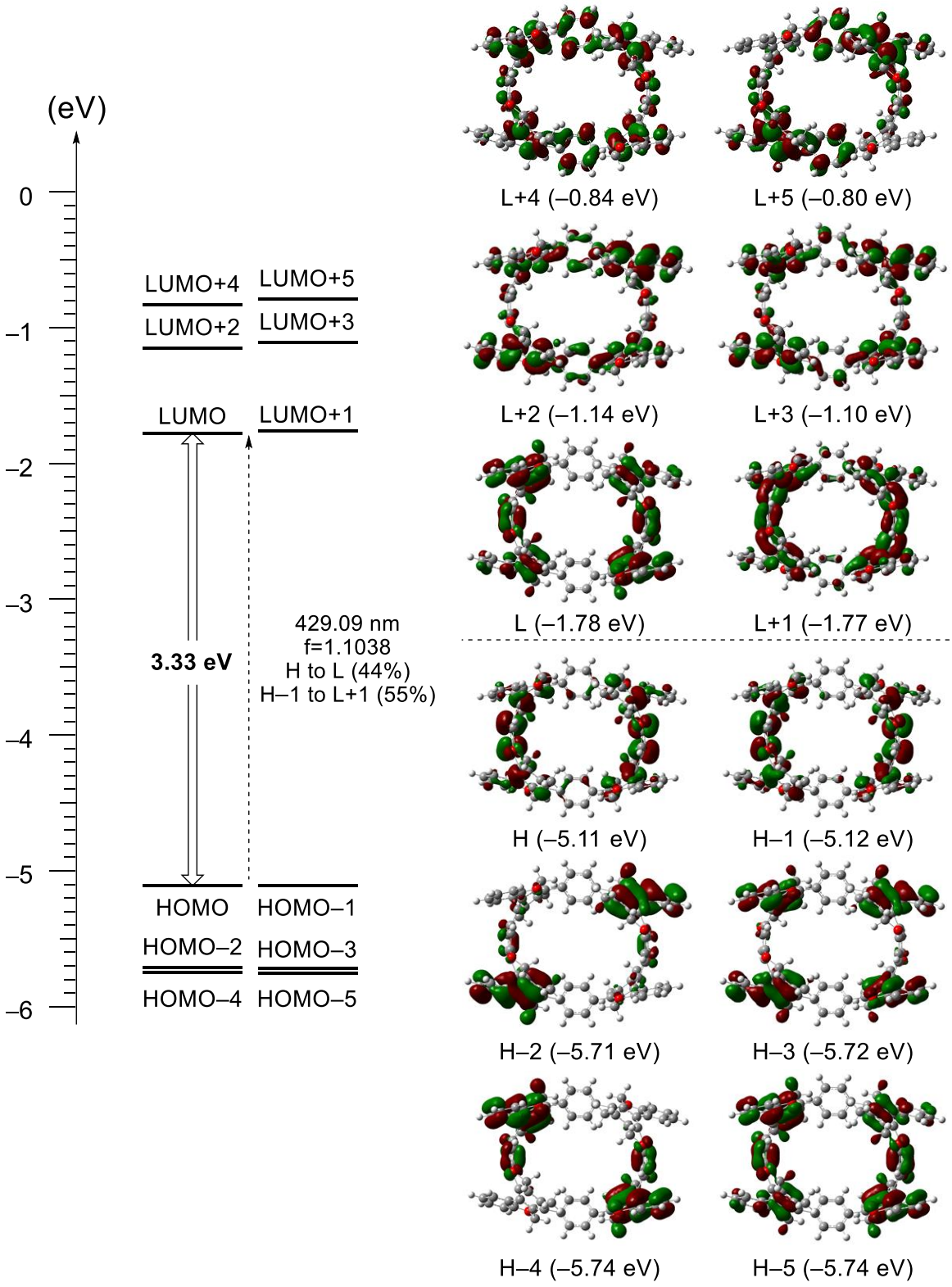


Fig. S3. Frontier molecular orbitals (MOs) and energy diagram of (*S*p,*S*p)-(*M*,*M*,*M*,*M*)-Me$_4$-**1a**.

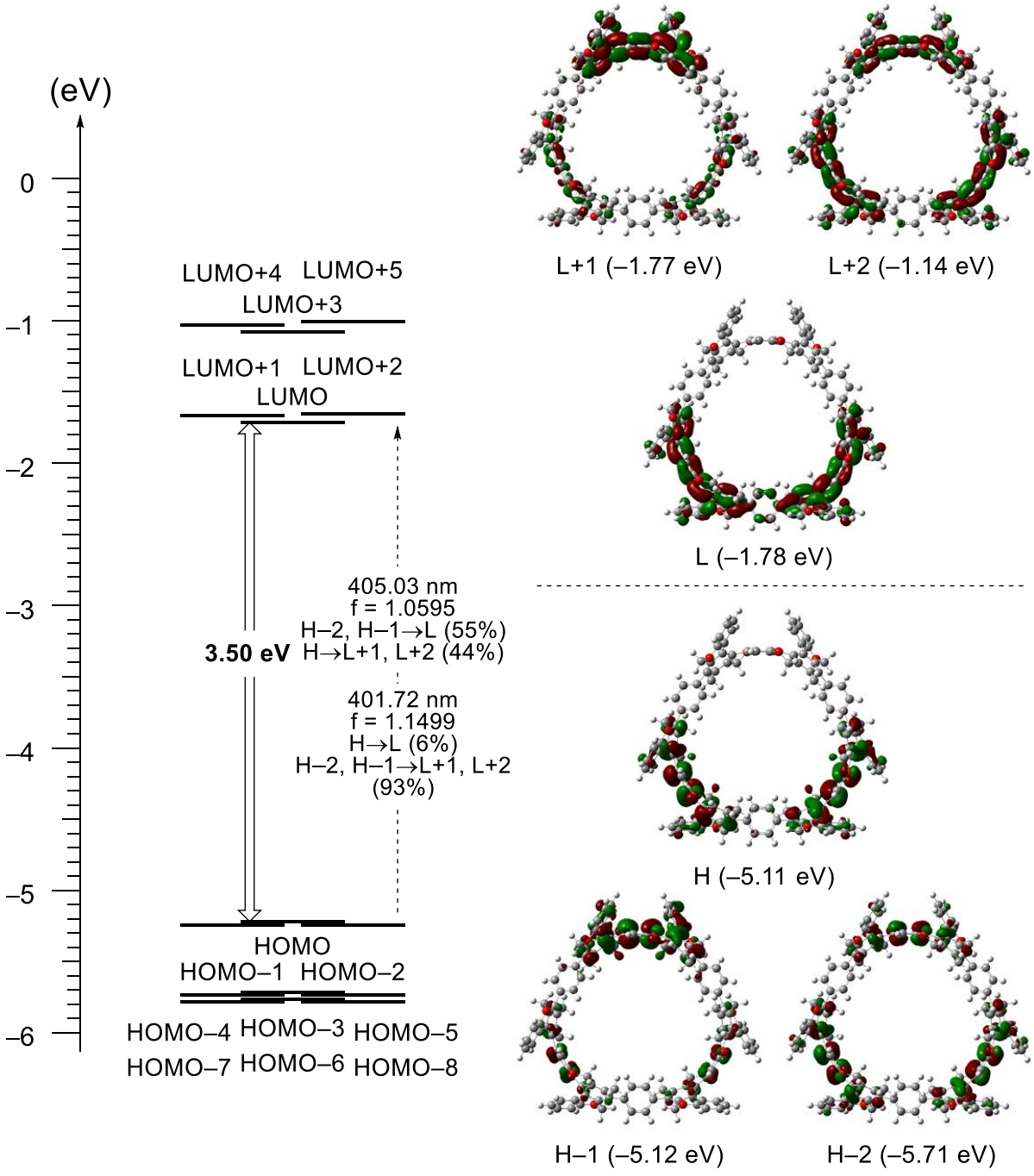


Fig. S4. Frontier molecular orbitals (MOs) and energy diagram of (*S*p,*S*p,*R*p)-(*M*,*M*,*M*,*M*,*P*,*P*)-Me$_6$-**1b**.

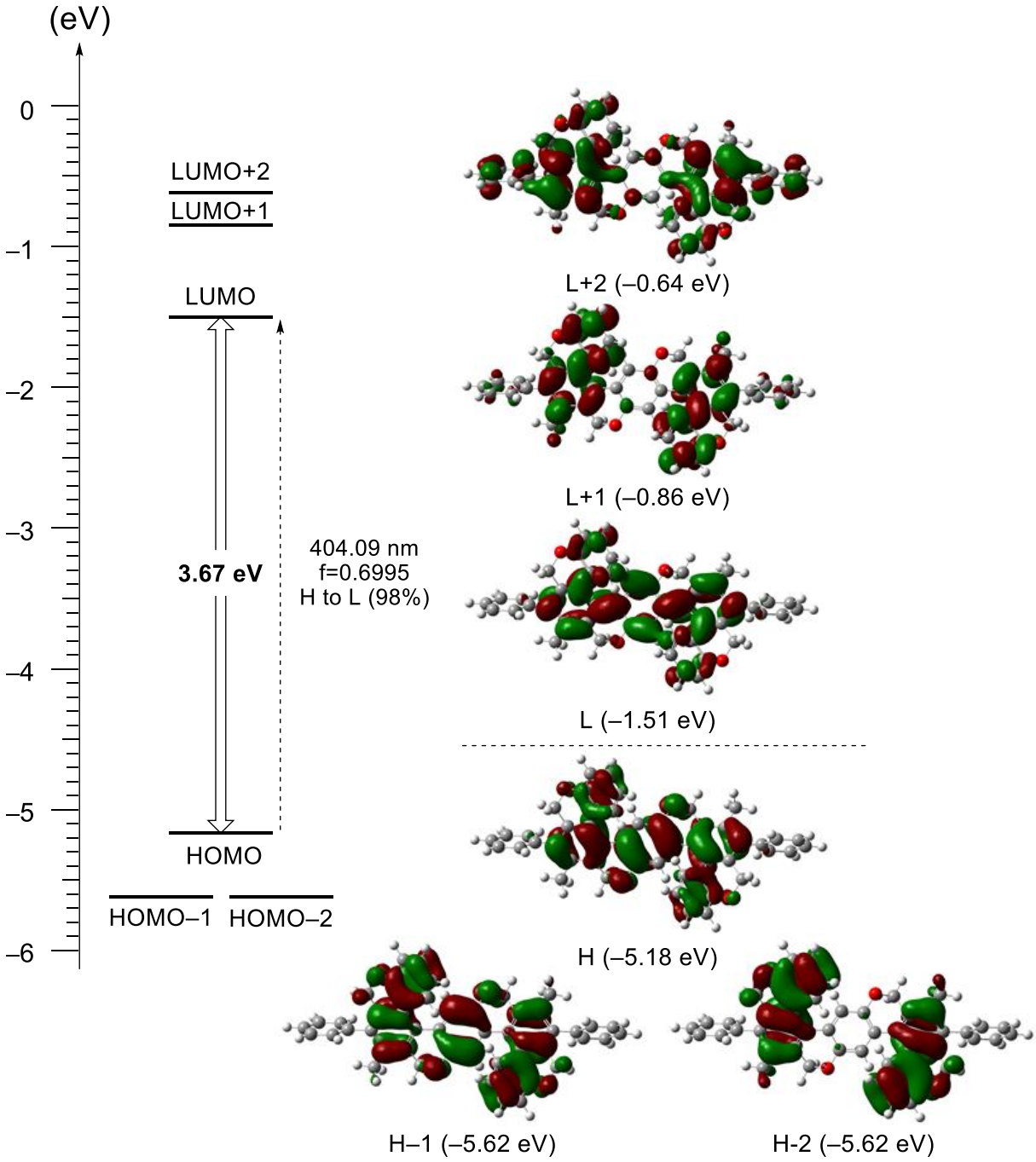


Fig. S5. Frontier molecular orbitals (MOs) and energy diagram of (*M*,*M*)-**8**.

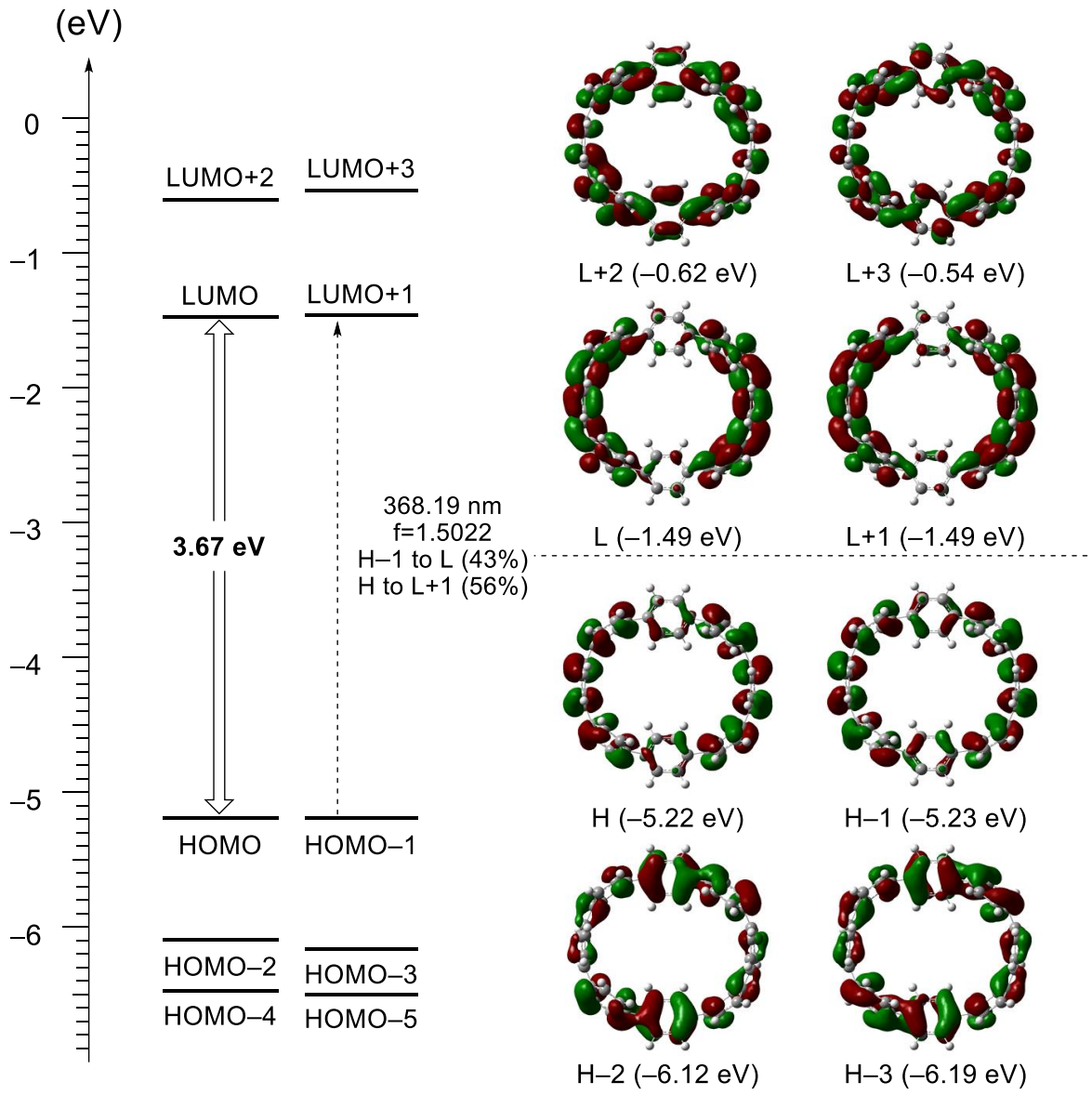


Fig. S6. Frontier molecular orbitals (MOs) and energy diagram of (*R*,*R*,*R*,*R*)-**9**.

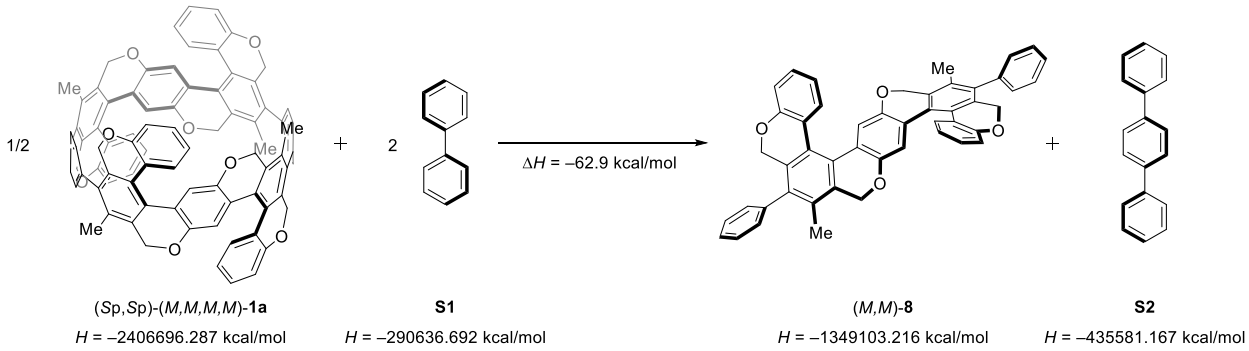


Fig. S7. Homodesmotic reaction for calculating the increase of the strain energy of (*S*p,*S*p)-(*M*,*M*,*M*,*M*)-Me$_4$-**1a** compared to that of (*M*,*M*)-**8**.

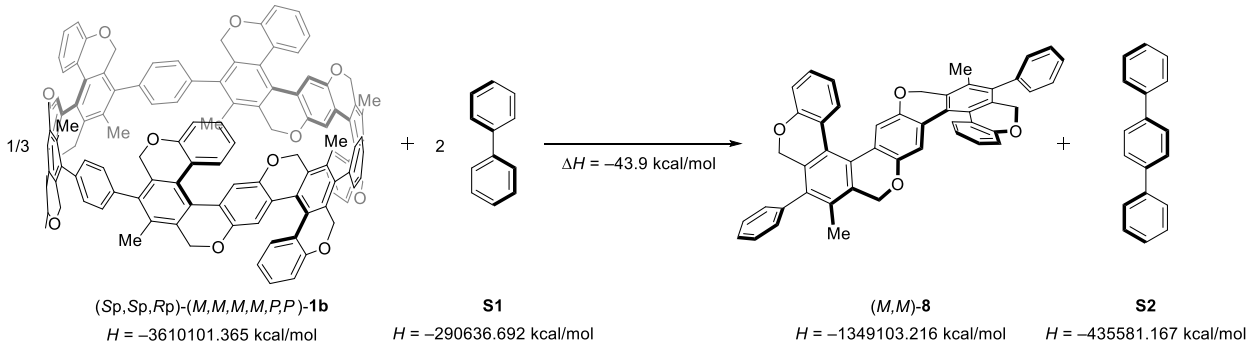


Fig. S8. Homodesmotic reaction for calculating the increase of the strain energy of (*S*p,*S*p,*R*p)-(*M*,*M*,*M*,*M*,*P*,*P*)-Me$_6$-**1b** compared to that of (*M*,*M*)-**8**.

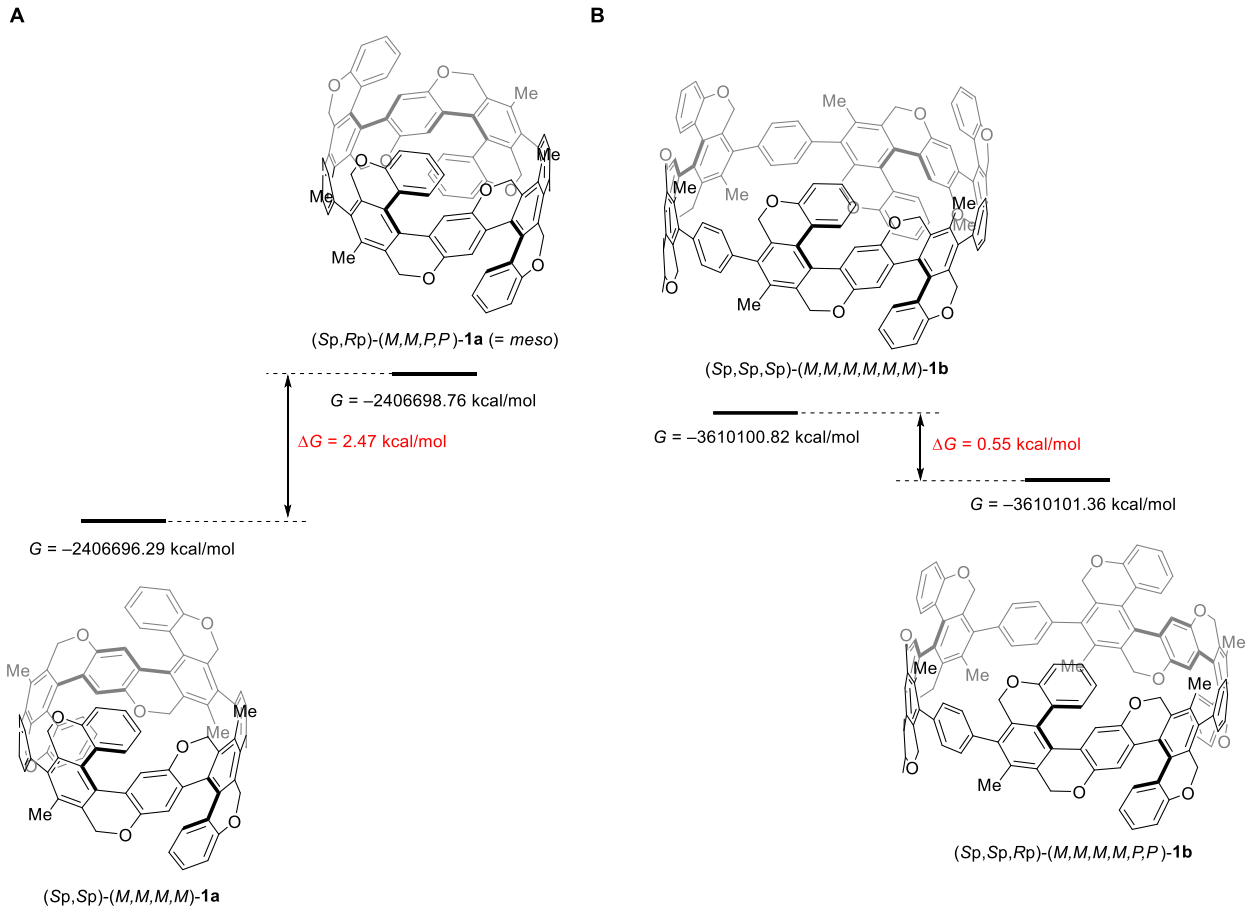


Fig. S9. The relative Gibbs energies of **1a** (**A**) and **1b** (**B**).

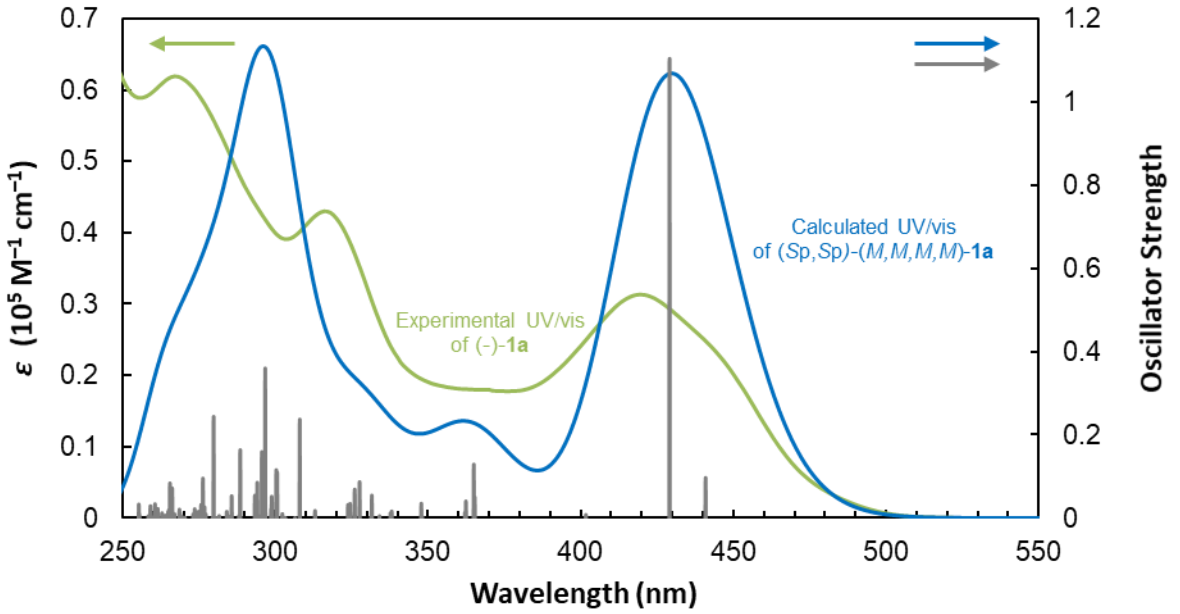


Fig. S10. Theoretical electronic absorption spectra of (*S*p,*S*p)-(*M*,*M*,*M*,*M*)-Me$_4$-**1a** (gray bar and blue line) calculated by the TD-DFT method at B3LYP/6-31G(d)/PCM(dichloromethane) level. The green line shows the experimental UV/vis spectra of (*S*p,*S*p)-(*M*,*M*,*M*,*M*)-(–)-**1a** in CH_2Cl_2.

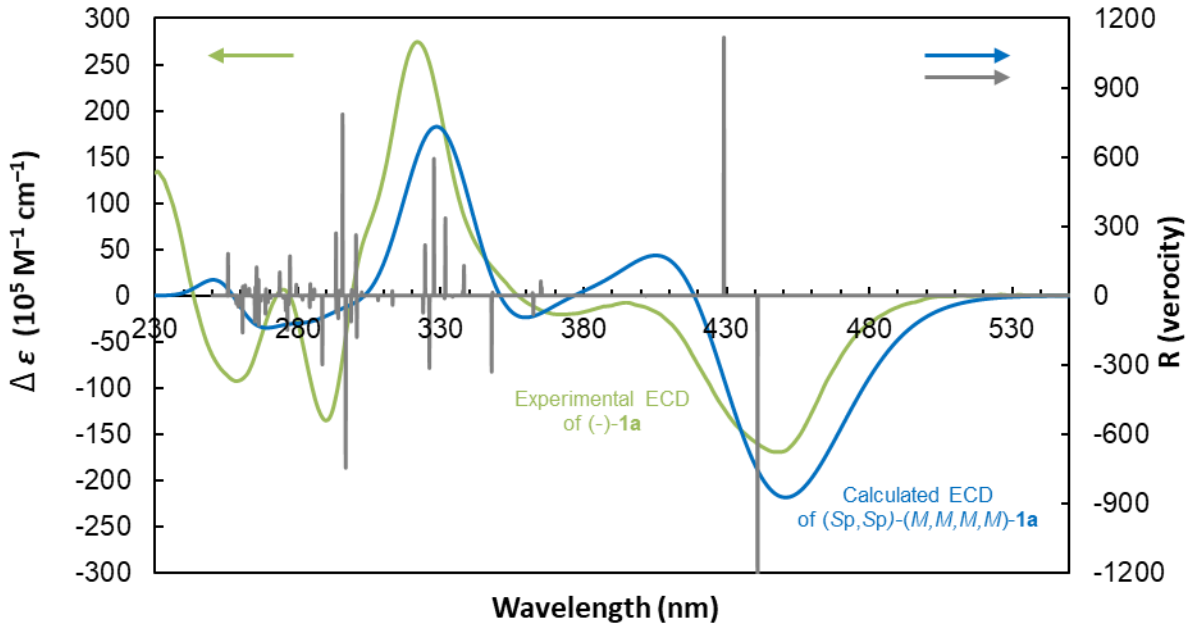


Fig. S11. Theoretical ECD spectra of (*S*p,*S*p)-(*M*,*M*,*M*,*M*)-Me$_4$-**1a** (gray bar and blue line) calculated by the TD-DFT method at B3LYP/6-31G(d)/PCM(dichloromethane). The green line shows the experimental ECD spectra of (*S*p,*S*p)-(*M*,*M*,*M*,*M*)-(–)-**1a** in CH_2Cl_2.

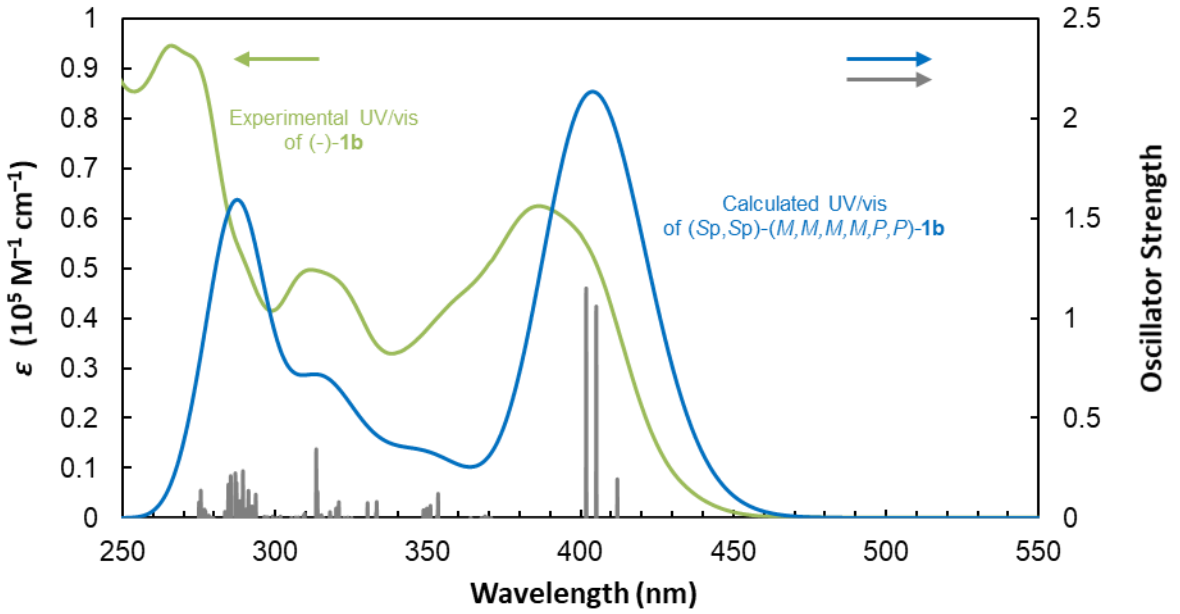


Fig. S12. Theoretical electronic absorption spectra of (*S*p,*S*p,*R*p)-(*M,M,M,M,P,P*)-Me$_6$-**1b** (gray bar and blue line) calculated by the TD-DFT method at B3LYP/6-31G(d)/PCM(dichloromethane). The green line shows the experimental UV/vis spectra of (*S*p,*S*p,*R*p)-(*M,M,M,M,P,P*)-(–)-**1b** in CH_2Cl_2.

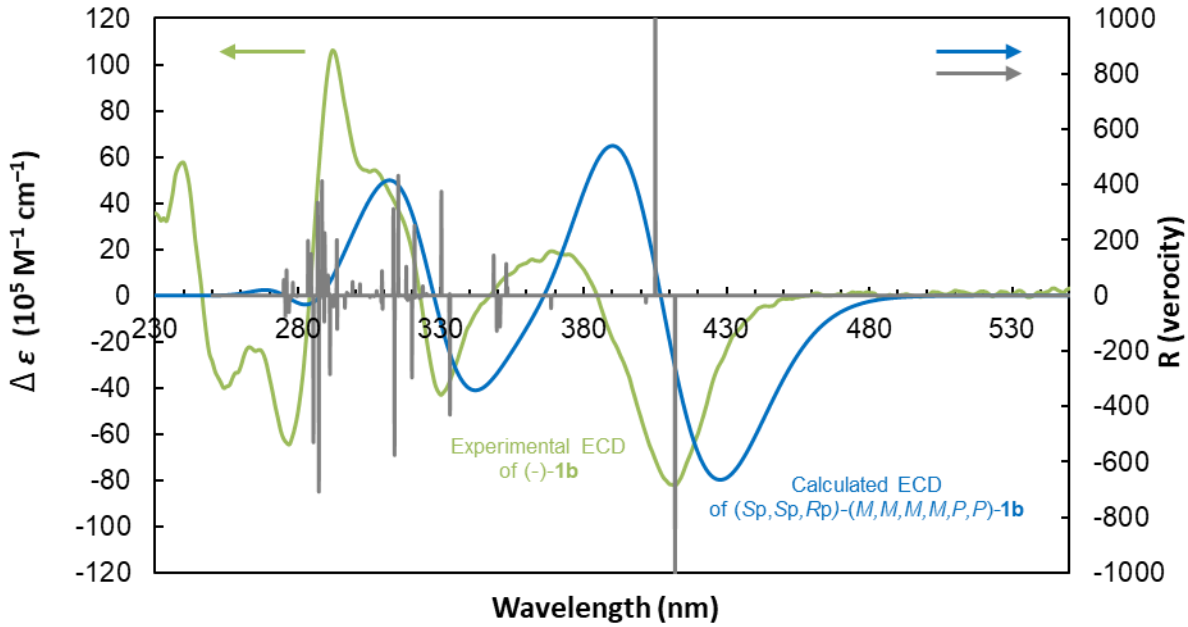
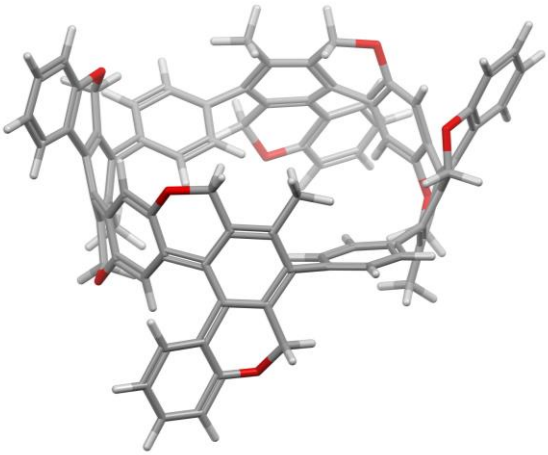


Fig. S13. Theoretical ECD spectra of (*S*p,*S*p,*R*p)-(*M,M,M,M,P,P*)-Me$_6$-**1b** (gray bar and blue line) calculated by the TD-DFT method at B3LYP/6-31G(d)/PCM(dichloromethane). The green line shows the experimental ECD spectra of (*S*p,*S*p,*R*p)-(*M,M,M,M,P,P*)-(–)-**1b** in CH_2Cl_2.

Table S2. Cartesian coordinates of optimized (*S*p,*S*p)-(*M*,*M*,*M*,*M*)-Me$_4$-**1a**.



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C	0.924012	5.653773	1.284708	C	4.230189	-6.494239	-4.262843
C	1.614356	5.671483	0.060627	C	-3.768639	-6.841724	2.275575
C	0.837408	5.906134	-1.091471	C	-3.885633	-7.488209	3.502805
C	-0.552174	5.906603	-1.063710	C	-4.242023	-6.761146	4.643746
C	2.954541	5.061369	-0.138233	C	-4.516263	-5.398199	4.548901
C	3.175614	4.483754	-1.407621	C	-4.802220	-1.281738	-0.434097
C	2.358358	4.950898	-2.595618	C	4.732091	-1.559986	-0.172040
O	1.473492	6.030501	-2.306358	C	-5.923244	-0.563830	0.011538
C	-2.623699	5.188580	0.247412	C	-5.886839	0.835230	0.146986
C	-2.861026	4.376485	1.379223	C	-3.644264	0.846170	-0.705743
C	-1.993648	4.541037	2.610750	C	-3.676522	-0.531131	-0.826629
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C	-4.384848	3.969230	-0.898817	C	3.867139	-2.375965	2.533419
C	-4.403976	3.000655	0.115873	C	-4.204420	-2.774235	-2.947592
C	-3.750684	3.291720	1.333899	C	-3.867139	2.375965	2.533419
C	-3.662260	6.084731	-1.918956	H	1.438290	5.483129	2.221366
C	-4.169371	5.643171	-3.158980	H	-1.071794	5.938627	-2.012644
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C	4.589157	3.508872	0.777047	H	-2.611766	4.726552	3.495648
C	4.574076	2.763623	-0.418030	H	-6.193670	4.346756	-2.010975
C	4.007284	3.367211	-1.567420	H	-5.439360	2.776976	-2.362777
C	4.000557	5.460853	2.159147	H	5.424660	1.967939	2.047350
C	4.417315	4.764068	3.310274	H	6.364448	3.473728	2.006292

O	4.703736	3.428166	3.232865	H	-2.945331	7.806102	-0.845622
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C	-3.301822	7.437829	-1.802619	H	-3.884632	8.488802	-4.984825
C	-3.380913	8.299689	-2.892793	H	-4.607309	6.103320	-5.202661
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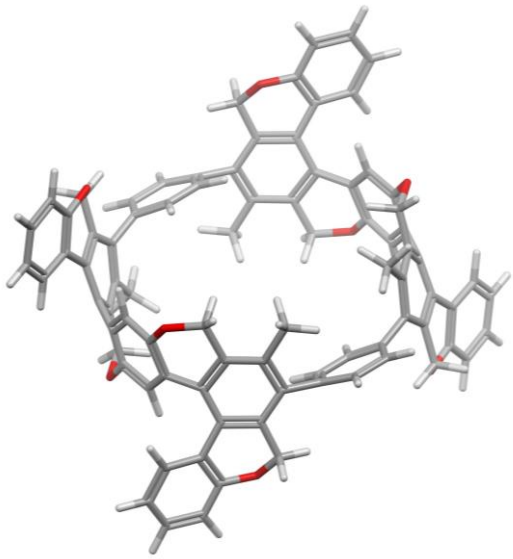
C	4.516263	5.398199	4.548901	H	6.759309	-1.351602	0.539618
C	4.802220	1.281738	-0.434097	H	2.740043	-1.386414	-0.971256
C	5.923244	0.563830	0.011538	H	2.789567	1.052089	-1.172918
C	5.886839	-0.835230	0.146986	H	-1.438290	-5.483129	2.221366
C	3.644264	-0.846170	-0.705743	H	1.071794	-5.938627	-2.012644
C	3.676522	0.531131	-0.826629	H	-3.011524	-5.317521	-3.395164
C	1.246692	-5.744405	0.148462	H	-1.776466	-4.111003	-3.011778
C	0.462348	-5.725287	1.318591	H	2.611766	-4.726552	3.495648
C	-0.924012	-5.653773	1.284708	H	1.418040	-3.619220	2.802063
C	-1.614356	-5.671483	0.060627	H	6.193670	-4.346756	-2.010975
C	-0.837408	-5.906134	-1.091471	H	5.439360	-2.776976	-2.362777
C	0.552174	-5.906603	-1.063710	H	-6.364448	-3.473728	2.006292
C	-2.954541	-5.061369	-0.138233	H	-5.424660	-1.967939	2.047350
C	-3.175614	-4.483754	-1.407621	H	2.945331	-7.806102	-0.845622
C	-2.358358	-4.950898	-2.595618	H	3.093940	-9.341042	-2.780311
O	-1.473492	-6.030501	-2.306358	H	3.884632	-8.488802	-4.984825
C	2.623699	-5.188580	0.247412	H	4.607309	-6.103320	-5.202661
C	2.861026	-4.376485	1.379223	H	-3.482397	-7.403313	1.391607
C	1.993648	-4.541037	2.610750	H	-3.698504	-8.555790	3.571192
O	1.097420	-5.645899	2.538135	H	-4.327576	-7.260638	5.604895
C	3.557598	-5.107667	-0.819129	H	-4.819753	-4.814581	5.412360
C	4.384848	-3.969230	-0.898817	H	-6.833570	-1.093144	0.281087
C	4.403976	-3.000655	0.115873	H	-6.759309	1.351602	0.539618
C	3.750684	-3.291720	1.333899	H	-2.740043	1.386414	-0.971256
C	3.662260	-6.084731	-1.918956	H	-2.789567	-1.052089	-1.172918
C	4.169371	-5.643171	-3.158980	H	3.275993	2.374427	-3.377318
O	4.589157	-4.348556	-3.311731	H	4.935325	1.964143	-2.935533
C	5.231055	-3.824911	-2.142327	H	4.567397	3.540654	-3.644245
C	-3.853902	-4.706701	0.900797	H	4.110260	-2.945039	3.439075
C	-4.589157	-3.508872	0.777047	H	2.928544	-1.842359	2.736879
C	-4.574076	-2.763623	-0.418030	H	4.645299	-1.624601	2.395641
C	-4.007284	-3.367211	-1.567420	H	-4.567397	-3.540654	-3.644245

C	-4.000557	-5.460853	2.159147	H	-4.935325	-1.964143	-2.935533
C	-4.417315	-4.764068	3.310274	H	-3.275993	-2.374427	-3.377318
O	-4.703736	-3.428166	3.232865	H	-4.110260	2.945039	3.439075
C	-5.344413	-3.054144	2.007318	H	-2.928544	1.842359	2.736879
C	3.301822	-7.437829	-1.802619	H	-4.645299	1.624601	2.395641

Table S3. Cartesian coordinates of optimized (*S*p,*R*p)-(*M*,*M*,*P*,*P*)-Me$_4$-**1a**.

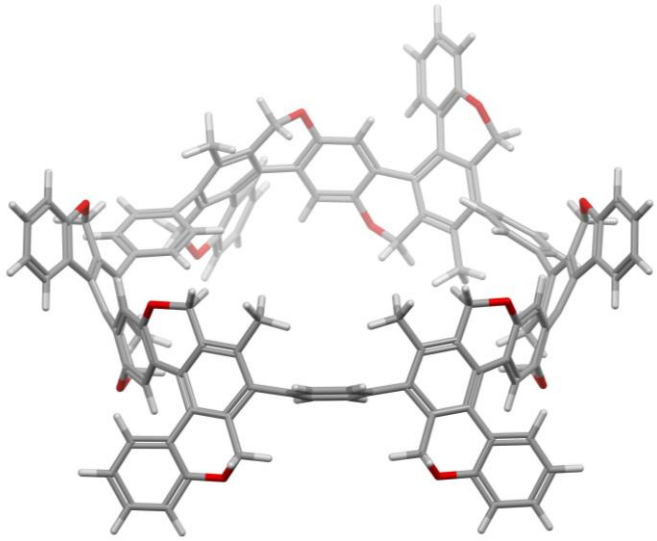


C	-4.356550	1.593734	2.855603	C	-4.356550	1.593734	-2.855603
C	-3.340583	2.517982	3.198777	C	-3.340583	2.517982	-3.198777
C	-2.486434	2.211136	4.271184	C	-4.292656	-0.755752	-5.808967
C	-2.621501	1.019219	5.014847	C	-5.178853	-1.734378	-5.311887
C	-3.845086	0.310600	4.892498	O	-5.647734	-1.652160	-4.027843
C	-4.659868	0.573579	3.774185	C	-5.880495	-0.301911	-3.607383
C	-4.292656	-0.755752	5.808967	C	-3.898312	-0.852529	-7.154281
C	-5.178853	-1.734378	5.311887	C	-4.314095	-1.915131	-7.951227
O	-5.647734	-1.652160	4.027843	C	-5.139966	-2.908714	-7.414546
C	-5.880495	-0.301911	3.607383	C	-5.580409	-2.816304	-6.096096
C	-3.898312	-0.852529	7.154281	C	-3.037878	3.748968	-2.371371
C	-4.314095	-1.915131	7.951227	C	3.037878	-3.748968	-2.371371
C	-5.139966	-2.908714	7.414546	C	-4.804950	1.511526	-1.423455
C	-5.580409	-2.816304	6.096096	C	-4.233266	0.452751	-0.693541
C	-1.273936	3.091257	4.503860	C	-4.233266	0.452751	0.693541
O	-0.493969	2.704472	5.631382	C	-4.804950	1.511526	1.423455
C	-0.253329	1.347984	5.648222	C	-5.528077	2.472172	0.701610
C	-1.351937	0.470776	5.561281	C	-5.528077	2.472172	-0.701610
C	1.062428	0.903046	5.623120	H	-6.193271	-0.365242	2.565027
C	1.351937	-0.470776	5.561281	H	-6.720430	0.105151	4.194894
C	0.253329	-1.347984	5.648222	H	-3.248659	-0.087756	7.568193
C	-1.062428	-0.903046	5.623120	H	-3.994272	-1.970633	8.987603
C	2.621501	-1.019219	5.014847	H	-5.460641	-3.744224	8.030795
C	2.486434	-2.211136	4.271184	H	-6.245700	-3.556244	5.662325
C	1.273936	-3.091257	4.503860	H	-0.630017	3.107638	3.607453
O	0.493969	-2.704472	5.631382	H	-1.579422	4.123541	4.703132

C	3.845086	-0.310600	4.892498	H	1.844351	1.648423	5.552662
C	4.659868	-0.573579	3.774185	H	-1.844351	-1.648423	5.552662
C	4.356550	-1.593734	2.855603	H	0.630017	-3.107638	3.607453
C	3.340583	-2.517982	3.198777	H	1.579422	-4.123541	4.703132
C	4.292656	0.755752	5.808967	H	6.720430	-0.105151	4.194894
C	5.178853	1.734378	5.311887	H	6.193271	0.365242	2.565027
O	5.647734	1.652160	4.027843	H	3.248659	0.087756	7.568193
C	5.880495	0.301911	3.607383	H	3.994272	1.970633	8.987603
C	3.898312	0.852529	7.154281	H	5.460641	3.744224	8.030795
C	4.314095	1.915131	7.951227	H	6.245700	3.556244	5.662325
C	5.139966	2.908714	7.414546	H	2.026697	-3.713959	1.944283
C	5.580409	2.816304	6.096096	H	3.087234	-4.654711	2.989467
C	3.037878	-3.748968	2.371371	H	3.735572	-3.876357	1.545681
C	-3.037878	3.748968	2.371371	H	-3.087234	4.654711	2.989467
C	4.804950	-1.511526	1.423455	H	-2.026697	3.713959	1.944283
C	4.233266	-0.452751	0.693541	H	-3.735572	3.876357	1.545681
C	4.233266	-0.452751	-0.693541	H	3.699244	0.328347	1.227600
C	4.804950	-1.511526	-1.423455	H	3.699244	0.328347	-1.227600
C	5.528077	-2.472172	-0.701610	H	6.043415	-3.270114	-1.230426
C	5.528077	-2.472172	0.701610	H	6.043415	-3.270114	1.230426
C	4.356550	-1.593734	-2.855603	H	6.720430	-0.105151	-4.194894
C	3.340583	-2.517982	-3.198777	H	6.193271	0.365242	-2.565027
C	2.486434	-2.211136	-4.271184	H	3.248659	0.087756	-7.568193
C	2.621501	-1.019219	-5.014847	H	3.994272	1.970633	-8.987603
C	3.845086	-0.310600	-4.892498	H	5.460641	3.744224	-8.030795
C	4.659868	-0.573579	-3.774185	H	6.245700	3.556244	-5.662325
C	4.292656	0.755752	-5.808967	H	1.579422	-4.123541	-4.703132
C	5.178853	1.734378	-5.311887	H	0.630017	-3.107638	-3.607453
O	5.647734	1.652160	-4.027843	H	-1.844351	-1.648423	-5.552662
C	5.880495	0.301911	-3.607383	H	1.844351	1.648423	-5.552662
C	3.898312	0.852529	-7.154281	H	-0.630017	3.107638	-3.607453
C	4.314095	1.915131	-7.951227	H	-1.579422	4.123541	-4.703132
C	5.139966	2.908714	-7.414546	H	-6.720430	0.105151	-4.194894
C	5.580409	2.816304	-6.096096	H	-6.193271	-0.365242	-2.565027
C	1.273936	-3.091257	-4.503860	H	-3.248659	-0.087756	-7.568193
O	0.493969	-2.704472	-5.631382	H	-3.994272	-1.970633	-8.987603
C	0.253329	-1.347984	-5.648222	H	-5.460641	-3.744224	-8.030795
C	1.351937	-0.470776	-5.561281	H	-6.245700	-3.556244	-5.662325
C	-1.062428	-0.903046	-5.623120	H	-3.735572	3.876357	-1.545681
C	-1.351937	0.470776	-5.561281	H	-2.026697	3.713959	-1.944283
C	-0.253329	1.347984	-5.648222	H	-3.087234	4.654711	-2.989467

C	1.062428	0.903046	-5.623120	H	3.735572	-3.876357	-1.545681
C	-2.621501	1.019219	-5.014847	H	2.026697	-3.713959	-1.944283
C	-2.486434	2.211136	-4.271184	H	3.087234	-4.654711	-2.989467
C	-1.273936	3.091257	-4.503860	H	-3.699244	-0.328347	-1.227600
O	-0.493969	2.704472	-5.631382	H	-3.699244	-0.328347	1.227600
C	-3.845086	0.310600	-4.892498	H	-6.043415	3.270114	1.230426
C	-4.659868	0.573579	-3.774185	H	-6.043415	3.270114	-1.230426

Table S6. Cartesian coordinates of optimized (*S*p,*S*p,*R*p)-(*M*,*M*,*M*,*M*,*P*,*P*)-Me_6-**1b**.



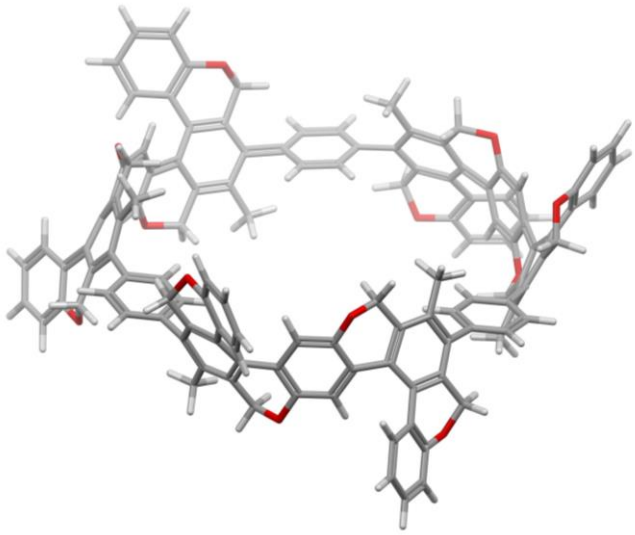
C	1.853861	7.687172	0.518071	C	-3.935218	4.715020	9.555684
C	1.789215	7.840720	-0.875499	C	-3.920748	3.979724	10.738672
C	0.650916	8.370891	-1.517287	C	-2.781036	3.252999	11.098872
C	-0.315523	9.028233	-0.713504	C	-1.676342	3.226934	10.252493
C	-0.284638	8.816020	0.679280	C	0.527187	6.114317	5.141260
C	0.744188	8.085823	1.296157	C	3.935218	-4.715020	9.555684
C	2.913765	7.290786	-1.729043	C	3.920748	-3.979724	10.738672
O	2.859848	7.731861	-3.083001	C	2.781036	-3.252999	11.098872
C	-1.393444	9.899011	-1.227712	C	1.676342	-3.226934	10.252493
C	-2.561067	10.040063	-0.449519	C	1.561322	-6.048536	7.290926
O	-2.651679	9.425048	0.771012	O	2.836147	-5.466484	7.589261
C	-1.408393	9.430202	1.483186	C	2.813004	-4.703861	8.726797
C	-1.320394	10.623035	-2.429965	C	1.680824	-3.919490	9.029668
C	-2.392676	11.391359	-2.874133	O	-2.517908	-1.105136	8.220463
C	-3.568088	11.454337	-2.118313	C	-2.639572	-2.058448	7.167594
C	-3.650991	10.786158	-0.898871	C	-0.602490	-5.154649	6.293445
C	-0.073768	1.421659	-7.693801	C	0.466066	-5.010667	7.193149
C	2.261595	7.236155	-7.898485	C	0.565613	-3.904013	8.059699
C	3.410677	7.915836	-8.292643	C	-0.373338	-2.850456	7.917640
C	4.570138	7.201703	-8.612868	C	-1.548796	-3.110110	7.183689
C	4.564778	5.808914	-8.580090	C	-1.680824	-4.245067	6.368573
C	2.241586	5.833888	-7.812050	C	-2.553196	2.747095	-6.759180
C	3.400480	5.136508	-8.207913	C	3.062549	7.002226	1.120334
O	3.406199	3.766997	-8.212846	C	-3.062549	-7.002226	1.120334
C	2.159268	3.207052	-8.641933	C	2.553196	-2.747095	-6.759180
C	1.074643	5.045763	-7.365039	C	-2.926870	-4.393844	5.521294
C	0.984557	3.720426	-7.838122	C	2.926870	4.393844	5.521294

C	-0.128275	2.912649	-7.550280	H	3.883948	7.629845	-1.355353
C	-1.248931	3.499897	-6.920713	H	2.918584	6.186405	-1.705338
C	0.084684	5.511025	-6.462678	H	-1.594252	8.877837	2.404235
C	-1.122632	4.786758	-6.378535	H	-1.162941	10.471697	1.750716
C	-2.260143	5.357966	-5.556677	H	-0.413533	10.570422	-3.023278
O	-2.099300	6.739851	-5.245659	H	-2.313513	11.938687	-3.808828
C	1.533008	6.827512	-4.834142	H	-4.410950	12.045245	-2.466302
C	0.285653	6.537130	-5.409290	H	-4.536061	10.844807	-0.273181
C	-0.852439	7.019345	-4.733426	H	1.366272	7.793253	-7.642351
C	-0.769452	7.705571	-3.528072	H	3.403687	9.000427	-8.348360
C	0.476996	7.966805	-2.935759	H	5.471769	7.729125	-8.912144
C	1.616559	7.529146	-3.638538	H	5.438857	5.226713	-8.854551
C	-0.036856	0.700403	-8.894807	H	2.025136	3.435935	-9.712445
C	0.036856	-0.700403	-8.894807	H	2.273536	2.127884	-8.537701
C	0.035547	-0.692041	-6.492327	H	-2.387768	4.785718	-4.620712
C	-0.035547	0.692041	-6.492327	H	-3.203807	5.297077	-6.106275
C	1.248931	-3.499897	-6.920713	H	2.452461	6.453612	-5.266225
C	1.122632	-4.786758	-6.378535	H	-1.694426	7.970142	-3.031400
C	-0.084684	-5.511025	-6.462678	H	-0.072295	1.230461	-9.843354
C	-1.074643	-5.045763	-7.365039	H	0.072295	-1.230461	-9.843354
C	-0.984557	-3.720426	-7.838122	H	0.057347	-1.229370	-5.548375
C	0.128275	-2.912649	-7.550280	H	-0.057347	1.229370	-5.548375
C	2.260143	-5.357966	-5.556677	H	3.203807	-5.297077	-6.106275
O	2.099300	-6.739851	-5.245659	H	2.387768	-4.785718	-4.620712
C	-2.241586	-5.833888	-7.812050	H	-2.025136	-3.435935	-9.712445
C	-3.400480	-5.136508	-8.207913	H	-2.273536	-2.127884	-8.537701
O	-3.406199	-3.766997	-8.212846	H	-1.366272	-7.793253	-7.642351
C	-2.159268	-3.207052	-8.641933	H	-3.403687	-9.000427	-8.348360
C	-2.261595	-7.236155	-7.898485	H	-5.471769	-7.729125	-8.912144
C	-3.410677	-7.915836	-8.292643	H	-5.438857	-5.226713	-8.854551
C	-4.570138	-7.201703	-8.612868	H	0.413533	-10.570422	-3.023278
C	-4.564778	-5.808914	-8.580090	H	2.313513	-11.938687	-3.808828
C	0.073768	-1.421659	-7.693801	H	4.410950	-12.045245	-2.466302
C	-0.594817	-7.552803	2.691702	H	4.536061	-10.844807	-0.273181
C	1.320394	-10.623035	-2.429965	H	1.162941	-10.471697	1.750716
C	2.392676	-11.391359	-2.874133	H	1.594252	-8.877837	2.404235
C	3.568088	-11.454337	-2.118313	H	-3.883948	-7.629845	-1.355353
C	3.650991	-10.786158	-0.898871	H	-2.918584	-6.186405	-1.705338
C	1.393444	-9.899011	-1.227712	H	1.694426	-7.970142	-3.031400
C	2.561067	-10.040063	-0.449519	H	-2.452461	-6.453612	-5.266225
O	2.651679	-9.425048	0.771012	H	-1.934447	-8.887600	3.728810

C	1.408393	-9.430202	1.483186	H	-1.875834	-7.637699	5.857035
C	0.315523	-9.028233	-0.713504	H	0.863902	-4.820507	4.125444
C	0.284638	-8.816020	0.679280	H	0.804805	-6.068732	1.999214
C	-0.744188	-8.085823	1.296157	H	1.875834	7.637699	5.857035
C	-1.853861	-7.687172	0.518071	H	1.934447	8.887600	3.728810
C	-0.650916	-8.370891	-1.517287	H	-0.804805	6.068732	1.999214
C	-1.789215	-7.840720	-0.875499	H	-0.863902	4.820507	4.125444
C	-2.913765	-7.290786	-1.729043	H	2.031389	-1.413954	8.208527
O	-2.859848	-7.731861	-3.083001	H	-2.031389	1.413954	8.208527
C	0.769452	-7.705571	-3.528072	H	3.621756	2.517754	7.309274
C	-0.476996	-7.966805	-2.935759	H	2.659003	1.529799	6.197887
C	-1.616559	-7.529146	-3.638538	H	-1.694769	6.583936	6.350968
C	-1.533008	-6.827512	-4.834142	H	-1.321318	6.785892	8.075290
C	-0.285653	-6.537130	-5.409290	H	-4.790886	5.317067	9.266464
C	0.852439	-7.019345	-4.733426	H	-4.788812	3.994771	11.392067
C	-1.309099	-8.002101	3.810905	H	-2.754876	2.706259	12.036896
C	-1.275911	-7.292820	5.018545	H	-0.797448	2.655504	10.532068
C	-0.527187	-6.114317	5.141260	H	4.790886	-5.317067	9.266464
C	0.261408	-5.721499	4.046761	H	4.788812	-3.994771	11.392067
C	0.228317	-6.424994	2.848757	H	2.754876	-2.706259	12.036896
C	1.275911	7.292820	5.018545	H	0.797448	-2.655504	10.532068
C	1.309099	8.002101	3.810905	H	1.321318	-6.785892	8.075290
C	0.594817	7.552803	2.691702	H	1.694769	-6.583936	6.350968
C	-0.228317	6.424994	2.848757	H	-3.621756	-2.517754	7.309274
C	-0.261408	5.721499	4.046761	H	-2.659003	-1.529799	6.197887
C	-1.254314	-0.561476	8.276654	H	-3.391451	3.330817	-7.160288
C	-0.141067	-1.424391	8.259104	H	-2.787997	2.541311	-5.706119
C	1.127076	-0.821851	8.271368	H	-2.536468	1.791364	-7.284257
C	1.254314	0.561476	8.276654	H	2.952380	6.843970	2.192764
C	0.141067	1.424391	8.259104	H	3.246233	6.023739	0.658185
C	-1.127076	0.821851	8.271368	H	3.971467	7.599181	0.966771
O	2.517908	1.105136	8.220463	H	-3.971467	-7.599181	0.966771
C	2.639572	2.058448	7.167594	H	-3.246233	-6.023739	0.658185
C	1.548796	3.110110	7.183689	H	-2.952380	-6.843970	2.192764
C	0.373338	2.850456	7.917640	H	3.391451	-3.330817	-7.160288
C	1.680824	4.245067	6.368573	H	2.536468	-1.791364	-7.284257
C	0.602490	5.154649	6.293445	H	2.787997	-2.541311	-5.706119
C	-0.466066	5.010667	7.193149	H	-2.868823	-5.253825	4.854577
C	-0.565613	3.904013	8.059699	H	-3.818079	-4.523336	6.149814
C	-1.561322	6.048536	7.290926	H	-3.104374	-3.505429	4.901628
O	-2.836147	5.466484	7.589261	H	2.868823	5.253825	4.854577

C	-2.813004	4.703861	8.726797	H	3.818079	4.523336	6.149814
C	-1.680824	3.919490	9.029668	H	3.104374	3.505429	4.901628

Table S7. Cartesian coordinates of optimized (*S*p,*S*p,*S*p)-(*M*,*M*,*M*,*M*,*M*,*M*)-Me_6-**1b**.



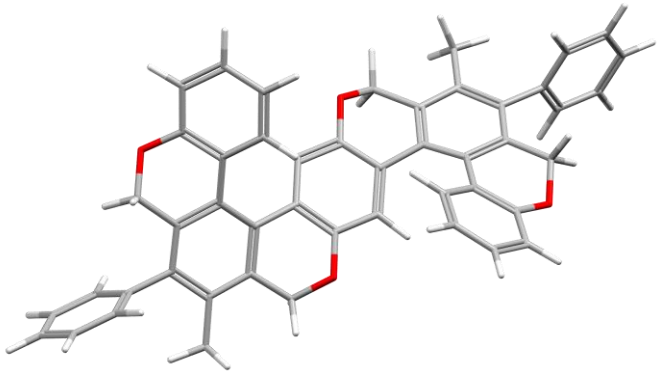
C	1.178816	0.743979	8.407461	C	-0.813735	8.680194	0.665757
C	-0.045662	1.431382	8.387890	C	0.261694	8.010601	1.272658
C	-1.213816	0.644676	8.420115	C	1.415076	7.740966	0.502369
C	-1.178816	-0.743979	8.407461	C	1.967102	5.935394	-7.815752
C	0.045662	-1.431382	8.387890	C	3.162103	5.294151	-8.199171
C	1.213816	-0.644676	8.420115	O	3.233718	3.926451	-8.202312
C	-0.183854	2.862269	8.016709	C	2.019489	3.307348	-8.643705
C	-1.355514	3.191546	7.303272	C	1.920387	7.336867	-7.904702
C	-2.529339	2.234742	7.343865	C	3.039274	8.070643	-8.288660
O	-2.440092	1.269367	8.388313	C	4.234958	7.412813	-8.595983
C	0.837328	3.842878	8.099657	C	4.296319	6.021420	-8.560862
C	0.816161	4.916251	7.185138	C	-1.967134	9.735028	-1.232413
C	-0.260079	5.107962	6.302974	C	-3.162002	9.746771	-0.485156
C	-1.414131	4.307243	6.456220	O	-3.233688	9.065442	0.700757
C	0.183854	-2.862269	8.016709	C	-2.019328	9.137564	1.457451
C	1.355514	-3.191546	7.303272	C	-1.920360	10.512962	-2.401531
C	2.529339	-2.234742	7.343865	C	-3.039062	11.212841	-2.844721
O	2.440092	-1.269367	8.388313	C	-4.234629	11.150445	-2.121141
C	-0.837328	-3.842878	8.099657	C	-4.296035	10.424176	-0.933811
C	-0.816161	-4.916251	7.185138	C	0.136160	7.391983	2.632337
C	0.260079	-5.107962	6.302974	C	0.070159	8.072925	3.855359
C	1.414131	-4.307243	6.456220	C	-0.064203	7.375065	5.064838
C	1.969889	3.799577	9.047415	C	-0.135149	5.975649	5.086980
C	3.165152	4.451129	8.682716	C	-0.067984	5.298499	3.856451
O	3.236717	5.136437	7.499096	C	0.063514	5.988025	2.661408
C	2.022943	5.829013	7.183591	C	2.682560	7.203364	1.133548
C	1.923216	3.177195	10.306261	C	-2.683156	2.620884	-6.808128

C	3.042364	3.143010	11.133361	H	2.121549	1.272205	8.343771
C	4.238263	3.736932	10.716318	H	-2.121549	-1.272205	8.343771
C	4.299613	4.400907	9.493062	H	-3.462151	2.773921	7.532137
C	-1.969889	-3.799577	9.047415	H	-2.640093	1.715647	6.375277
C	-3.165152	-4.451129	8.682716	H	3.462151	-2.773921	7.532137
O	-3.236717	-5.136437	7.499096	H	2.640093	-1.715647	6.375277
C	-2.022943	-5.829013	7.183591	H	2.187185	6.271930	6.201004
C	-1.923216	-3.177195	10.306261	H	1.890166	6.647466	7.910834
C	-3.042364	-3.143010	11.133361	H	0.999422	2.707938	10.628726
C	-4.238263	-3.736932	10.716318	H	2.983688	2.652562	12.100576
C	-4.299613	-4.400907	9.493062	H	5.116616	3.704283	11.355149
C	0.135149	-5.975649	5.086980	H	5.203576	4.899264	9.157218
C	0.067984	-5.298499	3.856451	H	-1.890166	-6.647466	7.910834
C	-0.063514	-5.988025	2.661408	H	-2.187185	-6.271930	6.201004
C	-0.136160	-7.391983	2.632337	H	-0.999422	-2.707938	10.628726
C	-0.070159	-8.072925	3.855359	H	-2.983688	-2.652562	12.100576
C	0.064203	-7.375065	5.064838	H	-5.116616	-3.704283	11.355149
C	2.682446	-4.586326	5.676815	H	-5.203576	-4.899264	9.157218
C	-2.682446	4.586326	5.676815	H	0.115974	-4.213184	3.848757
C	1.178455	-7.651398	-3.558373	H	-0.107483	-5.438409	1.725314
C	-0.046401	-7.977593	-2.953785	H	-0.130740	-9.158290	3.872068
C	-1.214166	-7.611527	-3.651550	H	0.120649	-7.932560	5.996491
C	-1.178455	-6.906686	-4.848065	H	2.614157	-5.517184	5.112735
C	0.046420	-6.546683	-5.433143	H	2.918386	-3.784712	4.963947
C	1.214171	-6.967963	-4.767247	H	3.543490	-4.670557	6.351933
C	-0.185233	-8.371459	-1.529028	H	-3.543490	4.670557	6.351933
C	-1.356438	-7.916780	-0.887383	H	-2.614157	5.517184	5.112735
C	-2.529438	-7.471995	-1.736636	H	-2.918386	3.784712	4.963947
O	-2.440724	-7.895017	-3.094567	H	2.120852	-7.860781	-3.068604
C	0.835122	-8.934991	-0.721142	H	-2.120891	-6.587116	-5.274137
C	0.813735	-8.680194	0.665757	H	-2.638097	-6.373380	-1.702762
C	-0.261694	-8.010601	1.272658	H	-3.463076	-7.902653	-1.363613
C	-1.415076	-7.740966	0.502369	H	2.638970	-4.661494	-4.670667
C	0.185380	-5.510216	-6.487037	H	3.463281	-5.133371	-6.164682
C	1.356711	-4.727363	-6.414542	H	1.884893	-10.176758	1.801511
C	2.529783	-5.240504	-5.604863	H	2.183831	-8.509155	2.333056
O	2.440724	-6.627868	-5.291593	H	0.996838	-10.556148	-2.969691
C	-0.834981	-5.092525	-7.379041	H	2.980299	-11.804387	-3.753625
C	-0.813631	-3.764138	-7.852082	H	5.112651	-11.687910	-2.468822
C	0.261921	-2.903747	-7.576016	H	5.199726	-10.383896	-0.333794
C	1.415422	-3.436060	-6.957536	H	-2.183946	-2.234829	-8.537478

C	1.967134	-9.735028	-1.232413	H	-1.885456	-3.529238	-9.715701
C	3.162002	-9.746771	-0.485156	H	-0.996793	-7.850526	-7.658295
O	3.233688	-9.065442	0.700757	H	-2.980574	-9.153562	-8.346349
C	2.019328	-9.137564	1.457451	H	-5.113119	-7.982673	-8.887130
C	1.920360	-10.512962	-2.401531	H	-5.200103	-5.481664	-8.825696
C	3.039062	-11.212841	-2.844721	H	0.126324	-1.226259	-9.869395
C	4.234629	-11.150445	-2.121141	H	-0.126324	1.226259	-9.869395
C	4.296035	-10.424176	-0.933811	H	-0.112231	1.225745	-5.574475
C	-1.967102	-5.935394	-7.815752	H	0.112231	-1.225745	-5.574475
C	-3.162103	-5.294151	-8.199171	H	2.614349	-1.666292	-7.330982
O	-3.233718	-3.926451	-8.202312	H	3.544669	-3.162307	-7.219173
C	-2.019489	-3.307348	-8.643705	H	2.918670	-2.405588	-5.757130
C	-1.920387	-7.336867	-7.904702	H	-3.544360	-7.829674	0.870240
C	-3.039274	-8.070643	-8.288660	H	-2.917601	-6.185438	0.794432
C	-4.234958	-7.412813	-8.595983	H	-2.613710	-7.178822	2.221667
C	-4.296319	-6.021420	-8.560862	H	2.120891	6.587116	-5.274137
C	0.136278	-1.416920	-7.719877	H	-2.120852	7.860781	-3.068604
C	0.067524	-0.698154	-8.920916	H	-3.463281	5.133371	-6.164682
C	-0.067524	0.698154	-8.920916	H	-2.638970	4.661494	-4.670667
C	-0.136278	1.416920	-7.719877	H	2.638097	6.373380	-1.702762
C	-0.066054	0.689821	-6.518365	H	3.463076	7.902653	-1.363613
C	0.066054	-0.689821	-6.518365	H	2.183946	2.234829	-8.537478
C	2.683156	-2.620884	-6.808128	H	1.885456	3.529238	-9.715701
C	-2.682560	-7.203364	1.133548	H	0.996793	7.850526	-7.658295
C	1.178455	6.906686	-4.848065	H	2.980574	9.153562	-8.346349
C	-0.046420	6.546683	-5.433143	H	5.113119	7.982673	-8.887130
C	-1.214171	6.967963	-4.767247	H	5.200103	5.481664	-8.825696
C	-1.178455	7.651398	-3.558373	H	-1.884893	10.176758	1.801511
C	0.046401	7.977593	-2.953785	H	-2.183831	8.509155	2.333056
C	1.214166	7.611527	-3.651550	H	-0.996838	10.556148	-2.969691
C	-0.185380	5.510216	-6.487037	H	-2.980299	11.804387	-3.753625
C	-1.356711	4.727363	-6.414542	H	-5.112651	11.687910	-2.468822
C	-2.529783	5.240504	-5.604863	H	-5.199726	10.383896	-0.333794
O	-2.440724	6.627868	-5.291593	H	0.130740	9.158290	3.872068
C	0.834981	5.092525	-7.379041	H	-0.120649	7.932560	5.996491
C	0.813631	3.764138	-7.852082	H	-0.115974	4.213184	3.848757
C	-0.261921	2.903747	-7.576016	H	0.107483	5.438409	1.725314
C	-1.415422	3.436060	-6.957536	H	2.613710	7.178822	2.221667
C	0.185233	8.371459	-1.529028	H	2.917601	6.185438	0.794432
C	1.356438	7.916780	-0.887383	H	3.544360	7.829674	0.870240
C	2.529438	7.471995	-1.736636	H	-2.614349	1.666292	-7.330982

O	2.440724	7.895017	-3.094567	H	-3.544669	3.162307	-7.219173
C	-0.835122	8.934991	-0.721142	H	-2.918670	2.405588	-5.757130

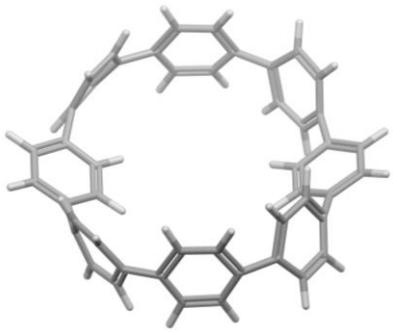
Table S8. Cartesian coordinates of optimized (*M*,*M*)-**8**.



C	-0.083440	1.422992	-0.166690	H	-1.673928	10.063309	0.479728
C	-1.233906	0.611050	-0.248113	H	-1.068951	10.916294	-1.776146
C	-1.159890	-0.776429	-0.228658	H	1.068951	-10.916294	-1.776146
C	0.083440	-1.422992	-0.166690	H	-1.483846	7.645810	0.985282
C	1.233906	-0.611050	-0.248113	C	-0.769431	7.110717	-0.974908
C	1.159890	0.776429	-0.228658	C	-0.985852	9.856735	-1.552968
C	0.270067	-2.892700	-0.148945	C	0.985852	-9.856735	-1.552968
C	1.438485	-3.370489	-0.776904	C	-1.324269	9.377706	-0.286798
C	2.459684	-2.339491	-1.206298	C	-1.215507	8.016011	-0.000295
O	2.471736	-1.197976	-0.345125	C	-0.432909	7.605082	-2.244732
C	-0.270067	2.892700	-0.148945	C	-0.539473	8.966558	-2.531270
C	-1.438485	3.370489	-0.776904	C	2.912002	-5.189163	-1.728665
C	-2.459684	2.339491	-1.206298	C	-2.912002	5.189163	-1.728665
O	-2.471736	1.197976	-0.345125	H	-2.083430	-1.339823	-0.268096
C	0.640990	3.835062	0.392859	H	2.083430	1.339823	-0.268096
C	0.477110	5.192571	0.053446	H	2.273422	-2.008844	-2.242741
C	-0.640990	5.649650	-0.661355	H	3.472802	-2.741035	-1.161476
C	-1.644886	4.733755	-1.036281	H	-2.273422	2.008844	-2.242741
C	1.754796	3.528882	1.322527	H	-3.472802	2.741035	-1.161476
C	2.859132	4.404519	1.332428	H	1.334869	6.547273	1.514888
O	2.846640	5.522580	0.540326	H	1.654290	6.991464	-0.172082
C	1.557633	6.148370	0.511740	H	-1.654290	-6.991464	-0.172082
C	-0.640990	-3.835062	0.392859	H	-1.334869	-6.547273	1.514888
C	-0.477110	-5.192571	0.053446	H	0.900496	1.816871	2.310233
C	0.640990	-5.649650	-0.661355	H	2.844770	1.409017	3.768246
C	1.644886	-4.733755	-1.036281	H	4.845924	2.886340	3.623787
C	-1.754796	-3.528882	1.322527	H	4.810501	4.859445	2.080733
C	-2.859132	-4.404519	1.332428	H	-0.900496	-1.816871	2.310233
O	-2.846640	-5.522580	0.540326	H	-2.844770	-1.409017	3.768246

C	-1.557633	-6.148370	0.511740	H	-4.845924	-2.886340	3.623787
C	1.763054	2.469262	2.245396	H	-4.810501	-4.859445	2.080733
C	2.861603	2.239046	3.068990	H	0.082654	-6.914867	-3.006973
C	3.982137	3.071673	2.992206	H	0.272268	-9.331634	-3.518790
C	3.977125	4.166695	2.131813	H	1.673928	-10.063309	0.479728
C	-1.763054	-2.469262	2.245396	H	1.483846	-7.645810	0.985282
C	-2.861603	-2.239046	3.068990	H	-0.082654	6.914867	-3.006973
C	-3.982137	-3.071673	2.992206	H	-0.272268	9.331634	-3.518790
C	-3.977125	-4.166695	2.131813	H	3.050399	-4.688724	-2.694036
C	0.769431	-7.110717	-0.974908	H	3.798459	-4.964521	-1.122813
C	0.432909	-7.605082	-2.244732	H	2.904980	-6.262965	-1.912516
C	0.539473	-8.966558	-2.531270	H	-2.904980	6.262965	-1.912516
C	1.324269	-9.377706	-0.286798	H	-3.798459	4.964521	-1.122813
C	1.215507	-8.016011	-0.000295	H	-3.050399	4.688724	-2.694036

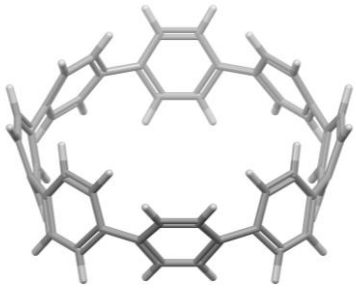
Table S9. Cartesian coordinates of optimized (*R*,*R*,*R*,*R*)-**9**.



C	-1.488707	5.686602	0.223677	C	-3.861197	-3.532157	-1.491663
C	-0.704315	5.700442	1.393724	C	-4.744263	-1.482641	-0.358181
C	0.683851	5.687102	1.359909	C	4.795173	-1.359486	-0.096200
C	1.372937	5.733584	0.135848	C	-5.895019	-0.813137	0.086931
C	0.586766	5.935279	-1.016312	C	-5.918207	0.586206	0.222320
C	-0.801546	5.877641	-0.988493	C	-3.677667	0.692513	-0.629310
C	2.737571	5.180455	-0.062835	C	-3.651251	-0.684866	-0.750097
C	2.982830	4.612308	-1.332084	C	-4.795173	1.359486	-0.096200
C	-2.841204	5.073411	0.322534	H	-1.171670	5.721828	2.344892
C	-3.044282	4.252152	1.454473	H	1.204724	5.538259	2.296650
C	-3.770716	4.953125	-0.744115	H	1.052255	6.139370	-1.946510
C	-4.549089	3.780679	-0.823789	H	-1.322055	5.887763	-1.937525
C	-4.527399	2.812253	0.190873	H	2.497999	5.002603	-2.190111
C	-3.887185	3.130691	1.408992	H	-2.554205	4.476885	2.367117
C	3.651251	4.864506	0.976241	H	-3.875467	5.651436	-1.534678
C	4.436719	3.698945	0.852661	H	-5.170966	3.613569	-1.665776
C	4.453322	2.953568	-0.342191	H	-3.941582	2.486505	2.249031
C	3.861197	3.532157	-1.491663	H	3.732323	5.498700	1.821713
C	4.744263	1.482641	-0.358181	H	4.978598	3.403363	1.714403
C	5.895019	0.813137	0.086931	H	4.016570	3.123080	-2.457124
C	5.918207	-0.586206	0.222320	H	6.782062	1.380726	0.356149
C	3.677667	-0.692513	-0.629310	H	6.812041	-1.065040	0.614504
C	3.651251	0.684866	-0.750097	H	2.797107	-1.270824	-0.894327
C	1.488707	-5.686602	0.223677	H	2.742719	1.167754	-1.095883
C	0.704315	-5.700442	1.393724	H	1.171670	-5.721828	2.344892
C	-0.683851	-5.687102	1.359909	H	-1.204724	-5.538259	2.296650
C	-1.372937	-5.733584	0.135848	H	-1.052255	-6.139370	-1.946510
C	-0.586766	-5.935279	-1.016312	H	1.322055	-5.887763	-1.937525
C	0.801546	-5.877641	-0.988493	H	-2.497999	-5.002603	-2.190111
C	-2.737571	-5.180455	-0.062835	H	2.554205	-4.476885	2.367117
C	-2.982830	-4.612308	-1.332084	H	3.875467	-5.651436	-1.534678

C	2.841204	-5.073411	0.322534	H	5.170966	-3.613569	-1.665776
C	3.044282	-4.252152	1.454473	H	3.941582	-2.486505	2.249031
C	3.770716	-4.953125	-0.744115	H	-3.732323	-5.498700	1.821713
C	4.549089	-3.780679	-0.823789	H	-4.978598	-3.403363	1.714403
C	4.527399	-2.812253	0.190873	H	-4.016570	-3.123080	-2.457124
C	3.887185	-3.130691	1.408992	H	-6.782062	-1.380726	0.356149
C	-3.651251	-4.864506	0.976241	H	-6.812041	1.065040	0.614504
C	-4.436719	-3.698945	0.852661	H	-2.797107	1.270824	-0.894327
C	-4.453322	-2.953568	-0.342191	H	-2.742719	-1.167754	-1.095883

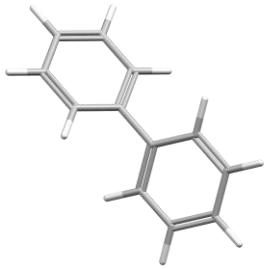
Table S10. Cartesian coordinates of optimized [8]CPP.



C	1.424629	5.376385	0.055950	C	4.621740	3.636958	1.057039
C	0.695093	5.141362	1.235326	C	3.636958	4.621740	1.057039
C	-0.695093	5.141362	1.235326	C	5.376385	1.424629	0.055950
C	-1.424629	5.376385	0.055950	C	5.839782	0.696346	-1.057039
C	-0.696346	5.839782	-1.057039	C	5.839782	-0.696346	-1.057039
C	0.696346	5.839782	-1.057039	C	5.376385	-1.424629	0.055950
C	-2.794314	4.809043	-0.055950	C	5.141362	-0.695093	1.235326
C	-3.636958	4.621740	1.057039	C	5.141362	0.695093	1.235326
C	-4.621740	3.636958	1.057039	H	1.213045	4.798527	2.125893
C	-4.809043	2.794314	-0.055950	H	-1.213045	4.798527	2.125893
C	-4.126997	3.143987	-1.235326	H	-1.222763	6.126912	-1.963687
C	-3.143987	4.126997	-1.235326	H	1.222763	6.126912	-1.963687
C	-5.376385	1.424629	0.055950	H	-3.467757	5.197005	1.963687
C	-5.141362	0.695093	1.235326	H	-5.197005	3.467757	1.963687
C	-5.141362	-0.695093	1.235326	H	-4.250823	2.535319	-2.125893
C	-5.376385	-1.424629	0.055950	H	-2.535319	4.250823	-2.125893
C	-5.839782	-0.696346	-1.057039	H	-4.798527	1.213045	2.125893
C	-5.839782	0.696346	-1.057039	H	-4.798527	-1.213045	2.125893
C	-4.809043	-2.794314	-0.055950	H	-6.126912	-1.222763	-1.963687
C	-4.621740	-3.636958	1.057039	H	-6.126912	1.222763	-1.963687
C	-3.636958	-4.621740	1.057039	H	-5.197005	-3.467757	1.963687
C	-2.794314	-4.809043	-0.055950	H	-3.467757	-5.197005	1.963687
C	-3.143987	-4.126997	-1.235326	H	-2.535319	-4.250823	-2.125893
C	-4.126997	-3.143987	-1.235326	H	-4.250823	-2.535319	-2.125893
C	-1.424629	-5.376385	0.055950	H	-1.213045	-4.798527	2.125893
C	-0.695093	-5.141362	1.235326	H	1.213045	-4.798527	2.125893
C	0.695093	-5.141362	1.235326	H	1.222763	-6.126912	-1.963687
C	1.424629	-5.376385	0.055950	H	-1.222763	-6.126912	-1.963687
C	0.696346	-5.839782	-1.057039	H	3.467757	-5.197005	1.963687
C	-0.696346	-5.839782	-1.057039	H	5.197005	-3.467757	1.963687
C	2.794314	-4.809043	-0.055950	H	4.250823	-2.535319	-2.125893
C	3.636958	-4.621740	1.057039	H	2.535319	-4.250823	-2.125893

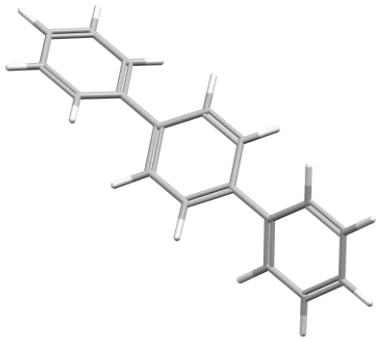
C	4.621740	-3.636958	1.057039	H	2.535319	4.250823	-2.125893
C	4.809043	-2.794314	-0.055950	H	4.250823	2.535319	-2.125893
C	4.126997	-3.143987	-1.235326	H	5.197005	3.467757	1.963687
C	3.143987	-4.126997	-1.235326	H	3.467757	5.197005	1.963687
C	2.794314	4.809043	-0.055950	H	6.126912	1.222763	-1.963687
C	3.143987	4.126997	-1.235326	H	6.126912	-1.222763	-1.963687
C	4.126997	3.143987	-1.235326	H	4.798527	-1.213045	2.125893
C	4.809043	2.794314	-0.055950	H	4.798527	1.213045	2.125893

Table S11. Cartesian coordinates of optimized biphenyl **S1**.



C	-5.090882	-0.859933	0.020594	C	-8.062704	1.291154	0.589096
C	-4.552508	-2.103503	0.348146	H	-4.435804	-0.065870	-0.327060
C	-5.376859	-3.122323	0.829224	H	-3.484851	-2.273622	0.235639
C	-6.744517	-2.885384	0.978713	H	-4.957499	-4.091595	1.085157
C	-7.282170	-1.641924	0.649549	H	-7.397502	-3.673702	1.344303
C	-6.465499	-0.606142	0.164811	H	-8.351992	-1.477392	0.744082
C	-7.038913	0.719195	-0.185170	H	-5.800711	1.002488	-1.928756
C	-6.573051	1.436813	-1.299965	H	-6.739085	3.213400	-2.500078
C	-7.110248	2.680680	-1.628334	H	-8.546894	4.204644	-1.105561
C	-8.127540	3.235375	-0.849611	H	-9.387349	2.960033	0.879375
C	-8.601524	2.534315	0.260720	H	-8.420300	0.766892	1.471026

Table S12. Cartesian coordinates of optimized terphenyl **S2**.



C	-1.201132	0.695611	-0.000547	C	-0.959061	-5.025953	-0.730382
C	-1.201121	-0.695632	0.000599	C	-0.958261	-3.631988	-0.730916
C	0.000018	-1.424493	0.000038	H	-2.148649	1.226975	-0.019489
C	1.201145	-0.695612	-0.000563	H	-2.148628	-1.227012	0.019581
C	1.201134	0.695630	0.000504	H	2.148660	-1.226979	-0.019515
C	-0.000005	1.424492	-0.000042	H	2.148642	1.227009	0.019416
C	0.000028	-2.908670	0.000080	H	-1.692278	3.094980	1.325428
C	-0.000021	2.908669	-0.000082	H	-1.705974	5.563137	1.309308
C	-0.958322	3.631969	0.730918	H	-0.000075	6.816502	-0.000182
C	-0.959149	5.025934	0.730388	H	1.705857	5.563119	-1.309607
C	-0.000060	5.729821	-0.000154	H	1.692231	3.094961	-1.325602
C	0.959048	5.025923	-0.730659	H	1.692291	-3.094922	1.325591
C	0.958260	3.631959	-0.731119	H	1.705963	-5.563083	1.309605
C	0.958327	-3.631938	0.731116	H	0.000050	-6.816500	0.000189
C	0.959141	-5.025902	0.730659	H	-1.705877	-5.563174	-1.309299
C	0.000044	-5.729820	0.000158	H	-1.692231	-3.095013	-1.325421

Table S13. TD-DFT vertical one-electron excitations calculated for (*S*p,*S*p)-(*M*,*M*,*M*,*M*)-Me$_4$-**1a**.

exited state	energy (eV)	wavelength (nm)	oscillator strength (*f*) [a]	description [b]
1	2.8125	440.84	0.0966	HOMO–1 → LUMO (0.49657) (49.5%) HOMO → LUMO+1 (0.49519) (49.2%)
2	3.0822	429.09	1.1038	HOMO → LUMO (0.46569) (43.5%) HOMO–1 → LUMO+1 (0.52429) (55.1%)
5	3.0822	365.23	0.0498	HOMO–5 → LUMO+1 (0.37161) (27.8%) HOMO–4 → LUMO+1 (0.45276) (41.3%) HOMO–3 → LUMO (–0.28443) (16.3%) HOMO–1 → LUMO+2 (–0.09189) (1.7%) HOMO–1 → LUMO+4 (–0.12466) (3.1%) HOMO → LUMO+3 (–0.13457) (3.6%) HOMO → LUMO+5 (–0.09151) (1.7%)
6	3.2011	364.93	0.1288	HOMO–5 → LUMO+1 (0.37836) (28.8%) HOMO–4 → LUMO (0.47339) (45.1%) HOMO–3 → LUMO+1 (–0.25100) (12.7%) HOMO–1 → LUMO+3 (–0.10815) (2.4%) HOMO–1 → LUMO+5 (–0.08940) (1.6%) HOMO → LUMO+2 (–0.08866) (1.6%) HOMO → LUMO+4 (–0.12574) (3.2%)
7	3.2011	362.39	0.0402	HOMO–5 → LUMO (0.27589) (15.3%) HOMO–3 → LUMO (0.33548) (22.7%) HOMO–2 → LUMO+1 (0.42505) (36.4%) HOMO–1 → LUMO+2 (0.23263) (10.9%) HOMO → LUMO+3 (0.17679) (6.3%) HOMO → LUMO+5 (–0.09411) (1.8%)
10	3.2011	347.79	0.0347	HOMO–4 → LUMO+1 (0.00717) (1.4%) HOMO–3 → LUMO (0.07148) (14.4%) HOMO–2 → LUMO+1 (0.03258) (6.6%) HOMO–1 → LUMO+2 (0.21526) (43.3%) HOMO → LUMO+3 (0.15363) (30.9%)

[a] Excitation energies with oscillator strength larger than 0.02 are listed. [b] Relative contribution larger than 1% is listed.

Table S14. TD-DFT vertical one-electron excitations calculated for (*S*p,*S*p,*R*p)-(*M*,*M*,*M*,*M*,*P*,*P*)-Me$_6$-**1b**.

exited state	energy (eV)	wavelength (nm)	oscillator strength (*f*) [a]	description [b]
1	3.0094	411.99	0.1942	HOMO–2 → LUMO+1 (–0.26994) (14.7%) HOMO–1 → LUMO+2 (0.27242) (15.0%) HOMO → LUMO (0.54169) (59.1%)
2	3.0611	405.03	1.0595	HOMO–2 → LUMO (0.43731) (38.5%) HOMO–1 → LUMO (0.28564) (16.4%) HOMO → LUMO+1 (–0.25055) (12.6%) HOMO → LUMO+2 (0.39379) (31.2%)
3	3.0864	401.72	1.1499	HOMO–2 → LUMO+1 (–0.24558) (12.1%) HOMO–2 → LUMO+2 (–0.26089) (13.7%) HOMO–1 → LUMO+1 (0.52437) (55.3%) HOMO–1 → LUMO+2 (0.23837) (11.4%) HOMO → LUMO (–0.17520) (6.2%)
10	3.5101	353.22	0.1213	HOMO–7 → LUMO+1 (0.20100) (8.2%) HOMO–7 → LUMO+2 (0.31629) (20.2%) HOMO–6 → LUMO (–0.48090) (46.8%) HOMO–5 → LUMO (–0.20314) (8.4%) HOMO–4 → LUMO+1 (–0.08165) (1.3%) HOMO–4 → LUMO+2 (–0.12947) (3.4%) HOMO–3 → LUMO (–0.10696) (2.3%)

[a] Excitation energies with oscillator strength larger than 0.02 are listed. [b] Relative contribution larger than 1% is listed.

Table S15. TD-DFT vertical one-electron excitations calculated for (*M*,*M*)-**8**.

exited state	energy (eV)	wavelength (nm)	oscillator strength (*f*) [a]	description [b]
1	3.0682	404.09	0.6995	HOMO → LUMO (0.70030) (98.4%)
2	3.4827	356.00	0.0434	HOMO–1 → LUMO (0.68521) (94.3%) HOMO → LUMO+2 (0.10032) (2.0%)
3	3.5356	350.67	0.0541	HOMO–2 → LUMO (0.67406) (91.3%) HOMO–1 → LUMO+1 (0.09009) (1.6%) HOMO → LUMO+1 (0.14400) (4.2%)
4	3.7304	332.36	0.0920	HOMO–2 → LUMO (–0.15375) (4.7%) HOMO–2 → LUMO+2 (–0.08578) (1.5%) HOMO → LUMO+1 (0.67507) (91.5%)
5	3.7982	326.43	0.0629	HOMO–4 → LUMO+1 (0.07969) (1.3%) HOMO–3 → LUMO (0.65112) (85.2%) HOMO → LUMO+2 (–0.20219) (8.2%) HOMO → LUMO+7 (–0.10397) (2.2%)
6	3.9670	312.54	0.2391	HOMO–5 → LUMO (–0.15223) (4.7%) HOMO–3 → LUMO (0.20096) (8.1%) HOMO–1 → LUMO (–0.11362) (2.6%) HOMO → LUMO+2 (0.62951) (79.7%) HOMO → LUMO+6 (0.07060) (1.0%)
8	4.1825	296.43	0.0323	HOMO–2 → LUMO (–0.09358) (1.8%) HOMO–2 → LUMO+2 (0.09704) (1.9%) HOMO–1 → LUMO+1 (0.65337) (85.8%) HOMO → LUMO+3 (0.18786) (7.1%) HOMO → LUMO+8 (0.06979) (1.0%)
10	4.2052	294.84	0.0686	HOMO–5 → LUMO (0.27836) (15.6%) HOMO–2 → LUMO+1 (0.58237) (68.3%) HOMO–1 → LUMO+2 (0.19728) (7.8%) HOMO → LUMO+2 (0.10435) (2.2%)
11	4.3073	287.84	0.3401	HOMO–5 → LUMO (0.53806) (68.5%) HOMO–3 → LUMO+2 (0.07659) (1.2%) HOMO–2 → LUMO+1 (–0.30240) (18.4%) HOMO → LUMO+2 (0.13725) (3.8%) HOMO → LUMO+7 (–0.12065) (2.9%)

14	4.4428	279.07	0.1371	HOMO–5 → LUMO (–0.07244) (1.1%) HOMO–3 → LUMO+2 (0.13573) (3.7%) HOMO–2 → LUMO+1 (–0.15197) (4.6%) HOMO–2 → LUMO+3 (0.17053) (5.9%) HOMO–1 → LUMO+2 (0.59052) (70.2%) HOMO → LUMO+4 (–0.14238) (4.1%) HOMO → LUMO+7 (0.14909) (4.5%)

[a] Excitation energies with oscillator strength larger than 0.02 are listed. [b] Relative contribution larger than 1% is listed.

Table S16. TD-DFT vertical one-electron excitations calculated for (*R*,*R*,*R*,*R*)-**9**.

exited state	energy (eV)	wavelength (nm)	oscillator strength (*f*) [a]	description [b]
2	3.3674	368.19	1.5022	HOMO–1 → LUMO (0.46467) (43.0%) HOMO → LUMO+1 (0.53039) (56.1%)
5	3.9745	311.95	0.0456	HOMO–4 → LUMO (–0.12393) (3.1%) HOMO–5 → LUMO+1 (0.19420) (7.6%) HOMO–4 → LUMO (0.15377) (4.7%) HOMO–3 → LUMO (–0.09315) (1.7%) HOMO–2 → LUMO+1 (0.10955) (2.4%) HOMO–1 → LUMO+2 (0.41348) (34.3%) HOMO–1 → LUMO+5 (–0.19976) (8.0%) HOMO–1 → LUMO+6 (–0.08192) (1.3%) HOMO → LUMO+3 (0.19195) (7.4%) HOMO → LUMO+4 (–0.34415) (23.8%) HOMO → LUMO+7 (0.07042) (1.0%)
9	4.2222	293.65	0.0843	HOMO–5 → LUMO+1 (–0.18338) (6.7%) HOMO–4 → LUMO (–0.18832) (7.1%) HOMO–3 → LUMO (0.42048) (35.4%) HOMO–1 → LUMO+2 (–0.19654) (7.7%) HOMO–1 → LUMO+6 (–0.21183) (9.0%) HOMO → LUMO+3 (0.31901) (20.4%) HOMO → LUMO+7 (0.15444) (4.8%)
11	4.2584	291.15	0.7020	HOMO–7 → LUMO+1 (0.09074) (1.7%) HOMO–5 → LUMO+1 (–0.07636) (1.2%) HOMO–5 → LUMO+1 (–0.07043) (1.0%) HOMO–4 → LUMO (–0.11190) (2.5%) HOMO–3 → LUMO (0.12564) (3.2%) HOMO–2 → LUMO+1 (0.39013) (30.6%) HOMO–1 → LUMO+2 (0.36188) (26.3%) HOMO–1 → LUMO+5 (0.23195) (10.8%) HOMO → LUMO+4 (0.29713) (17.7%)

[a] Excitation energies with oscillator strength larger than 0.02 are listed. [b] Relative contribution larger than 1% is listed.

Table S17. TD-DFT vertical one-electron excitations calculated for [8]CPP.

exited state	energy (eV)	wavelength (nm)	oscillator strength (*f*) [a]	description [b]
1	2.8766	431.01	0.0000	HOMO → LUMO (0.54169) (96.7%)
2	3.5634	347.94	0.8773	HOMO–1 → LUMO (0.70375) (99.0%)
3	3.5634	347.94	0.8773	HOMO–2 → LUMO (0.70375) (99.0%)
4	3.5823	346.10	0.7364	HOMO–1 → LUMO+2 (0.49411) (98.8%)
5	3.5823	346.10	0.7364	HOMO–1 → LUMO+1 (0.49411) (98.8%)

[a] Excitation energies (>340 nm) are listed. [b] Relative contribution larger than 1% is listed.

Table S18. Transition moments of (*S*p,*S*p)-(*M*,*M*,*M*,*M*)-Me$_4$-**1a**.

Ground to excited state transition electric dipole moments (Au):						
state	X	Y	Z	Dip. S.	Osc.	
1	0	0	-1.1839	1.4016	0.0966	
Ground to excited state transition velocity dipole moments (Au):						
state	X	Y	Z	Dip. S.	Osc.	
1	0	0	0.1265	0.016	0.1032	
Ground to excited state transition magnetic dipole moments (Au):						
state	X	Y	Z			
1	0	0	-5.9221			
Ground to excited state transition velocity quadrupole moments (Au):						
state	XX	YY	ZZ	XY	XZ	YZ
1	0.6387	-0.9235	0.0975	-2.7771	0	0
<0|del|b> * <b|rxdel|0> + <0|del|b> * <b|delr+rdel|0>						
Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)						
state	XX	YY	ZZ	R(velocity)	E-M Angle	
1	-3764.7392	-1361.0518	0	-1708.597	90	
1/2[<0|r|b>*<b|rxdel|0> + (<0|rxdel|b>*<b|r|0>)*]						
Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)						
state	XX	YY	ZZ	R(length)		
1	0	0	-4957.9895	-1652.6632		
1/2[<0|del|b>*<b|r|0> + (<0|r|b>*<b|del|0>)*] (Au)						
state	X	Y	Z	Dip. S.	Osc.(frdel)	
1	0	0	-0.1498	0.1498	0.0998	

Table S19. Transition moments of (*S*p,*S*p,*R*p)-(*M*,*M*,*M*,*M*,*P*,*P*)-Me_6-**1b**.

Ground to excited state transition electric dipole moments (Au):						
state	X	Y	Z	Dip. S.	Osc.	
1	0.8591	-1.3769	0	2.6339	0.1942	
Ground to excited state transition velocity dipole moments (Au):						
state	X	Y	Z	Dip. S.	Osc.	
1	-0.0967	0.1511	0	0.0322	0.1939	
Ground to excited state transition magnetic dipole moments (Au):						
state	X	Y	Z			
1	9.9405	0.8674	0			
Ground to excited state transition velocity quadrupole moments (Au):						
state	XX	YY	ZZ	XY	XZ	YZ
1	0	0	0	0	1.981	1.1516
<0|del|b> * <b|rxdel|0> + <0|del|b> * <b|delr+rdel|0>						
Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)						
state	XX	YY	ZZ	R(velocity)	E-M Angle	
1	-537.9379	-3427.6936	-1339.9567	-1768.5294	117.62	
1/2[<0|r|b>*<b|rxdel|0> + (<0|rxdel|b>*<b|r|0>)*]						
Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)						
state	XX	YY	ZZ	R(length)		
1	-6039.2876	844.6066	0	-1731.5604		
1/2[<0|del|b>*<b|r|0> + (<0|r|b>*<b|del|0>)*] (Au)						
state	X	Y	Z	Dip. S.	Osc.(frdel)	
1	-0.083	-0.208	0	0.2911	0.1941	

Table S20. Transition moments of (*M*,*M*)-**8**.

Ground to excited state transition electric dipole moments (Au):						
state	X	Y	Z	Dip. S.	Osc.	
1	-0.8077	-2.9417	0	9.3059	0.6995	
Ground to excited state transition velocity dipole moments (Au):						
state	X	Y	Z	Dip. S.	Osc.	
1	0.0914	0.3317	0	0.1184	0.6999	
Ground to excited state transition magnetic dipole moments (Au):						
state	X	Y	Z			
1	0.7535	0.0714	0			
Ground to excited state transition velocity quadrupole moments (Au):						
state	XX	YY	ZZ	XY	XZ	YZ
1	0	0	0	0	0.6153	0.0833
<0|del|b> * <b|rxdel|0> + <0|del|b> * <b|delr+rdel|0>						
Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)						
state	XX	YY	ZZ	R(velocity)	E-M Angle	
1	-565.7807	239.8525	906.3415	193.4711	69.18	
1/2[<0|r|b>*<b|rxdel|0> + (<0|rxdel|b>*<b|r|0>)*]						
Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)						
state	XX	YY	ZZ	R(length)		
1	430.3829	148.4484	0	192.9438		
1/2[<0|del|b>*<b|r|0> + (<0|r|b>*<b|del|0>)*] (Au)						
state	X	Y	Z	Dip. S.	Osc.(frdel)	
1	-0.0738	-0.9758	0	1.0496	0.6997	

Table S21. Transition moments of (*R*,*R*,*R*,*R*)-**9**.

Ground to excited state transition electric dipole moments (Au):						
state	X	Y	Z	Dip. S.	Osc.	
1	0	0	-0.108	0.0117	0.0009	
Ground to excited state transition velocity dipole moments (Au):						
state	X	Y	Z	Dip. S.	Osc.	
1	0	0	0.0108	0.0001	0.0007	
Ground to excited state transition magnetic dipole moments (Au):						
state	X	Y	Z			
1	0	0	8.5507			
Ground to excited state transition velocity quadrupole moments (Au):						
state	XX	YY	ZZ	XY	XZ	YZ
1	-0.3613	0.4983	0.01	-2.1131	0	0
<0|del|b> * <b|rxdel|0> + <0|del|b> * <b|delr+rdel|0>						
Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)						
state	XX	YY	ZZ	R(velocity)	E-M Angle	
1	208.3988	345.2072	0	184.5353	90	
1/2[<0|r|b>*<b|rxdel|0> + (<0|rxdel|b>*<b|r|0>)*]						
Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)						
state	XX	YY	ZZ	R(length)		
1	0	0	653.0537	217.6846		
1/2[<0|del|b>*<b|r|0> + (<0|r|b>*<b|del|0>)*] (Au)						
state	X	Y	Z	Dip. S.	Osc.(frdel)	
1	0	0	-0.0012	0.0012	0.0008	

Table S22. Calculated chiroptical properties of (*S*p,*S*p)-(*M*,*M*,*M*,*M*)-Me$_4$-**1a**.

compound	$\|\mu\|$ /10^{-20} esu·cm [a]	$\|m\|$ /10^{-20} erg·G^{-1} [b]	cosθ (E-M Angle) [c]	g_{calcd} (4R/D) [d]
(*S*p,*S*p)-(*M*,*M*,*M*,*M*)-Me$_4$-**1a**	300.92	5.492	-1.00	-0.07298
(*S*p,*S*p,*R*p)-(*M*,*M*,*M*,*M*,*P*,*P*)-Me$_6$-**1b**	412.51	9.254	-0.45	-0.04068
(*M*,*M*)-**8**	775.38	0.702	0.35	0.001284
(*R*,*R*,*R*,*R*)-**9**	27.45	7.930	1.00	1.067

[a] μ: Transition electronic 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 S23. 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
(*S*p,*S*p)-(*M*,*M*,*M*,*M*)-Me_4-**1a**	-3835.209343	-3835.140418	-3835.139473	-3835.311449
(*S*p,*R*p)-(*M*,*M*,*P*,*P*)-Me_4-**1a**	-3835.213718	-3835.144919	-3835.143975	-3835.315382
(*S*p,*S*p,*R*p)-(*M*,*M*,*M*,*M*,*P*,*P*)-Me_6-**1b**	-5752.911506	-5752.806607	-5752.805662	-5753.057903
(*S*p,*S*p,*S*p)-(*M*,*M*,*M*,*M*,*M*,*M*)-Me_6-**1b**	-5752.910592	-5752.805669	-5752.804725	-5753.057033
(*M*,*M*)-**8**	-2149.856969	-2149.816957	-2149.816013	-2149.931023
(*R*,*R*,*R*,*R*)-**9**	-1847.613391	-1847.582397	-1847.581452	-1847.67065
biphenyl **S1**	-463.124102	-463.115232	-463.114287	-463.158662
terphenyl **S2**	-694.100704	-694.087153	-694.086209	-694.142192

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