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Electronic Supplementary Information

Bottom-up synthesis and structures of π-lengthened tubular macrocycles

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General

Analytical thin-layer chromatography (TLC) was performed on a glass plate coated with silica gel (230-400 mesh, 0.25 mm thickness) containing a fluorescent indicator (silica gel 60F_{254}, Merck). Flash silica gel column chromatography was performed on silica gel 60N (spherical and neutral gel, 40-50 μm, Kanto).[1] Gel permeation chromatography (GPC) was performed on Japan Analytical Industry LC-9104 with JAIGEL 1H, 2H and 2.5H polystyrene columns (eluent: chloroform). High pressure liquid chromatography (HPLC) was performed with cholesterylated columns (COSMOSIL® Cholester, 4.6 ϕ × 250 + 250 + 250 mm for analytical scales and 20ϕ × 250 + 250 mm for preparative scales, Nacalai Tesque). The analysis was performed on a HPLC system at 40 °C in a column oven (JASCO CO-2060PLUS) under the detection with UV-vis (JASCO MD2018PLUS) and CD (JASCO CD-2095) detectors at flow rate of 1.0 mL/min, and the preparative isolation was performed on Japan Analytical Industry LC-908. IR spectra were recorded on Thermo Scientific Nicolet iS10 FT-IR equipped with an attenuated total reflection (ATR; neat), and were reported as wavenumbers (ν) in cm^{-1}. Proton (^1H) and carbon (^{13}C) nuclear magnetic resonance (NMR) spectra were recorded on Bruker AVANCE 400 (^1H: 400 MHz; ^{13}C: 100 MHz) or JEOL JNM-ECS 400 (^1H: 400 MHz; ^{13}C: 100 MHz) spectrometers. Chemical shift values were given in ppm relative to internal $CHCl_3$ (for ^1H NMR: δ 7.26), $CDCl_3$ (for ^{13}C NMR: δ 77.16). Time-of-flight (TOF) mass spectra were obtained on a JEOL JMS-T100 instrument using

1. Still, W. C.; Kahn, M.; Mitra, A. *J. Org. Chem.* **1978**, *43*, 2923-2925.

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Direct Analysis in Real Time (DART) ionization or a Bruker Daltonics microflex instrument using Matrix Assisted Laser Desorption Ionization (MALDI) with tetracyanoquinodimethane as the matrix (*ca.* 500 weight%). The melting points were determined by Stuart SMP30 instrument and were uncorrected. UV-visible absorption spectra were recorded with JASCO V-670 or V-630BIO spectrophotometer. Circular dichroism (CD) spectra were obtained on JASCO J-820 spectropolarimeter. X-ray diffraction analysis was carried out on a Bruker APEX II CCD diffractometer.

Materials

Pigment red 168 (4,10-dibromoanthanthrone) was obtained from Clariant Japan. Tin(II) chloride dihydrate, *N*,*N*,*N*′,*N*′-tetramethylethylenediamine, cesium fluoride, triphenylphosphine, triisopropylsilylacetylene and potassium phosphate were purchased from Wako. Palladium on carbon (10%), $[Ir(cod)OMe]_2$ and 4,4′-di-*tert*-butyl-2,2′-dipyridyl were purchased from Aldrich. 1-Hexyne, $PdCl_2(dppf)•CH_2Cl_2$ and bis(pinacolato)diboron were purchased from TCI. *o*-Dichlorobenzene and sodium borohydride were purchased from Kanto. Cyclohexane was purchased from Nacalai. $PtCl_2(cod)$ was synthesized as reported in literature.[2] Anhydrous THF (stabilizer free, Kanto) and toluene (Kanto) was purified by a solvent purification system (GlassContour) equipped with columns of activated alumina and supported copper catalyst (Q-5).[3] Other solvents were purified by distillation and dried over 4-Å molecular sieves. Butyllithium in hexane was purchased from Kanto and titrated before use.

2. McDermott, J. X.; White, J. F.; Whitesides, G. M. *J. Am. Chem. Soc.* **1976**, *98*, 6521-6528.

3. Pangborn, A. B.; Giardello, M. A.; Grubbs, R. H.; Rosen, R. K.; Timmers, F. J. *Organometallics* **1996**, *15*, 1518-1520.

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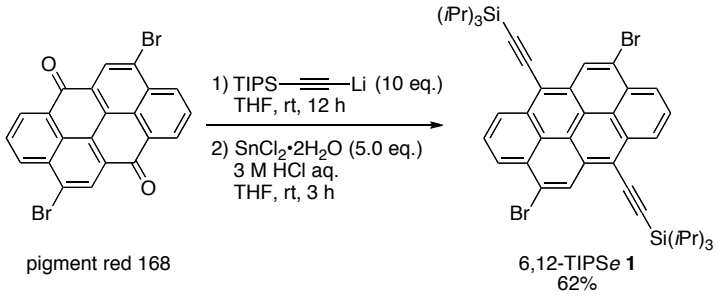
Synthesis

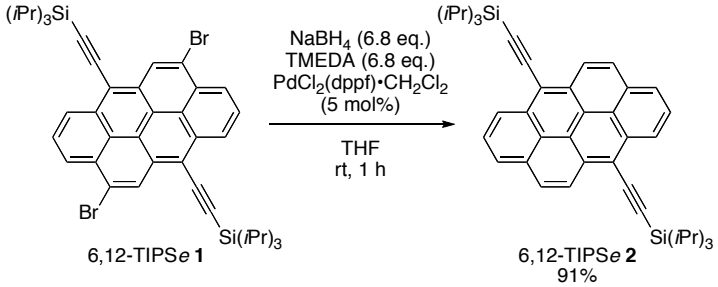
4,10-Dibromo-6,12-bis(triisopropylsilylethynyl)anthanthrene (6,12-TIPS*e* **1**)



pigment red 168 — 6,12-TIPS*e* **1** 62%

To a solution of triisopropylsilylacetylene (24.0 mL, 108 mmol) in THF (1.0 L) was dropwise added butyllithium (1.59 M in hexane, 67.0 mL, 107 mmol) at 0 °C over 10 min under nitrogen. After string the mixture for 1 h at 0 °C, pigment red 168 (5.00 g, 10.8 mmol) was added. After being stirred for 12 h, tin(II) chloride dihydrate (12.2 g, 54.0 mmol) in 3 M aqueous hydrogen chloride (60 mL) was added at ambient temperature and stirred for 3 h. Ice water (ca. 200 mL) was added to quench the reaction, and the insoluble material was filtered off. Organic materials were extracted with chloroform (100 mL × 5), and the organic layer was washed with brine, dried over magnesium sulfate and concentrated in vacuo. The crude material was washed with ethanol (200 mL) and hexane (300 mL) to afford the title compound in 62% yield (5.28 g, 6.64 mmol) as a dark red solid. Physical data of 6,12-TIPS*e* **1**: mp 239 °C, IR (neat) 677 (s), 725 (s), 753 (m), 840 (m), 879 (s), 995 (w), 1016 (m), 1184 (m), 1463 (w), 2130 (w), 2865 (w), 2941 (w) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 1.34-1.40 (m, 6H), 1.36 (d, J = 4.8 Hz, 36H), 8.31 (dd, J = 8.2, 8.2 Hz, 2H), 8.74 (d, J = 8.2 Hz, 2H), 9.15 (d, J = 8.2 Hz, 2H), 9.16 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.8, 19.1, 103.4, 105.7, 117.0, 120.9, 123.0, 125.7, 126.4, 127.1, 127.5, 130.1, 130.6, 130.8, 132.6; HRMS (DART-TOF) calcd for $C_{44}H_{50}Br_2Si_2$ $[M+H]^+$ 793.1896, found 793.1892.

6,12-Bis(triisopropylsilylethynyl)anthanthrene (6,12-TIPS*e* **2**)

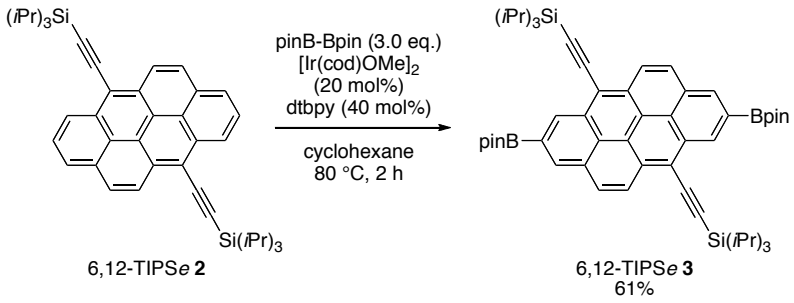


6,12-TIPS*e* **1** — 6,12-TIPS*e* **2** 91%

To a mixture of 6,12-TIPS*e* **1** (1.01 g, 1.27 mmol) and $Pd(dppf)Cl_2•CH_2Cl_2$ (51.8 mg, 63.4 μmol) in THF (125 mL) was added *N*,*N*,*N'*,*N'*-tetramethylethylenediamine (1.29 mL, 8.66 mmol) and sodium borohydride (0.327 g, 8.63 mmol) at ambient temperature under nitrogen. After string 1 h, the reaction mixture was filtrated to remove insoluble materials, and to the filtrate

was added 1 M aqueous hydrogen chloride (*ca.* 30 mL). Organic materials were extracted by chloroform (100 mL × 4), washed with brine, dried over magnesium sulfate and concentrated in vacuo. The crude material was purified by silica gel (*ca.* 10 g) column chromatography and recrystallization from dichloromethane/methanol to afford the title compound in 91% yield (734 mg, 1.15 mmol) as a red solid. Physical data of 6,12-TIPS*e* **2**[4]: mp 243 °C (lit.,[4] 244-245 °C); IR (neat) 674 (s), 724 (s), 825 (m), 882 (m), 994 (w), 1016 (w), 1191 (w), 1464 (w), 2139 (w), 2864 (w), 2941 (w) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 1.33-1.42 (m, 6H), 1.35 (d, J = 4.8 Hz, 36H), 8.22 (d, J = 7.2 Hz, 2H), 8.23 (dd, J = 9.2, 9.2 Hz, 2H), 8.30 (d, J = 7.2 Hz, 2H), 8.82 (d, J = 9.2 Hz, 2H), 9.13 (d, J = 9.2, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.8, 19.1, 104.2, 104.3, 117.2, 122.1, 122.5, 125.5, 125.8, 126.8, 126.9, 130.0, 131.2, 131.5, 132.9; HRMS (DART-TOF) calcd for $C_{44}H_{52}Si_2[M+H]^+$ 637.3686, found 637.3687.

2,8-Bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-6,12-bis(triisopropylsilylethynyl)anthanthrene (6,12-TIPS*e* **3**)



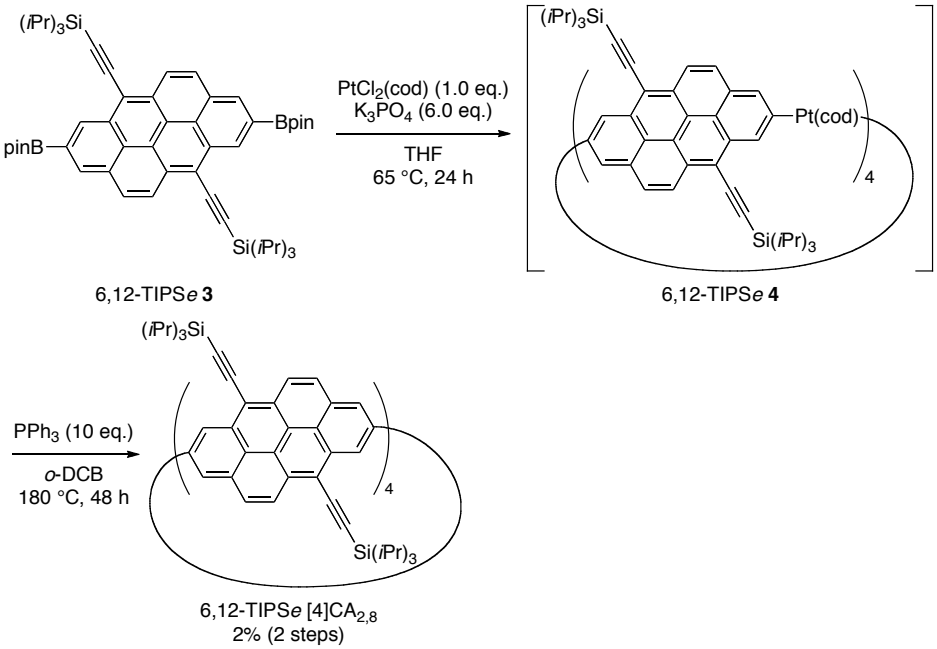
6,12-TIPS*e* **2** → 6,12-TIPS*e* **3** 61%

A mixture of 6,12-TIPS*e* **2** (2.50 g, 3.92 mmol), $[Ir(cod)OMe]_2$ (520 mg, 0.784 mmol), 4,4'-di-*tert*-butyl-2,2'-bipyridine (dtbpy; 421 mg, 1.57 mmol) and bis(pinacolato)diboron (2.98 g, 11.7 mmol) in cyclohexane (39 mL) was stirred at 80 °C under nitrogen. After 2 h, the solvent was removed in vacuo, and the residue was dissolved in chloroform (*ca.* 50 mL) and passed through a pad of silica gel (*ca.* 50 g) with chloroform (*ca.* 1 L). The crude material was further purified by silica gel column chromatography (eluent: 50% chloroform/hexane) and gel permeation chromatography to afford the title compound in 61% (2.10 g, 2.36 mmol) as an orange solid. Physical data of 6,12-TIPS*e* **3**: mp 310 °C (decomp.); IR (neat) 671 (s), 835 (m), 969 (m), 1141 (s), 1249 (m), 1307 (m), 1370 (s), 1464 (m), 2132 (w), 2864 (w), 2942 (w); ^1H NMR (400 MHz, $CDCl_3$) δ 1.30-1.41 (m, 6H), 1.37 (d, J = 4.0 Hz, 36H), 1.48 (s, 24H), 8.21 (d, J = 8.8 Hz, 2H), 8.66 (s, 2H), 8.76 (d, J = 8.8 Hz, 2H), 9.70 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.8, 19.2, 25.2, 84.3, 104.1, 104.6, 117.6, 122.6, 124.0, 126.7, 130.2, 130.7, 130.8, 132.9, 133.5. One quaternary carbon

4. The product was fully characterized by the spectra, but the characterization data were slightly different from the values reported for the same compound from a different synthesis route. Zhang, L.; Walker, B.; Liu, F.; Colella, N. S.; Mannsdeld, S. C. B.; Watkins, J. J.; Nguyen, T.-Q.; Briseno, A. L. *J. Matter. Chem.* **2012**, *22*, 4266-4286.

resonance should be overlapped with other resonance. HRMS (DART-TOF) calcd for $C_{56}H_{74}B_2O_4Si_2$ $[M+H]^+$ 889.5408, found 889.5430.

6,12-TIPS*e* [4]cyclo-2,8-anthanthrenylene (6,12-TIPS*e* [4]$CA_{2,8}$)



A mixture of 6,12-TIPS*e* **3** (2.00 g, 2.25 mmol), $PtCl_2$(cod) (842 mg, 2.25 mmol) and K_3PO_4 (2.87 g, 13.5 mmol) in THF (113 mL) was heated at reflux for 24 h. After the addion of water (*ca.* 100 mL), the precipitates were filtered and washed with methanol (*ca.* 20 mL). The solid material containing Pt-intermediate **4** was then dissolved in *o*-dichlorobenzene (190 mL), and triphenylphosphine (5.90 g, 22.5 mmol) was added. The mixture was stirred at ambient temperature for 30 min and at 180 °C for 48 h. After removal of volatile materials in vacuo, the residual materials were purified by silica gel column chromatography (eluent: 20% chloroform/hexane) and gel permeation chromatography to afford the racemic mixture of 6,12-TIPS*e* (12,8)-[4]$CA_{2,8}$ in 2% yield (27.8 mg, 10.9 mmol) as a red solid. Due to highly insoluble nature of the product, we could not obtain the ^{13}C NMR spectra. Physical data of 6,12-TIPS*e* (12,8)-[4]$CA_{2,8}$; IR (neat) 676 (s), 703 (s), 881 (s), 995 (m), 1071 (m), 1182 (m), 1462 (m), 1577 (m), 2130 (w), 2864 (m), 2941 (m); ^1H NMR (400 MHz, $CDCl_3$) δ 1.30-1.45 (m, 168H), 7.92 (d, J = 9.6 Hz, 8H), 8.43 (d, J = 9.6 Hz, 8H), 8.68 (d, J = 1.2 Hz, 8H), 9.03 (d, J = 1.2 Hz, 8H); MS (MALDI-TOF) calcd. for $C_{176}H_{200}Si_8$ $[M]^+$ 2537, found 2537. See Fig. 2 for HPLC analysis.

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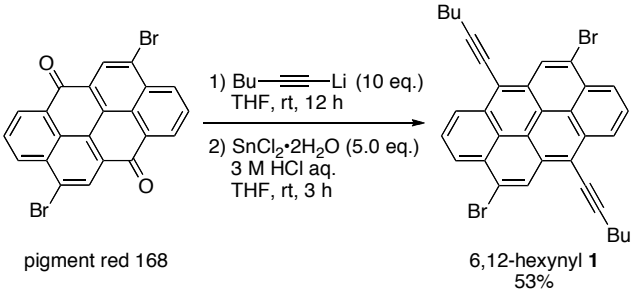
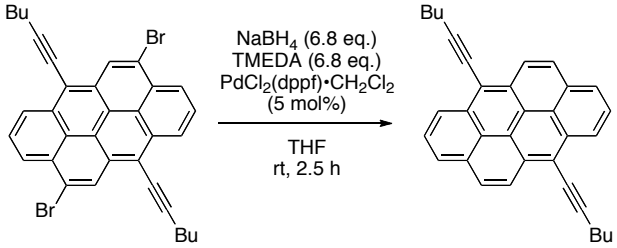
4,10-Dibromo-6,12-bis(1-hexynyl)anthanthrene (6,12-hexynyl **1**)



pigment red 168 — 6,12-hexynyl **1** 53%

The same synthesis procedure for 6,12-TIPSe **1** was adopted with 1-hexyne to convert pigment red 168 (10.0 g, 21.5 mmol) to 6,12-hexynyl **1** in 53% yield (6.78 g, 11.4 mmol) as an orange solid. Physical data of 6,12-hexynyl **1**: mp 214-215 °C; IR (neat) 685 (m), 728 (m), 759 (s), 812 (s), 876 (m), 1351 (m), 1463 (w), 1483 (m), 1579 (m), 1608 (w), 2869 (w), 2930 (m), 2953 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 1.15 (t, J = 7.4 Hz, 6H), 1.77 (qt, J = 7.4, 7.6 Hz, 4H), 1.94 (tt, J = 7.6, 6.8 Hz, 4H), 2.89 (t, J = 6.8 Hz, 4H), 8.15 (dd, J = 8.4, 7.2 Hz, 2H), 8.58 (d, J = 7.2 Hz, 2H), 8.86 (s, 2H), 8.92 (d, J = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.0, 20.3, 22.6, 31.3, 77.6, 104.1, 117.4, 120.2, 122.8, 125.0, 125.8, 126.8, 126.9, 129.9, 130.3, 130.7, 131.5; HRMS (DART-TOF) calcd for $C_{34}H_{26}Br_2$ $[M+H]^+$ 593.0480, found 593.0473.

6,12-Bis(1-hexynyl)anthanthrene (6,12-hexynyl **2**)



6,12-hexynyl **1** — 6,12-hexynyl **2** 80%

The same synthesis procedure for 6,12-TIPSe **2** was adopted to convert 6,12-hexynyl **1** (6.26 g, 10.5 mmol) to 6,12-hexynyl **2** in 80% yield (3.70 g, 8.47 mmol) as a red solid. Physical data of 6,12-hexynyl **2**: mp 149 °C; IR (neat) 731 (s), 757 (m), 795 (m), 812 (s), 830 (s), 1464 (m), 1496 (m), 1582 (m), 1618 (w), 2858 (w), 2929 (m), 2954 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 1.10 (t, J = 7.4 Hz, 6H), 1.78 (qt, J = 7.4, 7.2 Hz, 4H), 1.91 (tt, J = 7.2, 7.0 Hz, 4H), 2.88 (t, J = 7.0 Hz, 4H), 8.16 (d, J = 9.2 Hz, 2H), 8.20 (dd, J = 8.0, 6.4 Hz, 2H), 8.27 (d, J = 6.4 Hz, 2H), 8.74 (d, J = 9.2 Hz, 2H), 9.06 (d, J = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.0, 20.2, 22.5, 31.4, 78.1, 103.1, 117.5, 121.8, 122.6, 125.1, 125.5, 126.6, 126.9, 129.4, 131.1, 131.6, 132.1; HRMS (DART-TOF) calcd for $C_{34}H_{28}$ $[M+H]^+$ 437.2269, found 437.2263.

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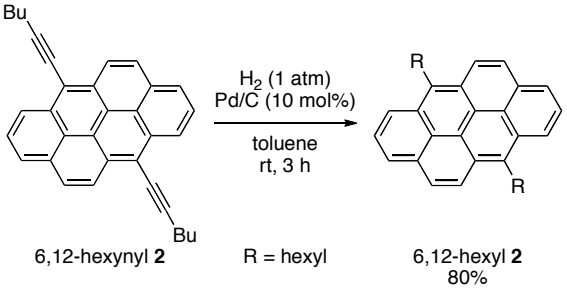
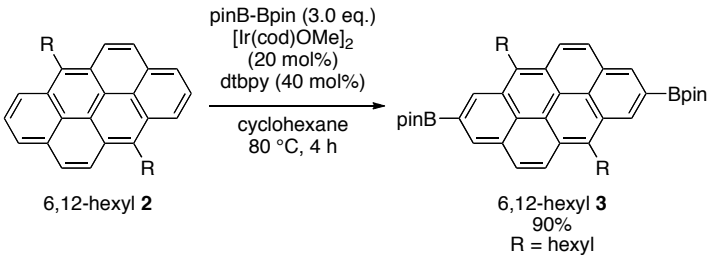
6,12-Dihexylanthanthrene (6,12-hexyl **2**)



A mixture of 6,12-hexyl-**2** (3.70 g, 8.47 mmol) and 10% palladium on carbon (902 mg) in toluene (280 mL) under atmospheric pressure of hydrogen was stirred for 3 h at ambient temperature. Palladium on carbon was filtrated off, and the filtrate was concentrated in vacuo. The crude material was washed with hexane (*ca.* 100 mL) and recrystallized from ethyl acetate to afford the title compound in 80% yield (3.00 g, 6.75 mmol) as a yellow solid. Physical data of 6,12-hexyl-**2**: mp 163-164 °C; IR (neat) 734 (s), 788 (m), 824 (s), 879 (w), 955 (w), 1114 (w), 1186 (w), 1396 (w), 1467 (m), 1494 (w), 1545 (w), 1585 (w), 1622 (w), 1757 (w), 2851 (w), 2918 (m), 2949 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 0.94 (t, J = 7.2 Hz, 6H), 1.33-1.54 (m, 8H), 1.70 (tt, J = 7.2, 7.2 Hz, 4H), 2.00 (tt, J = 8.0, 7.2 Hz, 4H), 3.90 (t, J = 8.0 Hz, 4H), 8.12 (d, J = 9.6 Hz, 2H), 8.17 (dd, J = 8.0, 8.0 Hz, 2H), 8.22 (d, J = 8.0 Hz, 2H), 8.48 (d, J = 9.6 Hz, 2H), 8.78 (d, J = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.3, 22.9, 28.9, 30.3, 31.8, 32.1, 121.9, 122.7, 123.5, 123.8, 124.8, 125.8, 127.8, 128.6, 129.6, 131.8, 133.6; HRMS (DART-TOF) calcd for $C_{34}H_{37}$ $[M+H]^+$ 445.2895, found 445.2904.

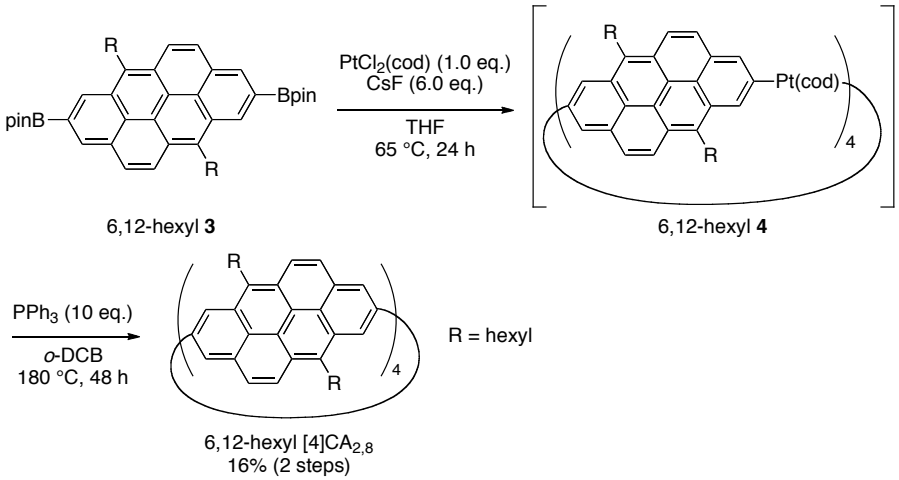
6,12-Dihexyl-2,8-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)anthanthrene (6,12-hexyl **3**)



The same diborylation procedure for 6,12-TIPS*e* **2** was adopted to convert 6,12-hexyl **2** (580 mg, 1.31 mmol) to 6,12-hexyl **3** in 90% yield (817 mg, 1.17 mmol) as a yellow solid. Physical data of 6,12-hexyl **3**: mp 215-216 °C; IR (neat) 693 (s), 857 (m), 970 (m), 1144 (s), 1248 (m), 1306 (s), 1334 (m), 1368 (s), 1406 (m), 1464 (m), 2858 (w), 2924 (w), 2948 (w), 2979 (w); ^1H NMR (400 MHz, $CDCl_3$) δ 0.96 (t, J = 7.2 Hz, 6H), 1.35-1.55 (m, 8H), 1.50 (s, 24H), 1.71 (tt, J = 7.2, 7.2 Hz, 4H), 2.01 (tt, J = 7.2, 7.2 Hz, 4H), 3.95 (t, J = 7.2 Hz, 4H), 8.13 (d, J = 9.6 Hz, 2H), 8.45 (d, J = 9.6 Hz, 2H), 8.60 (s, 2H), 9.25 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.3, 22.9, 25.2,

28.6, 30.0, 31.7, 31.9, 84.3, 122.4, 124.7, 125.0, 128.1, 128.8, 129.1, 129.2, 129.9, 131.1, 134.3; HRMS (DART-TOF) calcd for $C_{46}H_{59}B_2O_4$ $[M+H]^+$ 697.4614, found 697.4606.

6,12-Hexyl [4]cyclo-2,8-anthanthrenylne (6,12-hexyl [4]$CA_{2,8}$)



The same macrocyclization procedure for 6,12-hexyl [4]$CA_{2,8}$ was adopted to convert 6,12-hexyl **3** (260 mg, 0.373 mmol) to 6,12-hexyl [4]$CA_{2,8}$. As can be seen in the chromatograph for the compounds after silica gel column chromatography (Fig. 2), the compounds at this stage contained a small amount of impurities (R_t <20 min). The isomers were thus separated by preparative HPLC (eulent: 70% CH_2Cl_2/MeOH) to afford the total yield of 16% for 6,12-hexyl [4]$CA_{2,8}$. The yields for each isomer are as follows: 6,12-hexyl (*P*)-(12,8)-[4]$CA_{2,8}$ (3.2 mg, 2% yield), 6,12-hexyl (*M*)-(12,8)-[4]$CA_{2,8}$ (4.3 mg, 3% yield), 6,12-hexyl (*P*)-(11,9)-[4]$CA_{2,8}$ (5.9 mg, 4% yield), 6,12-hexyl (*M*)-(11,9)-[4]$CA_{2,8}$ (4.2 mg, 3% yield), 6,12-hexyl $(10,10)_{AABB}$-[4]$CA_{2,8}$ (4.8 mg, 3% yield) and 6,12-hexyl $(10,10)_{ABAB}$-[4]$CA_{2,8}$ (1.6 mg, 1% yield). Physical data of 6,12-hexyl (*P*)-(12,8)-[4]$CA_{2,8}$: IR (neat) 647 (m), 689 (m), 786 (w), 835 (m), 856 (s), 1457 (w), 1541 (w), 1577 (w), 1615 (w), 2852 (w), 2924 (w), 2952 (w) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 0.92 (t, *J* = 8.0 Hz, 24H), 1.30-1.44 (m, 32H), 1.55-1.70 (m, 16H), 1.74-1.83 (m, 16H), 3.62-3.69 (m, 16H), 7.89 (d, *J* = 9.6 Hz, 8H), 8.12 (d, *J* = 9.6 Hz, 8H), 8.58 (s, 8H), 8.62 (s, 8H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.4, 22.9, 29.0, 30.1, 31.6, 31.9, 120.6, 121.3, 122.6, 123.2, 124.6, 127.5, 127.7, 130.4, 132.1, 133.4, 135.4; MS (MALDI-TOF) calcd for $C_{136}H_{136}$ $[M]^+$ 1769, found 1769. Physical data of 6,12-hexyl (*M*)-(12,8)-[4]$CA_{2,8}$: IR (neat) 647 (m), 689 (s), 786 (w), 835 (m), 857 (s), 1457 (w), 1541 (w), 1578 (w), 1614 (w), 2854 (w), 2924 (w), 2952 (w) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 0.92 (t, *J* = 8.0 Hz, 24H), 1.30-1.44 (m, 32H), 1.55-1.70 (m, 16H), 1.74-1.83 (m, 16H), 3.62-3.69 (m, 16H), 7.89 (d, *J* = 9.6 Hz, 8H), 8.12 (d, *J* = 9.6 Hz, 8H), 8.58 (s, 8H), 8.62 (s, 8H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.4, 22.9, 29.0, 30.1, 31.6, 32.0, 120.6, 121.3, 122.6, 123.2, 124.6, 127.5, 127.7, 130.4, 132.1, 133.4, 135.4; MS (MALDI-TOF) calcd for $C_{136}H_{136}$ $[M]^+$ 1769,

found 1769. Physical data of 6,12-hexyl (*P*)-(11,9)-[4]$CA_{2,8}$: IR (neat) 644 (w), 690 (s), 786 (w), 836 (w), 856 (s), 1457 (w), 1540 (w), 1576 (w), 1616 (w), 2853 (w), 2923 (w), 2952 (w) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 0.85 (dd, *J* = 7.2, 7.2 Hz, 6H), 0.88 (dd, *J* = 7.2, 7.2 Hz, 6H), 0.94 (dd, *J* = 7.2, 7.2 Hz, 6H), 0.95 (dd, *J* = 7.2, 7.2 Hz, 6H), 1.27-1.45 (m, 32H), 1.55-1.70 (m, 16H), 1.71-1.85 (m, 16H), 3.60-3.75 (m, 16H), 7.83 (d, *J* = 9.6 Hz, 2H), 7.86 (d, *J* = 10 Hz, 2H), 7.88 (d, *J* = 10 Hz, 2H), 7.91 (d, *J* = 10 Hz, 2H), 8.09 (d, *J* = 9.6 Hz, 2H), 8.12 (d, *J* = 9.6 Hz, 2H × 2), 8.15 (d, *J* = 10 Hz, 2H), 8.32 (s, 2H), 8.41 (s, 2H), 8.43 (s, 2H), 8.44 (s, 2H), 8.64 (s, 2H), 8.66 (s, 2H), 8.70 (s, 2H), 8.83 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.2, 14.3, 14.3, 14.3, 22.9 (overlapped), 22.9, 22.9, 28.9, 29.0, 29.1, 29.1, 30.1 (overlapped), 30.2, 30.3, 31.6, 31.7, 31.8, 31.9 (overlapped), 32.0 (overlapped), 32.0, 120.9, 121.3, 121.4 (3C overlapped), 121.8 (overlapped), 122.0, 122.5 (overlapped), 122.6, 122.6 (overlapped), 122.7, 122.7, 123.4, 124.6 (4C overlapped), 127.5 (overlapped), 127.5 (overlapped), 127.7, 127.7 (overlapped), 127.8, 130.6, 130.6, 130.6, 130.7, 131.8, 131.9, 132.0, 132.0, 133.3, 133.3, 133.4, 133.5, 135.9, 135.9, 136.1 (overlapped); MS (MALDI-TOF) calcd for $C_{136}H_{136}$ $[M]^+$ 1769, found 1769. Physical data of 6,12-hexyl (*M*)-(11,9)-[4]$CA_{2,8}$: IR (neat) 642 (w), 690 (s), 786 (w), 836 (w), 856 (s), 1456 (w), 1540 (w), 1576 (w), 1615 (w), 2854 (w), 2924 (w), 2952 (w) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 0.85 (dd, *J* = 7.2, 7.2 Hz, 6H), 0.88 (dd, *J* = 7.2, 7.2 Hz, 6H), 0.94 (dd, *J* = 7.2, 7.2 Hz, 6H), 0.95 (dd, *J* = 7.2, 7.2 Hz, 6H), 1.27-1.45 (m, 32H), 1.55-1.70 (m, 16H), 1.71-1.85 (m, 16H), 3.60-3.75 (m, 16H), 7.83 (d, *J* = 9.6 Hz, 2H), 7.86 (d, *J* = 10 Hz, 2H), 7.88 (d, *J* = 10 Hz, 2H), 7.91 (d, *J* = 10 Hz, 2H), 8.09 (d, *J* = 9.6 Hz, 2H), 8.12 (d, *J* = 9.6 Hz, 2H × 2), 8.15 (d, *J* = 10 Hz, 2H), 8.32 (s, 2H), 8.41 (s, 2H), 8.43 (s, 2H), 8.44 (s, 2H), 8.64 (s, 2H), 8.66 (s, 2H), 8.71 (s, 2H), 8.83 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.2, 14.3, 14.3, 14.4, 22.9 (overlapped), 22.9, 22.9, 28.9, 29.0, 29.1, 29.1, 30.1 (overlapped), 30.2, 30.3, 31.6, 31.7, 31.8, 31.9 (overlapped), 32.0 (overlapped), 32.0, 120.9, 121.3, 121.4 (3C overlapped), 121.8 (overlapped), 122.0, 122.5 (overlapped), 122.6, 122.6 (overlapped), 122.7, 122.7, 123.4, 124.6 (4C overlapped), 127.5 (overlapped), 127.5 (overlapped), 127.7, 127.7 (overlapped), 127.8, 130.6, 130.6, 130.6, 130.7, 131.8, 131.9, 132.0, 132.0, 133.3, 133.3, 133.4, 133.5, 135.9, 135.9, 136.1 (overlapped); MS (MALDI-TOF) calcd for $C_{136}H_{136}$ $[M]^+$ 1769, found 1769. Physical data of 6,12-hexyl $(10,10)_{AABB}$-[4]$CA_{2,8}$: IR (neat) 645 (w), 690 (s), 786 (w), 836 (w), 856 (s), 1465 (w), 1540 (w), 1577 (w), 1615 (w), 2854 (w), 2925 (w), 1953 (w) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 0.82 (t, *J* = 7.6 Hz, 12H), 0.96 (t, *J* = 7.2 Hz, 12H), 1.21-1.49 (m, 32H), 1.53-1.70 (m, 16H), 1.73-1.85 (m, 16H), 3.56-3.76 (m, 16H), 7.82 (d, *J* = 9.6 Hz, 4H), 7.90 (d, *J* = 10 Hz, 4H), 8.09 (d, *J* = 10 Hz, 4H), 8.15 (d, *J* = 9.6 Hz, 4H), 8.35 (s, 4H), 8.38 (s, 4H), 8.70 (s, 4H), 8.74 (s, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.2, 14.4, 22.9, 22.9, 28.9, 29.1, 30.1, 30.2, 31.6, 31.8, 31.9, 31.9, 121.4, 121.4, 121.6, 122.2, 122.4, 122.5 (overlapped), 123.2, 124.6, 124.6, 127.5 (overlapped), 127.7, 127.7, 130.6, 130.7, 131.8, 131.9, 133.2, 133.4, 136.0, 136.3; MS

(MALDI-TOF) calcd for $C_{136}H_{136}$ $[M]^+$ 1769, found 1769. Physical data of $(10,10)_{ABAB}$-[4]$CA_{2,8}$: IR (neat) 690 (s), 786 (m), 856 (s), 1398 (w), 1456 (m), 1576 (w), 1615 (w), 2854 (m), 2924 (m), 2953 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 0.88 (t, J = 7.2 Hz, 24H), 1.25-1.42 (m, 32H), 1.54-1.65 (m, 16H), 1.67-1.81 (m, 16H), 3.58-3.74 (m, 16H), 7.87 (d, J = 9.6 Hz, 8H), 8.11 (d, J = 9.6 Hz, 8H), 8.31 (s, 8H), 8.70 (s, 8H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.3, 22.9, 29.0, 30.3, 31.8, 32.0, 121.4, 121.8, 122.5, 123.3, 124.6, 127.5, 127.7, 130.7, 131.9, 133.3, 136.6; MS (MALDI-TOF) calcd for $C_{136}H_{136}$ $[M]^+$ 1769, found 1769.

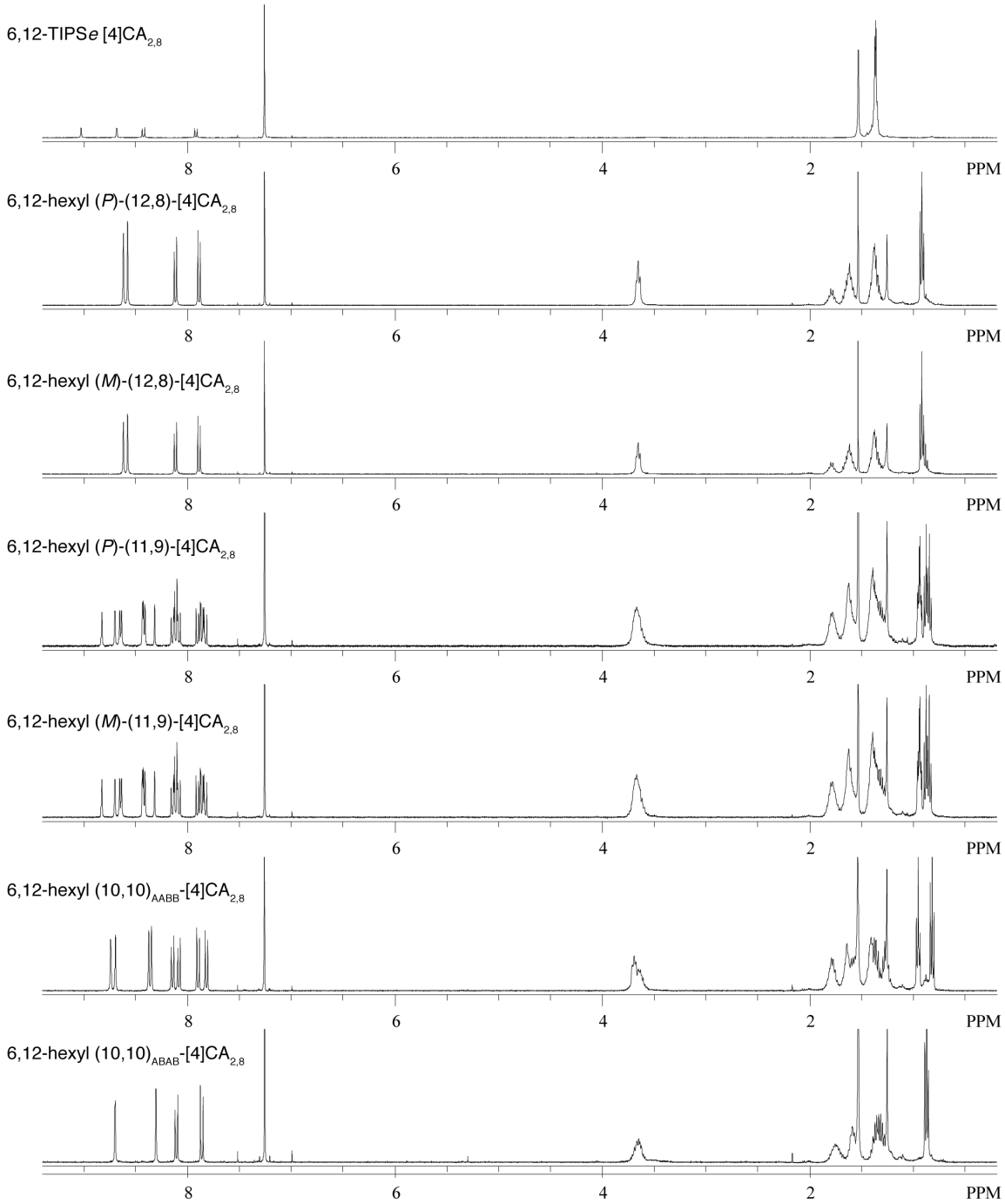


Fig. S1. ^1H NMR spectra of [4]$CA_{2,8}$ in $CDCl_3$. Enlarged views for aromatic region are shown in Fig. 2.

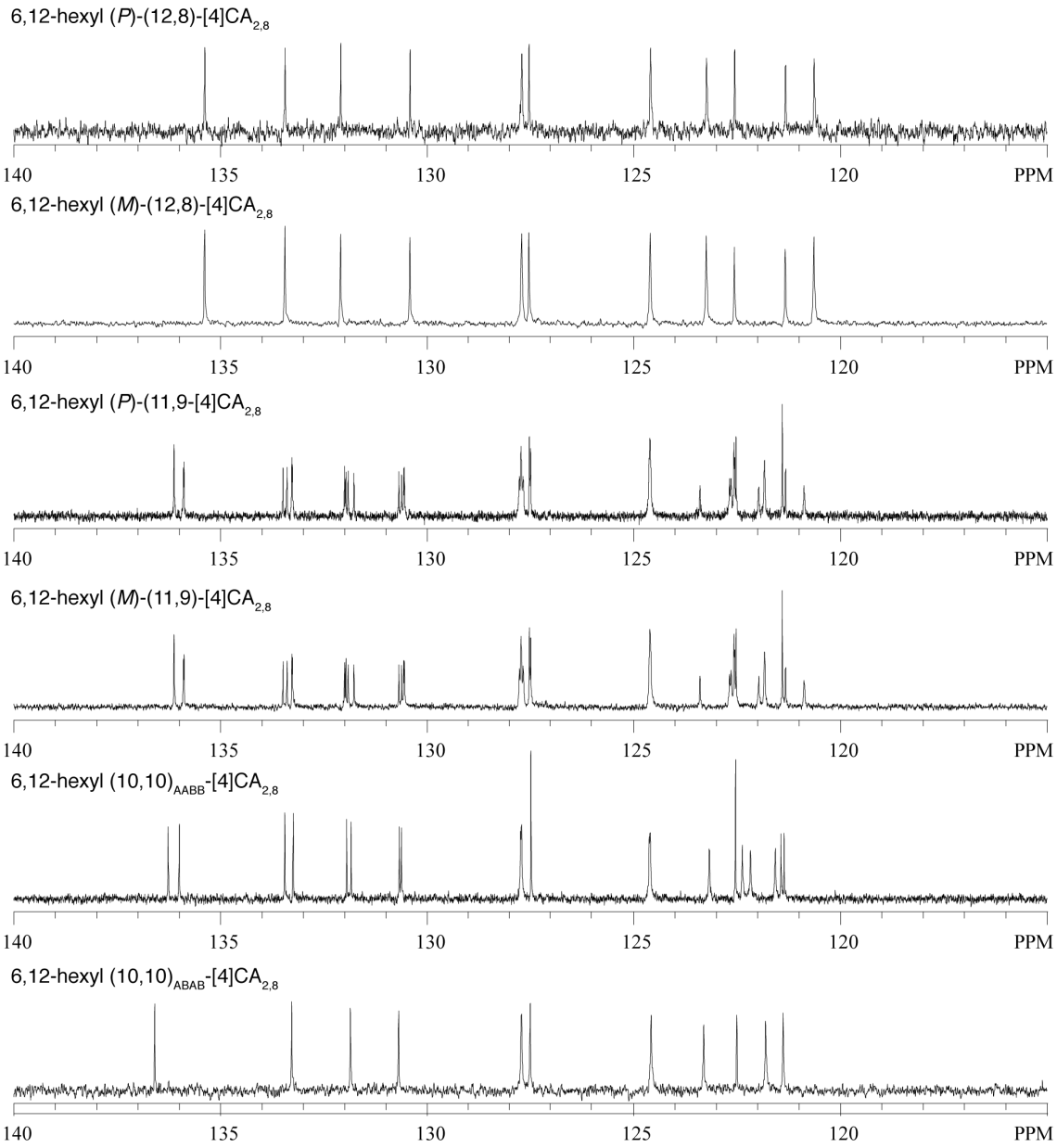


Fig. S2. Aromatic region of ^{13}C NMR spectra of $[4]CA_{2,8}$ in $CDCl_3$.

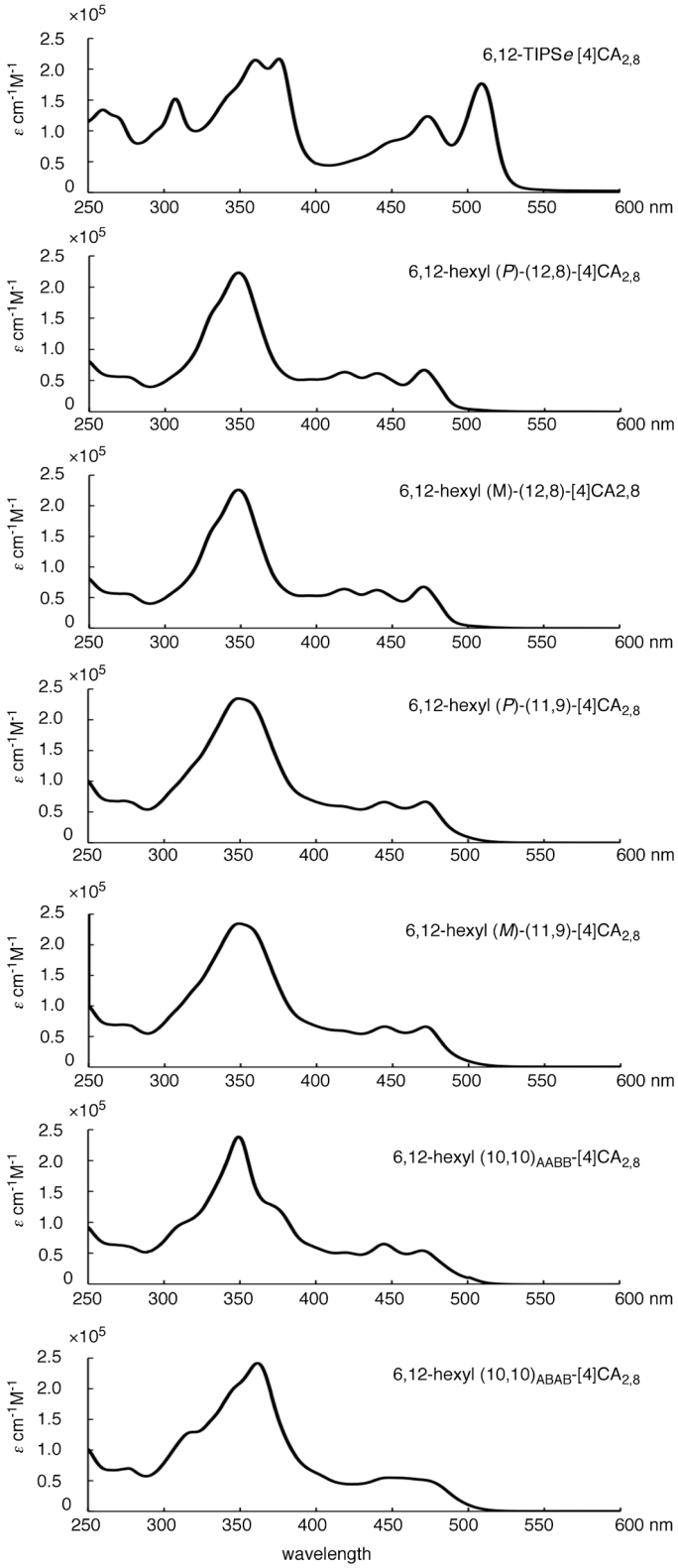


Fig. S3. UV-vis absorption spectra of [4]$CA_{2,8}$ isomers in chloroform. Concentrations are as follows: 6,12-TIPS*e* (*P*)/(*M*)-(12,8)-[4]$CA_{2,8}$ = 1.11 × 10^{-6} M, 6,12-hexyl (*P*)-(12,8)-[4]$CA_{2,8}$ = 4.23 × 10^{-6} M, 6,12-hexyl (*M*)-(12,8)-[4]$CA_{2,8}$ = 4.15 × 10^{-6} M, 6,12-hexyl (*P*)-(11,9)-[4]$CA_{2,8}$ = 4.04 × 10^{-6} M, 6,12-hexyl (*M*)-(12,8)-[4]$CA_{2,8}$ = 4.22 × 10^{-6} M, 6,12-hexyl $(10,10)_{AABB}$-[4]$CA_{2,8}$ = 3.82 × 10^{-6} M, 6,12-hexyl $(10,10)_{ABAB}$-[4]$CA_{2,8}$ = 4.04 × 10^{-6} M.

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Theoretical calculations

Computational methods

The Gaussian 09 program suite was used in all calculations,[5,6] and the results were visualized on GaussView 5.0.9.[7] Semiempirical calculations were performed at the PM6 level,[8] and DFT calculations were performed by the B3LYP functional, the gradient correction of the exchange functional by Becke[9] and the correlation functional by Lee, Yang and Parr[10] with the 6-31G(d,p) split valence plus polarization basis set.[11]

As reported,[12] theoretical CD spectra of 6,12-methyl [4]$CA_{2,8}$ were obtained by time-dependent DFT for the first 30 singlet–singlet transitions with an extra keyword of IOP(9/40 = 2) to output information on smaller contributions to each electronic transition. Cartesian coordinates for the optimized geometries are shown in Tables S1 and S2.

Energy profiles of single-bond rotation of biaryls were obtained by a relaxed potential energy surface scan method with the PM6 semiempirical calculations. Results are shown in Fig. 3 and S4. Cartesian coordinates of biaryls for the representative dihedral angles are shown in Tables S3-S12.

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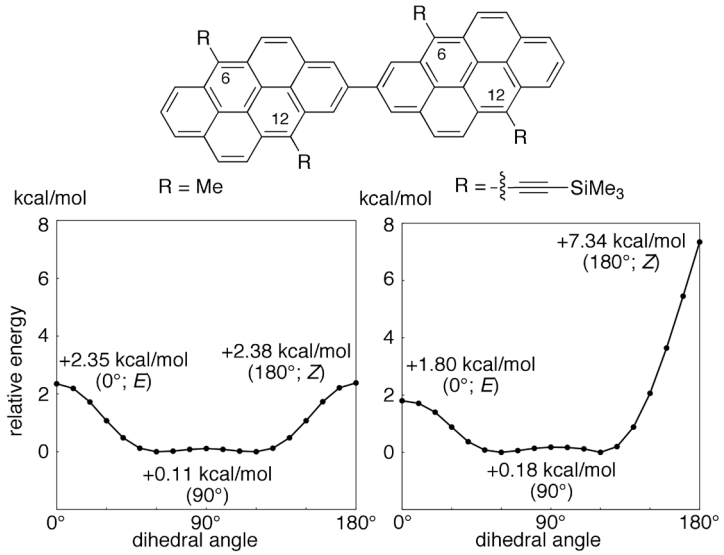

Fig. S4. Energy profile for rotation of biphenyl and 2,2'-bichrysenyl from PM6 calculations.

Cartesian coordinates

Table S1. Cartesian coordinate of 6,12-methyl (*P*)-(12,8)-[4]$CA_{2,8}$.

SCF Done: E(RB3LYP) = -3692.27490811 A.U. after 14 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.742611	1.938383	2.811806
2	6	0	-6.866325	0.598696	2.997032
3	6	0	-6.758428	-0.336600	1.897166
4	6	0	-6.735146	0.226541	0.567042
5	6	0	-6.605009	1.624266	0.378083
6	6	0	-6.494418	2.496932	1.505144
7	6	0	-6.575298	-1.710127	2.079640
8	6	0	-6.710810	-0.617276	-0.567087
9	6	0	-6.499497	-2.005098	-0.378329
10	6	0	-6.308534	-2.534136	0.935844
11	6	0	-6.338428	-2.869807	-1.505387
12	6	0	-6.619124	-2.326706	-2.811986
13	6	0	-6.820929	-0.996503	-2.997059
14	6	0	-6.767256	-0.056571	-1.897143

15	6	0	-6.664147	1.325203	-2.079915
16	6	0	-6.445738	2.163422	-0.936260
17	1	0	-6.766463	2.611732	3.664737
18	1	0	-6.603970	-3.000336	-3.664915
19	1	0	-6.964055	-0.622671	-4.004197
20	6	0	-5.704123	-3.809966	1.049285
21	6	0	-5.798081	-4.140795	-1.328885
22	1	0	-5.638998	-4.756895	-2.208161
23	6	0	-5.338119	-4.572175	-0.062577
24	1	0	-5.376706	-4.122599	2.031695
25	1	0	-6.986578	0.217251	4.004290
26	6	0	-5.916487	3.472261	-1.049774
27	6	0	-6.029329	3.797265	1.328413
28	6	0	-5.595179	4.254398	0.062018
29	1	0	-5.607749	3.803558	-2.032089
30	1	0	-5.906352	4.421903	2.207458
31	6	0	-6.675248	1.943801	-3.459186
32	1	0	-7.309093	1.383939	-4.149584
33	1	0	-7.063369	2.964648	-3.428596
34	1	0	-5.670824	1.985462	-3.901172
35	6	0	-6.550581	-2.329838	3.458181
36	1	0	-5.543546	-2.322923	3.896213
37	1	0	-7.208575	-1.803096	4.151929
38	1	0	-6.887825	-3.368625	3.427021
39	6	0	1.938280	6.742462	2.812162
40	6	0	0.598586	6.866168	2.997344
41	6	0	-0.336668	6.758326	1.897437
42	6	0	0.226522	6.735111	0.567333
43	6	0	1.624255	6.604982	0.378421
44	6	0	2.496878	6.494334	1.505509
45	6	0	-1.710202	6.575186	2.079850
46	6	0	-0.617251	6.710833	-0.566829
47	6	0	-2.005081	6.499512	-0.378134
48	6	0	-2.534168	6.308482	0.936009
49	6	0	-2.869748	6.338502	-1.505233

50	6	0	-2.326596	6.619266	-2.811797
51	6	0	-0.996386	6.821078	-2.996810
52	6	0	-0.056495	6.767347	-1.896861
53	6	0	1.325285	6.664246	-2.079586
54	6	0	2.163460	6.445778	-0.935910
55	1	0	2.611597	6.766271	3.665120
56	1	0	-3.000194	6.604158	-3.664753
57	1	0	-0.622517	6.964255	-4.003926
58	6	0	-3.810003	5.704064	1.049371
59	6	0	-4.140743	5.798147	-1.328808
60	1	0	-4.756813	5.639112	-2.208114
61	6	0	-4.572169	5.338119	-0.062539
62	1	0	-4.122674	5.376594	2.031751
63	1	0	0.217102	6.986372	4.004593
64	6	0	3.472303	5.916533	-1.049401
65	6	0	3.797216	6.029252	1.328804
66	6	0	4.254397	5.595166	0.062404
67	1	0	3.803639	5.607849	-2.031720
68	1	0	4.421819	5.906231	2.207867
69	6	0	1.943936	6.675414	-3.458833
70	1	0	1.384099	7.309288	-4.149222
71	1	0	2.964781	7.063536	-3.428186
72	1	0	1.985617	5.671011	-3.900864
73	6	0	-2.329966	6.550398	3.458366
74	1	0	-2.323070	5.543340	3.896345
75	1	0	-1.803250	7.208355	4.152169
76	1	0	-3.368751	6.887645	3.427182
77	6	0	2.326802	-6.619269	-2.811650
78	6	0	0.996606	-6.821083	-2.996760
79	6	0	0.056634	-6.767356	-1.896879
80	6	0	0.617293	-6.710843	-0.566807
81	6	0	2.005108	-6.499522	-0.378010
82	6	0	2.869858	-6.338509	-1.505045
83	6	0	-1.325133	-6.664258	-2.079706
84	6	0	-0.226564	-6.735123	0.567294

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85	6	0	-1.624283	-6.604995	0.378279
86	6	0	-2.163392	-6.445791	-0.936091
87	6	0	-2.496988	-6.494347	1.505303
88	6	0	-1.938486	-6.742475	2.811997
89	6	0	-0.598805	-6.866181	2.997277
90	6	0	0.336529	-6.758339	1.897439
91	6	0	1.710050	-6.575202	2.079952
92	6	0	2.534100	-6.308496	0.936173
93	1	0	3.000462	-6.604157	-3.664556
94	1	0	-2.611865	-6.766283	3.664905
95	1	0	-0.217396	-6.986383	4.004554
96	6	0	-3.472228	-5.916548	-1.049678
97	6	0	-3.797314	-6.029266	1.328503
98	1	0	-4.421982	-5.906246	2.207520
99	6	0	-4.254403	-5.595180	0.062069
100	1	0	-3.803491	-5.607863	-2.032022
101	1	0	0.622810	-6.964258	-4.003904
102	6	0	3.809927	-5.704080	1.049629
103	6	0	4.140840	-5.798154	-1.328526
104	6	0	4.572174	-5.338131	-0.062224
105	1	0	4.122526	-5.376612	2.032033
106	1	0	4.756974	-5.639117	-2.207786
107	6	0	2.329712	-6.550419	3.458514
108	1	0	2.322783	-5.543364	3.896498
109	1	0	1.802946	-7.208380	4.152275
110	1	0	3.368500	-6.887666	3.427406
111	6	0	-1.943682	-6.675430	-3.458999
112	1	0	-2.964531	-7.063544	-3.428426
113	1	0	-1.985321	-5.671030	-3.901040
114	1	0	-1.383798	-7.309314	-4.149341
115	6	0	6.742406	-1.938407	2.812294
116	6	0	6.866107	-0.598721	2.997535
117	6	0	6.758289	0.336579	1.897665
118	6	0	6.735105	-0.226555	0.567537
119	6	0	6.604981	-1.624280	0.378562

120	6	0	6.494309	-2.496951	1.505611
121	6	0	6.575146	1.710106	2.080131
122	6	0	6.710852	0.617266	-0.566590
123	6	0	6.499526	2.005087	-0.377842
124	6	0	6.308466	2.534120	0.936319
125	6	0	6.338540	2.869801	-1.504908
126	6	0	6.619333	2.326706	-2.811489
127	6	0	6.821150	0.996504	-2.996553
128	6	0	6.767395	0.056567	-1.896644
129	6	0	6.664299	-1.325206	-2.079430
130	6	0	6.445807	-2.163430	-0.935795
131	1	0	6.766196	-2.611760	3.665224
132	1	0	6.604243	3.000339	-3.664416
133	1	0	6.964349	0.622676	-4.003682
134	6	0	5.704045	3.809949	1.049721
135	6	0	5.798180	4.140788	-1.328441
136	1	0	5.639162	4.756892	-2.207725
137	6	0	5.338123	4.572162	-0.062165
138	1	0	5.376555	4.122578	2.032108
139	1	0	6.986286	-0.217280	4.004803
140	6	0	5.916565	-3.472269	-1.049353
141	6	0	6.029234	-3.797283	1.328841
142	6	0	5.595176	-4.254411	0.062412
143	1	0	5.607899	-3.803562	-2.031692
144	1	0	5.906194	-4.421926	2.207874
145	6	0	6.675499	-1.943798	-3.458704
146	1	0	7.309394	-1.383934	-4.149053
147	1	0	7.063616	-2.964646	-3.428092
148	1	0	5.671107	-1.985455	-3.900762
149	6	0	6.550330	2.329812	3.458673
150	1	0	5.543264	2.322896	3.896632
151	1	0	7.208274	1.803067	4.152466
152	1	0	6.887577	3.368599	3.427540

Table S2. Cartesian coordinate of 6,12-methyl (*P*)-(11,9)-[4]$CA_{2,8}$.

SCF Done: E(RB3LYP) = -3692.27443644 A.U. after 15 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.247268	-7.907335	2.165271
2	6	0	1.109402	-7.837580	2.176957
3	6	0	1.849217	-7.179213	1.120151
4	6	0	1.098801	-6.803478	-0.056061
5	6	0	-0.315191	-6.904553	-0.076785
6	6	0	-1.022157	-7.343199	1.086846
7	6	0	3.191750	-6.808534	1.247679
8	6	0	1.750363	-6.195937	-1.153897
9	6	0	3.088705	-5.758936	-0.992447
10	6	0	3.778576	-5.964449	0.244858
11	6	0	3.706988	-4.972175	-2.011751
12	6	0	3.036352	-4.858997	-3.282976
13	6	0	1.768242	-5.310383	-3.454776
14	6	0	1.019384	-5.894926	-2.363379
15	6	0	-0.367222	-6.055289	-2.404256
16	6	0	-1.055846	-6.428378	-1.203888
17	1	0	-0.777732	-8.344448	3.007310
18	1	0	3.552162	-4.352216	-4.094346
19	1	0	1.279463	-5.159029	-4.410098
20	6	0	4.939504	-5.189187	0.493231
21	6	0	4.836932	-4.220656	-1.705575
22	1	0	5.193986	-3.515755	-2.448519
23	6	0	5.394764	-4.221999	-0.407578
24	1	0	5.406402	-5.258973	1.468277
25	1	0	1.645964	-8.223608	3.035850
26	6	0	-2.434799	-6.165007	-1.022534
27	6	0	-2.388906	-7.092280	1.198399
28	6	0	-3.082280	-6.376544	0.195277
29	1	0	-2.954006	-5.612220	-1.795220
30	1	0	-2.896449	-7.365039	2.119478

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31	6	0	-1.164839	-5.729458	-3.646208
32	1	0	-0.608179	-5.963006	-4.556123
33	1	0	-2.089620	-6.309944	-3.681409
34	1	0	-1.439411	-4.667356	-3.695710
35	6	0	3.999965	-7.172392	2.472022
36	1	0	3.918872	-6.414682	3.262934
37	1	0	3.679734	-8.123594	2.900908
38	1	0	5.059541	-7.275640	2.225328
39	6	0	-7.630361	0.182570	-2.353240
40	6	0	-7.564894	-1.174171	-2.373876
41	6	0	-7.001764	-1.929277	-1.273744
42	6	0	-6.714700	-1.191548	-0.064675
43	6	0	-6.800486	0.223176	-0.041284
44	6	0	-7.149540	0.944001	-1.226027
45	6	0	-6.641854	-3.276600	-1.379055
46	6	0	-6.216000	-1.859491	1.077037
47	6	0	-5.799956	-3.208533	0.949014
48	6	0	-5.905520	-3.887523	-0.307950
49	6	0	-5.135868	-3.852982	2.036871
50	6	0	-5.117901	-3.186494	3.314665
51	6	0	-5.541139	-1.904110	3.447959
52	6	0	-6.005476	-1.138795	2.311665
53	6	0	-6.138082	0.251254	2.345572
54	6	0	-6.404332	0.951624	1.124103
55	1	0	-7.997751	0.723468	-3.221554
56	1	0	-4.704084	-3.718485	4.167245
57	1	0	-5.461216	-1.420413	4.414380
58	6	0	-5.143904	-5.070006	-0.488515
59	6	0	-4.402409	-5.011972	1.801640
60	1	0	-3.786485	-5.401977	2.605303
61	6	0	-4.295036	-5.562477	0.505868
62	1	0	-5.121835	-5.531868	-1.468878
63	1	0	-7.883155	-1.699731	-3.266692
64	6	0	-6.119932	2.330305	0.974378
65	6	0	-6.896784	2.312485	-1.301479

66	6	0	-6.250718	2.996125	-0.244889
67	1	0	-5.622908	2.836023	1.791953
68	1	0	-7.115172	2.829208	-2.231360
69	6	0	-5.897563	1.035895	3.615047
70	1	0	-4.835463	1.274613	3.759330
71	1	0	-6.448423	1.979058	3.604273
72	1	0	-6.228533	0.485896	4.498462
73	6	0	-6.908531	-4.071351	-2.636942
74	1	0	-7.053949	-5.129870	-2.407775
75	1	0	-7.810172	-3.730395	-3.148732
76	1	0	-6.080328	-4.001479	-3.354877
77	6	0	6.702240	3.832912	-2.146601
78	6	0	7.224884	2.589047	-2.304585
79	6	0	7.078803	1.564558	-1.291315
80	6	0	6.547861	1.988445	-0.015844
81	6	0	6.030620	3.297298	0.155683
82	6	0	5.989264	4.205611	-0.949069
83	6	0	7.322610	0.209751	-1.538241
84	6	0	6.410643	1.061641	1.043218
85	6	0	6.587239	-0.317267	0.766639
86	6	0	6.938370	-0.758095	-0.549214
87	6	0	6.267114	-1.288903	1.763509
88	6	0	6.009794	-0.826672	3.104485
89	6	0	5.879953	0.495002	3.383228
90	6	0	5.959523	1.498813	2.344355
91	6	0	5.513594	2.809321	2.529651
92	6	0	5.418586	3.675320	1.391856
93	1	0	6.767957	4.557973	-2.953733
94	1	0	5.868886	-1.567880	3.886759
95	1	0	5.635577	0.798719	4.394388
96	6	0	6.732797	-2.124216	-0.868100
97	6	0	6.060317	-2.612720	1.388368
98	1	0	5.667984	-3.296040	2.133687
99	6	0	6.168506	-3.023647	0.041221
100	1	0	6.896815	-2.445488	-1.889606

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101	1	0	7.703463	2.338403	-3.244173
102	6	0	4.584710	4.819426	1.392933
103	6	0	5.176091	5.335626	-0.883079
104	6	0	4.362774	5.582635	0.246521
105	1	0	3.965213	4.999415	2.262391
106	1	0	5.100408	5.978519	-1.755689
107	6	0	5.022673	3.295798	3.873948
108	1	0	3.954633	3.089884	4.024787
109	1	0	5.563485	2.823951	4.696676
110	1	0	5.166305	4.373960	3.976340
111	6	0	7.867242	-0.268309	-2.864467
112	1	0	8.457819	-1.179146	-2.738512
113	1	0	7.068882	-0.491511	-3.584909
114	1	0	8.522005	0.473022	-3.325812
115	6	0	0.323595	7.413312	2.492231
116	6	0	-1.029850	7.313481	2.547651
117	6	0	-1.809414	6.847030	1.419575
118	6	0	-1.105737	6.698344	0.165553
119	6	0	0.304607	6.831081	0.104812
120	6	0	1.057406	7.074884	1.297198
121	6	0	-3.146062	6.450851	1.529086
122	6	0	-1.798394	6.288492	-0.997079
123	6	0	-3.130564	5.821139	-0.866266
124	6	0	-3.775370	5.802960	0.412116
125	6	0	-3.790352	5.231186	-1.986968
126	6	0	-3.165090	5.342512	-3.280469
127	6	0	-1.903845	5.824558	-3.416351
128	6	0	-1.116389	6.218556	-2.268807
129	6	0	0.265088	6.414334	-2.337581
130	6	0	1.001117	6.587445	-1.120699
131	1	0	0.885127	7.702276	3.376932
132	1	0	-3.710506	4.982619	-4.148916
133	1	0	-1.451004	5.845319	-4.400617
134	6	0	-4.941599	5.010657	0.556476
135	6	0	-4.923795	4.449529	-1.782479

136	1	0	-5.318636	3.894591	-2.626676
137	6	0	-5.444352	4.230219	-0.488640
138	1	0	-5.381584	4.911501	1.541472
139	1	0	-1.531401	7.525706	3.484581
140	6	0	2.395656	6.351228	-1.051989
141	6	0	2.434251	6.859193	1.300936
142	6	0	3.097670	6.368233	0.153074
143	1	0	2.894495	5.973770	-1.935554
144	1	0	2.981492	6.982423	2.231438
145	6	0	1.009969	6.333703	-3.650477
146	1	0	0.408010	6.709740	-4.480149
147	1	0	1.921515	6.935017	-3.622056
148	1	0	1.301473	5.304577	-3.898950
149	6	0	-3.909178	6.579382	2.827557
150	1	0	-3.835961	5.671813	3.441728
151	1	0	-3.547075	7.411157	3.433707
152	1	0	-4.970536	6.761255	2.640076

Table S3. Cartesian coordinates of 6,12-methyl 2,2'-bianthanthrenyl (dihedral angle = 0°).

SCF Done: E(RPM6) = 0.240258928185 A.U. after 23 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.304744	-2.866164	0.167215
2	6	0	-4.643881	-3.028504	0.168004
3	6	0	-5.566688	-1.896917	0.099311
4	6	0	-4.988646	-0.571089	0.029127
5	6	0	-3.562018	-0.400425	0.025643
6	6	0	-2.697137	-1.541957	0.094517
7	6	0	-6.941361	-2.064011	0.101589
8	6	0	-5.816965	0.559849	-0.034709
9	6	0	-7.244627	0.389393	-0.032189
10	6	0	-7.810784	-0.911259	0.034698

11	6	0	-8.105849	1.535547	-0.096980
12	6	0	-7.495999	2.858085	-0.163655
13	6	0	-6.156742	3.018680	-0.165081
14	6	0	-5.236080	1.884849	-0.101014
15	6	0	-3.861254	2.051360	-0.102222
16	6	0	-2.991964	0.897233	-0.039268
17	1	0	-2.630362	-3.720519	0.219546
18	1	0	-5.077265	-4.027984	0.221928
19	1	0	-8.169662	3.713629	-0.211990
20	1	0	-5.721896	4.017542	-0.215161
21	6	0	-9.228655	-1.033264	0.034447
22	6	0	-10.043530	0.078709	-0.028881
23	1	0	-11.127302	-0.031280	-0.028139
24	6	0	-9.484907	1.372705	-0.094992
25	1	0	-10.145147	2.236691	-0.143937
26	6	0	-1.320583	-1.378905	0.093411
27	6	0	-0.737241	-0.086737	0.008093
28	6	0	-1.577081	1.018704	-0.038246
29	1	0	-0.670827	-2.253496	0.154141
30	1	0	-1.148944	2.027111	-0.080367
31	1	0	-9.668894	-2.032314	0.085893
32	6	0	-7.541265	-3.433703	0.173548
33	1	0	-7.229543	-4.050854	-0.682003
34	1	0	-7.238040	-3.953831	1.094160
35	1	0	-8.642243	-3.423337	0.167727
36	6	0	-3.261507	3.421425	-0.169681
37	1	0	-3.564751	3.944223	-1.088796
38	1	0	-3.573519	4.035539	0.687972
39	1	0	-2.160638	3.410713	-0.163706
40	6	0	0.737244	0.070598	0.053322
41	6	0	1.580201	-1.030609	-0.028230
42	6	0	1.316515	1.366385	0.100064
43	6	0	2.994710	-0.904866	-0.030083
44	1	0	1.154982	-2.039365	-0.089387
45	6	0	2.692574	1.533568	0.100917

46	1	0	0.664038	2.240020	0.140476
47	6	0	3.867409	-2.056019	-0.100576
48	6	0	3.560895	0.394353	0.037692
49	6	0	3.296162	2.860090	0.163297
50	6	0	5.241730	-1.885396	-0.099363
51	6	0	3.271735	-3.427617	-0.173258
52	6	0	4.986981	0.569512	0.036493
53	6	0	4.634811	3.026398	0.164844
54	1	0	2.619199	3.712693	0.210093
55	6	0	6.165760	-3.016285	-0.167155
56	6	0	5.818664	-0.558804	-0.030165
57	1	0	3.575293	-3.945438	-1.095115
58	1	0	3.586800	-4.044576	0.681257
59	1	0	2.170847	-3.420276	-0.165707
60	6	0	5.561029	1.897296	0.101923
61	1	0	5.065173	4.027446	0.213130
62	6	0	7.504528	-2.851655	-0.166343
63	1	0	5.733894	-4.016343	-0.219309
64	6	0	7.245796	-0.383944	-0.030399
65	6	0	6.935186	2.068602	0.102156
66	6	0	8.110427	-1.527375	-0.098068
67	1	0	8.180733	-3.705053	-0.217259
68	6	0	7.808056	0.918432	0.035763
69	6	0	7.530970	3.440271	0.170249
70	6	0	9.488982	-1.360315	-0.098003
71	6	0	9.225543	1.044790	0.033215
72	1	0	7.215982	4.054640	-0.686093
73	1	0	7.227603	3.961406	1.090239
74	1	0	8.631965	3.433285	0.162672
75	6	0	10.043733	-0.064662	-0.031707
76	1	0	10.151793	-2.222222	-0.148995
77	1	0	9.662787	2.045191	0.083872
78	1	0	11.127161	0.048657	-0.032776

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Table S4. Cartesian coordinates of 6,12-methyl 2,2'-bianthanthrenyl (dihedral angle = 60°).

SCF Done: E(RPM6) = 0.236594695853 A.U. after 28 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.416356	-2.424224	1.682018
2	6	0	-4.760608	-2.534770	1.691487
3	6	0	-5.626559	-1.569527	1.016993
4	6	0	-4.986246	-0.469265	0.326377
5	6	0	-3.553420	-0.353310	0.315330
6	6	0	-2.746351	-1.328609	0.991078
7	6	0	-7.006618	-1.684216	1.028461
8	6	0	-5.760712	0.494949	-0.337127
9	6	0	-7.193943	0.378572	-0.326831
10	6	0	-7.820342	-0.701871	0.349124
11	6	0	-8.000193	1.356066	-1.000780
12	6	0	-7.330115	2.454894	-1.685656
13	6	0	-5.985848	2.565330	-1.695166
14	6	0	-5.120098	1.596974	-1.024570
15	6	0	-3.740147	1.712561	-1.035099
16	6	0	-2.926481	0.728593	-0.357184
17	1	0	-2.783549	-3.151003	2.191396
18	1	0	-5.241333	-3.362593	2.214300
19	1	0	-7.962666	3.185041	-2.190398
20	1	0	-5.504797	3.395675	-2.213462
21	6	0	-9.241384	-0.778178	0.333695
22	6	0	-10.002720	0.169568	-0.319358
23	1	0	-11.089654	0.097342	-0.322046
24	6	0	-9.384377	1.244869	-0.991908
25	1	0	-10.002841	1.982024	-1.500647
26	6	0	-1.363323	-1.220814	0.982504
27	6	0	-0.738780	-0.150693	0.296543
28	6	0	-1.507491	0.809496	-0.339743
29	1	0	-0.744943	-1.950616	1.503536

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30	1	0	-1.021252	1.644737	-0.851989
31	1	0	-9.727513	-1.608081	0.852879
32	6	0	-7.669934	-2.821138	1.741849
33	1	0	-7.354785	-3.790105	1.327408
34	1	0	-7.424760	-2.816086	2.814179
35	1	0	-8.768351	-2.792549	1.671581
36	6	0	-3.076491	2.850651	-1.745977
37	1	0	-3.332367	2.856704	-2.815755
38	1	0	-3.379774	3.818175	-1.319841
39	1	0	-1.977193	2.812878	-1.688816
40	6	0	0.737585	-0.025523	0.335413
41	6	0	1.536422	-0.937289	-0.334485
42	6	0	1.323792	1.079890	0.998486
43	6	0	2.952004	-0.809775	-0.349399
44	1	0	1.077663	-1.774584	-0.868344
45	6	0	2.702570	1.232490	1.010402
46	1	0	0.679906	1.796115	1.507219
47	6	0	3.797957	-1.758083	-1.038671
48	6	0	3.542421	0.285625	0.334056
49	6	0	3.334887	2.349725	1.702025
50	6	0	5.173406	-1.597804	-1.024883
51	6	0	3.172596	-2.909407	-1.762746
52	6	0	4.970438	0.450392	0.344815
53	6	0	4.674861	2.503305	1.715463
54	1	0	2.677616	3.054889	2.210848
55	6	0	6.071116	-2.530757	-1.703747
56	6	0	5.776828	-0.481978	-0.326265
57	1	0	3.428735	-2.894755	-2.832442
58	1	0	3.507755	-3.871146	-1.347526
59	1	0	2.072642	-2.908794	-1.705607
60	6	0	5.573207	1.568433	1.040478
61	1	0	5.127220	3.345504	2.240472
62	6	0	7.411030	-2.376477	-1.691527
63	1	0	5.618088	-3.371447	-2.230462
64	6	0	7.205351	-0.317747	-0.314783

65	6	0	6.948675	1.728832	1.053648
66	6	0	8.043942	-1.262216	-0.996441
67	1	0	8.067703	-3.080717	-2.202350
68	6	0	7.795094	0.778024	0.369280
69	6	0	7.573273	2.883585	1.773146
70	6	0	9.423660	-1.105170	-0.985856
71	6	0	9.212791	0.901775	0.355074
72	1	0	7.226081	3.843585	1.363547
73	1	0	7.327930	2.864804	2.845316
74	1	0	8.672057	2.892095	1.703227
75	6	0	10.005570	-0.015248	-0.304534
76	1	0	10.066517	-1.817141	-1.500298
77	1	0	9.670750	1.743759	0.880271
78	1	0	11.089482	0.093221	-0.306222

Table S5. Cartesian coordinates of 6,12-methyl 2,2'-bianthanthrenyl (dihedral angle = 90°).

SCF Done: E(RPM6) = 0.236731379916 A.U. after 19 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.490820	2.320238	1.899905
2	6	0	-4.837574	2.336325	1.972832
3	6	0	-5.670184	1.407087	1.211402
4	6	0	-4.993400	0.450954	0.359653
5	6	0	-3.557817	0.432740	0.284571
6	6	0	-2.784506	1.366085	1.052984
7	6	0	-7.052864	1.425822	1.286852
8	6	0	-5.734879	-0.465895	-0.401467
9	6	0	-7.170817	-0.448629	-0.325423
10	6	0	-7.832915	0.487951	0.511920
11	6	0	-7.943579	-1.379539	-1.097343
12	6	0	-7.237319	-2.328585	-1.949434
13	6	0	-5.890529	-2.344843	-2.022230

14	6	0	-5.058028	-1.419050	-1.256309
15	6	0	-3.675353	-1.437419	-1.332642
16	6	0	-2.895489	-0.502476	-0.553580
17	1	0	-2.882857	3.020199	2.473213
18	1	0	-5.345756	3.058109	2.613567
19	1	0	-7.844860	-3.025422	-2.526716
20	1	0	-5.382045	-3.063021	-2.666630
21	6	0	-9.255245	0.469452	0.557149
22	6	0	-9.984138	-0.432634	-0.190704
23	1	0	-11.072534	-0.434253	-0.145221
24	6	0	-9.330299	-1.364471	-1.024442
25	1	0	-9.923467	-2.067202	-1.606650
26	6	0	-1.398950	1.353021	0.982482
27	6	0	-0.741317	0.405198	0.162286
28	6	0	-1.474467	-0.486715	-0.600167
29	1	0	-0.803866	2.062864	1.555584
30	1	0	-0.959545	-1.199436	-1.250632
31	1	0	-9.768781	1.188715	1.200267
32	6	0	-7.753809	2.413389	2.167176
33	1	0	-7.460733	2.287350	3.219930
34	1	0	-7.519359	3.446843	1.872266
35	1	0	-8.850290	2.319161	2.133706
36	6	0	-2.974111	-2.420775	-2.217127
37	1	0	-3.208066	-3.455730	-1.927702
38	1	0	-3.265710	-2.289323	-3.269563
39	1	0	-1.877178	-2.326616	-2.182616
40	6	0	0.738940	0.436033	0.065127
41	6	0	1.507212	-0.448292	0.801834
42	6	0	1.352339	1.326396	-0.847954
43	6	0	2.924620	-0.463630	0.690591
44	1	0	1.023994	-1.148770	1.488894
45	6	0	2.733178	1.339253	-0.982121
46	1	0	0.727797	1.999082	-1.434357
47	6	0	3.742295	-1.371285	1.463381
48	6	0	3.544629	0.441643	-0.210304

49	6	0	3.395847	2.254320	-1.903875
50	6	0	5.119956	-1.353242	1.323407
51	6	0	3.085542	-2.324430	2.412566
52	6	0	4.974924	0.456511	-0.354782
53	6	0	4.737844	2.270622	-2.038196
54	1	0	2.759377	2.926720	-2.479336
55	6	0	5.989805	-2.249637	2.083001
56	6	0	5.753658	-0.430677	0.404494
57	1	0	3.309178	-3.368495	2.148520
58	1	0	3.424802	-2.156276	3.445316
59	1	0	1.987904	-2.232968	2.425361
60	6	0	5.608198	1.377043	-1.276142
61	1	0	5.213171	2.964234	-2.732808
62	6	0	7.331748	-2.234169	1.947717
63	1	0	5.513851	-2.944631	2.775727
64	6	0	7.184376	-0.415507	0.260435
65	6	0	6.985795	1.394131	-1.416688
66	6	0	7.994898	-1.316346	1.029531
67	1	0	7.967455	-2.908873	2.521119
68	6	0	7.803984	0.488789	-0.642191
69	6	0	7.641812	2.345679	-2.368246
70	6	0	9.376658	-1.302716	0.891612
71	6	0	9.222702	0.469760	-0.753071
72	1	0	7.299609	2.177220	-3.399998
73	1	0	7.418930	3.390085	-2.104365
74	1	0	8.738881	2.253354	-2.382958
75	6	0	9.988263	-0.402388	-0.006162
76	1	0	9.998301	-1.982683	1.471304
77	1	0	9.703589	1.164059	-1.446727
78	1	0	11.073341	-0.404828	-0.102334

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Table S6. Cartesian coordinates of 6,12-methyl 2,2'-bianthanthrenyl (dihedral angle = 120°).

SCF Done: E(RPM6) = 0.236685025642 A.U. after 19 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.553558	2.736688	-1.333434
2	6	0	4.901909	2.752407	-1.366265
3	6	0	5.707181	1.657717	-0.828086
4	6	0	5.000818	0.534381	-0.247583
5	6	0	3.563722	0.516786	-0.216481
6	6	0	2.817786	1.616879	-0.757582
7	6	0	7.091524	1.676170	-0.861510
8	6	0	5.714871	-0.547162	0.290968
9	6	0	7.152460	-0.530545	0.258232
10	6	0	7.843667	0.570347	-0.313686
11	6	0	7.897383	-1.628524	0.805034
12	6	0	7.161503	-2.744177	1.387634
13	6	0	5.813103	-2.760007	1.420051
14	6	0	5.008217	-1.667894	0.875800
15	6	0	3.623838	-1.686323	0.909652
16	6	0	2.871910	-0.583755	0.354396
17	1	0	2.966342	3.560649	-1.738887
18	1	0	5.432287	3.599532	-1.803178
19	1	0	7.748223	-3.566257	1.797355
20	1	0	5.282310	-3.604358	1.861515
21	6	0	9.266542	0.544911	-0.325626
22	6	0	9.968524	-0.518845	0.203519
23	1	0	11.057753	-0.523417	0.186972
24	6	0	9.285714	-1.614242	0.773450
25	1	0	9.857901	-2.443126	1.185993
26	6	0	1.431001	1.605545	-0.726649
27	6	0	0.741846	0.495272	-0.180117
28	6	0	1.450512	-0.563453	0.362430
29	1	0	0.858115	2.439034	-1.131234

30	1	0	0.914652	-1.404385	0.811829
31	1	0	9.802466	1.390161	-0.765005
32	6	0	7.823101	2.836301	-1.461991
33	1	0	7.558847	2.968900	-2.521567
34	1	0	7.586998	3.772426	-0.934817
35	1	0	8.917617	2.722843	-1.423838
36	6	0	2.892083	-2.842069	1.518055
37	1	0	3.116436	-3.779551	0.988709
38	1	0	3.166471	-2.975958	2.574933
39	1	0	1.797638	-2.720931	1.493631
40	6	0	-0.738761	0.518700	-0.117819
41	6	0	-1.478469	-0.550014	-0.596345
42	6	0	-1.389548	1.607829	0.511253
43	6	0	-2.897171	-0.566788	-0.507493
44	1	0	-0.970575	-1.397283	-1.065799
45	6	0	-2.772223	1.622466	0.621131
46	1	0	-0.790648	2.427027	0.907359
47	6	0	-3.682760	-1.665786	-1.022218
48	6	0	-3.551814	0.531880	0.108684
49	6	0	-3.469559	2.734236	1.256776
50	6	0	-5.062893	-1.643879	-0.909738
51	6	0	-2.990437	-2.820438	-1.676752
52	6	0	-4.984445	0.550949	0.225513
53	6	0	-4.813837	2.753716	1.365449
54	1	0	-2.857062	3.550292	1.640485
55	6	0	-5.900907	-2.730638	-1.413669
56	6	0	-5.731485	-0.525102	-0.278618
57	1	0	-3.187147	-3.759948	-1.139959
58	1	0	-3.325014	-2.948410	-2.716942
59	1	0	-1.896038	-2.702149	-1.714240
60	6	0	-5.652508	1.668786	0.859117
61	1	0	-5.315252	3.595723	1.844114
62	6	0	-7.245188	-2.711590	-1.304336
63	1	0	-5.398826	-3.573547	-1.889850
64	6	0	-7.164651	-0.506036	-0.161982

65	6	0	-7.032496	1.689793	0.972940
66	6	0	-7.943036	-1.598329	-0.672804
67	1	0	-7.856902	-3.529558	-1.685042
68	6	0	-7.818402	0.591305	0.458369
69	6	0	-7.724481	2.844644	1.627626
70	6	0	-9.327150	-1.581295	-0.560956
71	6	0	-9.238246	0.568765	0.552460
72	1	0	-7.398115	2.965399	2.671177
73	1	0	-7.517287	3.785957	1.097455
74	1	0	-8.819621	2.733463	1.652675
75	6	0	-9.972715	-0.489001	0.056029
76	1	0	-9.924574	-2.405796	-0.945903
77	1	0	-9.745387	1.411269	1.029384
78	1	0	-11.059142	-0.491486	0.135694

Table S7. Cartesian coordinates of 6,12-methyl 2,2'-bianthanthrenyl (dihedral angle = 180°).

SCF Done: E(RPM6) = 0.240077140934 A.U. after 10 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.587416	3.074210	0.000002
2	6	0	-4.936143	3.094177	0.000043
3	6	0	-5.734255	1.869655	-0.000039
4	6	0	-5.019469	0.610373	-0.000053
5	6	0	-3.582807	0.591028	-0.000104
6	6	0	-2.843295	1.819683	-0.000059
7	6	0	-7.118842	1.890814	-0.000078
8	6	0	-5.723911	-0.603201	-0.000001
9	6	0	-7.161628	-0.584212	0.000075
10	6	0	-7.861832	0.651101	0.000024
11	6	0	-7.897138	-1.816318	0.000200
12	6	0	-7.151193	-3.068752	0.000297
13	6	0	-5.802466	-3.087243	0.000192

14	6	0	-5.006542	-1.861090	-0.000017
15	6	0	-3.621802	-1.881608	-0.000179
16	6	0	-2.879028	-0.640998	-0.000170
17	1	0	-3.006809	3.996390	0.000019
18	1	0	-5.472666	4.043693	0.000161
19	1	0	-7.730868	-3.991738	0.000476
20	1	0	-5.264812	-4.035888	0.000287
21	6	0	-9.284617	0.622886	0.000053
22	6	0	-9.977702	-0.570379	0.000152
23	1	0	-11.067029	-0.575229	0.000181
24	6	0	-9.285715	-1.799809	0.000238
25	1	0	-9.851120	-2.729803	0.000295
26	6	0	-1.457376	1.803167	-0.000070
27	6	0	-0.741701	0.576996	-0.000130
28	6	0	-1.459063	-0.612383	-0.000203
29	1	0	-0.902933	2.743609	-0.000038
30	1	0	-0.926984	-1.570156	-0.000286
31	1	0	-9.827797	1.571214	-0.000043
32	6	0	-7.859923	3.191347	-0.000001
33	1	0	-7.616100	3.788738	0.890751
34	1	0	-7.612036	3.791478	-0.887770
35	1	0	-8.953650	3.064872	-0.002785
36	6	0	-2.881161	-3.182710	-0.000265
37	1	0	-3.126532	-3.780168	0.890045
38	1	0	-3.129045	-3.781630	-0.888880
39	1	0	-1.787843	-3.055747	-0.001924
40	6	0	0.741704	0.576998	-0.000151
41	6	0	1.459078	-0.612378	-0.000234
42	6	0	1.457369	1.803169	-0.000033
43	6	0	2.879036	-0.640997	-0.000178
44	1	0	0.926979	-1.570147	-0.000396
45	6	0	2.843294	1.819681	0.000013
46	1	0	0.902948	2.743619	0.000013
47	6	0	3.621802	-1.881611	-0.000220
48	6	0	3.582809	0.591032	-0.000083

49	6	0	3.587418	3.074205	0.000152
50	6	0	5.006541	-1.861088	-0.000103
51	6	0	2.881149	-3.182709	-0.000219
52	6	0	5.019472	0.610379	-0.000053
53	6	0	4.936145	3.094174	0.000119
54	1	0	3.006810	3.996385	0.000291
55	6	0	5.802468	-3.087236	0.000018
56	6	0	5.723910	-0.603200	-0.000048
57	1	0	3.129407	-3.781948	-0.888513
58	1	0	3.126129	-3.779849	0.890416
59	1	0	1.787834	-3.055732	-0.002447
60	6	0	5.734258	1.869653	-0.000017
61	1	0	5.472661	4.043695	0.000211
62	6	0	7.151191	-3.068747	0.000133
63	1	0	5.264815	-4.035884	0.000024
64	6	0	7.161620	-0.584213	0.000032
65	6	0	7.118850	1.890806	-0.000063
66	6	0	7.897136	-1.816318	0.000143
67	1	0	7.730866	-3.991733	0.000219
68	6	0	7.861825	0.651093	0.000027
69	6	0	7.859942	3.191341	0.000010
70	6	0	9.285701	-1.799812	0.000259
71	6	0	9.284612	0.622878	0.000125
72	1	0	7.612075	3.791476	-0.887753
73	1	0	7.616113	3.788732	0.890770
74	1	0	8.953669	3.064861	-0.002776
75	6	0	9.977693	-0.570379	0.000245
76	1	0	9.851113	-2.729801	0.000367
77	1	0	9.827782	1.571209	0.000093
78	1	0	11.067019	-0.575244	0.000316

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Table S8. Cartesian coordinates of 6,12-TMS*e* 2,2'-bianthanthrenyl (dihedral angle = 0°).

SCF Done: E(RPM6) = 0.319105292949 A.U. after 26 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.042073	1.684567	0.166965
2	6	0	5.364286	1.414797	0.167191
3	6	0	5.874201	0.047879	0.097295
4	6	0	4.911223	-1.028791	0.026683
5	6	0	3.505153	-0.735901	0.024021
6	6	0	3.046116	0.620103	0.093846
7	6	0	7.233996	-0.234017	0.098694
8	6	0	5.344642	-2.363267	-0.038050
9	6	0	6.751697	-2.656320	-0.036338
10	6	0	7.700603	-1.602918	0.030860
11	6	0	7.204916	-4.015770	-0.102153
12	6	0	6.207326	-5.077901	-0.169223
13	6	0	4.885474	-4.806651	-0.170059
14	6	0	4.379217	-3.438433	-0.104785
15	6	0	3.019789	-3.155940	-0.105111
16	6	0	2.554076	-1.785474	-0.041186
17	1	0	3.672057	2.709092	0.220099
18	1	0	6.104590	2.217197	0.221101
19	1	0	6.575197	-6.102936	-0.218350
20	1	0	4.143443	-5.607555	-0.220091
21	6	0	9.085439	-1.924470	0.030582
22	6	0	9.504318	-3.239289	-0.033879
23	1	0	10.567559	-3.477350	-0.033594
24	6	0	8.566597	-4.291783	-0.100459
25	1	0	8.922456	-5.319426	-0.150119
26	6	0	1.686713	0.894792	0.092944
27	6	0	0.727047	-0.149215	0.007218
28	6	0	1.172506	-1.465418	-0.040123
29	1	0	1.342374	1.930375	0.154312

30	1	0	0.449503	-2.286732	-0.082532
31	1	0	9.816677	-1.115593	0.082331
32	6	0	2.055048	-4.193659	-0.168937
33	6	0	1.215000	-5.069965	-0.222756
34	6	0	8.192859	0.809249	0.166968
35	6	0	9.015029	1.702104	0.225287
36	14	0	-0.071981	-6.353033	-0.301881
37	14	0	10.250338	3.035274	0.312306
38	6	0	0.119712	-7.465076	1.180024
39	1	0	-0.645140	-8.255635	1.189921
40	1	0	1.107284	-7.951610	1.186113
41	1	0	0.024842	-6.892510	2.116430
42	6	0	0.152505	-7.309041	-1.884609
43	1	0	-0.614360	-8.090133	-1.993675
44	1	0	0.082381	-6.643343	-2.759623
45	1	0	1.138398	-7.797950	-1.916640
46	6	0	-1.727061	-5.493097	-0.275848
47	1	0	-1.849786	-4.901811	0.644505
48	1	0	-1.831663	-4.812950	-1.135030
49	1	0	-2.550908	-6.220995	-0.320605
50	6	0	9.974461	3.976676	1.895985
51	1	0	10.704115	4.792207	2.008821
52	1	0	8.967014	4.419371	1.925186
53	1	0	10.072412	3.313421	2.770066
54	6	0	10.012710	4.141198	-1.167855
55	1	0	10.743498	4.963466	-1.174221
56	1	0	10.133823	3.575331	-2.105210
57	1	0	9.005519	4.585383	-1.174864
58	6	0	11.942480	2.255541	0.291596
59	1	0	12.075627	1.576176	1.147791
60	1	0	12.097663	1.671208	-0.628621
61	1	0	12.733021	3.019096	0.342255
62	6	0	-0.721976	0.164742	0.052976
63	6	0	-1.678877	-0.884046	0.099605
64	6	0	-1.171770	1.477967	-0.028147

65	6	0	-3.039100	-0.613446	0.101177
66	1	0	-1.331623	-1.919610	0.139504
67	6	0	-2.554301	1.793849	-0.028909
68	1	0	-0.451450	2.300580	-0.089021
69	6	0	-4.031939	-1.681446	0.163408
70	6	0	-3.502169	0.741508	0.038598
71	6	0	-3.024226	3.162612	-0.098740
72	6	0	-5.354946	-1.415601	0.165355
73	1	0	-3.658891	-2.705169	0.209776
74	6	0	-4.909158	1.029961	0.037632
75	6	0	-4.384493	3.441035	-0.097351
76	6	0	-2.062676	4.203049	-0.166732
77	6	0	-5.868924	-0.049878	0.102892
78	1	0	-6.092878	-2.220531	0.213235
79	6	0	-5.346631	2.363059	-0.028320
80	6	0	-4.894915	4.807615	-0.164643
81	6	0	-1.225340	5.081706	-0.224691
82	6	0	-7.229578	0.227846	0.103281
83	6	0	-6.754586	2.651764	-0.028318
84	6	0	-6.217578	5.074875	-0.163436
85	1	0	-4.155331	5.610686	-0.216284
86	14	0	0.057601	6.368415	-0.310669
87	6	0	-7.700309	1.595429	0.037571
88	6	0	-8.185320	-0.818526	0.167251
89	6	0	-7.211935	4.009774	-0.095358
90	1	0	-6.588568	6.098727	-0.213877
91	6	0	-0.135715	7.486005	1.166882
92	6	0	-0.171729	7.317188	-1.897101
93	6	0	1.715347	5.513676	-0.282969
94	6	0	-9.086127	1.912723	0.036055
95	6	0	-9.004780	-1.714067	0.222147
96	6	0	-8.574456	4.281615	-0.094581
97	1	0	0.626724	8.278956	1.172593
98	1	0	-1.124766	7.969537	1.172142
99	1	0	-0.037967	6.917600	2.105553

100	1	0	0.592598	8.100198	-2.010318
101	1	0	-0.100608	6.648083	-2.769455
102	1	0	-1.159161	7.802927	-1.929973
103	1	0	1.840953	4.926593	0.639713
104	1	0	1.821043	4.830272	-1.139451
105	1	0	2.536902	6.243928	-0.331706
106	6	0	-9.508988	3.226264	-0.028421
107	1	0	-9.814922	1.101575	0.086572
108	14	0	-10.235886	-3.051394	0.304356
109	1	0	-8.933436	5.308137	-0.145034
110	1	0	-10.572956	3.461054	-0.029144
111	6	0	-9.959001	-3.995699	1.886113
112	6	0	-9.992802	-4.152972	-1.178122
113	6	0	-11.930506	-2.277068	0.283265
114	1	0	-10.686163	-4.813832	1.996040
115	1	0	-8.950171	-4.435217	1.915565
116	1	0	-10.060210	-3.334875	2.761641
117	1	0	-10.720924	-4.977558	-1.187413
118	1	0	-10.114539	-3.585251	-2.114263
119	1	0	-8.984176	-4.593894	-1.184884
120	1	0	-12.066955	-1.600187	1.140886
121	1	0	-12.086381	-1.691050	-0.635752
122	1	0	-12.718642	-3.043271	0.331063

Table S9. Cartesian coordinates of 6,12-TMS*e* 2,2'-bianthanthrenyl (dihedral angle = 60°).

SCF Done: E(RPM6) = 0.316313373964 A.U. after 20 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.889899	1.529165	1.693738
2	6	0	5.222564	1.318444	1.705192
3	6	0	5.830521	0.186266	1.011612
4	6	0	4.955624	-0.719860	0.300575

5	6	0	3.536994	-0.490790	0.289204
6	6	0	2.981927	0.635021	0.983150
7	6	0	7.201717	-0.033517	1.022788
8	6	0	5.488556	-1.827327	-0.379503
9	6	0	6.907694	-2.056253	-0.368880
10	6	0	7.769536	-1.168294	0.326165
11	6	0	7.461641	-3.184263	-1.060611
12	6	0	6.552877	-4.081149	-1.765697
13	6	0	5.220182	-3.870091	-1.777097
14	6	0	4.613045	-2.735198	-1.087166
15	6	0	3.241485	-2.516483	-1.097126
16	6	0	2.673888	-1.379773	-0.402549
17	1	0	3.445190	2.376738	2.215754
18	1	0	5.896883	1.992828	2.239354
19	1	0	6.996183	-4.931463	-2.284033
20	1	0	4.545028	-4.546792	-2.307326
21	6	0	9.168609	-1.420687	0.318620
22	6	0	9.684802	-2.511656	-0.353319
23	1	0	10.758255	-2.698281	-0.354324
24	6	0	8.834273	-3.399173	-1.046322
25	1	0	9.265664	-4.251791	-1.567797
26	6	0	1.611257	0.852206	0.970880
27	6	0	0.754918	-0.028348	0.265005
28	6	0	1.275731	-1.132349	-0.392291
29	1	0	1.178332	1.699031	1.502984
30	1	0	0.610547	-1.819307	-0.920781
31	1	0	9.832468	-0.738558	0.853032
32	6	0	2.370739	-3.398047	-1.787416
33	6	0	1.626534	-4.153922	-2.380179
34	6	0	8.073548	0.845536	1.715423
35	6	0	8.821018	1.597899	2.308577
36	14	0	0.508315	-5.281605	-3.269369
37	14	0	9.943605	2.721503	3.196179
38	6	0	1.332019	-6.950642	-3.367929
39	1	0	0.689472	-7.680582	-3.882476

40	1	0	2.283110	-6.892401	-3.918545
41	1	0	1.549287	-7.343089	-2.362277
42	6	0	0.218231	-4.583315	-4.971310
43	1	0	-0.452670	-5.226242	-5.560019
44	1	0	-0.240274	-3.583147	-4.912420
45	1	0	1.163654	-4.483275	-5.526639
46	6	0	-1.086711	-5.385215	-2.313123
47	1	0	-0.913895	-5.759904	-1.292366
48	1	0	-1.562108	-4.394879	-2.230222
49	1	0	-1.803605	-6.060567	-2.803348
50	6	0	9.464340	2.714888	4.996206
51	1	0	10.119716	3.371682	5.587257
52	1	0	8.428342	3.061217	5.132991
53	1	0	9.534739	1.699934	5.418546
54	6	0	9.754560	4.424487	2.464949
55	1	0	10.421397	5.147461	2.957767
56	1	0	9.996553	4.420592	1.390391
57	1	0	8.722013	4.790698	2.572613
58	6	0	11.683733	2.094047	2.971987
59	1	0	11.791525	1.074889	3.374486
60	1	0	11.960022	2.065857	1.906608
61	1	0	12.409004	2.738727	3.490539
62	6	0	-0.709600	0.195753	0.312383
63	6	0	-1.533672	-0.758147	0.958388
64	6	0	-1.274383	1.285775	-0.332275
65	6	0	-2.910790	-0.588042	0.986112
66	1	0	-1.070196	-1.618539	1.440707
67	6	0	-2.680122	1.485777	-0.326043
68	1	0	-0.637876	2.003432	-0.855403
69	6	0	-3.784054	-1.542472	1.660767
70	6	0	-3.507760	0.545490	0.340875
71	6	0	-3.291049	2.622878	-0.982513
72	6	0	-5.122864	-1.376912	1.688118
73	1	0	-3.307941	-2.395599	2.144827
74	6	0	-4.933540	0.723646	0.364761

75	6	0	-4.669066	2.794773	-0.956673
76	6	0	-2.455676	3.554934	-1.649828
77	6	0	-5.772873	-0.238767	1.043948
78	1	0	-5.770849	-2.095210	2.196968
79	6	0	-5.508357	1.834686	-0.274465
80	6	0	-5.319117	3.930592	-1.605059
81	6	0	-1.741843	4.353744	-2.223352
82	6	0	-7.150725	-0.066888	1.069271
83	6	0	-6.934487	2.013711	-0.249696
84	6	0	-6.658077	4.095763	-1.578856
85	1	0	-4.670992	4.647124	-2.116351
86	14	0	-0.669531	5.545684	-3.084890
87	6	0	-7.761164	1.072558	0.417487
88	6	0	-7.987949	-1.000975	1.731870
89	6	0	-7.531092	3.144953	-0.899739
90	1	0	-7.133536	4.947308	-2.065976
91	6	0	-1.554256	7.185550	-3.135098
92	6	0	-0.361300	4.905087	-4.806299
93	6	0	0.924710	5.681811	-2.131038
94	6	0	-9.168127	1.276605	0.425232
95	6	0	-8.705783	-1.800343	2.299561
96	6	0	-8.910172	3.311859	-0.871359
97	1	0	-0.941221	7.952306	-3.631856
98	1	0	-2.505113	7.107363	-3.683865
99	1	0	-1.781098	7.542423	-2.118337
100	1	0	0.283073	5.588079	-5.379331
101	1	0	0.133782	3.921112	-4.776189
102	1	0	-1.304788	4.785539	-5.361288
103	1	0	0.742559	6.021748	-1.099743
104	1	0	1.436555	4.707689	-2.076929
105	1	0	1.614178	6.396404	-2.604704
106	6	0	-9.725504	2.372068	-0.205495
107	1	0	-9.804977	0.553417	0.938076
108	14	0	-9.784085	-2.994276	3.149395
109	1	0	-9.373786	4.166500	-1.361140

110	1	0	-10.804736	2.521421	-0.195072
111	6	0	-9.295072	-3.038033	4.946431
112	6	0	-9.540878	-4.661473	2.354311
113	6	0	-11.545996	-2.419333	2.956050
114	1	0	-9.924117	-3.738602	5.515379
115	1	0	-8.247013	-3.353271	5.065768
116	1	0	-9.397866	-2.042459	5.406670
117	1	0	-10.179735	-5.424845	2.822645
118	1	0	-9.788964	-4.625973	1.281637
119	1	0	-8.495783	-4.995674	2.443865
120	1	0	-11.686518	-1.420114	3.396744
121	1	0	-11.829052	-2.361137	1.893573
122	1	0	-12.245761	-3.107540	3.453222

Table S10. Cartesian coordinates of 6,12-TMS*e* 2,2'-bianthanthrenyl (dihedral angle = 90°).

SCF Done: E(RPM6) = 0.316535703812 A.U. after 38 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.776935	-2.135946	-1.507677
2	6	0	-5.116240	-2.166768	-1.347014
3	6	0	-5.793712	-1.333899	-0.357174
4	6	0	-4.981632	-0.460114	0.460838
5	6	0	-3.555678	-0.427973	0.284694
6	6	0	-2.931277	-1.263691	-0.699808
7	6	0	-7.171856	-1.365057	-0.188788
8	6	0	-5.582982	0.358605	1.430895
9	6	0	-7.009424	0.327227	1.606783
10	6	0	-7.809698	-0.527345	0.804567
11	6	0	-7.632906	1.159369	2.594937
12	6	0	-6.786500	2.026761	3.406468
13	6	0	-5.447198	2.058187	3.244996
14	6	0	-4.770454	1.229182	2.251404

15	6	0	-3.391941	1.259918	2.083797
16	6	0	-2.754588	0.425147	1.087267
17	1	0	-3.280053	-2.761994	-2.249164
18	1	0	-5.743748	-2.822127	-1.956581
19	1	0	-7.282042	2.649719	4.151118
20	1	0	-4.818930	2.710339	3.857337
21	6	0	-9.217642	-0.536351	1.001423
22	6	0	-9.801231	0.272236	1.957318
23	1	0	-10.881046	0.259537	2.102160
24	6	0	-9.012181	1.124146	2.759135
25	1	0	-9.496039	1.751250	3.505817
26	6	0	-1.553527	-1.232347	-0.864775
27	6	0	-0.761852	-0.364013	-0.074811
28	6	0	-1.347481	0.434980	0.893240
29	1	0	-1.066460	-1.867433	-1.604062
30	1	0	-0.728256	1.085886	1.514895
31	1	0	-9.834165	-1.193334	0.385097
32	6	0	-2.582427	2.107489	2.882631
33	6	0	-1.891195	2.833975	3.568889
34	6	0	-7.982548	-2.216077	-0.983194
35	6	0	-8.677617	-2.944737	-1.663285
36	14	0	-0.852022	3.919789	4.595894
37	14	0	-9.721608	-4.034605	-2.679484
38	6	0	-1.930531	4.659088	5.924346
39	1	0	-1.349701	5.322413	6.582484
40	1	0	-2.748728	5.251186	5.486959
41	1	0	-2.380408	3.873346	6.550648
42	6	0	-0.145706	5.248838	3.499101
43	1	0	0.490772	5.942451	4.068195
44	1	0	0.468893	4.810700	2.696415
45	1	0	-0.944973	5.837297	3.022462
46	6	0	0.503380	2.883740	5.342405
47	1	0	0.088133	2.068702	5.955520
48	1	0	1.127025	2.426054	4.557942
49	1	0	1.162007	3.487057	5.984574

50	6	0	-9.178320	-5.792366	-2.387896
51	1	0	-9.785588	-6.500714	-2.970733
52	1	0	-8.125240	-5.935600	-2.675034
53	1	0	-9.273343	-6.062476	-1.324232
54	6	0	-9.491198	-3.555951	-4.464997
55	1	0	-10.109921	-4.177838	-5.128822
56	1	0	-9.772158	-2.503772	-4.629985
57	1	0	-8.441474	-3.672940	-4.775379
58	6	0	-11.492429	-3.792907	-2.152341
59	1	0	-11.626298	-4.044531	-1.088849
60	1	0	-11.807849	-2.747502	-2.292928
61	1	0	-12.172122	-4.430743	-2.736891
62	6	0	0.712943	-0.389455	-0.237365
63	6	0	1.462788	-1.365943	0.461442
64	6	0	1.351344	0.573656	-1.001694
65	6	0	2.846573	-1.389126	0.356321
66	1	0	0.938223	-2.096887	1.076159
67	6	0	2.766004	0.576212	-1.130277
68	1	0	0.767902	1.339780	-1.517804
69	6	0	3.647829	-2.390467	1.051838
70	6	0	3.522148	-0.412791	-0.449109
71	6	0	3.456056	1.561317	-1.936686
72	6	0	4.992939	-2.413956	0.948438
73	1	0	3.112566	-3.121239	1.658830
74	6	0	4.954924	-0.433027	-0.559784
75	6	0	4.840705	1.538820	-2.044591
76	6	0	2.691424	2.545439	-2.613950
77	6	0	5.721736	-1.440478	0.139572
78	1	0	5.586825	-3.167924	1.471502
79	6	0	5.607298	0.529477	-1.348227
80	6	0	5.569640	2.514799	-2.850399
81	6	0	2.038743	3.389512	-3.195417
82	6	0	7.106200	-1.461962	0.032434
83	6	0	7.040415	0.508757	-1.460019
84	6	0	6.914875	2.491594	-2.953631

85	1	0	4.975681	3.270710	-3.370774
86	14	0	1.057716	4.652320	-4.065229
87	6	0	7.796013	-0.479365	-0.776699
88	6	0	7.872818	-2.443614	0.711490
89	6	0	7.715853	1.487209	-2.263000
90	1	0	7.449541	3.224729	-3.557954
91	6	0	2.199093	5.577979	-5.212437
92	6	0	0.328827	5.796546	-2.789285
93	6	0	-0.282740	3.783100	-5.022526
94	6	0	9.211765	-0.474525	-0.906585
95	6	0	8.530135	-3.284285	1.292645
96	6	0	9.101212	1.460924	-2.366723
97	1	0	1.654735	6.352737	-5.772783
98	1	0	3.007866	6.072759	-4.653206
99	1	0	2.661976	4.896910	-5.943211
100	1	0	-0.274857	6.587616	-3.258166
101	1	0	-0.322855	5.244586	-2.092823
102	1	0	1.117481	6.281728	-2.193256
103	1	0	0.144022	3.072679	-5.747720
104	1	0	-0.943274	3.214491	-4.348286
105	1	0	-0.906828	4.498373	-5.578477
106	6	0	9.845571	0.475112	-1.684559
107	1	0	9.793971	-1.233997	-0.381420
108	14	0	9.517689	-4.541756	2.160846
109	1	0	9.624293	2.198343	-2.973288
110	1	0	10.931044	0.472109	-1.779080
111	6	0	8.981051	-6.219259	1.553536
112	6	0	9.201968	-4.365048	3.988423
113	6	0	11.313480	-4.237821	1.766714
114	1	0	9.555536	-7.022687	2.037945
115	1	0	7.914421	-6.395059	1.762107
116	1	0	9.127006	-6.309175	0.465316
117	1	0	9.784331	-5.096899	4.567604
118	1	0	9.479492	-3.358757	4.340428
119	1	0	8.137680	-4.518906	4.224450

120	1	0	11.498395	-4.309989	0.683624
121	1	0	11.626508	-3.234561	2.095252
122	1	0	11.960562	-4.972913	2.268090

Table S11. Cartesian coordinates of 6,12-TMS*e* 2,2'-bianthanthrenyl (dihedral angle = 120°).

SCF Done: E(RPM6) = 0.318888369959 A.U. after 26 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.680721	2.685609	-1.015419
2	6	0	5.024798	2.705791	-0.898970
3	6	0	5.758589	1.626652	-0.243681
4	6	0	4.997952	0.515739	0.284923
5	6	0	3.566858	0.496348	0.155942
6	6	0	2.885863	1.579224	-0.492927
7	6	0	7.141658	1.646413	-0.120056
8	6	0	5.654544	-0.546927	0.927223
9	6	0	7.086168	-0.527761	1.056479
10	6	0	7.836000	0.559894	0.537793
11	6	0	7.765839	-1.607991	1.711230
12	6	0	6.970516	-2.712283	2.235949
13	6	0	5.626549	-2.733460	2.117083
14	6	0	4.893471	-1.656082	1.458081
15	6	0	3.510089	-1.675891	1.334807
16	6	0	2.815908	-0.590237	0.674597
17	1	0	3.141933	3.495946	-1.506866
18	1	0	5.613991	3.537510	-1.293868
19	1	0	7.508289	-3.521528	2.729958
20	1	0	5.036804	-3.564123	2.513486
21	6	0	9.250422	0.550758	0.680747
22	6	0	9.888477	-0.498165	1.313804
23	1	0	10.972906	-0.497706	1.419485
24	6	0	9.149790	-1.582871	1.832426

25	1	0	9.676083	-2.397067	2.327395
26	6	0	1.503245	1.559920	-0.609975
27	6	0	0.759147	0.463181	-0.109007
28	6	0	1.402739	-0.582480	0.534301
29	1	0	0.975913	2.379003	-1.097977
30	1	0	0.823352	-1.414112	0.942547
31	1	0	9.828213	1.386845	0.282364
32	6	0	2.750855	-2.757256	1.850521
33	6	0	2.102349	-3.684513	2.293367
34	6	0	7.902365	2.728225	-0.633403
35	6	0	8.554648	3.654417	-1.073020
36	14	0	1.124467	-5.069519	2.956413
37	14	0	9.534810	5.039306	-1.730229
38	6	0	2.309470	-6.328006	3.654418
39	1	0	1.769998	-7.193128	4.067901
40	1	0	2.996094	-6.698847	2.878202
41	1	0	2.917362	-5.893018	4.462481
42	6	0	0.132901	-5.796275	1.557261
43	1	0	-0.482643	-6.641259	1.899174
44	1	0	-0.543340	-5.042764	1.121521
45	1	0	0.788639	-6.159533	0.750442
46	6	0	0.006523	-4.401480	4.287376
47	1	0	0.587907	-3.930228	5.095189
48	1	0	-0.676727	-3.638613	3.880859
49	1	0	-0.607485	-5.197573	4.733732
50	6	0	8.968346	6.600328	-0.886259
51	1	0	9.537516	7.473872	-1.237248
52	1	0	7.901982	6.792635	-1.080657
53	1	0	9.100450	6.528107	0.204912
54	6	0	9.242363	5.134048	-3.567454
55	1	0	9.820858	5.951406	-4.022973
56	1	0	9.538015	4.195346	-4.062145
57	1	0	8.178783	5.308075	-3.792134
58	6	0	11.329869	4.701495	-1.361898
59	1	0	11.501411	4.613062	-0.277944

60	1	0	11.660313	3.762599	-1.832451
61	1	0	11.972557	5.510956	-1.739058
62	6	0	-0.719677	0.490320	-0.206310
63	6	0	-1.424776	1.602201	0.316584
64	6	0	-1.409940	-0.590912	-0.732780
65	6	0	-2.811474	1.634027	0.273787
66	1	0	-0.863545	2.427569	0.753901
67	6	0	-2.828756	-0.586944	-0.795502
68	1	0	-0.863306	-1.456110	-1.115826
69	6	0	-3.565007	2.769415	0.795098
70	6	0	-3.538375	0.533596	-0.290992
71	6	0	-3.570019	-1.696157	-1.359072
72	6	0	-4.913162	2.802103	0.749895
73	1	0	-2.991641	3.592212	1.223108
74	6	0	-4.974322	0.563728	-0.339171
75	6	0	-4.957827	-1.663928	-1.408295
76	6	0	-2.851993	-2.812196	-1.859715
77	6	0	-5.693093	1.705853	0.181354
78	1	0	-5.471116	3.656537	1.141562
79	6	0	-5.676623	-0.520162	-0.892148
80	6	0	-5.737617	-2.762662	-1.972338
81	6	0	-2.238838	-3.769401	-2.288999
82	6	0	-7.080691	1.737107	0.133601
83	6	0	-7.113045	-0.489445	-0.942211
84	6	0	-7.085837	-2.729679	-2.018756
85	1	0	-5.179499	-3.619393	-2.358909
86	14	0	-1.314204	-5.200160	-2.930976
87	6	0	-7.821661	0.630572	-0.434613
88	6	0	-7.800644	2.849889	0.639378
89	6	0	-7.839270	-1.591179	-1.505486
90	1	0	-7.658653	-3.554997	-2.442321
91	6	0	-2.549627	-6.475325	-3.500682
92	6	0	-0.258180	-5.869463	-1.550248
93	6	0	-0.260810	-4.616144	-4.351555
94	6	0	-9.241946	0.632347	-0.498334

95	6	0	-8.418018	3.802729	1.072331
96	6	0	-9.227554	-1.554413	-1.551084
97	1	0	-2.043289	-7.367600	-3.898094
98	1	0	-3.197822	-6.797387	-2.671211
99	1	0	-3.195001	-6.072572	-4.296407
100	1	0	0.327445	-6.740112	-1.880080
101	1	0	0.449927	-5.104800	-1.190506
102	1	0	-0.874236	-6.181130	-0.691959
103	1	0	-0.878641	-4.176500	-5.150192
104	1	0	0.453277	-3.844612	-4.020719
105	1	0	0.317837	-5.442891	-4.789363
106	6	0	-9.925040	-0.437109	-1.044798
107	1	0	-9.788079	1.493215	-0.108198
108	14	0	-9.345977	5.227640	1.719583
109	1	0	-9.788990	-2.384656	-1.976437
110	1	0	-11.013671	-0.428138	-1.090036
111	6	0	-8.814267	6.742005	0.773455
112	6	0	-8.947818	5.402679	3.531163
113	6	0	-11.162341	4.894269	1.469818
114	1	0	-9.354175	7.637329	1.115610
115	1	0	-7.736708	6.930509	0.897813
116	1	0	-9.009453	6.621668	-0.304100
117	1	0	-9.491709	6.246668	3.980674
118	1	0	-9.223281	4.490878	4.084738
119	1	0	-7.871506	5.574494	3.686794
120	1	0	-11.396615	4.758680	0.402429
121	1	0	-11.473958	3.981509	2.001169
122	1	0	-11.774812	5.727518	1.845345

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Table S12. Cartesian coordinates of 6,12-TMS*e* 2,2'-bianthanthrenyl (dihedral angle = 180°).

SCF Done: E(RPM6) = 0.327651880601 A.U. after 8 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.628776	2.934347	0.320428
2	6	0	-4.977965	2.942847	0.290283
3	6	0	-5.753633	1.718568	0.110972
4	6	0	-5.027119	0.482795	-0.077045
5	6	0	-3.592360	0.474475	-0.016531
6	6	0	-2.871348	1.692814	0.199969
7	6	0	-7.142441	1.715596	0.110825
8	6	0	-5.719032	-0.716098	-0.311599
9	6	0	-7.155850	-0.718293	-0.327513
10	6	0	-7.874252	0.484522	-0.100796
11	6	0	-7.871235	-1.935746	-0.579013
12	6	0	-7.104681	-3.146831	-0.849188
13	6	0	-5.755157	-3.142132	-0.859420
14	6	0	-4.985695	-1.934038	-0.575239
15	6	0	-3.595545	-1.927670	-0.568831
16	6	0	-2.870042	-0.735728	-0.179782
17	1	0	-3.058990	3.854685	0.446888
18	1	0	-5.540124	3.874122	0.396081
19	1	0	-7.669123	-4.057854	-1.047968
20	1	0	-5.188455	-4.052236	-1.072142
21	6	0	-9.295392	0.445531	-0.099973
22	6	0	-9.968512	-0.739243	-0.326469
23	1	0	-11.057851	-0.761155	-0.321548
24	6	0	-9.260554	-1.935076	-0.571745
25	1	0	-9.814914	-2.853373	-0.756627
26	6	0	-1.488649	1.668261	0.297293
27	6	0	-0.772407	0.441112	0.295122
28	6	0	-1.466393	-0.735560	0.029006
29	1	0	-0.940677	2.604388	0.427372

30	1	0	-0.934526	-1.689218	-0.033312
31	1	0	-9.850029	1.367904	0.081480
32	6	0	-2.879660	-3.048030	-1.061217
33	6	0	-2.313519	-3.979135	-1.599429
34	6	0	-7.871844	2.915268	0.312253
35	6	0	-8.497148	3.942514	0.485516
36	14	0	-1.559264	-5.309686	-2.587521
37	14	0	-9.437443	5.478251	0.744858
38	6	0	-2.944336	-6.403350	-3.190567
39	1	0	-2.557326	-7.217825	-3.820737
40	1	0	-3.489134	-6.857674	-2.349663
41	1	0	-3.667390	-5.829147	-3.790163
42	6	0	-0.365769	-6.278700	-1.541333
43	1	0	0.139575	-7.058410	-2.129927
44	1	0	0.411161	-5.617256	-1.122142
45	1	0	-0.882112	-6.768832	-0.701311
46	6	0	-0.679388	-4.504421	-4.017722
47	1	0	-1.372724	-3.895867	-4.619261
48	1	0	0.122225	-3.837831	-3.660715
49	1	0	-0.222948	-5.251867	-4.682808
50	6	0	-8.967766	6.677716	-0.600628
51	1	0	-9.517844	7.625116	-0.501387
52	1	0	-7.891759	6.908044	-0.570270
53	1	0	-9.191488	6.260686	-1.595194
54	6	0	-8.990440	6.153642	2.422121
55	1	0	-9.539141	7.082029	2.638851
56	1	0	-9.229712	5.427706	3.215179
57	1	0	-7.914062	6.375182	2.487427
58	6	0	-11.252277	5.064828	0.659433
59	1	0	-11.514190	4.634349	-0.319404
60	1	0	-11.528065	4.332281	1.433569
61	1	0	-11.872033	5.961376	0.809059
62	6	0	0.705863	0.452762	0.426395
63	6	0	1.396993	1.695521	0.397818
64	6	0	1.447821	-0.723212	0.429228

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65	6	0	2.778687	1.747898	0.305459
66	1	0	0.822352	2.624367	0.420001
67	6	0	2.866890	-0.703743	0.460108
68	1	0	0.944443	-1.694218	0.444698
69	6	0	3.493845	3.014007	0.179924
70	6	0	3.541619	0.535059	0.314182
71	6	0	3.654442	-1.905839	0.639101
72	6	0	4.833958	3.055088	0.026431
73	1	0	2.898434	3.926427	0.206504
74	6	0	4.970230	0.575435	0.176372
75	6	0	5.032499	-1.876084	0.457483
76	6	0	3.027211	-3.078174	1.131862
77	6	0	5.645642	1.841259	-0.002809
78	1	0	5.362024	4.006172	-0.079079
79	6	0	5.704690	-0.620902	0.206474
80	6	0	5.850874	-3.083226	0.527908
81	6	0	2.549415	-4.056822	1.671639
82	6	0	7.020979	1.874719	-0.191601
83	6	0	7.130068	-0.586547	0.026980
84	6	0	7.186252	-3.051243	0.335011
85	1	0	5.331686	-4.022606	0.734337
86	14	0	1.956067	-5.456580	2.674029
87	6	0	7.792993	0.649751	-0.188421
88	6	0	7.698190	3.105624	-0.386770
89	6	0	7.890652	-1.801628	0.071300
90	1	0	7.785910	-3.960591	0.374715
91	6	0	3.395067	-6.619252	2.910167
92	6	0	0.550905	-6.320402	1.814943
93	6	0	1.395558	-4.755651	4.306357
94	6	0	9.200901	0.648578	-0.384515
95	6	0	8.278655	4.159721	-0.554680
96	6	0	9.265887	-1.763602	-0.123577
97	1	0	3.105518	-7.484039	3.525522
98	1	0	3.763368	-6.999970	1.945931
99	1	0	4.232270	-6.112891	3.414763

100	1	0	0.085878	-7.070578	2.471781
101	1	0	-0.232171	-5.603341	1.518225
102	1	0	0.898292	-6.836695	0.906433
103	1	0	2.208483	-4.201276	4.800986
104	1	0	0.555516	-4.056706	4.165344
105	1	0	1.062110	-5.547955	4.992119
106	6	0	9.916017	-0.533074	-0.356017
107	1	0	9.712092	1.597331	-0.557447
108	14	0	9.151742	5.735870	-0.806889
109	1	0	9.853575	-2.679408	-0.096834
110	1	0	10.994646	-0.525522	-0.509889
111	6	0	8.852653	6.807632	0.686913
112	6	0	8.469511	6.534924	-2.344788
113	6	0	10.967123	5.364639	-1.002798
114	1	0	9.369561	7.774283	0.595171
115	1	0	7.779264	7.011021	0.821993
116	1	0	9.216737	6.316384	1.603008
117	1	0	8.969806	7.491921	-2.554123
118	1	0	8.608440	5.883074	-3.221707
119	1	0	7.391220	6.733078	-2.244923
120	1	0	11.367054	4.862754	-0.108269
121	1	0	11.145210	4.705259	-1.866211
122	1	0	11.547095	6.286408	-1.158616

Atropisomerism of 6,12-hexyl [4]$CA_{2,8}$

Atropisomerism of 6,12-hexyl [4]$CA_{2,8}$ was analyzed by the same method for 6,12-hexyl [4]$CC_{2,8}$.[13] Thus, a toluene solution of 6,12-hexyl (*P*)-(12,8)-[4]$CA_{2,8}$ in a sealed tube under dark conditions was heated at 120, 140, 160 and 180 °C, respectively (Fig. S5). The profile of the second (11,9)-isomer indicated one-by-one rotation of the anthanthrenylene panel (Fig. S6). The first-order decay constant of 6,12-hexyl (*P*)-(12,8)-[4]$CA_{2,8}$ was analyzed by Eyring plot (Fig. S7)[14,15] to give the approximate line with high degree of confidence. The activation enthalpy $\Delta H^{\ddagger}$

13. Hitosugi, S.; Nakanishi, W.; Isobe, H. *Chem. Asian J.* **2012**, *7*, 1550-1552.

14. Eyring, H. *Chem. Rev.* **1935**, *17*, 65-77.

was +21 kcal/mol, and the activation entropy $\Delta S^{\ddagger}$ was –15 cal/mol·K.

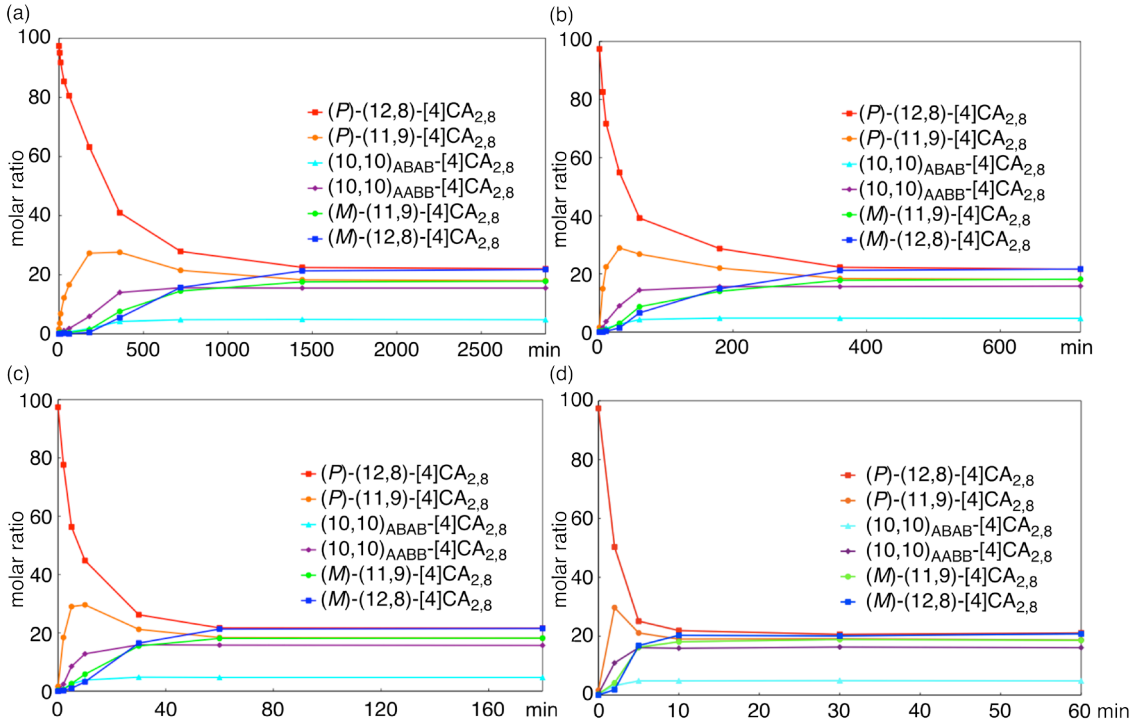

Fig. S5. Time-course analysis of isomerization of 6,12-hexyl (*P*)-(12,8)-[4]$CA_{2,8}$ in toluene at 120 °C (a), 140 °C (b), 160 °C (c) and 180 °C (d).

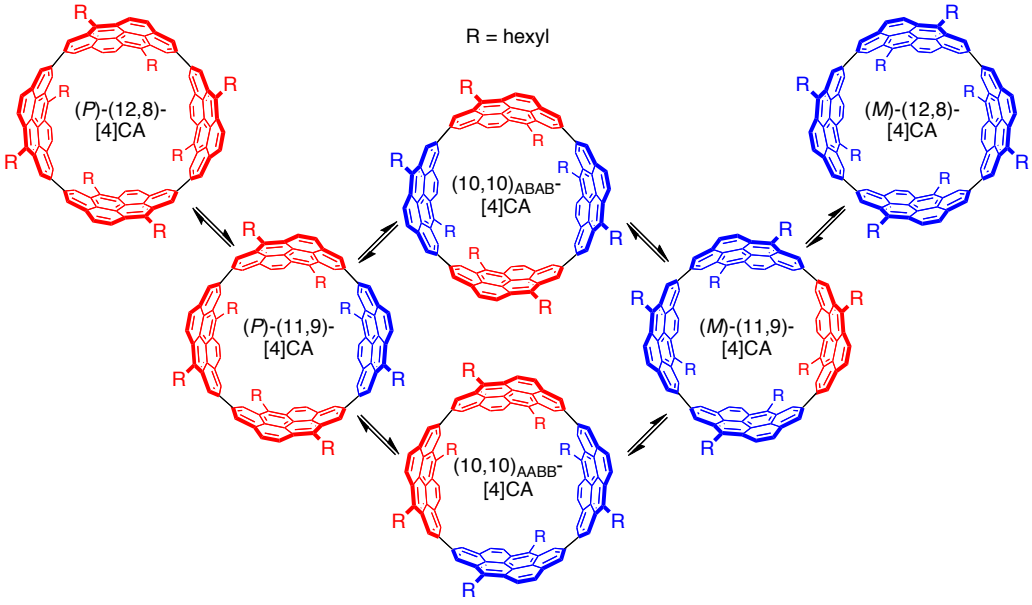

Fig. S6. Isomerization path of 6,12-hexyl [4]$CA_{2,8}$.

15. Newell, L. M.; Sekhar, V. C.; DeVries, K. M.; Staiger, T. L.; Finneman,J. I. *J. Chem. Soc., Perkin Trans 2*, **2001**, 961-963.

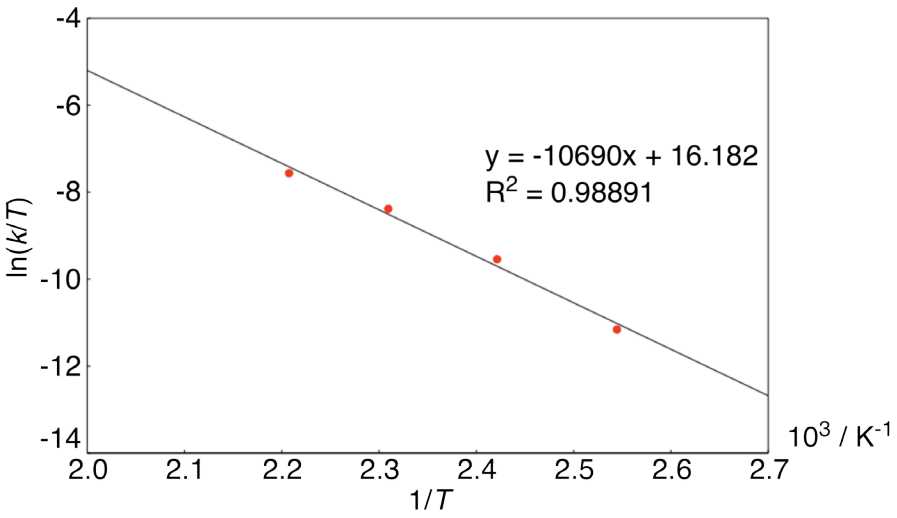

Fig. S7. Eyring plot of the first-order decay rate of 6,12-hexyl (*P*)-(12,8)-[4]$CA_{2,8}$.

X-ray crystallographic analysis of 6,12-TIPS*e* [4]$CA_{2,8}$

A single crystal (ca. 0.10 × 0.02 × 0.02 mm^3) suitable for X-ray analysis was obtained from toluene solution of racemic 6,12-TIPS*e* [4]$CA_{2,8}$ after diffusing vaporous hexane over 5 days. The structure was solved by SHELXS-97 and refined by SHELXL-97[16] through Yadokari-XG 2009 application.[17] Due to the insufficient data, the structures are refined with isotropic thermal factors on carbon atoms. Hydrogen atoms were included in calculated positions. The residual scattered electron densities, originating from disordered solvents in the tube void, were eliminated by the SQUEEZE protocol equipped in PLATON.[18] Several errors were found in CheckCIF routine of IUCR mostly because of the insufficient quality of the crystal, and, due to the insufficient data, the crystal data were used only for the discussion of overall molecular structures and packing motifs. Crystallographic data were deposited in the Cambridge Crystallographic Data Centre (CCDC 927603). The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif. Crystal data and structure refinement are listed in Table S13. Representative intermolecular contacts are shown in Fig. S8.

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Table S13. Crystal data and structure refinement for 6,12-TIPS*e* [4]$CA_{2,8}$ (CCDC927603).

Empirical formula	$C_{200}H_{256}Si_8$
Formula weight	2884.77
Temperature	100 K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2/n
Unit cell dimensions	*a* = 16.179(7) Å a = 90°.
	b = 17.461(8) Å b = 95.835(6)°.
	c = 32.012(15) Å g = 90°.
Volume	8997(7) $Å^3$
Z	2
Density (calculated)	1.065 Mg/m^3
Absorption coefficient	0.110 mm^{-1}
F(000)	3136.0
Crystal size	0.10 x 0.02 x 0.02 mm^3
Theta range for data collection	2.20 to 16.00°.
Index ranges	-12<=h<=12, -13<=k<=13, -24<=l<=24
Reflections collected	29996
Independent reflections	4437 [R(int) = 0.0863]
Completeness to theta = 25.00°	99.4 %
Absorption correction	Empirical
Max. and min. transmission	0.9978 and 0.9891
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4437 / 0 / 433
Goodness-of-fit on F^2	1.929
Final R indices [I>2sigma(I)]	*R*1 = 0.1535, *wR*2 = 0.4279
R indices (all data)	*R*1 = 0.1715, *wR*2 = 0.4429
Largest diff. peak and hole	1.132 and -0.899 e.$Å^{-3}$

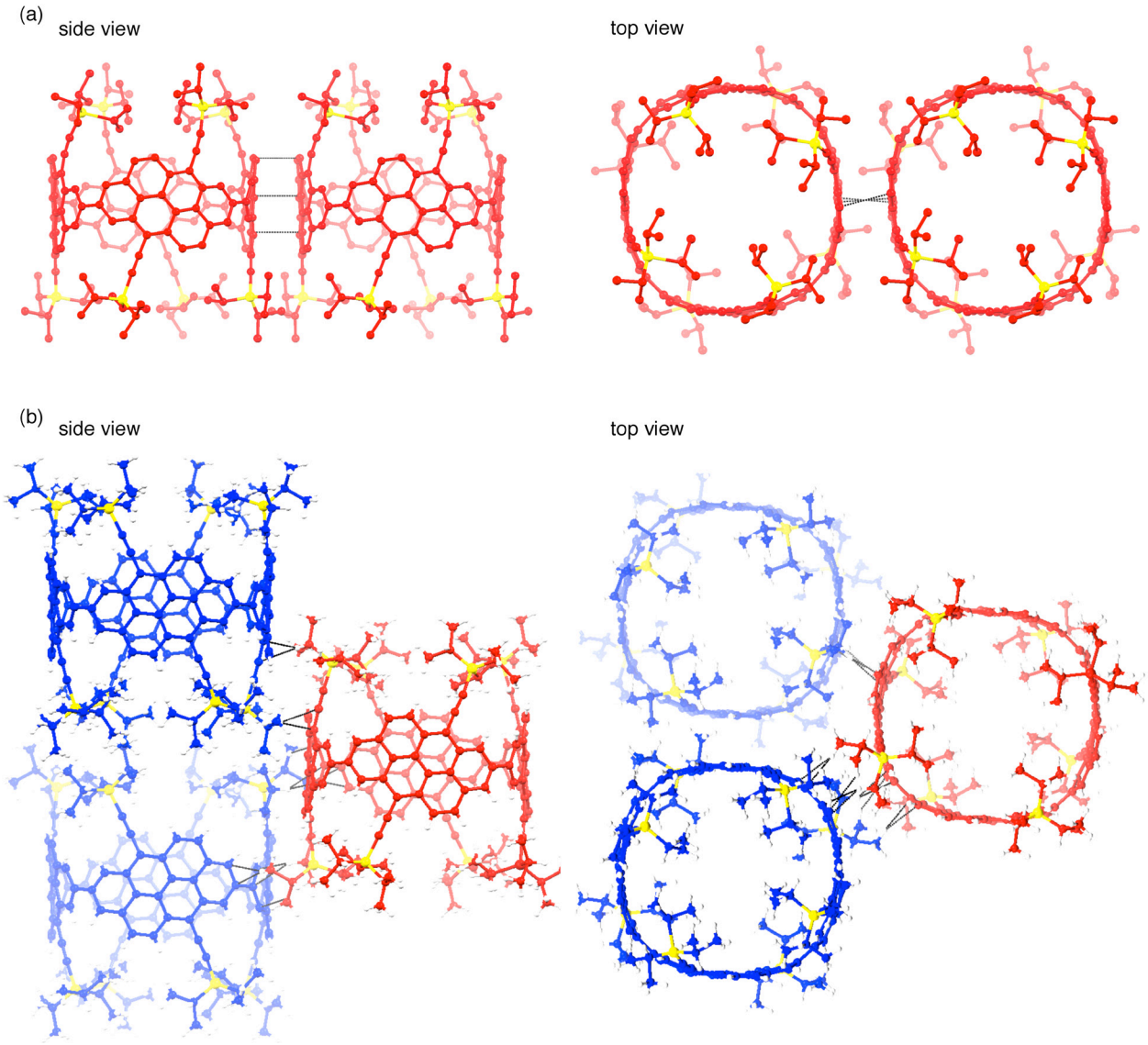

Fig. S8. Inter-columnar short contacts of (12,8)-[4]$CA_{2,8}$. Atomic distances within the sum of van der Waals radii are automatically selected by Mercury CSD. (a) Inter-columnar contacts between two (*P*)-isomers in the homohelical layer. The short contacts between sp^2-carbons on the wall are observed at 3.36(1), 3.257(19) and 3.24(1) Å. Hydrogen atoms are omitted for clarity. (b) Inter-columnar contacts between (*P*)- and (*M*)-isomers in heterohelical layers. The short contacts between isopropyl-H and sp^2-carbons on the wall are observed at 2.762(14), 2.724(13), 2.896(14), 2.733(13), 2.891(13), 2.822(12) and 2.881(12) Å.