Electronic Supplementary Material (ESI) for ChemComm.

Supplementary Information for:

A New Armchair Carbon Nanobelt Synthesized by Tuning the Regioselectivity of the Scholl Reaction of Quinquephenyl

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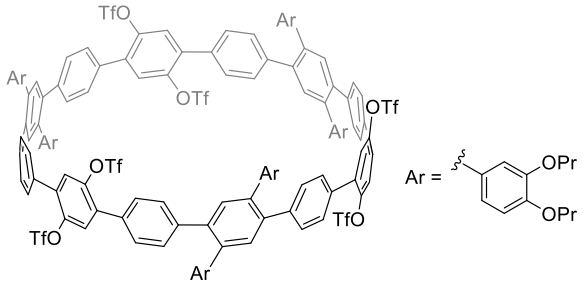
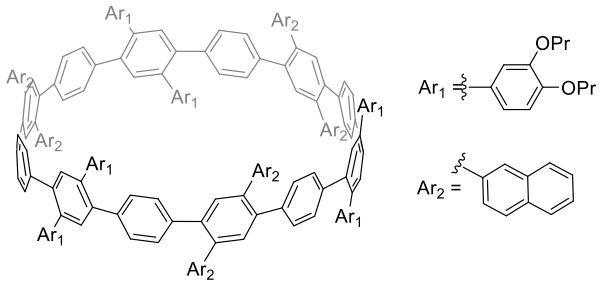
1. Synthesis

General: The reagents and starting materials employed were commercially available and used without any further purification or made following reported methods as indicated. Unless otherwise noted, all reactions were performed with dry solvents under an atmosphere of nitrogen in dried glassware with standard vacuum-line techniques. Anhydrous and oxygen-free diethyl ether, THF and CH_2Cl_2 were purified by an Innovative Technology Pure-Solv PS-MD-4 system. Gel permeation chromatography (GPC) were performed on a JAI LC-9160 II NEXT automatic recycling preparative HPLC system with a UV/VIS detector. NMR spectra were recorded on a Bruker AVANCE III 400MHz spectrometer (^{1}H NMR: 400 MHz, ^{13}C NMR: 100 MHz). Abbreviations: s = singlet, d = doublet, t = triplet, m = multiplet. Chemical shift values (δ) are expressed in parts per million using residual solvent protons (^{1}H NMR, δH = 5.32 for CD_2Cl_2, δH = 7.26 for $CDCl_3$, ^{13}C NMR, δC = 77.16 for $CDCl_3$) as internal standard. Mass spectra were recorded on Therno Finnigan MAT 95 XL spectrometer or a Bruker Autoflex speed MALDI-TOF spectrometer. UV-vis absorption spectra were recorded on a Shimadzu UV-3600 Plus UV-VIS-NIR Spectrophotometer. Fluorescence spectra were taken on a HITACHI F-4500 spectrofluorometer. Unless otherwise noted, melting points, without correction, were measured using a Nikon Polarized Light Microscope ECLIPSE 50i POL equipped with an INTEC HCS302 heating stage.



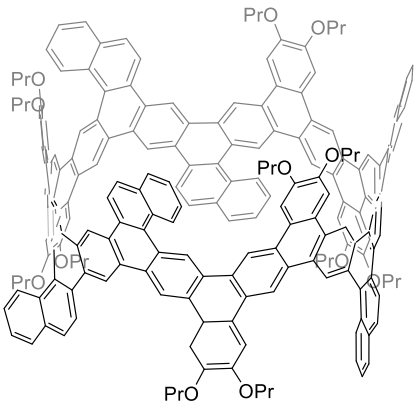
Compound **18** was synthesized following the reported procedures.[1]



Compound **4**

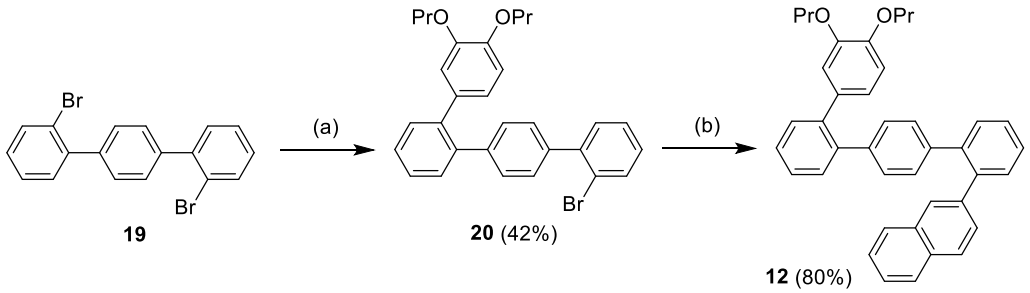
To a mixture of compound **18** (250 mg, 85 μmol), 2-naphthylboronic acid (218 mg, 1.3 mmol), $Pd(PPh_3)_4$ (49 mg, 42 μmol) and K_3PO_4 •1.5 H_2O (607 mg, 2.5 mmol) in a reaction flask filled with N_2 was added 20 ml of 1,4-dioxane, which had been bubbled with a flow of N_2 for 20 minutes. The reaction mixture was further bubbled with a flow of N_2 for 5 minutes. The reaction flask was then sealed and heated at 100 ℃ for 5 days. The mixture was cooled to room temperature, diluted with CH_2Cl_2, washed with a diluted aqueous solution of NaOH and brine subsequently, and dried with anhydrous Na_2SO_4. After concentrated under a reduced pressure, the crude product was triturated with methanol to give compound **4** as white solid (220 mg, 92%). mp: 117–121 ℃ ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.98 (s, 6H), 7.85 (d, *J* = 6.9 Hz, 6H), 7.77 (d, *J* = 7.0 Hz, 6H), 7.66 (d, *J* = 9.8 Hz, 12H), 7.46 (dt, *J* = 14.6, 7.6 Hz, 18H), 7.36 (s, 6H), 7.13 (d, *J* = 8.1 Hz, 12H), 7.03 (d, *J* = 8.2 Hz, 12H), 6.86 (d, *J* = 8.1 Hz, 6H), 6.73 (d,

J = 7.0 Hz, 12H), 3.86 (t, *J* = 6.6 Hz, 12H), 3.72 (t, *J* = 6.8 Hz, 12H), 1.83 (h, *J* = 7.2 Hz, 12H), 1.69 – 1.51 (m, 12H), 1.05 (t, *J* = 7.4 Hz, 15H), 0.87 (t, *J* = 7.4 Hz, 15H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.07, 147.93, 139.69, 138.90, 138.23, 138.14, 138.08, 138.04, 137.84, 133.84, 133.18, 133.16, 132.70, 132.00, 129.24, 129.11, 128.15, 127.74, 127.40, 127.28, 125.61, 125.49, 121.55, 115.59, 113.12, 70.17, 70.13, 22.27, 21.96, 10.22, 10.07. HRMS (MALDI-TOF): calcd. for $C_{204}H_{180}O_{12}$ ([M]$^+$): 2823.3542, found: 2823.3567.

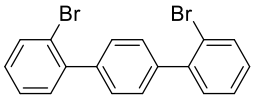


Compound **3**

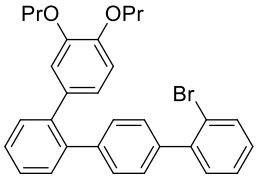
To a flask containing 20 mg (7.1 μmol) of **4** under an atmosphere or N_2 was added 10 ml of anhydrous CH_2Cl_2. 57 mg (0.35 mmol) of $FeCl_3$ was weighed and dissolved in 0.2 ml of nitromethane in a glove box. The solution of $FeCl_3$ was added dropwise into the above solution of **3**. After being stirred for 80 minutes at −20 ℃, the reaction was quenched by addition of methanol. The mixture was poured into water. The organic layer was washed with brine and dried with anhydrous Na_2SO_4. After concentrated under a reduced pressure, the crude product was first purified by flash column chromatography on silica gel using dichloromethane as eluent, the obtained solid was further purified by preparative TLC for five consecutive times using hexane/CH_2Cl_2 /Et_2O/ CS_2 2/1/1/1 (V/V/V/V) as eluent to give compound **3** as yellow solid (2.2 mg, 11%). mp: not melt when heated up to 300 ℃ ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.83 (s, 6H), 9.73 (s, 6H), 9.40 (s, 6H), 9.25 (d, *J* = 8.4 Hz, 6H), 9.19 (s, 6H), 8.84 (d, *J* = 8.9 Hz, 6H), 8.21 – 8.09 (m, 18H), 7.94 (s, 6H), 7.77 (t, *J* = 7.5 Hz, 6H), 7.67 (t, *J* = 7.4 Hz, 6H), 4.49 – 4.31 (m, 12H), 4.14 (dq, *J* = 22.5, 8.0, 7.5 Hz, 12H), 2.14 – 2.04 (m, 12H), 1.98 (h, *J* = 7.3 Hz, 12H). HRMS (MALDI-TOF): calcd. for $C_{204}H_{156}O_{12}$ ([M]$^+$): 2799.1658, found: 2799.1716.



Scheme S1. Synthesis of compound **12**. Reagents and conditions: (a) (3,4-dipropoxyphenyl)boronic acid, $Pd(PPh_3)_4$, K_2CO_3, toluene/EtOH/H_2O, 80 ℃; (b) 2-naphthaleneboronic acid, $Pd(PPh_3)_4$, K_2CO_3, toluene/EtOH/H_2O, 80 ℃.

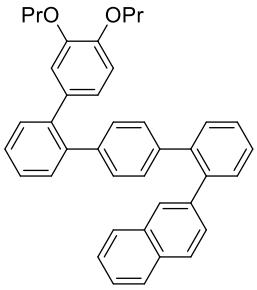


2,2″-dibromo-1,1′:4′,1″-terphenyl (**19**) was synthesized following the reported procedures.[2]



2-bromo-3‴,4‴-dipropoxy-1,1′:4′,1″:2″,1‴-quaterphenyl (**20**)

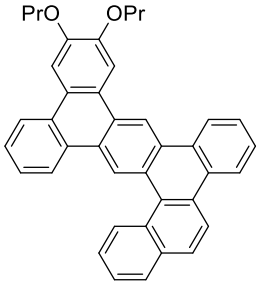
To a mixture of compound **19** (500 mg, 1.3 mol), (3,4-dipropoxyphenyl)boronic acid (307 mg, 1.3 mmol), $Pd(PPh_3)_4$ (149 mg, 0.13 mmol) and K_2CO_3 (1.8 g, 13 mmol) in a reaction flask filled with N_2 was added a mixture of 10 ml of toluene, 10 ml of EtOH and 5 ml of H_2O, which had been bubbled with a flow of N_2 for 20 minutes. The reaction mixture was further bubbled with a flow of N_2 for 5 minutes. The reaction flask was then sealed and heated at 80 ℃ for 12 h. The mixture was cooled to room temperature, diluted with CH_2Cl_2, washed with a diluted aqueous solution of NaOH and brine subsequently, and dried with anhydrous Na_2SO_4. After concentrated under a reduced pressure, the crude product was purified by flash column chromatography on silica gel using hexane/CH_2Cl_2 2/1(V/V) as eluent to give compound **20** as colourless oil (271 mg, 42%). ^{1}H NMR (400 MHz, Chloroform-d) δ 7.66 (dd, J = 8.0, 1.2 Hz, 1H), 7.47 (ddt, J = 8.8, 5.4, 2.9 Hz, 2H), 7.44 – 7.39 (m, 2H), 7.34 (td, J = 7.4, 1.2 Hz, 1H), 7.32 – 7.27 (m, 3H), 7.24 – 7.15 (m, 3H), 6.82 (d, J = 1.8 Hz, 2H), 6.57 (d, J = 1.5 Hz, 1H), 3.94 (t, J = 6.7 Hz, 2H), 3.63 (t, J = 6.7 Hz, 2H), 1.83 (h, J = 7.1 Hz, 2H), 1.65 (h, J = 7.2 Hz, 2H), 1.03 (t, J = 7.4 Hz, 3H), 0.91 (t, J = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.97, 147.83, 147.67, 140.66, 140.51, 140.12, 139.75, 138.88, 133.81, 130.31, 130.21, 130.01, 128.52, 127.35, 126.97, 126.69, 126.40, 121.75, 120.80, 115.97, 113.88, 113.01, 70.31, 70.12, 22.42, 22.01, 10.29, 10.14. HRMS (MALDI-TOF): calcd. for $C_{30}H_{29}BrO_2$ ($[M+H]^+$): 501.14237, found: 501.14254



2-[3‴,4‴-dipropoxy-1,1′:4′,1″:2″,1‴-quaterphenyl]-2-yl-naphthalene (**12**)

To a mixture of compound **20** (270 mg, 0.54 mol), 2-naphthylboronic acid (111 mg, 0.65 mmol), $Pd(PPh_3)_4$ (62 mg, 54 μmol) and K_2CO_3 (745 mg, 5.4 mmol) in a reaction flask filled with N_2 was added a mixture of 10 ml of toluene, 10 ml of EtOH and 5 ml of H_2O, which had been bubbled with a flow of N_2 for 20 minutes. The reaction mixture was further bubbled with a flow of N_2 for 5 minutes. The reaction flask was then sealed and heated at 80 ℃ for 12 h. The mixture was cooled to room temperature, diluted with CH_2Cl_2, washed with a diluted aqueous solution of NaOH and brine subsequently, and dried with anhydrous Na_2SO_4. After concentrated under a reduced pressure, the crude product was purified by flash column chromatography on silica gel using hexane/CH_2Cl_2 2/1(V/V) as eluent to give compound **12** as white solid (237 mg, 80%). mp: 81–84 ℃ ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.78 (q, *J* =

3.7 Hz, 3H), 7.61 (d, *J* = 8.5 Hz, 1H), 7.54 (td, *J* = 4.1, 1.8 Hz, 1H), 7.45 (t, *J* = 3.3 Hz, 5H), 7.41 – 7.32 (m, 4H), 7.14 – 7.08 (m, 1H), 7.05 (d, *J* = 8.2 Hz, 2H), 6.98 (d, *J* = 8.2 Hz, 2H), 6.66 (s, 2H), 6.59 (s, 1H), 3.90 (t, *J* = 6.7 Hz, 2H), 3.70 (t, *J* = 6.7 Hz, 2H), 1.86 (h, *J* = 7.2 Hz, 2H), 1.69 (h, *J* = 7.1 Hz, 2H), 1.06 (t, *J* = 7.4 Hz, 3H), 0.94 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.18, 147.81, 140.34, 140.27, 140.02, 139.97, 139.39, 139.29, 134.14, 133.41, 132.12, 131.06, 130.65, 130.54, 130.44, 129.48, 129.43, 128.47, 128.32, 127.93, 127.65, 127.62, 127.56, 127.39, 127.08, 127.01, 125.90, 125.71, 122.03, 115.98, 113.10, 70.57, 70.38, 22.70, 22.44, 10.58, 10.48. HRMS (MALDI-TOF): calcd. for $C_{40}H_{36}O_2$ ($[M+H]^+$): 549.27881, found: 549.27903.



13,14-dipropoxytriphenyleno[2,3-*g*]chrysene (**13**)

To a flask containing compound **12** (30 mg, 55 μmol) under an atmosphere of N_2 was added 10 ml of anhydrous CH_2Cl_2. 177 mg (1.0 mmol) of $FeCl_3$ was weighed and dissolved in 0.3 ml of nitromethane in a glove box. The solution of $FeCl_3$ was added dropwise into the above solution of **12**. After being stirred for 4 h at room temperature, the reaction was quenched by addition of methanol. The mixture was poured into water. The organic layer was washed with brine and dried with anhydrous Na_2SO_4. After concentrated under a reduced pressure, the crude product was purified by preparative TLC using hexane/CH_2Cl_2 3/1(V/V) as eluent to give compound **13** as white solid (25.5 mg, 85%) ^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.08 (s, 1H), 9.67 (s, 1H), 9.11 (d, *J* = 8.5 Hz, 1H), 8.99 – 8.90 (m, 1H), 8.73 – 8.68 (m, 1H), 8.68 – 8.64 (m, 1H), 8.62 (d, *J* = 8.8 Hz, 1H), 8.53 – 8.47 (m, 1H), 8.29 (s, 1H), 8.08 (dd, *J* = 8.1, 1.4 Hz, 1H), 8.04 (t, *J* = 4.4 Hz, 2H), 7.81 – 7.72 (m, 3H), 7.69 – 7.61 (m, 3H), 4.36 (t, *J* = 6.5 Hz, 2H), 4.25 (t, *J* = 6.6 Hz, 2H), 2.07 (m, *J* = 14.1, 7.0 Hz, 2H), 2.05 – 1.97 (m, 2H), 1.24 (t, *J* = 7.4 Hz, 3H), 1.18 (t, *J* = 7.4 Hz, 3H). 13C NMR (101 MHz, $CDCl_3$) δ 150.02, 149.70, 133.84, 130.50, 130.23, 130.11, 130.06, 129.64, 129.42, 128.38, 128.27, 128.22, 128.17, 127.71, 127.70, 127.67, 127.59, 127.37, 127.31, 127.24, 126.63, 126.46, 125.96, 124.81, 124.34, 124.28, 124.00, 123.58, 123.14, 123.01, 120.85, 116.89, 107.85, 107.12, 71.21, 70.80, 22.89, 22.76, 10.78, 10.68. HRMS (MALDI-TOF): calcd. for $C_{40}H_{32}O_2$ ($[M+H]^+$): 545.24751, found: 545.24764.

2. NMR spectra

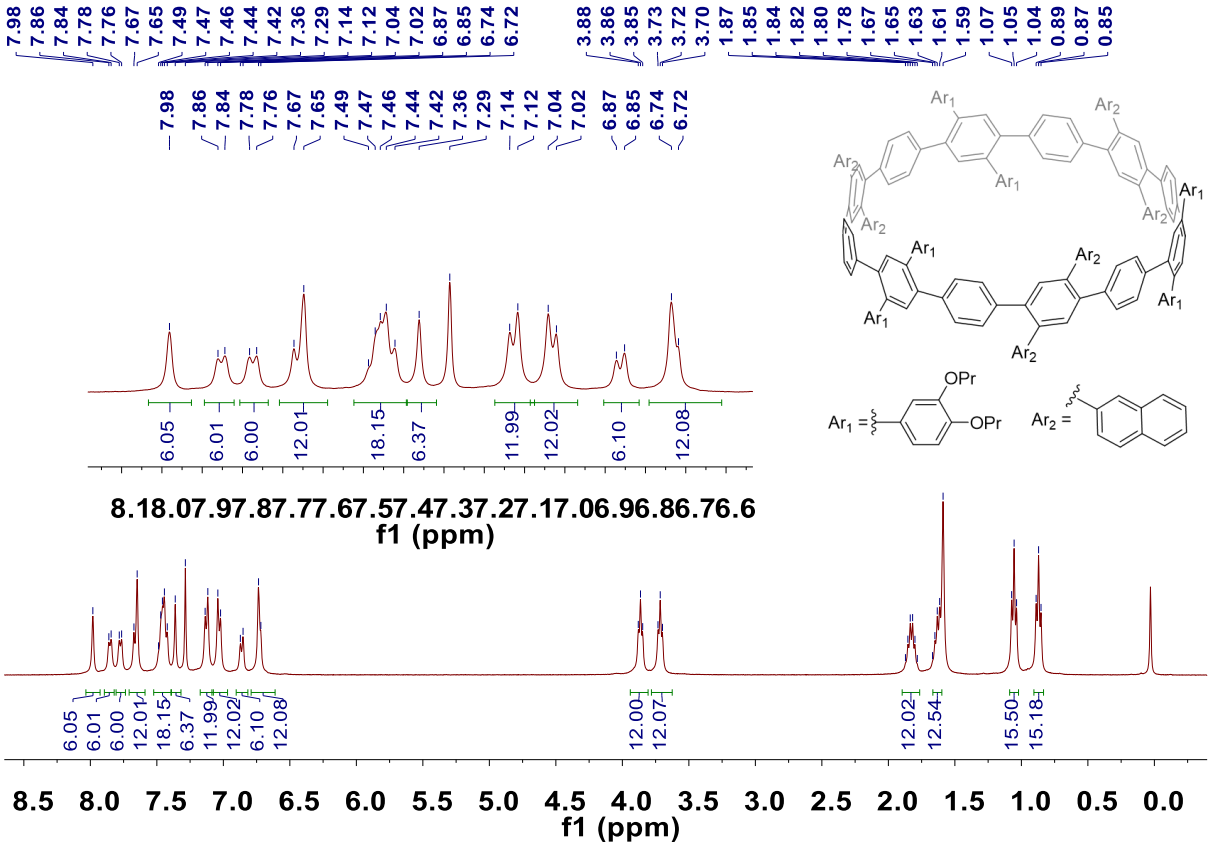


Figure S1. ^{1}H NMR spectrum of **4** in $CDCl_3$ at 298K.

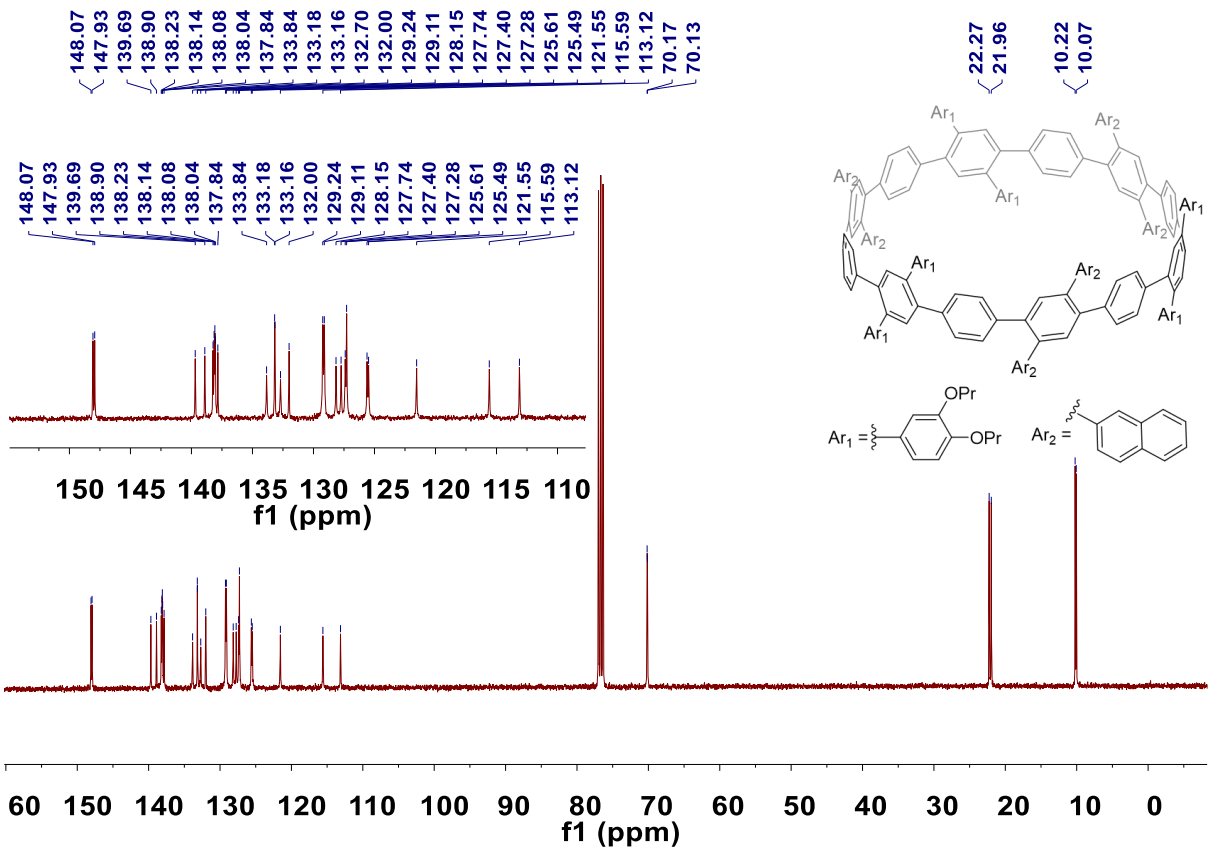


Figure S2. ^{13}C NMR spectrum of **4** in $CDCl_3$ at 298K.

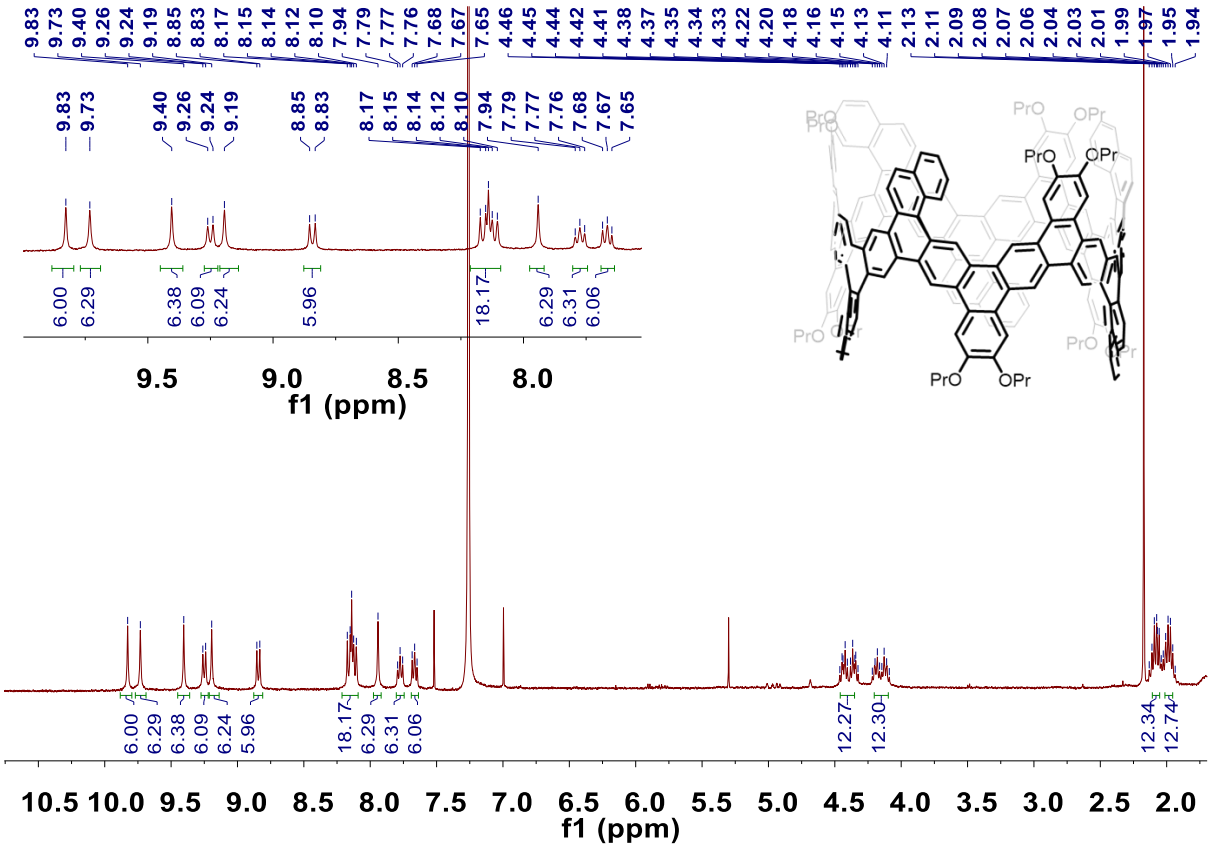


Figure S3. ^{1}H NMR spectrum of **3** in $CDCl_3$ at 298K.

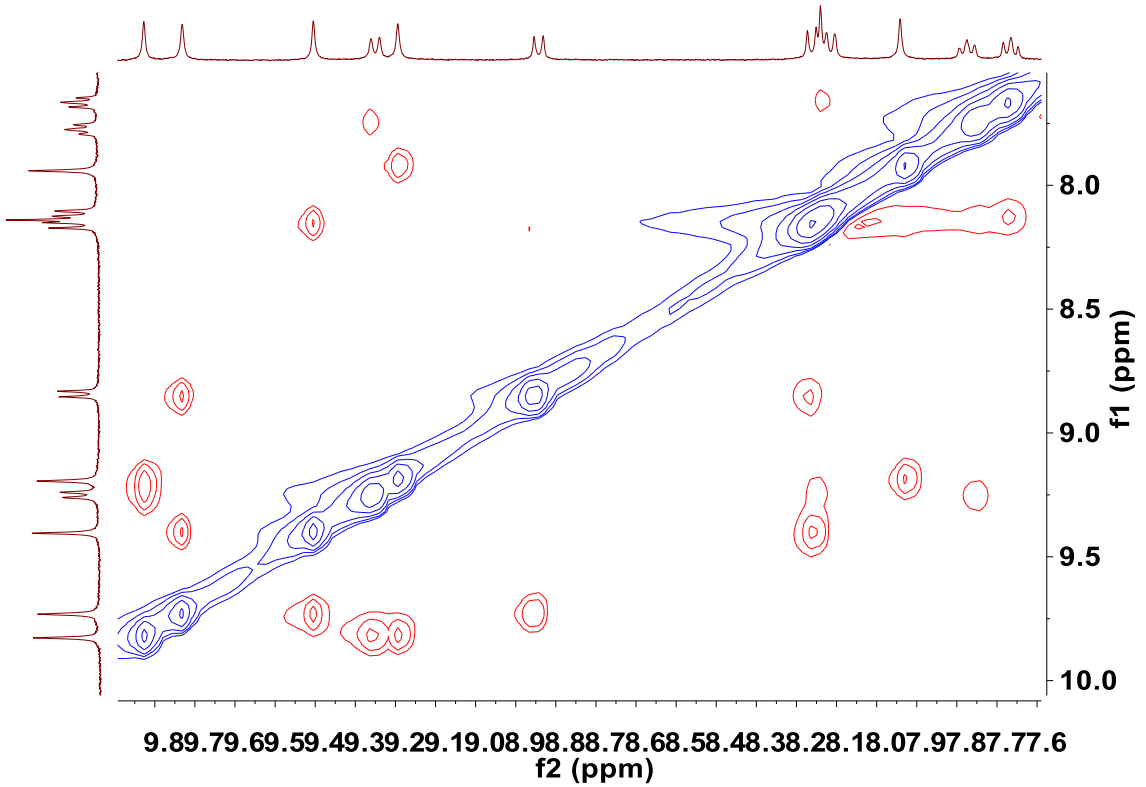


Figure S4. ROESY spectrum of **3** in $CDCl_3$, 298K (aromatic region).

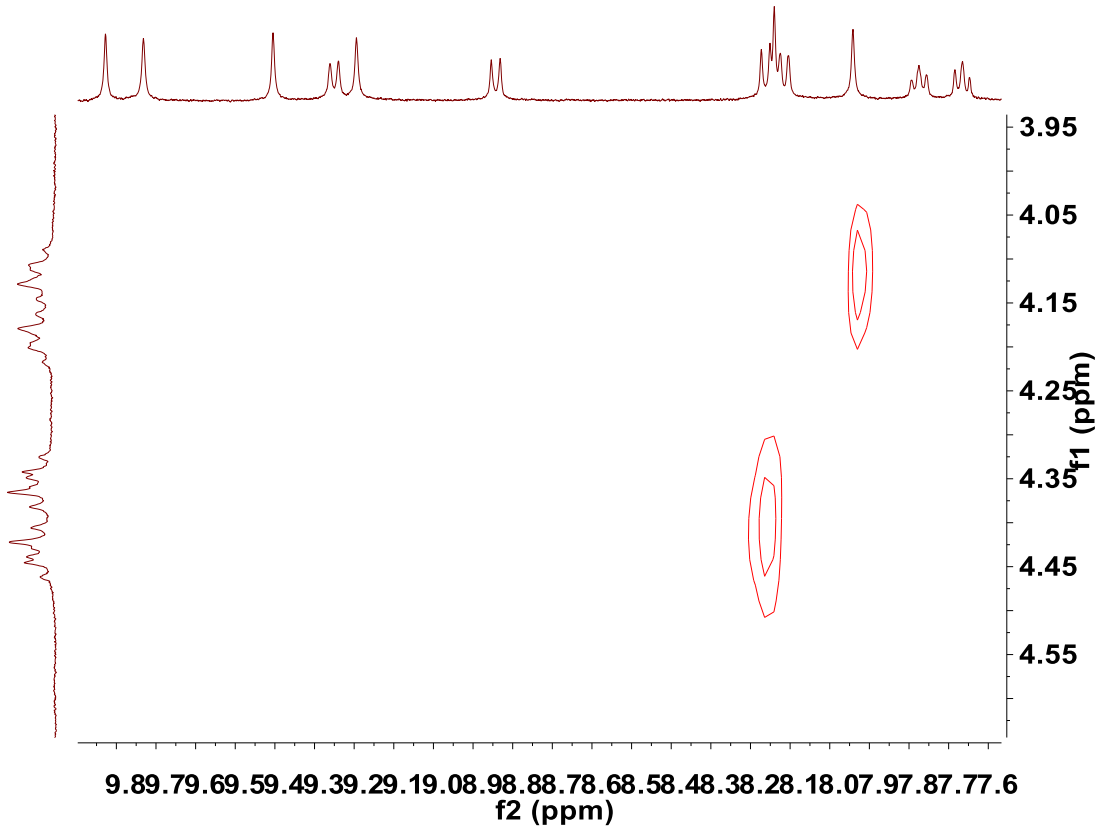


Figure S5. ROESY spectrum of **3** in $CDCl_3$, 298K (aromatic region versus aliphatic region).

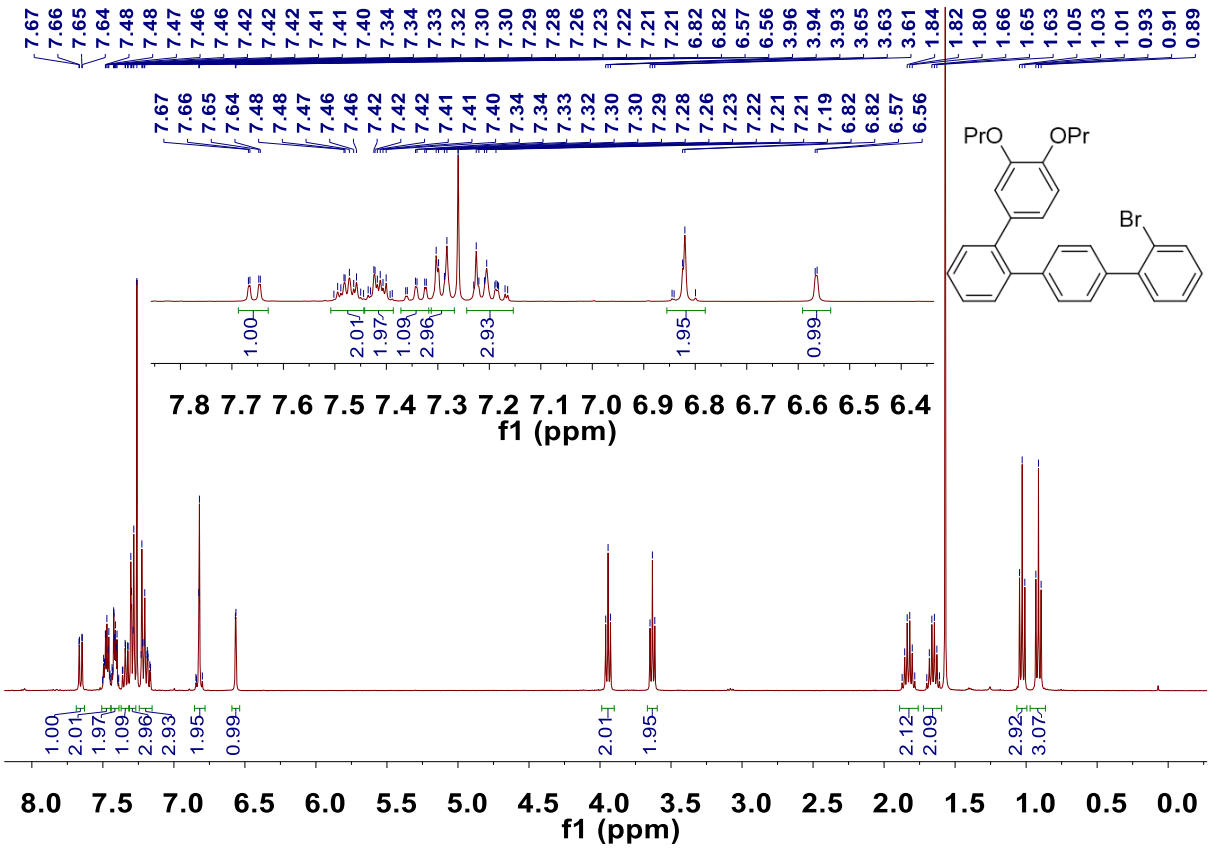


Figure S6. ^1H NMR spectrum of **20** in $CDCl_3$ at 298K.

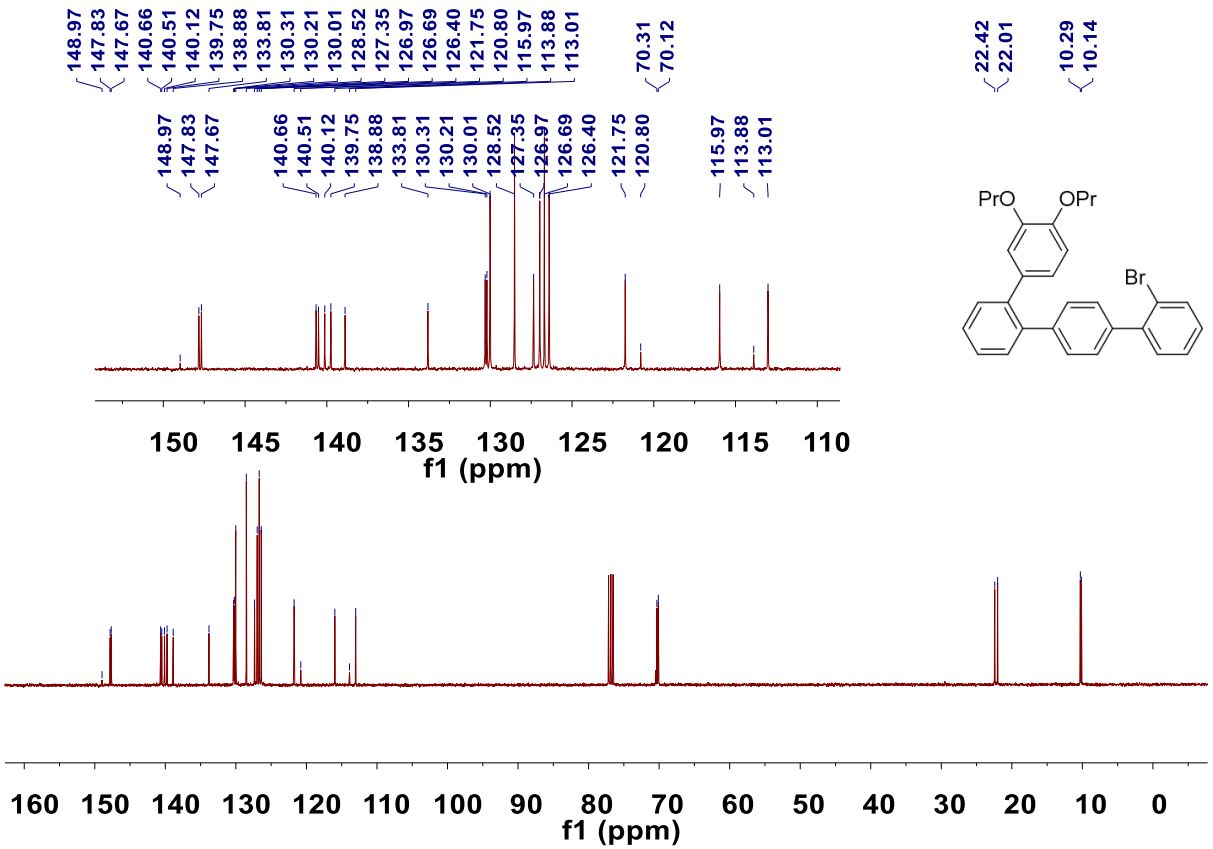


Figure S7. ^{13}C NMR spectrum of **20** in $CDCl_3$ at 298K.

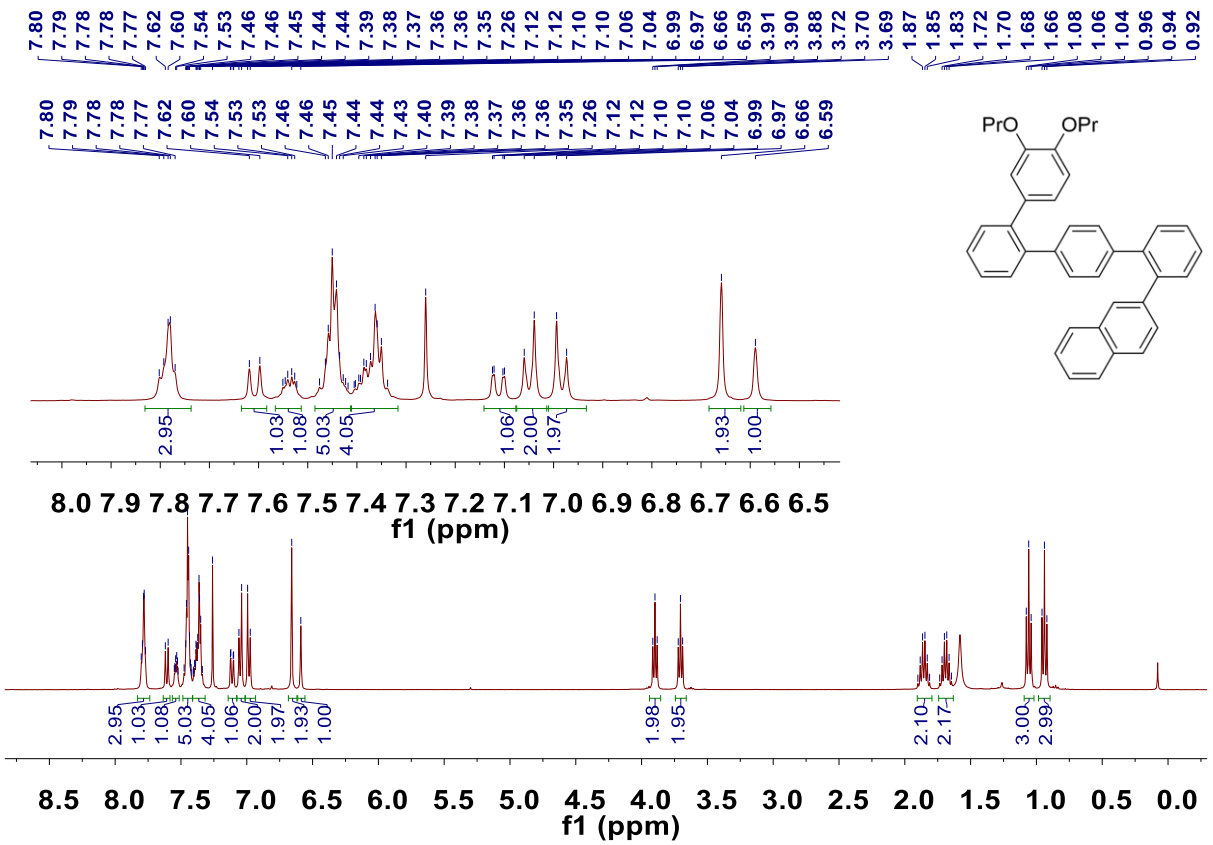


Figure S8. ^{1}H NMR spectrum of **12** in $CDCl_3$ at 298K.

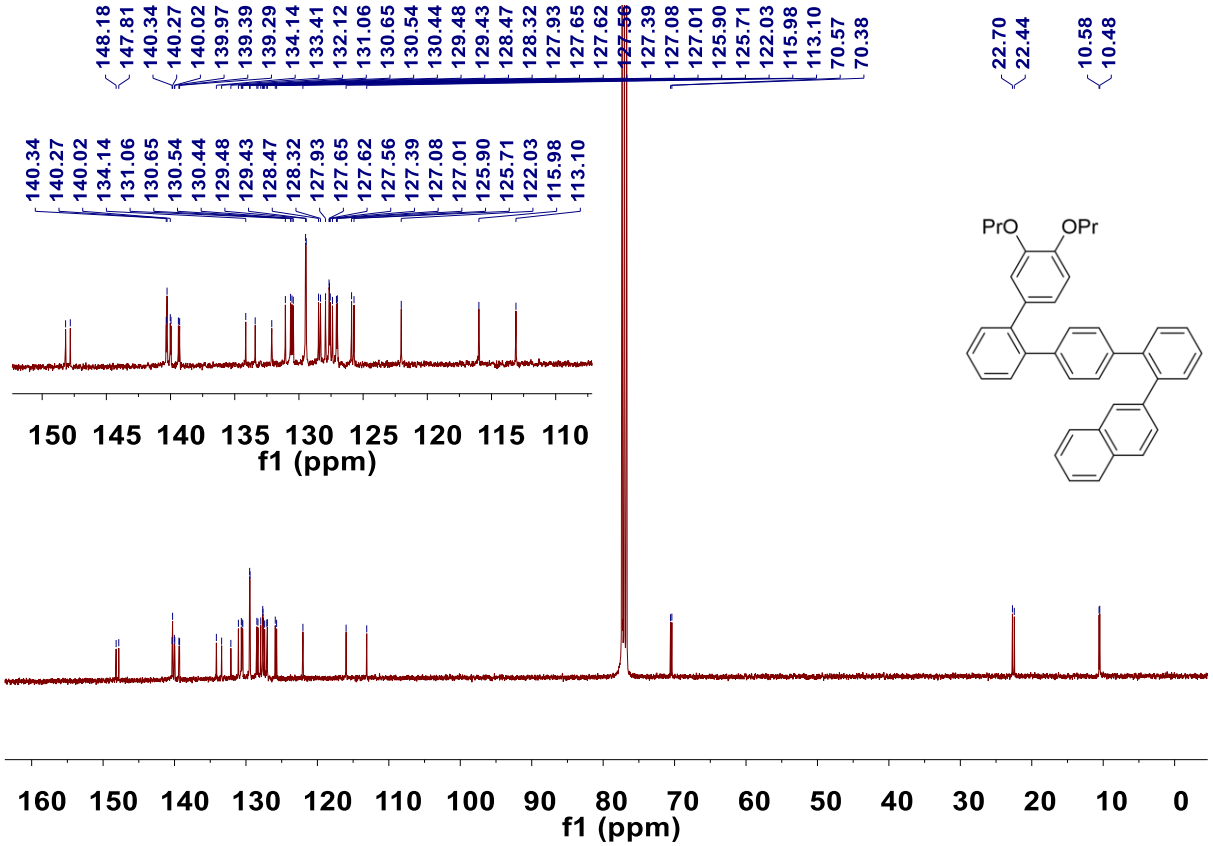


Figure S9. ^{13}C NMR spectrum of **12** in $CDCl_3$ at 298K.

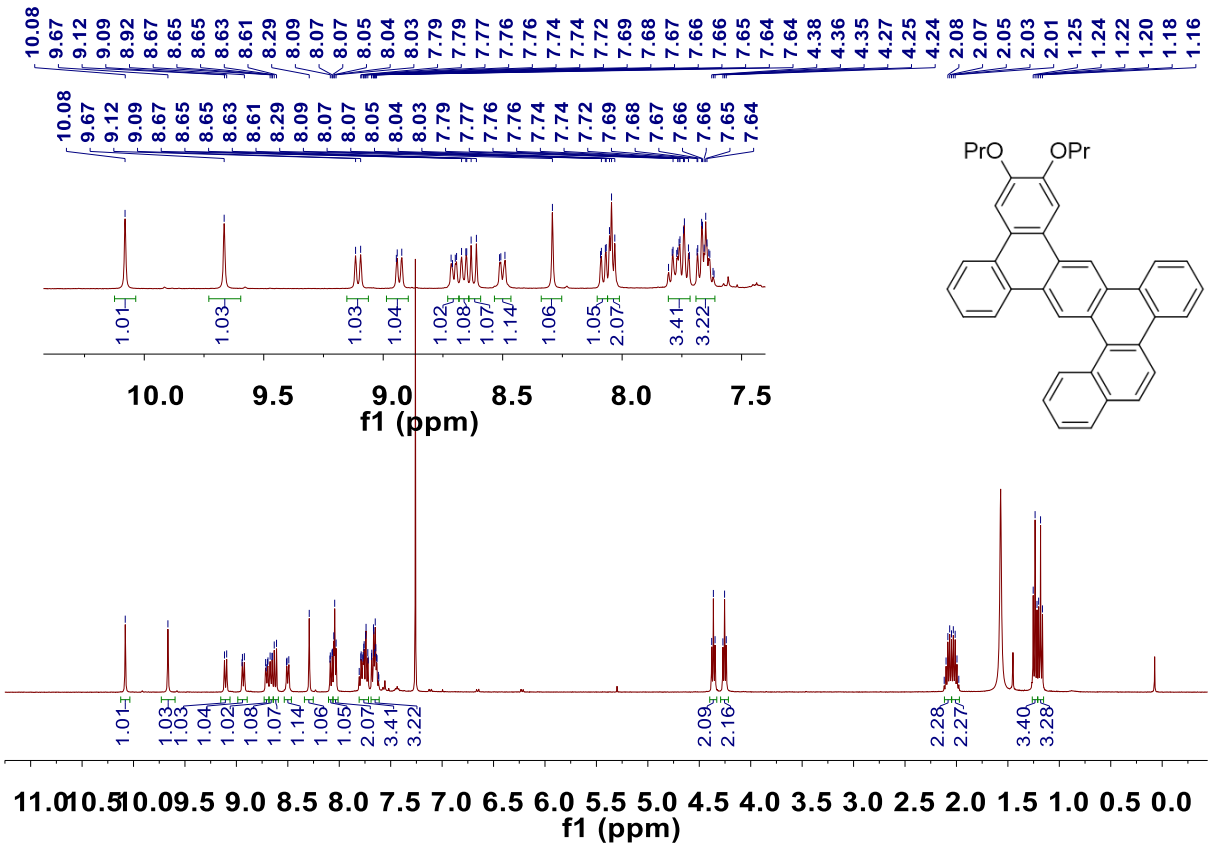


Figure S10. ^{1}H NMR spectrum of **13** in $CDCl_3$ at 298K.

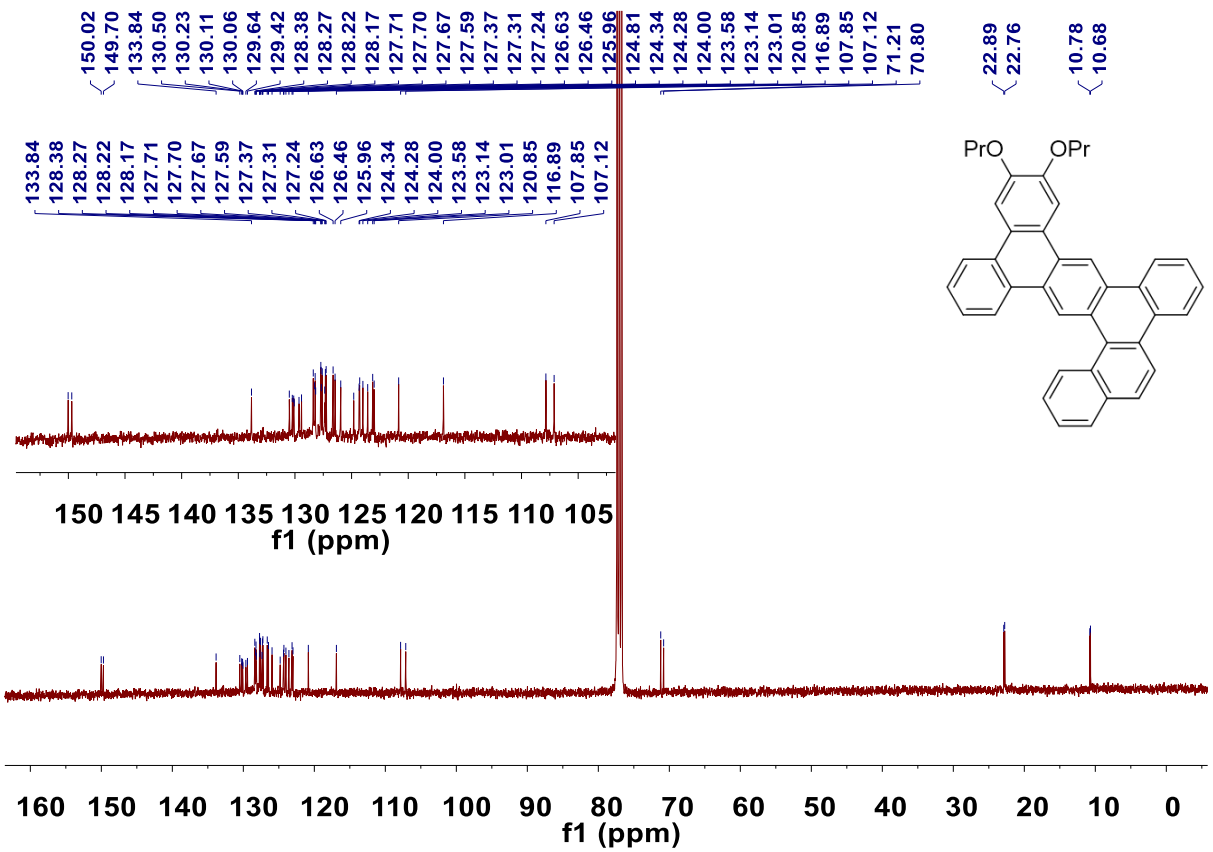


Figure S11. ^{13}C NMR spectrum of **13** in $CDCl_3$ at 298K.

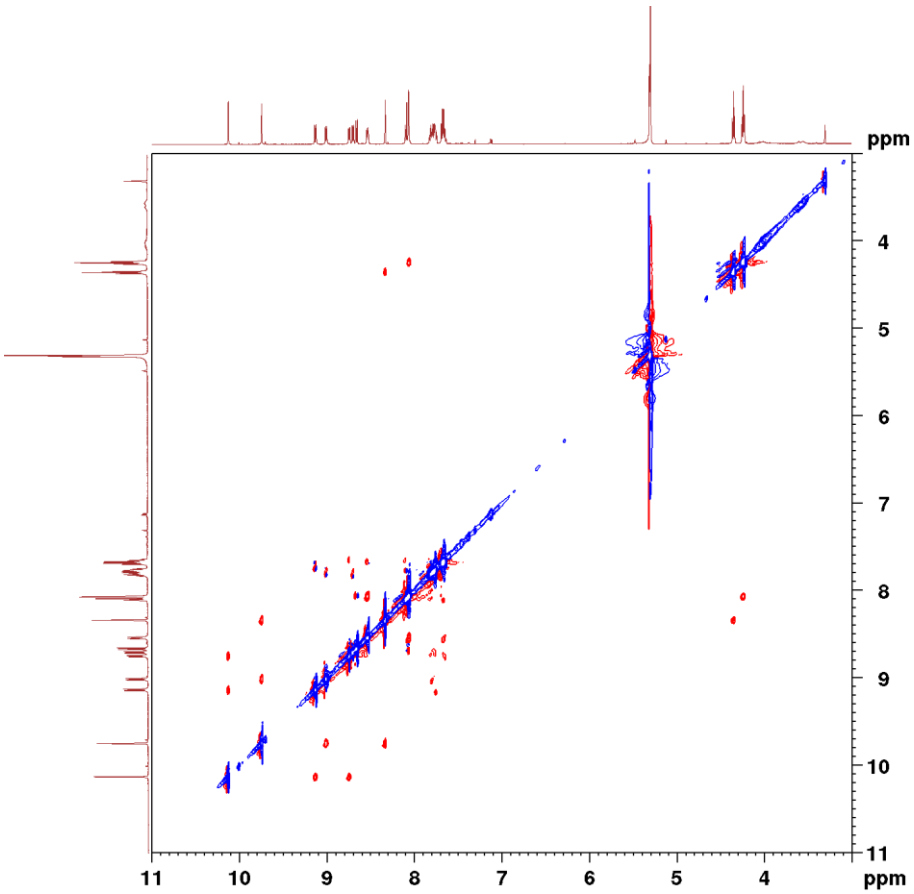


Figure S12. ROESY spectrum of 1**3** in CD_2Cl_2, 298K.

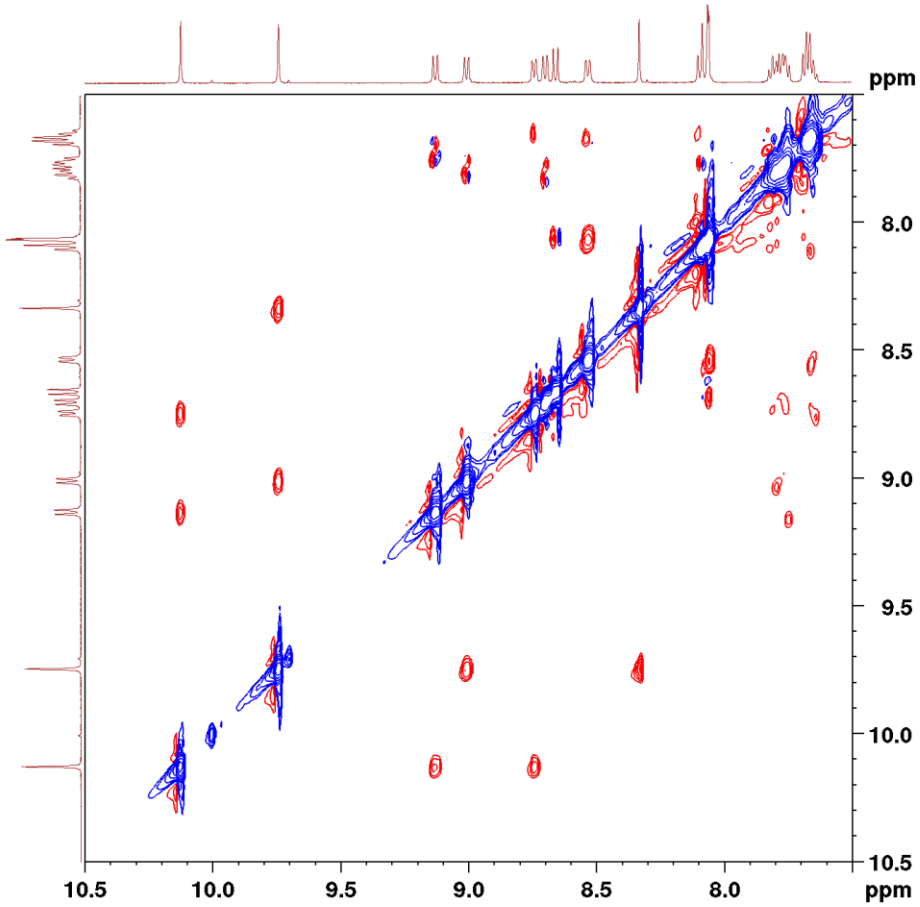


Figure S13. ROESY spectrum of 1**3** in CD_2Cl_2, 298K (aromatic region).

3. High resolution MALDI-TOF mass spectra

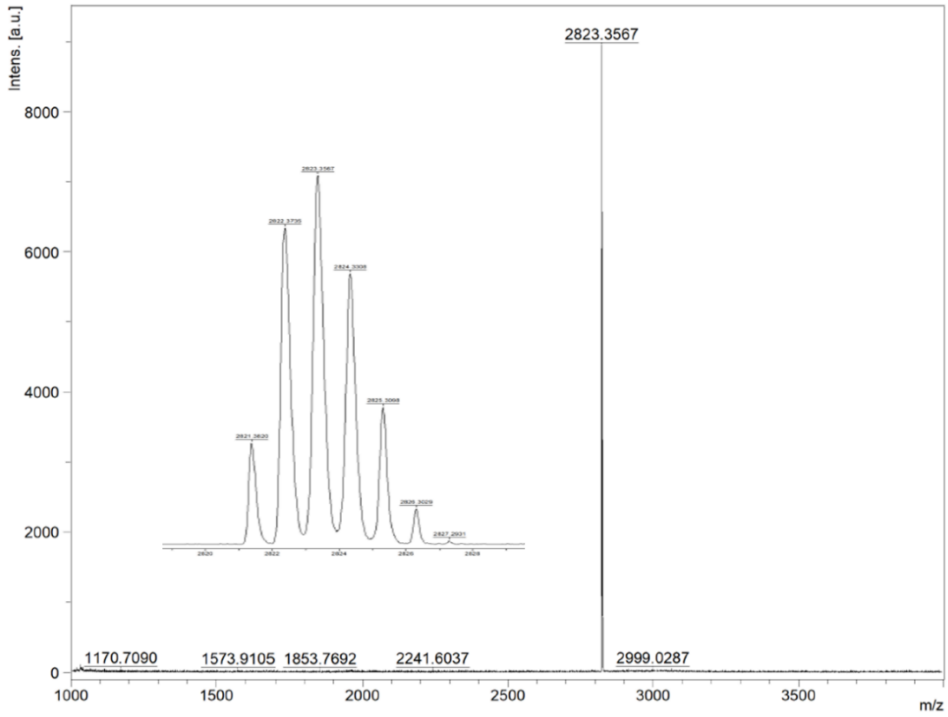


Figure S14. High resolution MALDI-TOF mass spectrum of **4**

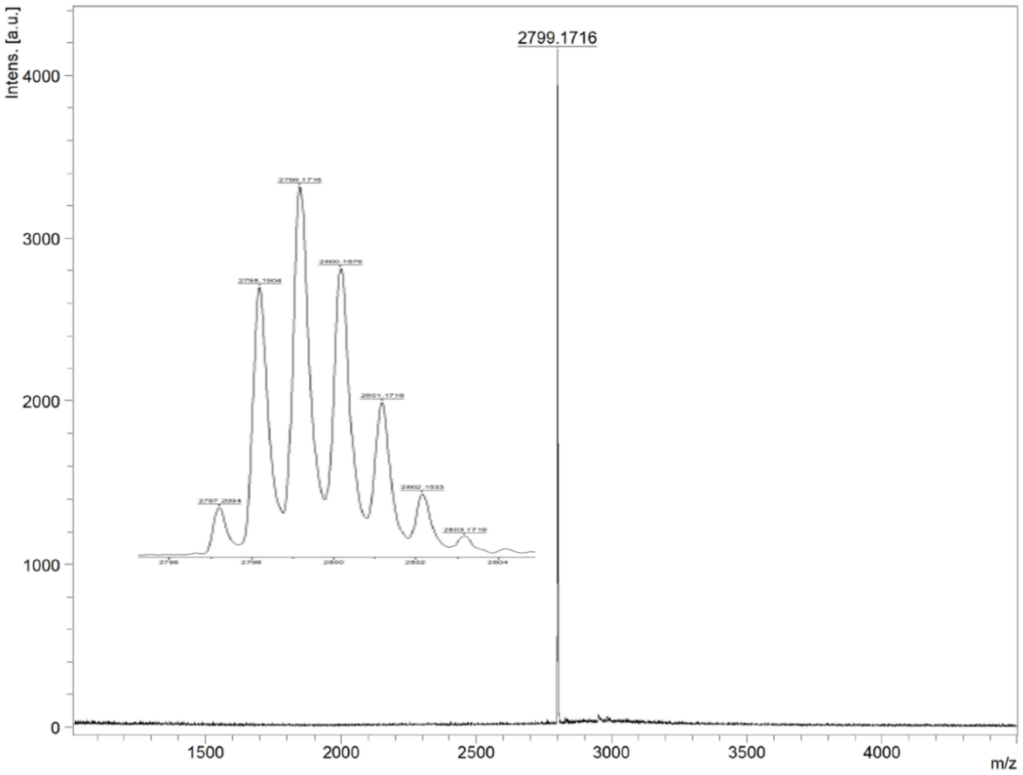


Figure S15. High resolution MALDI-TOF mass spectrum of **3**

4. Photophysical properties and florescence titration experiments

UV-vis absorption spectra were recorded on a Shimadzu UV-3600 Plus UV-VIS-NIR Spectrophotometer. Fluorescence spectra were taken on a Hitachi F-4500 spectrofluorometer.

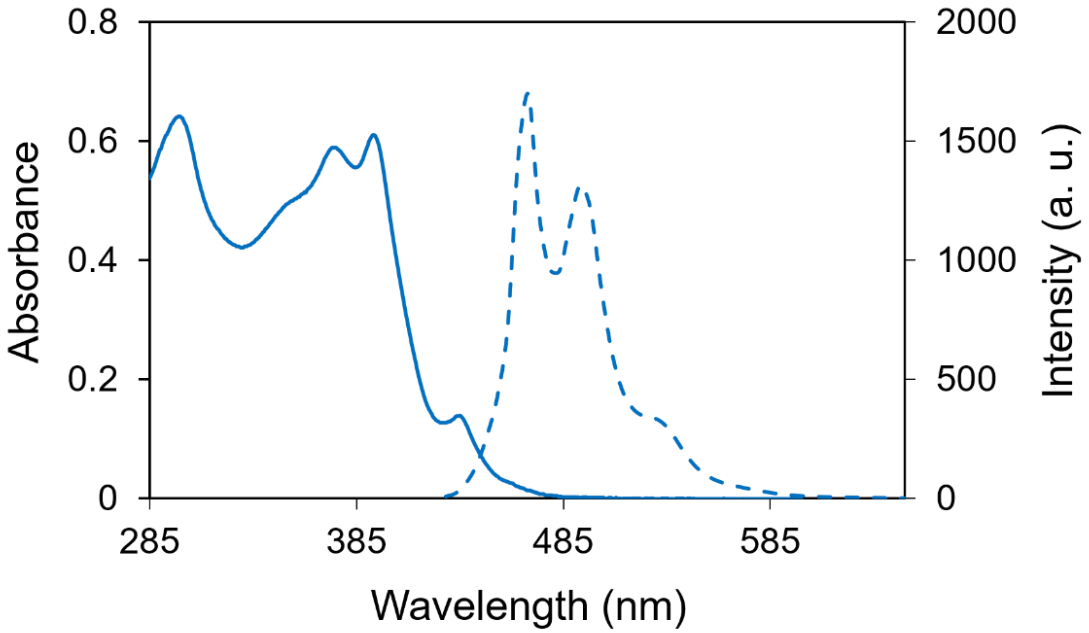


Figure S16. Absorption spectrum and photoluminescence spectrum of **3** in CH_2Cl_2 (5×10^{-6} mol/L). The photoluminescence spectrum of **3** was measured with excitation at 395 nm.

Determination of fluorescence quantum yield

The fluorescence quantum yields (Φ) of **3** were determined by comparing the photoluminescence (PL) integrated intensities (area) and absorbance intensities with 9,10-diphenylanthracene (DPA) as reference. The reported quantum yield for 9,10-diphenylanthracene (DPA) is 1 in toluene.[2] The quantum yield was calculated by using the following equation[3]:

$$\Phi_{sample} = \left(\frac{F_{sample}}{F_{ref}}\right)\left(\frac{A_{ref}}{A_{sample}}\right)\left(\frac{\eta_{sample}}{\eta_{ref}}\right)^2\Phi_{ref}$$

Where F is the integrated intensities (area under emission peak), A is the absorbance, η is the refractive index and Φ is the quantum yield, the subscript "ref" refers to reference. The reference 9,10-diphenylanthracene (DPA) and the nanobelt **3** were dissolved in toluene. The samples were measured by using UV-Vis spectrometer to obtain the absorbance values. The samples were then measured by PL spectrometer in order to get the PL emission intensity at the excitation wavelength of 380nm.

Table S1. Quantum yield of **3**

Sample	Integrated Intensities (F)	Absorbance Intensity (A)	Refractive Index (η)	Quantum Yield(Φ)
DPA	418288	0.055	1.496	1
3	88872	0.043	1.496	0.27

Florescence titration experiments

Job's plot

A solution of the hosts and fullerenes (C_{60} or C_{70}) in toluene were mixed in different ratios to prepare 11 samples with a fixed total concentration of 5×10^{-7} mol/L. The florescence of each sample was measured, and the changes of florescence intensity at 467nm were monitored for Job's plot analysis. Results showed that nanobelt **3** adopt 1:1 binding stoichiometry with C_{60} and C_{70} in toluene.

Determination of binding constant

Binding constant was determined by titrating a solution of the hosts with variable amounts of fullerenes in toluene. The change in the florescence (ΔF) of **3** at 467 nm was plotted against the concentration of fullerenes. On the basis of the 1:1 complex model, association constant K_a is calculated by non-linear curve fitting using the following equation:

$$\frac{F}{F_0} = (1 + (\frac{k_f}{k_s})K_a[L])/(1 + K_a[L])$$

where F, F_0, k_f, k_s, $[L]$ and K_a are fluorescence intensity, fluorescence intensity of the nanobelts before the addition of C_{60}, proportionality constant of the complex, proportionality constant of the host, the concentration of the guest, and the binding constant, respectively.[4] The binding constant of nanobelt **3** for C_{60} and C_{70} in toluene is determined as $(2.1\pm0.2)\times10^4$ M^{-1} and $(1.3\pm0.1)\times10^5$ M^{-1}, respectively.

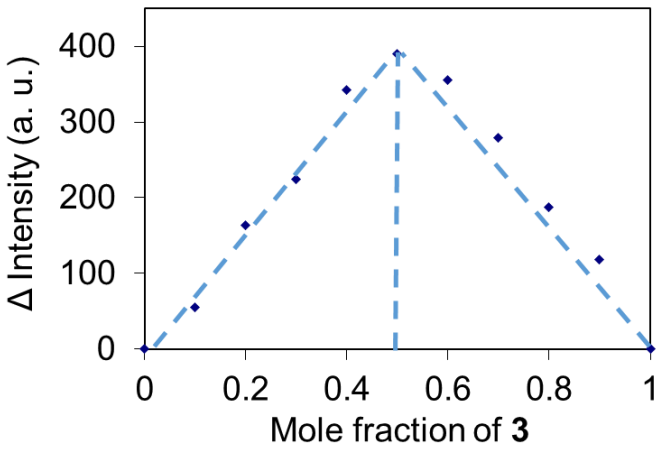


Figure S17. Job's plot based on the florescence change at 467 nm, indicating a 1:1 binding stoichiometry between **3** and C_{60} in toluene.

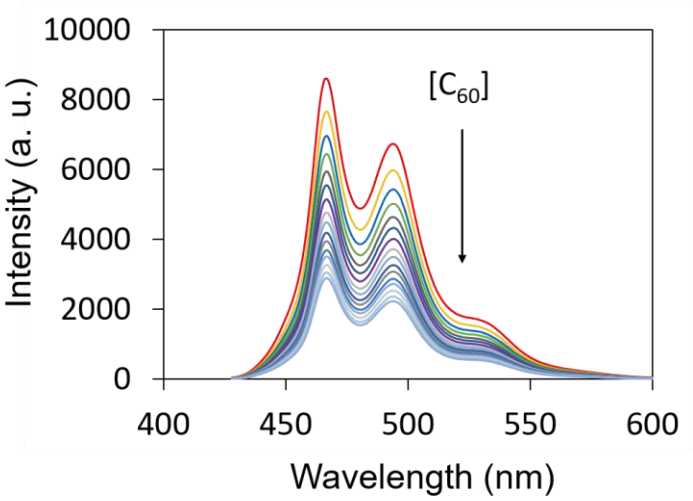


Figure S18. Florescence spectra of **3** in the presence of C_{60} (from 0 to 7.5×10^{-5} mol/L) in toluene.

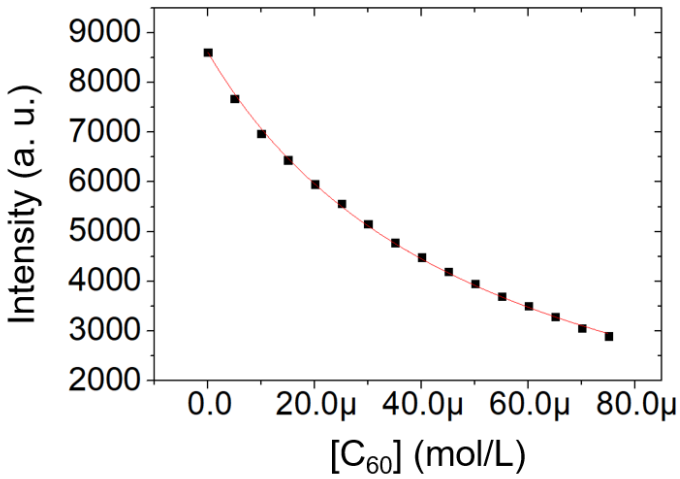


Figure S19. Nonlinear curve regression of the titration of **3** with C_{60} using 1:1 binding model. Based on this data set, K_a is calculated to be 1.9×10^4 M^{-1}.

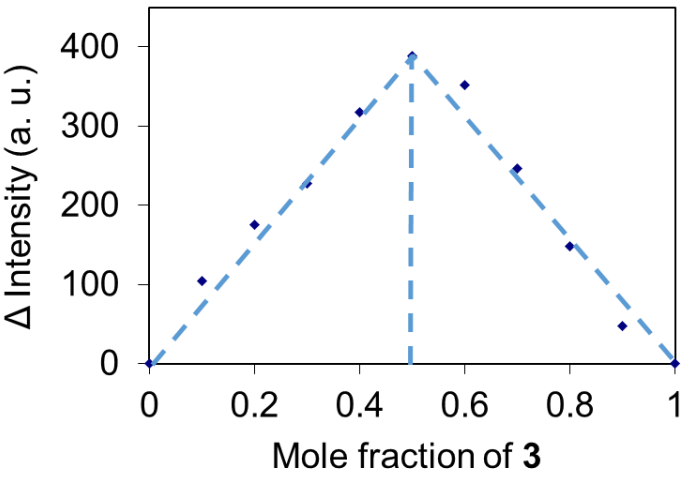


Figure S20. Job's plot based on the florescence change at 467 nm, indicating a 1:1 binding stoichiometry between **3** and C_{70} in toluene.

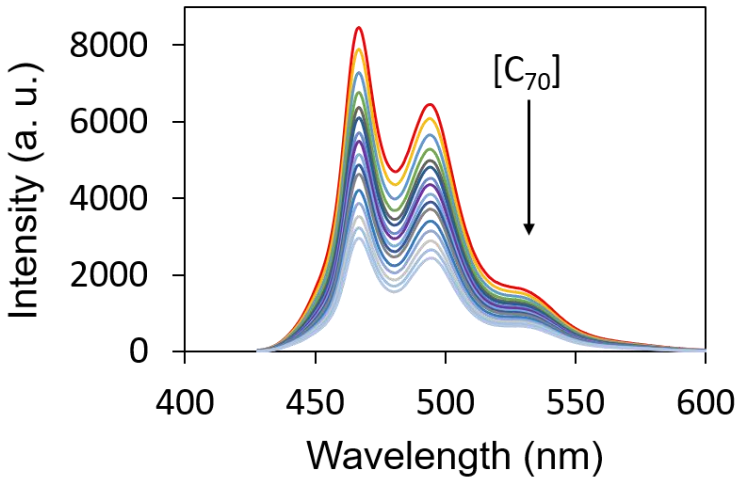


Figure S21. Florescence spectra of **3** in the presence of C_{70} (from 0.0 to 1.0×10^{-5} mol/L) in toluene.

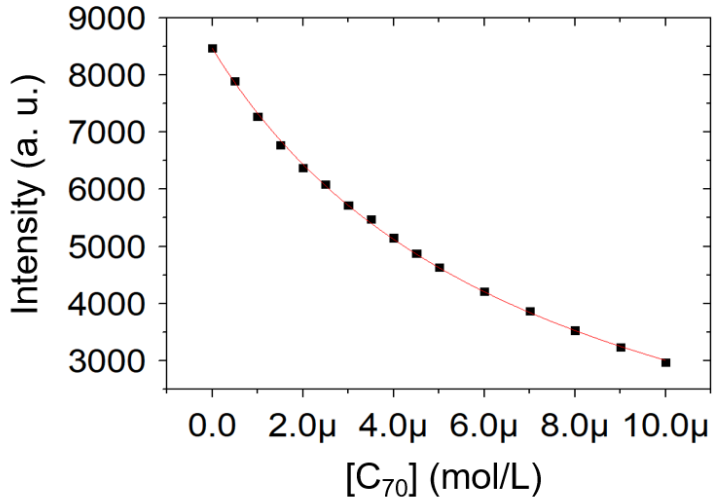


Figure S22. Nonlinear curve regression of the titration of **3** with C_{70} using 1:1 binding model. Based on this data set, K_a is calculated to be 1.4×10^5 M^{-1}.

5. Density Function Theory (DFT) Calculations

Gaussian 16 program [5] was used for the Density Function Theory (DFT) calculations.

The molecular geometry of nanobelt **3** was calculated at the B3LYP level of DFT with the 6-31g(d) basis set.

To study the reaction mechanism, calculations of compounds **15**–**17** and transition states **TS3** and **TS4** were carried out with the long-range corrected hybrid functional LC-wPBE [6] which has been found to successfully locate all transition states in conjunction with the def2-SVP basis set.[7]

Strain energy

The strain energy of the arylated [n]cycloparaphenylene (CPP) precursor (**4'**) was calculated using Itami's method,[8] which affords the strain energies of CNRs as a function of n^{-1} (n is the number of repeat unit in a CNR) by linear regression analysis of the total energy of CNRs per repeat unit as a function of n^{-2}. The strain energy of **3'** were calculated using Itami's modified method,[7] which combines linear regression analysis and homodesmotic reactions. Linear regression analysis was applied to helicene-free nanobelt $\mathbf{B_n}$ to determine its strain energies as a function of n^{-2} (n is the number of repeat unit in a nanobelt). The homodesmotic reaction shown in Figure S23c converts $\mathbf{B_6}$ to helicene-containing nanobelt **3'**. In order to reduce computational cost, a series of arylated CPPs ($\mathbf{A_n}$) and nanobelts ($\mathbf{B_n}$) without any substituents were calculated at the B3LYP level of density function theory (DFT) with the 6-31G(d) basis set. The strain energy of $\mathbf{A_n}$ is calculated as $146.1 \cdot n^{-1}$ kcal/mol. Therefore, the strain energy of **4'** (namely $\mathbf{A_3}$) is determined as 48.7 kcal/mol. The strain energy of $\mathbf{B_n}$ is calculated as $266.0 \cdot n^{-1}$ kcal/mol. By combining the strain of $\mathbf{B_6}$ (44.3 kcal/mol) and the enthalpy change of the hypothetical homodesmotic reaction (Figure S23c), the strain of **3'** is calculated to be 73.4 kcal/mol. Therefore, the ladderization step from **4'** to **3'** through the Scholl reaction is accompanied by an increase of strain of 24.7 kcal/mol.

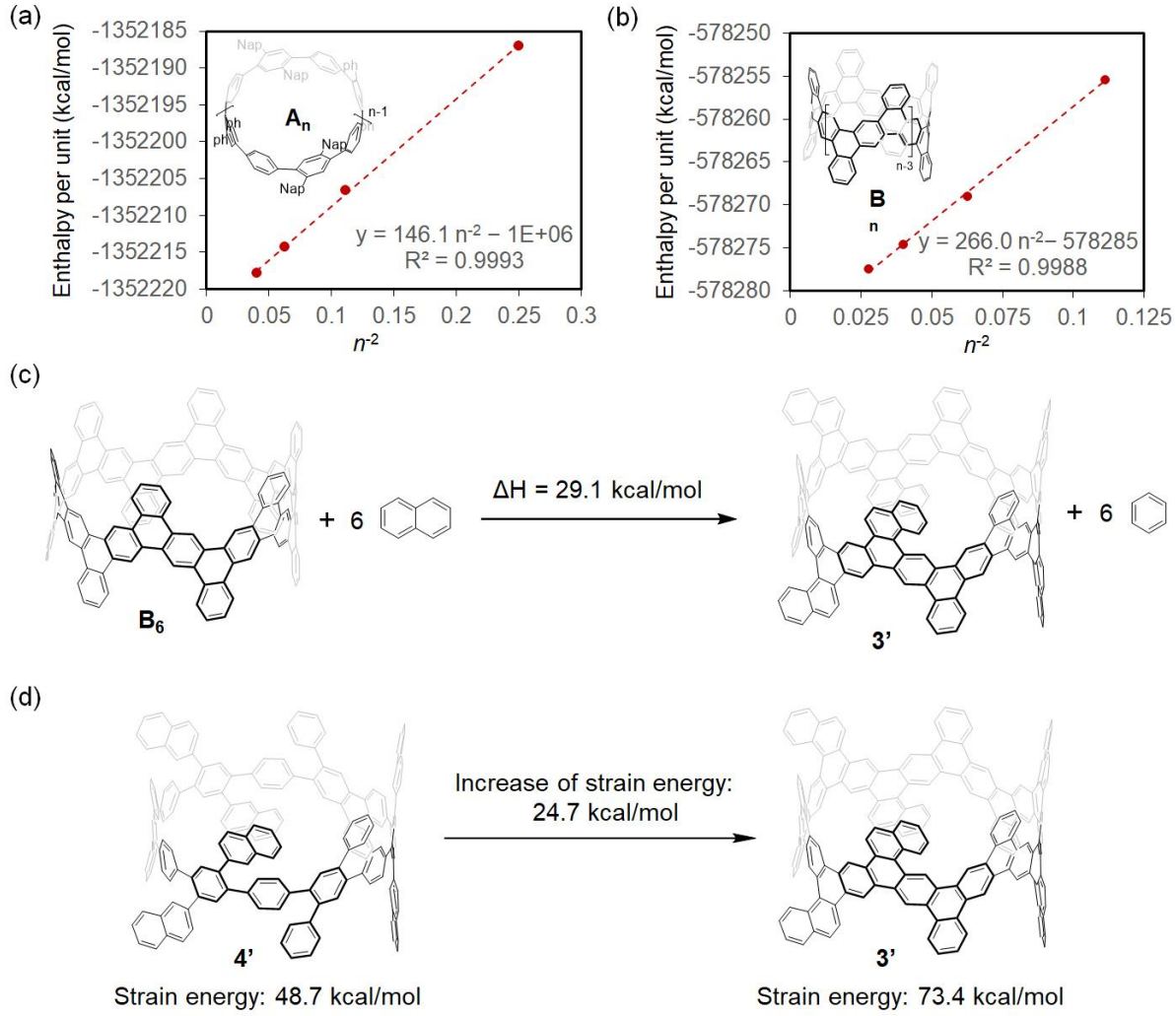


Figure S23. (a) Plot of enthalpy per unit of $\mathbf{A_n}$ as a function of n^{-2} with linear regression line; (b) plot of enthalpy per unit of $\mathbf{B_n}$ as a function of n^{-2} with linear regression line; (c) hypothetical homodesmotic reaction of **3'**; (d) the ladderization step from **3'** to **1'**.

Table S2. Uncorrected and thermal-corrected (298 K) energies of stationary points (Hartree): *E*: electronic energy; *ZPE*: zero-point energy; *H* (= *E* + *ZPE* + *E*vib + *E*rot + *E*trans + *RT*): sum of electronic and thermal enthalpies.

Molecule	*E* (Hartree)	*E+ZPE* (Hartree)	*H* (Hartree)	*H* (kcal/mol)
A_2	-4309.760385	-4309.844604	-4309.759441	-2704374.049
A_3	-6464.733852	-6464.861967	-6464.732908	-4056619.9
A_4	-8619.693222	-8619.864967	-8619.692277	-5408856.904
A_5	-10774.645419	-10774.860902	-10774.644475	-6761089.408
B_3	-2765.456291	-2764.614897	-2764.567701	-1734766.232
B_4	-3687.363982	-3686.240478	-3686.176782	-2313075.931
B_5	-4609.251666	-4607.846249	-4607.765865	-2891373.08
B_6	-5531.130272	-5529.443072	-5529.346034	-3469664.636
1'	-6450.868097	-6450.980319	-6450.867152	-4047919.138
Benzene	-232.143524	-232.147910	-232.142579	-145669.4683
Naphthalene	-385.738100	-385.744898	-385.737156	-242050.0654

Cartesian coordinates of compound **3** optimized at the B3LYP/6-31g(d) level of DFT

C	8.35840000	1.11670000	1.34030000
C	7.80490000	2.48280000	-1.08770000
C	8.34620000	0.40020000	0.10630000
C	7.88100000	2.43500000	1.32990000
C	7.52790000	3.11560000	0.15880000
C	8.15640000	1.12870000	-1.07410000
H	7.70520000	2.91010000	2.28490000
H	8.17690000	0.60390000	-2.02100000
C	8.31700000	-1.06370000	0.13720000
C	7.48560000	-3.77130000	0.26490000
C	8.21560000	-1.71500000	1.40120000
C	8.19710000	-1.84350000	-1.01850000
C	7.81930000	-3.19120000	-0.99390000
C	7.77350000	-3.04300000	1.42430000
H	8.32780000	-1.36430000	-1.97970000

H	7.57310000	-3.50030000	2.38410000
C	6.68960000	-5.00040000	0.27860000
C	4.50080000	-6.80000000	0.15330000
C	6.06940000	-5.47870000	1.43940000
C	6.35750000	-5.62180000	-0.96210000
C	5.22840000	-6.45180000	-0.99030000
C	5.02190000	-6.40650000	1.41950000
H	6.33400000	-5.03740000	2.39210000
H	4.86440000	-6.76670000	-1.95810000
C	3.17130000	-7.41660000	0.08450000
C	0.40260000	-8.06590000	-0.01330000
C	2.51100000	-7.63070000	-1.13020000
C	2.45500000	-7.67050000	1.28890000
C	1.09090000	-7.96900000	1.20220000
C	1.15760000	-7.97200000	-1.21850000
H	3.04350000	-7.43560000	-2.05150000
H	0.53100000	-8.04150000	2.12540000
C	-1.06320000	-8.10180000	-0.08250000
C	-3.82160000	-7.45770000	-0.22110000
C	-1.87280000	-8.10500000	1.05930000
C	-1.70090000	-7.98380000	-1.35100000
C	-3.05110000	-7.61900000	-1.37880000
C	-3.25320000	-7.86090000	1.02430000
H	-1.41050000	-8.21970000	2.02980000
H	-3.48060000	-7.35190000	-2.33610000
C	-5.07800000	-6.70510000	-0.21670000
C	-7.01600000	-4.63970000	-0.10590000
C	-5.63930000	-6.32730000	1.03790000
C	-5.65020000	-6.18140000	-1.38120000
C	-6.63170000	-5.18340000	-1.36640000
C	-6.57170000	-5.28340000	1.05430000
H	-5.26380000	-6.50740000	-2.33770000
H	-6.90600000	-4.90860000	2.01270000
H	5.00220000	6.30700000	-1.98870000
C	5.38450000	5.95440000	-1.03970000
C	6.27670000	4.93390000	1.35740000
C	4.80710000	6.43380000	0.14190000
C	6.36210000	4.95420000	-1.06210000

C	6.76210000	4.36760000	0.17300000
C	5.33100000	5.96450000	1.38090000
H	6.57640000	4.50320000	2.30390000
C	3.59980000	7.26870000	0.14250000
C	0.93830000	8.25140000	0.13910000
C	2.97760000	7.69320000	-1.03730000
C	2.94480000	7.54530000	1.37740000
C	1.61590000	7.98100000	1.33400000
C	1.69130000	8.25020000	-1.07280000
H	3.47010000	7.51400000	-1.98280000
H	1.06280000	8.00570000	2.26440000
C	-0.52260000	8.32330000	0.06710000
C	-3.27720000	7.69030000	-0.15250000
C	-1.34210000	8.23830000	1.19800000
C	-1.14200000	8.29150000	-1.21650000
C	-2.49650000	7.94470000	-1.28540000
C	-2.71200000	7.95950000	1.12820000
H	-0.88390000	8.31880000	2.17490000
H	-2.93890000	7.79440000	-2.26120000
C	-4.56070000	6.98800000	-0.21540000
C	-6.51410000	4.93130000	-0.18640000
C	-5.05340000	6.43230000	-1.40210000
C	-5.23830000	6.67590000	1.00100000
C	-6.14540000	5.60660000	0.98320000
C	-6.05490000	5.45580000	-1.42950000
H	-4.57180000	6.68680000	-2.33790000
H	-6.51010000	5.24450000	1.93460000
C	-7.21970000	3.64410000	-0.16890000
C	-8.04000000	0.91980000	-0.17340000
C	-7.48790000	2.98020000	-1.40070000
C	-7.50880000	2.96450000	1.02040000
C	-7.93400000	1.63190000	1.05620000
C	-7.87120000	1.63560000	-1.36420000
H	-7.31440000	3.45750000	1.96420000
H	-7.95510000	1.10980000	-2.30630000
C	-8.16380000	-0.54250000	-0.14970000
C	-7.68760000	-3.33850000	-0.08260000
C	-8.17930000	-1.31600000	-1.31630000

C	-8.12180000	-1.22440000	1.10040000
C	-7.83530000	-2.59390000	1.09380000
C	-8.01860000	-2.70900000	-1.31960000
H	-8.23550000	-0.81840000	-2.27430000
H	-7.61450000	-3.06720000	2.04220000
C	0.49340000	-8.16210000	-2.51170000
C	-0.80490000	-8.51590000	-4.99240000
C	-0.91870000	-8.15780000	-2.57530000
C	1.23300000	-8.34370000	-3.69980000
C	0.61270000	-8.50020000	-4.93220000
C	-1.53370000	-8.35160000	-3.82940000
H	2.31250000	-8.38300000	-3.64760000
H	-2.61350000	-8.39520000	-3.91950000
C	3.13890000	-7.54610000	2.57820000
C	4.47080000	-7.27830000	5.06390000
C	4.40130000	-6.91230000	2.64670000
C	2.58100000	-8.05360000	3.76950000
C	3.21260000	-7.92980000	4.99240000
C	5.04810000	-6.79700000	3.89620000
H	1.63180000	-8.57740000	3.76390000
H	6.03190000	-6.34840000	3.93920000
C	-7.29270000	3.69050000	-2.66650000
C	-6.88660000	5.07400000	-5.10460000
C	-6.57520000	4.90830000	-2.68470000
C	-7.81170000	3.20280000	-3.88350000
C	-7.62100000	3.86050000	-5.08390000
C	-6.39180000	5.58300000	-3.91110000
H	-8.39770000	2.29120000	-3.91650000
H	-5.87900000	6.53580000	-3.91490000
C	-8.20600000	0.94160000	2.31940000
C	-8.72410000	-0.41750000	4.75050000
C	-8.29230000	-0.46950000	2.34420000
C	-8.40300000	1.64360000	3.52660000
C	-8.65260000	0.99890000	4.72330000
C	-8.55880000	-1.12350000	3.56660000
H	-8.37850000	2.72720000	3.55420000
H	-8.66620000	-2.20020000	3.57340000
C	6.92820000	4.45700000	-2.31810000

C	8.02460000	3.46980000	-4.73820000
C	6.80460000	5.17190000	-3.52710000
C	7.63410000	3.23220000	-2.33490000
C	8.17660000	2.76450000	-3.55130000
C	7.32800000	4.70550000	-4.71790000
H	6.30030000	6.13110000	-3.56070000
H	8.75180000	1.84810000	-3.55020000
C	4.82460000	6.51720000	2.63910000
C	3.81730000	7.58210000	5.06340000
C	5.49160000	6.31460000	3.86460000
C	3.64090000	7.29020000	2.64100000
C	3.16300000	7.81550000	3.86100000
C	5.01510000	6.82170000	5.05880000
H	6.42150000	5.75910000	3.91030000
H	2.27880000	8.43920000	3.85320000
C	-0.34790000	8.59720000	-2.40980000
C	1.05380000	8.68070000	-2.32190000
C	-0.26830000	9.15920000	-4.78090000
C	1.80610000	9.17510000	-3.45670000
C	-0.98520000	8.84160000	-3.66200000
C	1.13700000	9.36050000	-4.71040000
C	3.17130000	9.57330000	-3.38970000
H	-2.06560000	8.78560000	-3.73070000
H	1.33560000	9.90760000	-6.78880000
H	-0.77280000	9.31680000	-5.73110000
C	3.85030000	10.02310000	-4.50380000
H	3.68200000	9.56650000	-2.43510000
H	4.88870000	10.32940000	-4.41010000
C	3.20390000	10.10920000	-5.75510000
H	3.75110000	10.44950000	-6.62990000
C	1.86540000	9.79890000	-5.84520000
C	-3.56640000	7.91550000	2.31810000
C	-4.86120000	7.37130000	2.23640000
C	-3.90110000	8.45230000	4.67240000
C	-5.76170000	7.51560000	3.36160000
C	-3.10940000	8.44950000	3.55890000
C	-5.25150000	8.01420000	4.60460000
C	-7.16220000	7.27010000	3.29140000

H	-2.11480000	8.87620000	3.62190000
H	-5.68700000	8.48460000	6.66560000
H	-3.52410000	8.84360000	5.61440000
C	-7.97870000	7.41230000	4.39470000
H	-7.61020000	7.00790000	2.34140000
H	-9.04530000	7.22800000	4.29810000
C	-7.44600000	7.81430000	5.63790000
H	-8.09400000	7.90910000	6.50480000
C	-6.10770000	8.12470000	5.72940000
C	-7.24900000	-4.67160000	-2.59340000
C	-8.02600000	-3.49930000	-2.55540000
C	-7.68300000	-4.92500000	-4.97880000
C	-8.78650000	-3.11590000	-3.72690000
C	-7.09260000	-5.36700000	-3.82870000
C	-8.56370000	-3.80940000	-4.96110000
C	-9.81630000	-2.13300000	-3.71650000
H	-6.49920000	-6.27340000	-3.86060000
H	-9.05600000	-3.94780000	-7.05780000
H	-7.52800000	-5.45600000	-5.91480000
C	-10.50230000	-1.79030000	-4.86400000
H	-10.10270000	-1.67120000	-2.78010000
H	-11.29030000	-1.04370000	-4.81360000
C	-10.20530000	-2.41460000	-6.09410000
H	-10.73980000	-2.12700000	-6.99520000
C	-9.26370000	-3.41870000	-6.13060000
C	-5.21010000	-7.01590000	2.25840000
C	-4.08410000	-7.85900000	2.23320000
C	-5.57620000	-7.51460000	4.61670000
C	-3.78760000	-8.67840000	3.39040000
C	-5.94090000	-6.86150000	3.47330000
C	-4.51170000	-8.45640000	4.60720000
C	-2.86530000	-9.76280000	3.37820000
H	-6.81420000	-6.21960000	3.49220000
H	-4.75390000	-9.00860000	6.67950000
H	-6.13290000	-7.36280000	5.53830000
C	-2.60360000	-10.50450000	4.51220000
H	-2.38720000	-10.04490000	2.44870000
H	-1.90190000	-11.33260000	4.46010000

C	-3.25410000	-10.21210000	5.72990000
H	-3.03030000	-10.79160000	6.62120000
C	-4.20390000	-9.21580000	5.76440000
C	7.73310000	-4.00460000	-2.21020000
C	7.09740000	-5.25910000	-2.17560000
C	8.26840000	-4.30090000	-4.57080000
C	7.18870000	-6.13090000	-3.32890000
C	8.31250000	-3.54860000	-3.43100000
C	7.73230000	-5.61730000	-4.55150000
C	6.84430000	-7.51230000	-3.30720000
H	8.81020000	-2.58600000	-3.45810000
H	8.18590000	-6.01670000	-6.62360000
H	8.69450000	-3.92220000	-5.49670000
C	6.93480000	-8.30020000	-4.43710000
H	6.54760000	-7.97240000	-2.37320000
H	6.68000000	-9.35500000	-4.37540000
C	7.38190000	-7.75610000	-5.66030000
H	7.44160000	-8.38120000	-6.54730000
C	7.78830000	-6.44100000	-5.70450000
C	8.54710000	-0.97720000	2.62330000
C	8.71820000	0.41850000	2.57920000
C	9.06150000	-1.00200000	5.00600000
C	9.23060000	1.10600000	3.74670000
C	8.72580000	-1.66510000	3.85960000
C	9.34720000	0.39020000	4.98290000
C	9.71020000	2.44620000	3.73030000
H	8.60420000	-2.74180000	3.89350000
H	9.85750000	0.49410000	7.07740000
H	9.16840000	-1.54280000	5.94320000
C	10.17360000	3.06390000	4.87410000
H	9.75520000	2.98470000	2.79210000
H	10.54250000	4.08460000	4.81910000
C	10.19280000	2.37680000	6.10640000
H	10.54460000	2.87660000	7.00460000
C	9.80200000	1.05710000	6.14850000
O	-8.78040000	1.73860000	5.87230000
O	-8.97180000	-0.97950000	5.96750000
O	-8.10700000	3.30180000	-6.23890000

O	-6.73830000	5.66160000	-6.32570000
O	5.68740000	6.53620000	6.21980000
O	3.40490000	8.04290000	6.27880000
O	7.12590000	5.42610000	-5.86820000
O	8.50890000	3.07410000	-5.94980000
O	2.58730000	-8.39850000	6.11990000
O	5.02850000	-7.19110000	6.30440000
O	-1.46940000	-8.64390000	-6.18610000
O	1.26800000	-8.65620000	-6.11700000
C	2.17160000	8.75570000	6.36130000
H	2.23030000	9.67900000	5.76550000
H	1.35930000	8.13920000	5.94910000
C	1.91450000	9.07690000	7.82730000
H	2.75580000	9.66740000	8.21050000
H	1.90360000	8.13790000	8.39350000
C	0.59930000	9.83610000	8.02910000
H	0.43670000	10.05780000	9.08880000
H	0.59800000	10.78940000	7.48670000
H	-0.25900000	9.25060000	7.67760000
C	6.35870000	7.63620000	6.86050000
H	7.03020000	8.11880000	6.13420000
H	5.62230000	8.37450000	7.19560000
C	7.14780000	7.08150000	8.03880000
H	6.44570000	6.58890000	8.72330000
H	7.57460000	7.93440000	8.58410000
C	-10.10360000	1.81980000	6.42800000
H	-10.47530000	0.81470000	6.65970000
H	-10.77950000	2.27410000	5.68750000
C	-10.02730000	2.67310000	7.68560000
H	-9.32130000	2.20360000	8.38150000
H	-9.60490000	3.65050000	7.42120000
C	-11.39520000	2.84720000	8.35310000
H	-11.82460000	1.88090000	8.64470000
H	-11.31480000	3.46020000	9.25710000
H	-12.10970000	3.33850000	7.68140000
C	-8.97340000	-2.40270000	6.08370000
H	-9.79120000	-2.82420000	5.48150000
H	-8.02400000	-2.80370000	5.69920000

C	-9.14980000	-2.75320000	7.55590000
H	-10.10220000	-2.33260000	7.90280000
H	-9.24430000	-3.84500000	7.62720000
C	-8.00070000	-2.26090000	8.44090000
H	-7.04730000	-2.70920000	8.13540000
H	-7.89620000	-1.17400000	8.37350000
H	-8.17350000	-2.52490000	9.48990000
C	9.13850000	1.79610000	-6.05000000
H	10.04360000	1.77630000	-5.42400000
H	8.45210000	1.02090000	-5.68100000
C	9.49140000	1.54890000	-7.51120000
H	8.56920000	1.59130000	-8.10360000
H	9.86850000	0.52020000	-7.58680000
C	10.52690000	2.52690000	-8.07380000
H	10.15560000	3.55570000	-8.03980000
H	11.46180000	2.48670000	-7.50110000
H	10.76320000	2.28820000	-9.11640000
C	8.27480000	6.11360000	-6.39320000
H	8.68780000	6.77130000	-5.61320000
H	9.04540000	5.38600000	-6.67330000
C	7.82710000	6.92440000	-7.60170000
H	7.40290000	6.23470000	-8.34230000
H	8.72380000	7.36590000	-8.05760000
C	6.81310000	8.02130000	-7.26290000
H	5.91390000	7.59450000	-6.80900000
H	7.23780000	8.74370000	-6.55420000
H	6.51400000	8.57170000	-8.16200000
C	8.25740000	6.10690000	7.63250000
H	7.84520000	5.25010000	7.09140000
H	8.99110000	6.59670000	6.97950000
H	8.79200000	5.73070000	8.51200000
C	6.25230000	-6.47230000	6.46350000
H	7.05400000	-6.97480000	5.90320000
H	6.13660000	-5.45630000	6.05800000
C	6.57930000	-6.42540000	7.95080000
H	6.68070000	-7.45450000	8.31830000
H	7.56610000	-5.95540000	8.05780000
C	5.53780000	-5.66780000	8.77980000

H	5.45810000	-4.62330000	8.45440000
H	4.55010000	-6.12670000	8.67710000
H	5.80730000	-5.66760000	9.84150000
C	3.16470000	-9.56670000	6.73120000
H	3.24030000	-10.36540000	5.97790000
H	4.17270000	-9.33480000	7.09250000
C	2.25930000	-9.99190000	7.87920000
H	2.19200000	-9.16050000	8.59230000
H	2.75520000	-10.81920000	8.40490000
C	0.85710000	-10.41600000	7.43200000
H	0.35040000	-9.59950000	6.90920000
H	0.90510000	-11.27450000	6.74990000
H	0.24140000	-10.70600000	8.29080000
C	-1.41430000	-9.94060000	-6.80900000
H	-0.37110000	-10.21270000	-7.00850000
H	-1.84270000	-10.68490000	-6.12220000
C	-2.21610000	-9.87430000	-8.10160000
H	-2.25450000	-10.88840000	-8.52230000
H	-3.24890000	-9.59430000	-7.85790000
C	-1.63670000	-8.89680000	-9.12850000
H	-1.59600000	-7.88380000	-8.71720000
H	-0.61740000	-9.18410000	-9.41500000
H	-2.24670000	-8.87310000	-10.03850000
C	2.69320000	-8.54160000	-6.13380000
H	2.99020000	-7.58570000	-5.67920000
H	3.13770000	-9.35350000	-5.54050000
C	3.15890000	-8.61570000	-7.58210000
H	2.84970000	-9.58160000	-8.00180000
H	4.25700000	-8.61260000	-7.57120000
C	2.63500000	-7.46880000	-8.45150000
H	1.54120000	-7.46210000	-8.47030000
H	2.97080000	-6.49800000	-8.06700000
H	2.99480000	-7.56300000	-9.48190000
C	-5.93880000	6.83990000	-6.43290000
H	-6.39920000	7.65540000	-5.85650000
H	-4.94070000	6.64580000	-6.01320000
C	-5.84110000	7.20850000	-7.90800000
H	-6.85390000	7.38830000	-8.29040000

H	-5.30580000	8.16500000	-7.97520000
C	-5.13670000	6.14520000	-8.75600000
H	-4.10620000	5.98720000	-8.41480000
H	-5.66080000	5.18700000	-8.69250000
H	-5.09810000	6.44610000	-9.80850000
C	-9.22400000	3.97220000	-6.85050000
H	-10.03100000	4.07400000	-6.10920000
H	-8.92180000	4.97460000	-7.17330000
C	-9.68300000	3.13390000	-8.03590000
H	-8.84370000	3.03740000	-8.73630000
H	-10.46720000	3.69830000	-8.55870000
C	-10.20300000	1.74750000	-7.64400000
H	-9.43030000	1.17330000	-7.12450000
H	-11.07000000	1.82750000	-6.97580000
H	-10.51430000	1.17980000	-8.52820000

Cartesian coordinates of compound **15** optimized at the LC-ωPBE/def2-SVP level of DFT

C	2.86807500	-2.19604300	-0.90283600
C	2.01087200	-4.58457800	-2.07092100
C	1.55931300	-2.29461400	-1.40629300
C	3.72473000	-3.30246300	-0.99760200
C	3.30722300	-4.48509900	-1.57411800
C	1.15425700	-3.50313500	-1.98554900
H	4.74333300	-3.24961800	-0.61505600
H	3.99126200	-5.33330000	-1.63720600
H	0.14630700	-3.61294800	-2.38213400
H	1.66617800	-5.51404600	-2.52839800
C	0.64851200	-1.14156300	-1.31793000
C	-1.11689600	1.08603600	-1.14800300
C	1.07539900	0.07284900	-0.72526600
C	-0.65702200	-1.20282500	-1.81394500
C	-1.51935600	-0.12757600	-1.73398100
C	0.16992000	1.16005300	-0.65996500
H	-1.02371900	-2.11366400	-2.28337700
H	-2.52829000	-0.21879000	-2.14044700
H	0.47259300	2.09979300	-0.20038600
C	-2.02557000	2.26333600	-1.09813600
C	-3.67315300	4.52217300	-1.13477600
C	-1.56060500	3.48497200	-1.59227500

C	-3.33956200	2.17507900	-0.60640900
C	-4.14567300	3.31483600	-0.64109400
C	-2.37190200	4.60973500	-1.61153800
H	-0.54957200	3.54233800	-2.00383000
H	-5.16367500	3.25011000	-0.24970200
H	-1.99201600	5.55163400	-2.01275000
H	-4.32479300	5.39846200	-1.14549500
C	3.31274700	-0.94298300	-0.28684300
C	4.13400100	1.51279600	0.91365400
C	4.58385200	-0.79997000	0.22156900
C	2.40926300	0.18329700	-0.19965200
C	2.86718200	1.37656500	0.40647200
C	5.04072000	0.38368300	0.82112500
H	5.31310700	-1.60665600	0.18650600
H	2.19475900	2.22526200	0.47926000
C	-3.90009100	0.91943500	-0.03349900
H	-2.37200700	0.68089600	1.44378400
C	-3.29060200	0.27416700	1.01290200
C	-5.65191700	-0.75653600	-0.04591200
C	-3.83374600	-0.91196700	1.57137500
C	-5.10965100	0.38681200	-0.55970900
C	-5.03050300	-1.44014700	1.03270000
C	-3.21357600	-1.58370200	2.65924900
H	-5.59928100	0.89943500	-1.39136200
H	-6.49932500	-3.03148800	1.17133700
H	-6.57853900	-1.15953700	-0.46191400
C	-3.75890800	-2.72484200	3.17664200
H	-2.29351300	-1.16989400	3.07963400
H	-3.27653300	-3.23223300	4.01505700
C	-4.95454000	-3.25510300	2.63420400
H	-5.38198700	-4.16629200	3.05822900
C	-5.57386800	-2.62828200	1.58965300
O	6.26919500	0.35509800	1.25072600
O	4.61311400	2.60239400	1.49151300
C	6.99759000	1.40213000	1.89543200
H	7.08073400	2.27446800	1.23762700
H	7.98713800	0.97697900	2.08965400
H	6.51327100	1.68423300	2.83694700

C	3.79743100	3.75274700	1.62800700
H	3.48939400	4.13059100	0.64186500
H	4.41071000	4.50698800	2.13115200
H	2.91231700	3.53171000	2.24269900

Cartesian coordinates of compound **16** optimized at the LC-ωPBE/def2-SVP level of DFT

C	-2.47874800	2.38856100	-0.11108600
C	-2.70617400	5.10171500	0.55549800
C	-1.32388000	3.17374300	0.05613500
C	-3.73917000	2.99305900	0.05916000
C	-3.85597200	4.32376200	0.38449800
C	-1.46434700	4.53303600	0.39251400
H	-4.64805100	2.40681700	-0.06804900
H	-4.84439500	4.76959400	0.51086700
H	-0.58751400	5.16195200	0.54723500
H	-2.79118400	6.15710800	0.82156900
C	-0.01384200	2.54642000	-0.10647800
C	2.62888300	1.42258200	-0.39907800
C	0.10007200	1.17073000	-0.34123700
C	1.16789300	3.30216700	-0.11961800
C	2.44855700	2.78234700	-0.30386100
C	1.44376300	0.52569600	-0.33336300
H	1.09177600	4.38480400	-0.00405800
H	3.29903700	3.46343300	-0.30103100
H	1.49826800	-0.14757500	-1.20318600
C	3.93643900	0.79133700	-0.47267900
C	6.40757700	-0.47528600	-0.71485600
C	5.05536900	1.49505000	-0.94640200
C	4.06467300	-0.57204600	-0.10330800
C	5.32080700	-1.18297600	-0.23658500
C	6.27947300	0.86973000	-1.07373500
H	4.95364000	2.53532200	-1.25977600
H	5.45158400	-2.22061000	0.07349500
H	7.13956000	1.42152000	-1.45689400
H	7.37691700	-0.97064600	-0.80348900

C	-2.34675400	0.97906100	-0.46906600
C	-2.07535500	-1.74532100	-1.20000100
C	-3.46813300	0.16370300	-0.66502600
C	-1.06283600	0.39024900	-0.59862800
C	-0.96905300	-0.96815900	-0.99274600
C	-3.36187400	-1.17479300	-0.98795700
H	-4.48155200	0.54394200	-0.55245800
H	-0.00791000	-1.45127300	-1.16681900
C	2.91066000	-1.26708200	0.43891100
H	2.18620200	0.30103200	1.68873500
C	1.78537300	-0.39175500	0.92817400
C	1.63075500	-3.28129100	0.88949400
C	0.64532300	-1.13045200	1.58306400
C	2.76689600	-2.64951800	0.41044100
C	0.57247300	-2.53510100	1.52308600
C	-0.32052900	-0.43101400	2.30246400
H	3.55724600	-3.25759400	-0.03359300
H	-0.56666900	-4.28071100	2.07272400
H	1.54254200	-4.36728000	0.82666400
C	-1.38215900	-1.09102200	2.90613900
H	-0.24616600	0.65642800	2.39344100
H	-2.12920100	-0.52359300	3.46480200
C	-1.48408400	-2.47795400	2.80450700
H	-2.31612600	-3.00275400	3.27888900
C	-0.51097400	-3.19116100	2.12849300
O	-4.48969600	-1.88034900	-1.15124600
O	-1.92815800	-3.03260400	-1.59150300
C	-4.66780600	-3.05669900	-0.37390400
H	-3.84209700	-3.76720700	-0.51222800
H	-5.60904800	-3.50849700	-0.70535300
H	-4.75174400	-2.79416300	0.69171700
C	-2.35805000	-3.32453000	-2.91165900
H	-3.42533600	-3.09535200	-3.05090800
H	-2.19184500	-4.39590300	-3.07175300
H	-1.76658500	-2.75589500	-3.64638800

Cartesian coordinates of compound **17** optimized at the LC-ωPBE/def2-SVP level of DFT

C	2.49295000	-2.21784800	-0.31183200
C	1.21323100	-4.67221900	-0.74784100
C	1.09785200	-2.26903500	-0.45325500
C	3.22322800	-3.41440300	-0.39733600
C	2.59987400	-4.62470200	-0.61174500
C	0.47823500	-3.50799200	-0.66933200
H	4.30747300	-3.40766100	-0.29831600
H	3.19210500	-5.53948500	-0.67534200
H	-0.60387100	-3.57635500	-0.78019400
H	0.70785500	-5.62475500	-0.91839800
C	0.31552000	-1.02258800	-0.36933400
C	-1.14869200	1.46318800	-0.19876400
C	0.98323300	0.24425200	-0.16017700
C	-1.03562100	-1.01321000	-0.47558500
C	-1.87590500	0.19188800	-0.44779300
C	0.21051600	1.43449100	-0.07837800
H	-1.57494800	-1.94457500	-0.64684900
H	-2.26747900	0.25520500	-1.48739600
H	0.73078900	2.36557500	0.12005700
C	-1.94379800	2.68832100	-0.09173000
C	-3.49238300	5.01738100	-0.01022300
C	-1.34102800	3.95604100	-0.09358200
C	-3.35712800	2.59699200	-0.04686300
C	-4.10892900	3.78113200	-0.01008400
C	-2.09947000	5.10882400	-0.05227100
H	-0.25636300	4.04963700	-0.15468200
H	-5.19649400	3.72218900	0.05455300
H	-1.61132600	6.08495900	-0.05754200
H	-4.09802700	5.92525900	0.03062200
C	3.15619100	-0.92538300	-0.08437000
C	4.45387600	1.56824200	0.31482700
C	4.54159300	-0.85284700	0.08586000

C	2.40387900	0.27575200	-0.02874400
C	3.09980600	1.50023600	0.16025200
C	5.19922700	0.35137800	0.29729300
H	5.13286900	-1.76334800	0.07106600
H	2.58210500	2.45596400	0.20448600
C	-3.99573300	1.28911300	-0.02666500
H	-2.78568400	0.39682700	1.48269200
C	-3.14299400	0.15210800	0.46646800
C	-5.80555400	-0.22093700	-0.60890500
C	-3.85144100	-1.17997100	0.54691500
C	-5.25584500	1.05209700	-0.55733100
C	-5.12695500	-1.35060200	-0.02427400
C	-3.27302500	-2.24198400	1.24021500
H	-5.81591500	1.88358400	-0.98975600
H	-6.73364100	-2.73881700	-0.40207700
H	-6.78630800	-0.37448100	-1.06258500
C	-3.90213700	-3.47833700	1.31799300
H	-2.31287500	-2.09840500	1.74568800
H	-3.43289200	-4.29553500	1.86976100
C	-5.13946100	-3.66509500	0.70336500
H	-5.63857900	-4.63475100	0.75778600
C	-5.74727700	-2.60906300	0.04953500
O	6.50003300	0.46770500	0.50542600
O	5.03841600	2.75510100	0.55631200
C	7.32478300	-0.67831800	0.55299600
H	7.01077900	-1.35596900	1.36107500
H	8.33866000	-0.32007800	0.75896900
H	7.31846300	-1.21216200	-0.40943500
C	5.98352400	3.23998900	-0.38163100
H	6.89138500	2.62276200	-0.40089200
H	6.24551900	4.25491200	-0.06234900
H	5.54394700	3.28570100	-1.39088400

Cartesian coordinates of compound **TS3** optimized at the LC-ωPBE/def2-SVP level of DFT

C	-2.40953000	2.40706900	-0.14127600

C	-2.57799600	5.11976500	0.54995900
C	-1.23765500	3.16568200	0.02872600
C	-3.65485000	3.03790100	0.03590200
C	-3.74340100	4.36863400	0.37367100
C	-1.34955700	4.52407500	0.37825000
H	-4.57682100	2.47412100	-0.09830000
H	-4.72241100	4.83411900	0.50306200
H	-0.45922000	5.13451500	0.52701900
H	-2.63880000	6.17521400	0.82221800
C	0.06412500	2.52038800	-0.15419800
C	2.64463200	1.33548600	-0.51796600
C	0.14662600	1.14865900	-0.45513300
C	1.25956300	3.24755100	-0.09524600
C	2.52190800	2.68492400	-0.29129900
C	1.45005300	0.50886700	-0.50627400
H	1.21852600	4.31889200	0.10285300
H	3.40807700	3.31656500	-0.21668600
H	1.49721200	-0.33806500	-1.19470000
C	3.95687600	0.67155500	-0.57620200
C	6.44349100	-0.58568100	-0.56829200
C	5.05952600	1.28667500	-1.16555100
C	4.09594500	-0.60281800	0.01189200
C	5.35036600	-1.21132500	0.01606500
C	6.29791800	0.65913200	-1.16851800
H	4.94340300	2.25774200	-1.65155500
H	5.47924900	-2.17950300	0.50396300
H	7.15381100	1.14616100	-1.63969200
H	7.41947100	-1.07507800	-0.55285400
C	-2.31373500	0.99148100	-0.50045000
C	-2.12255100	-1.74394400	-1.19664500
C	-3.45615200	0.19682000	-0.65566900
C	-1.04880000	0.38186500	-0.66990600
C	-0.99338300	-0.98062800	-1.03864800
C	-3.38736600	-1.14655600	-0.96868400
H	-4.45809400	0.59919300	-0.51855900

H	-0.04950600	-1.48955800	-1.23043500
C	2.90619800	-1.25522500	0.57661900
H	2.14648600	0.45445600	1.66078100
C	1.81817000	-0.39463400	1.04917200
C	1.53458100	-3.22601800	0.90609400
C	0.64029200	-1.05997100	1.62650800
C	2.70876200	-2.62800000	0.47655500
C	0.49105400	-2.45956100	1.50937500
C	-0.33171500	-0.32270200	2.31451000
H	3.48923400	-3.24596900	0.02861300
H	-0.77572900	-4.15696900	1.93913800
H	1.40534600	-4.30571100	0.80704400
C	-1.44598200	-0.94523000	2.84217200
H	-0.20746000	0.75729100	2.43021900
H	-2.19458300	-0.35827200	3.37803300
C	-1.61536400	-2.32884400	2.69290100
H	-2.49821800	-2.81659800	3.11157700
C	-0.65966900	-3.07575900	2.04041300
O	-4.53485300	-1.83697900	-1.09985400
O	-2.00333100	-3.04711300	-1.54695400
C	-4.73258900	-2.95034500	-0.24354900
H	-3.92007200	-3.68451700	-0.33530800
H	-5.68193900	-3.41004300	-0.54009600
H	-4.80966000	-2.61646400	0.80305900
C	-2.48565500	-3.38298700	-2.83851700
H	-3.55325200	-3.14090200	-2.94755800
H	-2.34175900	-4.46244700	-2.96223000
H	-1.91262900	-2.85324300	-3.61571700

Cartesian coordinates of compound **TS4** optimized at the LC-ωPBE/def2-SVP level of DFT

C	2.44275200	-2.11922700	-0.49598800
C	1.23841400	-4.57473300	-1.12542400
C	1.06759100	-2.17922200	-0.77825900
C	3.19088900	-3.30806500	-0.54697800
C	2.60663500	-4.51610000	-0.85759100

C	0.48643400	-3.42114500	-1.08315200
H	4.25980800	-3.29368900	-0.34035300
H	3.21410300	-5.42259000	-0.89098900
H	-0.58096400	-3.49670000	-1.28961600
H	0.76384700	-5.52745700	-1.36824000
C	0.26707400	-0.94733500	-0.74081100
C	-1.25286100	1.47439600	-0.64608000
C	0.88219000	0.29877100	-0.40177300
C	-1.07206000	-0.94213000	-1.05788100
C	-1.90368200	0.21435500	-0.96125300
C	0.07964800	1.47442000	-0.35928000
H	-1.55456100	-1.86026900	-1.39211600
H	-2.71284600	0.24514200	-1.69842600
H	0.53462600	2.41210400	-0.04835600
C	-2.09485700	2.67367500	-0.46394900
C	-3.69553500	4.91397300	-0.00562400
C	-1.61692100	3.95281800	-0.73867600
C	-3.40793200	2.51263100	0.02583200
C	-4.19044700	3.64405500	0.25625900
C	-2.41160100	5.06895100	-0.51368000
H	-0.61668100	4.07755400	-1.15890100
H	-5.19539300	3.52973400	0.66782700
H	-2.02586600	6.06539800	-0.73780000
H	-4.31897500	5.78953500	0.18634200
C	3.06361800	-0.83340500	-0.15175500
C	4.26667600	1.64575900	0.50212800
C	4.43030500	-0.74918800	0.14927400
C	2.28788400	0.34620100	-0.10837400
C	2.93225700	1.56607700	0.21541300
C	5.03952500	0.44880400	0.48393400
H	5.03843800	-1.64886700	0.13882300
H	2.39094700	2.50884800	0.26447500
C	-3.93003200	1.15321000	0.23476500
H	-2.21608200	0.37212700	1.29306700
C	-2.98440800	0.09882600	0.56089400

C	-5.69445800	-0.48500000	-0.03907800
C	-3.51231700	-1.25665800	0.75901100
C	-5.24419300	0.82076400	-0.09568900
C	-4.84703900	-1.54646400	0.40825800
C	-2.70746000	-2.26966600	1.29835100
H	-5.92179800	1.60622900	-0.43545000
H	-6.36360800	-3.08500700	0.28928400
H	-6.72505700	-0.71673700	-0.31689000
C	-3.20076800	-3.54943600	1.45486700
H	-1.68090200	-2.04124700	1.59696400
H	-2.56587500	-4.32948000	1.88027200
C	-4.51863900	-3.84908200	1.07712000
H	-4.90286300	-4.86354300	1.20159100
C	-5.33060700	-2.86220100	0.56611200
O	6.31982700	0.57705000	0.81726200
O	4.79582500	2.82989800	0.86355400
C	7.15407700	-0.55796100	0.87125100
H	6.78388600	-1.28756500	1.60789300
H	8.14126700	-0.20300800	1.18547400
H	7.24158900	-1.03743800	-0.11613600
C	5.81975500	3.37937700	0.05450900
H	6.73874700	2.78016000	0.09758100
H	6.02413500	4.38130800	0.44872600
H	5.48543200	3.46959700	-0.99165300

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