Tetrabenzocircumpyrene: A Nanographene Fragment with an Embedded Peripentacene Core

Electronic Supplementary Information

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1. Experimental Details

1.1. General Methods

Reactions under argon atmosphere were carried out in solvents dried by passing through an activated alumina column on a PureSolvTM solvent purification system (Innovative Technologies, Inc., MA).

Thin layer chromatography was carried out using TLC aluminum sheets coated with 0.2 mm of silica gel (Merck Gf234). Chromatographic purifications were carried out using flash grade silica gel (SDS Chromatogel 60 ACC, 40-60 μm).

NMR spectra were recorded at 25 ºC on a Bruker Avance 300, 400 Ultrashield and Bruker Avance 500 Ultrashield apparatus, or at 125 ºC on a Bruker Avance 500 Ultrashield apparatus. Solid State NMR spectra were recorded on a Bruker 400 AVANCE III WB spectrometer operating at ^{1}H and ^{13}C Larmor frequencies of 400 and 100.6MHz, respectively. ^{13}C-CPMAS spectra were collected by using a 7mm MAS double resonance (^{13}C-^{1}H) probe at a spinning of 6KHz.

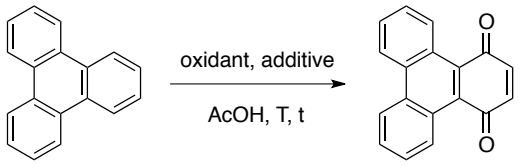
Mass spectra were recorded on a Waters LCT Premier Spectrometer (ESI and APCI) or on an Autoflex Broker Daltonics (MALDI and LDI).

Melting points were determined using a Büchi melting point apparatus.

Crystal structure determinations were carried out using a Bruker-Nonius diffractomer equipped with an APPEX 2 4K CCD area detector, a FR591 rotating anode with MoKa radiation, Montel mirrors as monochromator and a Kryoflex low temperature device (T = -173 ºC). Full-sphere data collection was used with w and j scans. Programs used: Data collection APEX-2, data reduction Bruker Saint V/.60A and absorption correction SADABS. Structure Solution and Refinement: Crystal structure solution was achieved using direct methods as implement in SHELXTL and visualized using the program XP. Missing atoms were subsequently located from difference Fourier synthesis and added to the atom list. Least-squares refinement on F2 using all measured intensities was carried out using the program SHELXTL. All non-hydrogen atoms were refined including anisotropic displacement parameters.

The molecules investigated by Scanning Tunneling Microscopy (STM) were sublimated on a Au(111) crystal surface which was previously cleaned using standard cleaning methods consisting of cycles of sputtering, using a beam of ionized Neon gas, and subsequent annealing. Evaporation parameters were adjusted to deposit minute amounts of molecules down to submonolayer coverages that are enough to result on the adsorption of single molecules on the substrate terraces. After preparation samples were cooled down and transferred to the STM chamber where they thermalized to temperatures down to about 7K, the base temperature of the LT-UHV-STM instrument used in all the experiments. The Elastic Scattering Quantum Chemistry (ESQC) calculated dI/dV STM images were calculated using a mono-electronic description of the tip apex – molecule – surface tunneling junction.

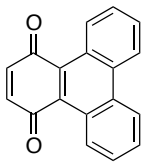
*1.2. Optimization of the Synthesis of **4***



4

Entry	Oxidant (eq.)	Additive (eq.)	Scale (mmol)	t (h)	T (ºC)	Yield (%)
1	H_2O_2 (12)	none	14	1	110	6
2	H_2O_2 (12)	none	14	16	110	5
3	H_2O_2 (12)	none	70	2	110	1
4	H_2O_2 (36)	none	14	1	110	5
5	CrO_3 (4)	none	2	4	70	22
6	CrO_3 (4)	18-crown-6 (0.1)	2	4	70	39
7	CrO_3 (8)	18-crown-6 (0.1)	2	4	70	37
8	CrO_3 (4)	18-crown-6 (0.1)	2	16	70	37
9	CrO_3 (4)	18-crown-6 (0.1)	20	4	70	41

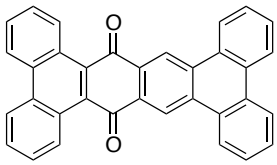
1.3. Synthetic Procedures and Analytical Data



Triphenylene-1,4-dione (4). A suspension of triphenylene (2.28 g, 10.00 mmol) in AcOH (50 mL) was slowly added to a suspension of CrO_3 (4.00 g, 40.00 mmol) and 18-crown-6 (400 mg) in AcOH (150 mL) at 0 ºC. Once the addition was complete the mixture was heated at 60 ºC for 4 hours and then cooled down to room temperature, diluted with CH_2Cl_2 (300 mL) and washed with water (3x200 mL) and saturated solution of $NaHCO_3$ (3x250 mL). The organic layer was dried over $MgSO_4$ and concentrated under reduced pressure. The product was obtained after purification by silica column eluted with a gradient of cyclohexane:CH_2Cl_2 (4:1 to 1:1) as an orange solid (1.06 g, 4.01 mmol, yield = 41%). Melting point = 174-176 ºC.

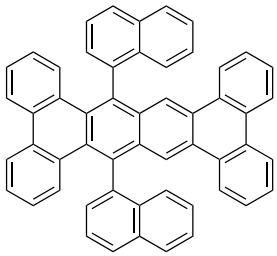
This reaction could be scaled up to obtain 5.0 grams of product.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.28 (dd, *J* = 8.7, 1.3 Hz, 2H), 8.71 (dd, *J* = 8.0, 1.2 Hz, 2H), 7.87 – 7.70 (m, 4H), 6.96 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 188.7, 137.8, 133.3, 130.2, 129.5, 129.2, 128.5, 126.8, 122.7. HRMS (APCI+) Calcd. for $C_{18}H_{11}O_2$ $[M+H]^+$: 259.0754. Found: 259.0747.



Tetrabenzo[*a*,*c*,*j*,*l*]tetracene-9,20-dione (3). 4 (2.69 g, 10.41 mmol), **6**[1] (5.69 g, 15.63 mmol) and KI (17.28 g, 104.10 mmol) were dissolved in DMF (300 mL) and the mixture was heated at 110 ºC for 20 hours. After cooling down to room temperature, the precipitate was filtered off and washed with water (2x200 mL), acetone (2x200 mL) and CH_2Cl_2 (2x200 mL) to afford the title compound mixed with variable amounts of partially reduced tetrabenzo[*a*,*c*,*j*,*l*]tetracene-9,20(10*H*,19*H*)-dione (**3'**) as an insoluble orange solid (3.33 g, 7.26 mmol, yield = 70%). Melting point > 300 ºC.

^{1}H NMR (500 MHz, $CDCl_2$-$CDCl_2$, 398 K) δ 8.99 (d, *J* = 8.3 Hz, 2H), 8.91 (s, 2H), 8.34-8.29 (m, 2H), 8.18 (d, *J* = 8.0 Hz, 2H), 8.13-8.07 (m, 2H), 7.28-7.17 (m, 8H). HRMS (LDI-) Calcd. for $C_{34}H_{18}O_2$ $[M]^+$: 458.1307. Found: 458.1300.



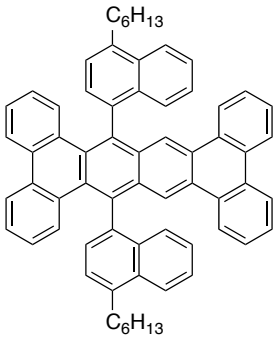
9,20-Di(naphthalen-1-yl)tetrabenzo[*a*,*c*,*j*,*l*]tetracene (2a). To a solution of 1-bromonaphthalene (677 mg, 3.3 mmol) in anhydrous Et_2O (20 mL) under Ar atmosphere at 0 ºC, a solution of *n*-BuLi 2.5 M in hexanes (1.3 mL, 3.3 mmol) was added. After stirring at this temperature for 30 minutes this solution was transferred via cannula to a suspension of **3+3'** (500 mg, ≈1.1 mmol) in anhydrous toluene (20 mL) under Ar atmosphere and the resulting mixture was stirred at room temperature for 3 hours. The reaction was quenched by addition of saturated solution of NH_4Cl (30 mL), the organic phase was separated and the aqueous phase extracted with CH_2Cl_2 (2x20 mL). The combined organic phases were dried over $MgSO_4$ and the solvents evaporated to afford the crude mixture of **7*syn***, **7*anti***, **7'*syn* and 7'*anti***. This mixture was directly suspended in AcOH (60 mL) and then HI (57% wt. % in H_2O, 1

[1] 9,10-Bis(bromomethyl)phenanthrene is commercially available (CAS: 57743-47-2). However, it was more practical in terms of price to prepare it from 9,10-dimethylphenanthrene following the reported procedure: Kotha, S.; Krishna, N. G.; Misra, S.; Khedkar, P. *Synthesis* **2011**, *18*, 2945-2950.

mL) was added. After stirring at 100 ºC for 16 hours and cooling down to room temperature, saturated solution of $Na_2S_2O_3$ (25 mL) was added followed by extraction with CH_2Cl_2 (3x60 mL). The combined organic phases were washed with saturated solution of $NaHCO_3$ (2x100 mL, CO_2 evolution), dried over $MgSO_4$, filtered and concentrated under reduced pressure. The crude solid was dissolved in toluene (80 mL) and treated with DDQ (500 mg, 2.2 mmol) at 70 ºC for 1 hour. After cooling down to room temperature, the mixture was diluted with EtOAc (50 mL) and washed with a solution of NaOH (10% wt., 3x60 mL) and water (3x60 mL). The organic phase was dried over $MgSO_4$ and the solvents removed under reduced pressure. Purification by silica column chromatography (gradient of cyclohexane:CH_2Cl_2 1:0 to 4:1) gave the title compound as an intense yellow solid (256.8 mg, 0.38 mmol, yield in 3 steps = 34%, mixture *syn*:*anti* ≈ 1:5). Melting point > 300 ºC.

X-ray quality single crystals were obtained by layering a solution of polyarene in $CHCl_3$ with MeOH followed by addition of small amounts of CH_2Cl_2 to redissolve the precipitate formed in the interface.

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.79 (s, 0.4H) (*syn*), 8.63 (s, 2H) (*anti*), 8.51 – 8.38 (m, 2.4H) (*syn*+*anti*), 8.35 – 8.24 (m, 2.4H) (*syn*+*anti*), 8.22 – 8.08 (m, 4.8H) (*syn*+*anti*), 7.87 – 7.43 (m, 16.8H) (*syn*+*anti*), 7.41 – 7.23 (m, 7.2H) (*syn*+*anti*), 6.88 – 6.79 (m, 2.4H) (*syn*+*anti*). ^{13}C NMR (75 MHz, $CDCl_3$) δ (*anti*) 140.1, 134.2, 134.1, 133.8, 131.9, 131.3, 130.9, 130.4, 130.1, 130.1, 129.9, 129.8, 128.8, 128.6, 127.8, 127.4, 127.4, 127.4, 127.2, 126.9, 126.6, 126.2, 126.2, 123.4, 123.4, 123.2, 122.1. HRMS (APCI+) Calcd. for $C_{54}H_{33}$ $[M+H]^+$: 681.2577. Found: 681.2573.

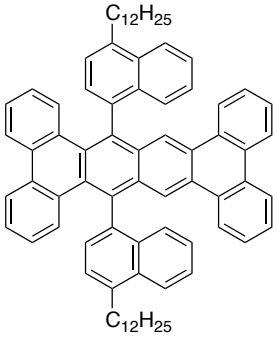


9,20-Bis(4-hexylnaphthalen-1-yl)tetrabenzo[*a*,*c*,*j*,*l*]tetracene (2b). Procedure described for **2a** starting from 1-bromo-4-hexylnaphthalene.[2] Yellow solid, yield in 3 steps = 32%, mixture *syn*:*anti* < 1:10. Melting point = 278-280 ºC.

X-ray quality single crystals were obtained by layering a solution of polyarene in $CHCl_3$ with MeOH followed by addition of small amounts of CH_2Cl_2 to redissolve the precipitate formed in the interface.

[2] 1-bromo-4-hexylnaphthalene and 1-bromo-4-dodecylnaphthalene were prepared according to: Cammidge, A. N.; Gopee, H. *Chem. Eur. J.* **2006**, *12*, 8609-8613.

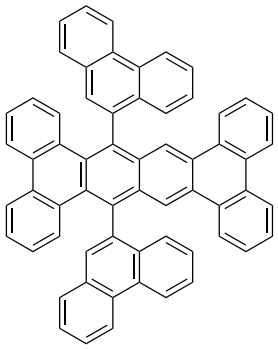
^{1}H NMR (300 MHz, $CDCl_3$) δ 8.61 (d, *J* = 1.8 Hz, 2H), 8.45 – 8.39 (m, 2H), 8.39 – 8.27 (m, 4H), 7.74 (dd, *J* = 8.5, 1.4 Hz, 2H), 7.72 – 7.59 (m, 4H), 7.61 – 7.44 (m, 8H), 7.36 – 7.23 (m, 6H), 6.81 (ddd, *J* = 8.4, 7.2, 1.4 Hz, 2H), 3.42 – 3.30 (m, 4H), 2.01 (p, *J* = 7.2 Hz, 4H), 1.68 – 1.39 (m, 12H), 0.99 (t, *J* = 6.9 Hz, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 139.5, 138.3, 134.5, 134.4, 132.3, 131.8, 131.5, 131.1, 130.3, 130.2, 130.0, 129.8, 129.5, 128.1, 127.6, 127.3, 127.3, 127.1, 126.7, 126.2, 126.1, 125.8, 124.7, 123.4, 123.3, 123.2, 122.2, 33.4, 31.9, 30.9, 29.5, 22.8, 14.2. HRMS (MALDI+) Calcd. for $C_{66}H_{56}$ $[M]^+$: 848.4382. Found: 848.4368.



9,20-Bis(4-dodecylnaphthalen-1-yl)tetrabenzo[*a*,*c*,*j*,*l*]tetracene (2c). Procedure described for **2a** starting from 1-bromo-4-dodecylnaphthalene. Orange solid, yield in 3 steps = 26%, mixture *syn*:*anti* ≈ 1:10. Melting point = 184-186 ºC.

X-ray quality single crystals were obtained by layering a solution of polyarene in $CHCl_3$ with MeOH followed by addition of small amounts of CH_2Cl_2 to redissolve the precipitate formed in the interface.

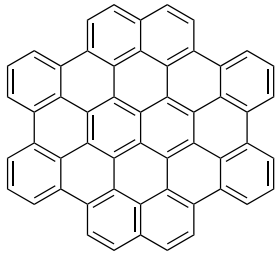
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.78 (s, 0.3H) (*syn*), 8.62 (s, 2H) (*anti*), 8.46 (d, *J* = 7.7 Hz, 0.3H) (*syn*), 8.43 (d, *J* = 7.4 Hz, 2H) (*anti*), 8.36 (d, *J* = 8.6 Hz, 2H) (*anti)*, 8.31 (d, *J* = 6.8 Hz, 2.3H) (*syn+anti)*, 8.29 (d, *J* = 7.9 Hz, 0.3H) (*syn*), 7.85 – 7.80 (m, 0.6H) (*syn*), 7.75 (dd, *J* = 8.6, 1.3 Hz, 2H) (*anti*), 7.68 (dd, *J* = 8.4, 1.2 Hz, 2H) (*anti*), 7.67 (d, *J* = 8.2 Hz, 0.3H) (*syn*), 7.66 – 7.63 (m, 2H), 7.62 – 7.51 (m, 6.9H) (*syn+anti*), 7.48 (ddd, *J* = 8.2, 7.0, 1.2 Hz, 2H) (*anti*), 7.38 – 7.23 (m, 7.2H) (*syn+anti*), 6.83 (ddd, *J* = 8.4, 7.0, 1.3 Hz, 2.3H) (*syn+anti*), 3.43 – 3.29 (m, 4.6H) (*syn+anti*), 2.08 – 1.92 (m, 4.6H) (*syn+anti*), 1.65 – 1.55 (m, 4.6H) (*syn+anti*), 1.55 – 1.47 (m, 4.6H) (*syn+anti*), 1.45 – 1.26 (m, 32.2H) (*syn+anti*), 0.96 – 0.90 (m, 6.9H) (*syn+anti*). ^{13}C NMR (126 MHz, $CDCl_3$) (*anti*) δ 139.5, 138.3, 134.5, 134.4, 132.3, 131.8, 131.5, 131.1, 130.3, 130.2, 130.0, 129.8, 129.5, 128.1, 127.6, 127.3, 127.3, 127.1, 127.0, 126.6, 126.2, 126.1, 125.8, 124.7, 123.4, 123.3, 123.1, 122.2, 33.4, 32.0, 30.9, 29.8, 29.8, 29.8, 29.8, 29.8, 29.7, 29.4, 22.7, 14.1. HRMS (MALDI+) Calcd. for $C_{78}H_{80}$ $[M]^+$: 1016.6260. Found: 1016.6276.



9,20-Di(phenanthren-9-yl)tetrabenzo[*a*,*c*,*j*,*l*]tetracene (2d). Procedure described for **2a** starting from 9-bromophenanthrene. Orange solid, yield in 3 steps = 38%, mixture *syn*:*anti* < 1:10. Melting point = 269-271 ºC.

X-ray quality single crystals were obtained by layering a solution of polyarene in $CHCl_3$ with MeOH followed by addition of small amounts of CH_2Cl_2 to redissolve the precipitate formed in the interface.

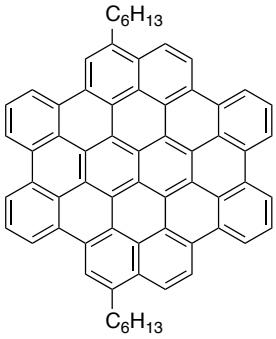
^{1}H NMR (300 MHz, $CDCl_3$) δ 9.04 (d, *J* = 8.3 Hz, 2H), 8.99 (d, *J* = 8.5 Hz, 2H), 8.66 (s, 2H), 8.38 (dd, *J* = 8.3, 1.2 Hz, 2H), 8.31 (dd, *J* = 8.2, 1.4 Hz, 2H), 7.96 (s, 2H), 7.90 – 7.78 (m, 8H), 7.78 – 7.73 (m, 2H), 7.67 (dd, *J* = 7.6, 1.1 Hz, 2H), 7.55 (dd, *J* = 8.4, 1.3 Hz, 2H), 7.43 (ddt, *J* = 8.2, 6.9, 1.3 Hz, 4H), 7.32 (ddd, *J* = 8.2, 7.1, 1.2 Hz, 2H), 7.22 (ddd, *J* = 8.2, 7.0, 1.2 Hz, 2H), 6.79 (ddd, *J* = 8.4, 7.1, 1.3 Hz, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 138.7, 134.1, 133.3, 132.5, 131.9, 131.2, 130.8, 130.8, 130.5, 130.5, 130.3, 130.0, 130.0, 129.2, 128.6, 127.8, 127.4, 127.4, 127.4, 127.2, 127.0, 126.9, 126.9, 126.9, 126.4, 123.5, 123.4, 123.4, 123.1, 122.8, 122.3. HRMS (APCI+) Calcd. for $C_{62}H_{37}$ $[M+H]^+$: 781.2890. Found: 781.2889.



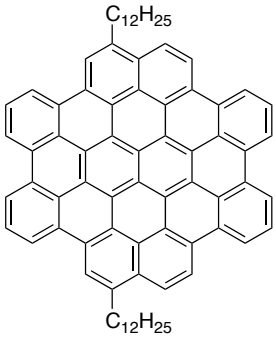
Tetrabenzocircumpyrene (1a). $FeCl_3$ (305.6 mg, 1.884 mmol) was dissolved in CH_3NO_2 (5 mL), the solution was degassed by bubbling Ar for 10 minutes and then transferred to a degassed solution of **2a** (70 mg, 0.105 mmol) in CH_2Cl_2 (5 mL) at 0 ºC. The resulting mixture was stirred at room temperature for 16 hours. Then the reaction was quenched by addition of 1 mL of MeOH and the suspended solid filtered off and washed by centrifuge with H_2O (3x10 mL), acetone (3x10mL), and CH_2Cl_2 (5x10 mL). After a soxhlet extraction with benzene for 2 hours the product was obtained as a highly insoluble black solid (67.3 mg, 0.101 mmol, yield = 96%). Melting point > 300 ºC.

This product could be obtained in up to 1-gram scale.

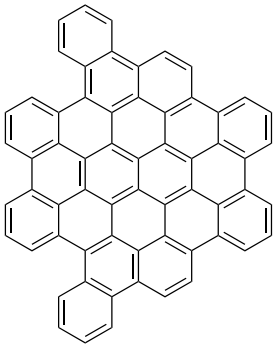
HRMS (LDI+) Calcd. for $C_{54}H_{20}$ $[M]^+$: 668.1560. Found: 668.1501.



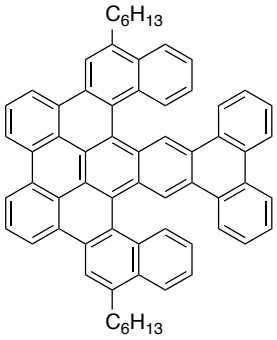
Dihexyltetrabenzocircumpyrene (1b). Procedure described for **1a** starting from **2b**. Insoluble black solid, yield = 85%, melting point > 300 ºC. HRMS (LDI+) Calcd. for $C_{66}H_{44}$ $[M]^+$: 836.3443. Found: 836.3411.



Didodecyltetrabenzocircumpyrene (1c). Procedure described for **1a** starting from **2c**. Insoluble black solid, yield = 54%, melting point > 300 ºC. HRMS (MALDI+) Calcd. for $C_{78}H_{68}$ $[M]^+$: 1004.5321. Found: 1004.5355.



Hexabenzocircumpyrene (1d). Procedure described for **1a** starting from **2d**. Insoluble black solid, yield = 64%, melting point > 300 ºC. HRMS (MALDI+) Calcd. for $C_{78}H_{68}$ $[M]^+$: 768.1878. Found: 768.1884.



10,19-Dihexyltetrabenzo[*a*,*fg*,*ij*,*o*]benzo[5,6]tetrapheno[8,9,10,11-*rst*]pentaphene (8). Procedure described for **1a** starting from **2b**. The resulting mixture was diluted 40 times with CH_2Cl_2, filtered and washed with water (x3). The organic layer was separated, dried over $MgSO_4$ and the solvent evaporated. The crude mixture was then filtered through a pad of silica eluting with copious amounts of CH_2Cl_2 (over 1 L every 0.1 mmol of starting material) due to the low solubility of the product. After evaporation of the solvent the title compound was obtained as a dark brown solid with poor solubility in standard organic solvents (yield = 17%). Melting point > 300 ºC.

X-ray quality single crystals were obtained by heating a suspension of polyarene in $(CDCl_2)_2$ over 100 ºC followed by slow cooling down to room temperature.

^{1}H NMR (500 MHz, $CDCl_2CDCl_2$, 398 K) δ 9.04 – 8.99 (m, 2H), 8.47 – 8.40 (m, 2H), 8.37 – 8.32 (m, 2H), 8.31 – 8.27 (m, 2H), 8.25 – 8.20 (m, 2H), 7.89 – 7.83 (m, 2H), 7.83 – 7.78 (m, 2H), 7.51 – 7.44 (m, 2H), 7.21 – 7.15 (m, 2H), 7.11 – 7.03 (m, 2H), 6.96 – 6.88 (m, 2H), 6.80 – 6.72 (m, 2H) + aliphatic protons. HRMS (MALDI+) Calcd. for $C_{66}H_{52}$ $[M]^+$: 844.4069. Found: 844.4059.

2. Crystal Data and Structure Refinement

*2.1. Triphenylene-1,4-dione (**4**)*

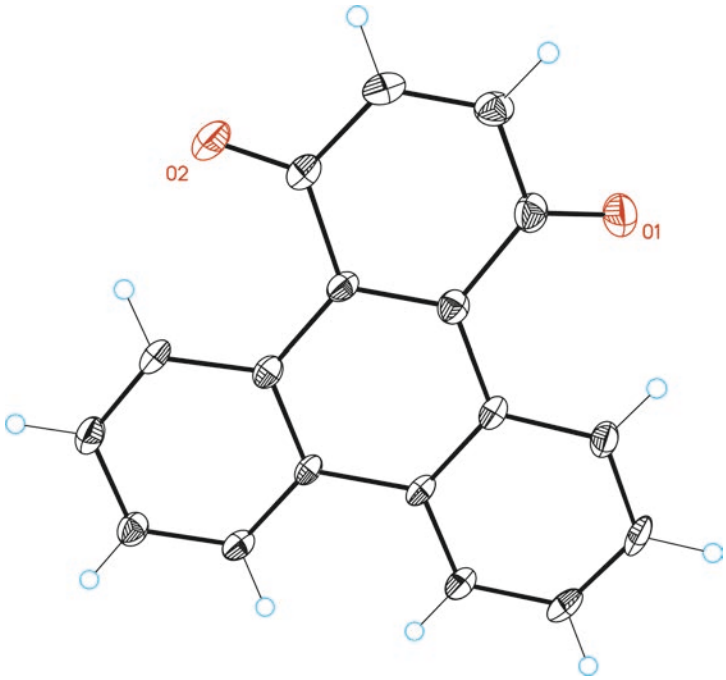


Table 1. Crystal data and structure refinement for **4**.

Identification code	mo_RD276_0m	
Empirical formula	C18 H10 O2	
Formula weight	258.26	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 5.2561(11) Å	a = 90.00 °.
	b = 9.121(2) Å	b = 90.00 °.
	c = 24.027(5) Å	g = 90.00 °.
Volume	1151.8(4) $Å^3$	
Z	4	
Density (calculated)	1.489 Mg/m^3	
Absorption coefficient	0.097 mm^{-1}	
F(000)	536	
Crystal size	0.30 x 0.15 x 0.05 mm^3	
Theta range for data collection	1.70 to 29.83 °.	
Index ranges	-7 <=h<=4 ,-12 <=k<=12 ,-30 <=l<=33	
Reflections collected	10774	

Independent reflections	3051 [R(int) = 0.0616]
Completeness to theta =29.83 °	95.8%
Absorption correction	Empirical
Max. and min. transmission	0.9952 and 0.9716
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3051 / 0 / 181
Goodness-of-fit on F^2	1.052
Final R indices [I>2sigma(I)]	R1 = 0.0555 , wR2 = 0.1338
R indices (all data)	R1 = 0.0730 , wR2 = 0.1431
Flack parameter	x =2(2)
Largest diff. peak and hole	0.266 and -0.320 e.$Å^{-3}$

Table 2. Bond lengths [Å] and angles [°] for **4**.

Bond lengths----	
C1-C6	1.387(3)
C1-C18	1.442(3)
C1-C2	1.499(3)
C2-O1	1.228(3)
C2-C3	1.459(3)
C3-C4	1.329(3)
C4-C5	1.469(3)
C5-O2	1.219(3)
C5-C6	1.503(3)
C6-C7	1.454(3)
C7-C12	1.414(3)
C7-C8	1.419(3)
C8-C9	1.374(3)
C9-C10	1.397(3)
C10-C11	1.375(3)
C11-C12	1.409(3)
C12-C13	1.453(3)
C13-C14	1.405(3)
C13-C18	1.416(3)
C14-C15	1.368(3)
C15-C16	1.397(3)
C16-C17	1.375(3)
C17-C18	1.416(3)

Angles----------	
C6-C1-C18	121.03(18)
C6-C1-C2	118.43(19)
C18-C1-C2	120.40(18)
O1-C2-C3	119.2(2)
O1-C2-C1	121.8(2)
C3-C2-C1	118.80(19)
C4-C3-C2	119.8(2)
C3-C4-C5	121.3(2)
O2-C5-C4	117.5(2)
O2-C5-C6	123.9(2)
C4-C5-C6	118.5(2)
C1-C6-C7	120.18(19)
C1-C6-C5	118.36(19)
C7-C6-C5	121.45(18)
C12-C7-C8	118.36(19)
C12-C7-C6	119.27(18)
C8-C7-C6	122.4(2)
C9-C8-C7	121.1(2)
C8-C9-C10	120.5(2)
C11-C10-C9	119.5(2)
C10-C11-C12	121.52(19)
C11-C12-C7	119.02(18)
C11-C12-C13	120.87(19)
C7-C12-C13	120.07(18)
C14-C13-C18	118.69(18)
C14-C13-C12	121.63(19)
C18-C13-C12	119.67(18)
C15-C14-C13	121.5(2)
C14-C15-C16	120.0(2)
C17-C16-C15	120.0(2)
C16-C17-C18	120.9(2)
C17-C18-C13	118.56(18)
C17-C18-C1	122.13(19)
C13-C18-C1	119.31(18)

Table 3. Torsion angles [°] for **4**.

C6-C1-C2-O1	-153.3(2)
C18-C1-C2-O1	22.4(3)
C6-C1-C2-C3	21.6(3)
C18-C1-C2-C3	-162.6(2)
O1-C2-C3-C4	155.2(2)
C1-C2-C3-C4	-19.9(3)
C2-C3-C4-C5	1.6(3)
C3-C4-C5-O2	-164.5(2)
C3-C4-C5-C6	14.8(3)
C18-C1-C6-C7	-2.4(3)
C2-C1-C6-C7	173.29(18)
C18-C1-C6-C5	178.90(18)
C2-C1-C6-C5	-5.4(3)
O2-C5-C6-C1	166.8(2)
C4-C5-C6-C1	-12.3(3)
O2-C5-C6-C7	-11.8(3)
C4-C5-C6-C7	169.03(18)
C1-C6-C7-C12	-3.4(3)
C5-C6-C7-C12	175.17(19)
C1-C6-C7-C8	177.2(2)
C5-C6-C7-C8	-4.2(3)
C12-C7-C8-C9	-1.6(3)
C6-C7-C8-C9	177.8(2)
C7-C8-C9-C10	0.6(3)
C8-C9-C10-C11	0.4(3)
C9-C10-C11-C12	-0.4(3)
C10-C11-C12-C7	-0.7(3)
C10-C11-C12-C13	177.13(19)
C8-C7-C12-C11	1.6(3)
C6-C7-C12-C11	-177.76(18)
C8-C7-C12-C13	-176.18(18)
C6-C7-C12-C13	4.4(3)
C11-C12-C13-C14	1.6(3)
C7-C12-C13-C14	179.33(18)
C11-C12-C13-C18	-177.35(19)
C7-C12-C13-C18	0.4(3)
C18-C13-C14-C15	2.8(3)

C12-C13-C14-C15	-176.13(19)
C13-C14-C15-C16	2.0(3)
C14-C15-C16-C17	-3.7(3)
C15-C16-C17-C18	0.4(3)
C16-C17-C18-C13	4.3(3)
C16-C17-C18-C1	-176.38(19)
C14-C13-C18-C17	-5.9(3)
C12-C13-C18-C17	173.08(19)
C14-C13-C18-C1	174.84(19)
C12-C13-C18-C1	-6.2(3)
C6-C1-C18-C17	-172.0(2)
C2-C1-C18-C17	12.4(3)
C6-C1-C18-C13	7.3(3)
C2-C1-C18-C13	-168.33(18)

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*2.2. 9,20-Di(naphthalen-1-yl)tetrabenzo[a,c,j,l]tetracene (**2a**)*

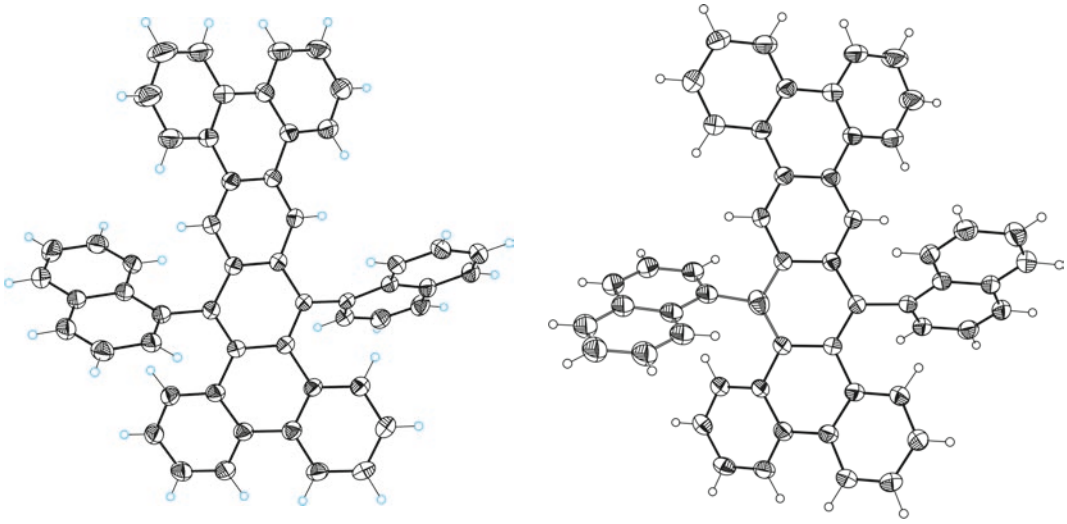

Table 4. Crystal data and structure refinement for **2a**.

Identification code	RD294P21c
Empirical formula	C54 H32
Formula weight	680.80
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic

Space group	P2(1)/c	
Unit cell dimensions	a = 9.2045(10) Å	a= 90.00 °.
	b = 16.8399(17) Å	b = 90.064(4)
°.		
	c = 22.397(2) Å	g = 90.00 °.
Volume	3471.6(6) $Å^3$	
Z	4	
Density (calculated)	1.303 Mg/m^3	
Absorption coefficient	0.074 mm^{-1}	
F(000)	1424	
Crystal size	0.20 x 0.08 x 0.08 mm^3	
Theta range for data collection	1.51 to 32.13 °.	
Index ranges	-11 <=h<=13 ,-25 <=k<=16 ,-18 <=l<=32	
Reflections collected	30518	
Independent reflections	10289 [R(int) = 0.0624]	
Completeness to theta =32.13 °	84.3%	
Absorption correction	Empirical	
Max. and min. transmission	0.9941 and 0.9854	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10289 / 225 / 586	
Goodness-of-fit on F^2	1.060	
Final R indices [I>2sigma(I)]	R1 = 0.0887 , wR2 = 0.1815	
R indices (all data)	R1 = 0.1572 , wR2 = 0.2101	
Largest diff. peak and hole	0.367 and -0.215 $e.Å^{-3}$	

Table 5. Bond lengths [Å] and angles [°] for **2a**.

Bond lengths----	
C1-C2	1.395(3)
C1-C34	1.428(3)
C1-C35	1.500(3)
C2-C15	1.447(3)
C2-C3	1.484(3)
C3-C4	1.407(3)
C3-C8	1.411(3)
C4-C5	1.379(3)
C5-C6	1.390(3)
C6-C7	1.375(4)

C7-C8	1.411(3)
C8-C9	1.468(3)
C9-C10	1.400(3)
C9-C14	1.404(3)
C10-C11	1.374(3)
C11-C12	1.395(4)
C12-C13	1.375(3)
C13-C14	1.411(3)
C14-C15	1.474(3)
C15-C16	1.393(4)
C15-C16'	1.416(8)
C16-C17	1.436(4)
C16-C45	1.506(4)
C16'-C17	1.411(9)
C16'-C45'	1.531(9)
C17-C18	1.405(3)
C17-C34	1.427(3)
C18-C19	1.386(3)
C19-C32	1.433(3)
C19-C20	1.468(3)
C20-C21	1.405(3)
C20-C25	1.412(3)
C21-C22	1.359(4)
C22-C23	1.386(4)
C23-C24	1.382(4)
C24-C25	1.392(4)
C25-C26	1.471(3)
C26-C31	1.407(4)
C26-C27	1.408(4)
C27-C28	1.378(4)
C28-C29	1.366(4)
C29-C30	1.379(4)
C30-C31	1.407(4)
C31-C32	1.466(3)
C32-C33	1.375(3)
C33-C34	1.414(3)
C35-C36	1.375(4)
C35-C44	1.427(3)

C36-C37	1.411(3)
C37-C38	1.362(4)
C38-C39	1.409(4)
C39-C40	1.417(4)
C39-C44	1.437(3)
C40-C41	1.348(4)
C41-C42	1.408(4)
C42-C43	1.364(3)
C43-C44	1.425(4)
C45-C46	1.372(4)
C45-C54	1.437(4)
C46-C47	1.404(5)
C47-C48	1.363(5)
C48-C49	1.425(5)
C49-C50	1.412(4)
C49-C54	1.436(4)
C50-C51	1.367(5)
C51-C52	1.411(5)
C52-C53	1.374(4)
C53-C54	1.413(4)
C45'-C46'	1.372(6)
C45'-C54'	1.435(5)
C46'-C47'	1.402(6)
C47'-C48'	1.366(7)
C48'-C49'	1.426(7)
C49'-C50'	1.412(6)
C49'-C54'	1.438(5)
C50'-C51'	1.367(6)
C51'-C52'	1.410(6)
C52'-C53'	1.373(6)
C53'-C54'	1.412(6)

Angles----------

C2-C1-C34	119.0(2)
C2-C1-C35	121.2(2)
C34-C1-C35	119.61(19)
C1-C2-C15	118.9(2)
C1-C2-C3	124.5(2)

C15-C2-C3	116.31(19)
C4-C3-C8	117.6(2)
C4-C3-C2	122.3(2)
C8-C3-C2	119.5(2)
C5-C4-C3	121.7(2)
C4-C5-C6	120.4(2)
C7-C6-C5	119.4(2)
C6-C7-C8	121.2(2)
C7-C8-C3	119.7(2)
C7-C8-C9	120.7(2)
C3-C8-C9	119.6(2)
C10-C9-C14	119.8(2)
C10-C9-C8	121.7(2)
C14-C9-C8	118.5(2)
C11-C10-C9	121.3(2)
C10-C11-C12	119.4(2)
C13-C12-C11	120.1(2)
C12-C13-C14	121.3(2)
C9-C14-C13	118.0(2)
C9-C14-C15	120.2(2)
C13-C14-C15	121.4(2)
C16-C15-C16'	16.0(12)
C16-C15-C2	119.1(2)
C16'-C15-C2	119.5(4)
C16-C15-C14	124.1(2)
C16'-C15-C14	120.7(5)
C2-C15-C14	116.8(2)
C15-C16-C17	118.2(3)
C15-C16-C45	118.9(3)
C17-C16-C45	122.9(3)
C17-C16'-C15	118.3(7)
C17-C16'-C45'	112.0(7)
C15-C16'-C45'	128.5(8)
C18-C17-C16'	123.6(4)
C18-C17-C34	117.9(2)
C16'-C17-C34	115.9(6)
C18-C17-C16	122.5(2)
C16'-C17-C16	15.8(12)

C34-C17-C16	119.6(2)
C19-C18-C17	122.8(2)
C18-C19-C32	118.6(2)
C18-C19-C20	122.4(2)
C32-C19-C20	119.0(2)
C21-C20-C25	118.0(2)
C21-C20-C19	121.5(2)
C25-C20-C19	120.5(2)
C22-C21-C20	121.8(2)
C21-C22-C23	120.5(3)
C24-C23-C22	118.9(3)
C23-C24-C25	121.9(2)
C24-C25-C20	118.8(2)
C24-C25-C26	121.3(2)
C20-C25-C26	119.8(2)
C31-C26-C27	118.3(2)
C31-C26-C25	120.1(2)
C27-C26-C25	121.6(2)
C28-C27-C26	121.5(3)
C29-C28-C27	120.0(3)
C28-C29-C30	120.2(3)
C29-C30-C31	121.2(3)
C30-C31-C26	118.6(2)
C30-C31-C32	121.4(2)
C26-C31-C32	119.9(2)
C33-C32-C19	118.7(2)
C33-C32-C31	121.5(2)
C19-C32-C31	119.8(2)
C32-C33-C34	122.7(2)
C33-C34-C17	118.2(2)
C33-C34-C1	122.1(2)
C17-C34-C1	119.6(2)
C36-C35-C44	119.6(2)
C36-C35-C1	118.6(2)
C44-C35-C1	121.8(2)
C35-C36-C37	121.4(2)
C38-C37-C36	119.9(3)
C37-C38-C39	121.1(2)

C38-C39-C40	122.1(2)
C38-C39-C44	119.3(2)
C40-C39-C44	118.6(2)
C41-C40-C39	121.5(2)
C40-C41-C42	120.2(3)
C43-C42-C41	120.9(3)
C42-C43-C44	120.5(2)
C43-C44-C35	123.2(2)
C43-C44-C39	118.2(2)
C35-C44-C39	118.6(2)
C46-C45-C54	118.8(3)
C46-C45-C16	117.2(3)
C54-C45-C16	124.0(3)
C45-C46-C47	122.9(3)
C48-C47-C46	119.5(3)
C47-C48-C49	120.9(3)
C50-C49-C48	121.5(3)
C50-C49-C54	119.2(4)
C48-C49-C54	119.3(3)
C51-C50-C49	120.7(3)
C50-C51-C52	120.2(3)
C53-C52-C51	120.7(3)
C52-C53-C54	120.6(3)
C53-C54-C49	118.5(3)
C53-C54-C45	122.8(3)
C49-C54-C45	118.6(3)
C46'-C45'-C54'	118.7(6)
C46'-C45'-C16'	120.2(11)
C54'-C45'-C16'	120.9(11)
C45'-C46'-C47'	123.1(7)
C48'-C47'-C46'	119.6(7)
C47'-C48'-C49'	120.4(6)
C50'-C49'-C48'	121.2(6)
C50'-C49'-C54'	119.0(6)
C48'-C49'-C54'	119.5(6)
C51'-C50'-C49'	120.7(6)
C50'-C51'-C52'	120.2(6)
C53'-C52'-C51'	120.6(7)

C52'-C53'-C54'	120.7(6)
C53'-C54'-C45'	123.0(6)
C53'-C54'-C49'	118.3(6)
C45'-C54'-C49'	118.5(5)

Table 6. Torsion angles [°] for **2a**.

C34-C1-C2-C15	10.9(3)
C35-C1-C2-C15	-164.5(2)
C34-C1-C2-C3	-163.1(2)
C35-C1-C2-C3	21.5(4)
C1-C2-C3-C4	21.1(4)
C15-C2-C3-C4	-153.1(2)
C1-C2-C3-C8	-167.8(2)
C15-C2-C3-C8	18.1(3)
C8-C3-C4-C5	-0.8(4)
C2-C3-C4-C5	170.6(2)
C3-C4-C5-C6	0.5(4)
C4-C5-C6-C7	0.2(4)
C5-C6-C7-C8	-0.7(4)
C6-C7-C8-C3	0.4(4)
C6-C7-C8-C9	-179.4(2)
C4-C3-C8-C7	0.3(4)
C2-C3-C8-C7	-171.3(2)
C4-C3-C8-C9	-179.9(2)
C2-C3-C8-C9	8.5(3)
C7-C8-C9-C10	-22.2(4)
C3-C8-C9-C10	158.0(2)
C7-C8-C9-C14	159.6(2)
C3-C8-C9-C14	-20.2(3)
C14-C9-C10-C11	-0.7(4)
C8-C9-C10-C11	-178.9(2)
C9-C10-C11-C12	1.0(4)
C10-C11-C12-C13	0.5(4)
C11-C12-C13-C14	-2.4(4)
C10-C9-C14-C13	-1.2(3)
C8-C9-C14-C13	177.1(2)
C10-C9-C14-C15	-173.5(2)

C8-C9-C14-C15	4.7(3)
C12-C13-C14-C9	2.8(4)
C12-C13-C14-C15	175.0(2)
C1-C2-C15-C16	-26.4(4)
C3-C2-C15-C16	148.0(4)
C1-C2-C15-C16'	-8.0(12)
C3-C2-C15-C16'	166.4(12)
C1-C2-C15-C14	152.7(2)
C3-C2-C15-C14	-32.9(3)
C9-C14-C15-C16	-159.0(4)
C13-C14-C15-C16	28.9(5)
C9-C14-C15-C16'	-177.6(12)
C13-C14-C15-C16'	10.3(12)
C9-C14-C15-C2	21.9(3)
C13-C14-C15-C2	-150.1(2)
C16'-C15-C16-C17	-74.2(17)
C2-C15-C16-C17	21.8(6)
C14-C15-C16-C17	-157.3(3)
C16'-C15-C16-C45	109.8(18)
C2-C15-C16-C45	-154.2(3)
C14-C15-C16-C45	26.8(6)
C16-C15-C16'-C17	79(2)
C2-C15-C16'-C17	-14(2)
C14-C15-C16'-C17	-174.2(11)
C16-C15-C16'-C45'	-88(3)
C2-C15-C16'-C45'	179.1(15)
C14-C15-C16'-C45'	19(3)
C15-C16'-C17-C18	-166.2(11)
C45'-C16'-C17-C18	3(2)
C15-C16'-C17-C34	33(2)
C45'-C16'-C17-C34	-158.5(11)
C15-C16'-C17-C16	-74.7(17)
C45'-C16'-C17-C16	94(3)
C15-C16-C17-C18	177.0(3)
C45-C16-C17-C18	-7.2(7)
C15-C16-C17-C16'	78.2(18)
C45-C16-C17-C16'	-106.0(18)
C15-C16-C17-C34	-2.5(6)

C45-C16-C17-C34	173.3(3)
C16'-C17-C18-C19	-153.7(12)
C34-C17-C18-C19	7.0(4)
C16-C17-C18-C19	-172.5(4)
C17-C18-C19-C32	2.4(4)
C17-C18-C19-C20	-176.8(2)
C18-C19-C20-C21	-0.5(4)
C32-C19-C20-C21	-179.8(2)
C18-C19-C20-C25	178.2(2)
C32-C19-C20-C25	-1.0(3)
C25-C20-C21-C22	-1.3(4)
C19-C20-C21-C22	177.5(3)
C20-C21-C22-C23	0.5(5)
C21-C22-C23-C24	-0.3(5)
C22-C23-C24-C25	1.0(4)
C23-C24-C25-C20	-1.8(4)
C23-C24-C25-C26	174.9(3)
C21-C20-C25-C24	1.9(4)
C19-C20-C25-C24	-176.9(2)
C21-C20-C25-C26	-174.8(2)
C19-C20-C25-C26	6.4(3)
C24-C25-C26-C31	-179.5(2)
C20-C25-C26-C31	-2.9(4)
C24-C25-C26-C27	-2.8(4)
C20-C25-C26-C27	173.9(3)
C31-C26-C27-C28	3.8(5)
C25-C26-C27-C28	-172.9(3)
C26-C27-C28-C29	-0.4(6)
C27-C28-C29-C30	-2.5(6)
C28-C29-C30-C31	2.0(5)
C29-C30-C31-C26	1.5(4)
C29-C30-C31-C32	-180.0(3)
C27-C26-C31-C30	-4.3(4)
C25-C26-C31-C30	172.5(2)
C27-C26-C31-C32	177.2(2)
C25-C26-C31-C32	-6.0(4)
C18-C19-C32-C33	-8.3(3)
C20-C19-C32-C33	170.9(2)

C18-C19-C32-C31	172.9(2)
C20-C19-C32-C31	-7.8(3)
C30-C31-C32-C33	14.2(4)
C26-C31-C32-C33	-167.3(2)
C30-C31-C32-C19	-167.1(2)
C26-C31-C32-C19	11.4(3)
C19-C32-C33-C34	4.8(3)
C31-C32-C33-C34	-176.5(2)
C32-C33-C34-C17	4.7(4)
C32-C33-C34-C1	-173.3(2)
C18-C17-C34-C33	-10.4(3)
C16'-C17-C34-C33	151.8(10)
C16-C17-C34-C33	169.1(3)
C18-C17-C34-C1	167.7(2)
C16'-C17-C34-C1	-30.2(11)
C16-C17-C34-C1	-12.8(4)
C2-C1-C34-C33	-173.7(2)
C35-C1-C34-C33	1.7(3)
C2-C1-C34-C17	8.3(3)
C35-C1-C34-C17	-176.3(2)
C2-C1-C35-C36	58.5(3)
C34-C1-C35-C36	-116.8(2)
C2-C1-C35-C44	-120.1(3)
C34-C1-C35-C44	64.6(3)
C44-C35-C36-C37	2.3(3)
C1-C35-C36-C37	-176.4(2)
C35-C36-C37-C38	-1.0(4)
C36-C37-C38-C39	-0.6(4)
C37-C38-C39-C40	-179.6(2)
C37-C38-C39-C44	0.9(4)
C38-C39-C40-C41	178.4(3)
C44-C39-C40-C41	-2.1(4)
C39-C40-C41-C42	2.0(4)
C40-C41-C42-C43	0.6(4)
C41-C42-C43-C44	-2.9(4)
C42-C43-C44-C35	-178.4(2)
C42-C43-C44-C39	2.7(3)
C36-C35-C44-C43	179.2(2)

C1-C35-C44-C43	-2.1(3)
C36-C35-C44-C39	-1.9(3)
C1-C35-C44-C39	176.74(19)
C38-C39-C44-C43	179.3(2)
C40-C39-C44-C43	-0.3(3)
C38-C39-C44-C35	0.4(3)
C40-C39-C44-C35	-179.2(2)
C15-C16-C45-C46	65.9(6)
C17-C16-C45-C46	-109.8(5)
C15-C16-C45-C54	-113.0(4)
C17-C16-C45-C54	71.2(6)
C54-C45-C46-C47	0.8(6)
C16-C45-C46-C47	-178.2(4)
C45-C46-C47-C48	1.7(7)
C46-C47-C48-C49	-1.5(7)
C47-C48-C49-C50	-179.3(5)
C47-C48-C49-C54	-1.1(9)
C48-C49-C50-C51	179.0(5)
C54-C49-C50-C51	0.8(9)
C49-C50-C51-C52	-0.6(6)
C50-C51-C52-C53	0.6(6)
C51-C52-C53-C54	-0.8(7)
C52-C53-C54-C49	1.0(7)
C52-C53-C54-C45	178.1(4)
C50-C49-C54-C53	-1.0(9)
C48-C49-C54-C53	-179.2(5)
C50-C49-C54-C45	-178.2(5)
C48-C49-C54-C45	3.5(8)
C46-C45-C54-C53	179.5(4)
C16-C45-C54-C53	-1.6(5)
C46-C45-C54-C49	-3.4(6)
C16-C45-C54-C49	175.6(5)
C17-C16'-C45'-C46'	73(2)
C15-C16'-C45'-C46'	-119(2)
C17-C16'-C45'-C54'	-111.6(16)
C15-C16'-C45'-C54'	56(3)
C54'-C45'-C46'-C47'	-2(3)
C16'-C45'-C46'-C47'	172.8(18)

C45'-C46'-C47'-C48'	1(3)
C46'-C47'-C48'-C49'	2(3)
C47'-C48'-C49'-C50'	-179(3)
C47'-C48'-C49'-C54'	-5(4)
C48'-C49'-C50'-C51'	179(2)
C54'-C49'-C50'-C51'	6(4)
C49'-C50'-C51'-C52'	-1(3)
C50'-C51'-C52'-C53'	0(3)
C51'-C52'-C53'-C54'	-3(3)
C52'-C53'-C54'-C45'	-179.4(18)
C52'-C53'-C54'-C49'	7(3)
C46'-C45'-C54'-C53'	-174.0(19)
C16'-C45'-C54'-C53'	11(2)
C46'-C45'-C54'-C49'	0(3)
C16'-C45'-C54'-C49'	-175(2)
C50'-C49'-C54'-C53'	-8(4)
C48'-C49'-C54'-C53'	178(3)
C50'-C49'-C54'-C45'	178(2)
C48'-C49'-C54'-C45'	4(4)

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*2.3. 9,20-Bis(4-hexylnaphthalen-1-yl)tetrabenzo[a,c,j,l]tetracene (**2b**)*

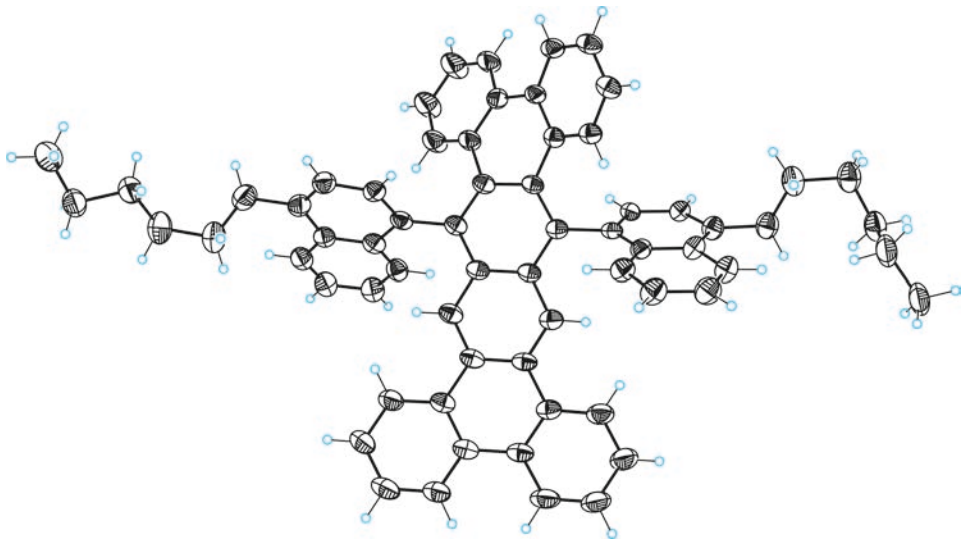

Table 7. Crystal data and structure refinement for **2b**.

Identification code	RD470_0m

Empirical formula	C66.15 H56.83 Cl0.45	
Formula weight	867.69	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 9.3755(6)Å	a= 90°.
	b = 26.1158(14)Å	b = 101.625(2)°.
	c = 20.0039(14)Å	g = 90°.
Volume	4797.5(5) $Å^3$	
Z	4	
Density (calculated)	1.201 Mg/m^3	
Absorption coefficient	0.092 mm^{-1}	
F(000)	1846	
Crystal size	0.04 x 0.005 x 0.005 mm^3	
Theta range for data collection	1.874 to 25.042°.	
Index ranges	-11<=h<=7,-27<=k<=27,-23<=l<=22	
Reflections collected	22882	
Independent reflections	7790[R(int) = 0.0418]	
Completeness to theta =25.042°	97.899994%	
Absorption correction	Empirical	
Max. and min. transmission	1.000 and 0.887	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7790/ 1192/ 1015	
Goodness-of-fit on F^2	1.056	
Final R indices [I>2sigma(I)]	R1 = 0.0769, wR2 = 0.2148	
R indices (all data)	R1 = 0.1286, wR2 = 0.2486	
Largest diff. peak and hole	0.665 and -0.531 $e.Å^{-3}$	

Table 8. Bond lengths [Å] and angles [°] for **2b**.

Bond lengths----	
C1-C34	1.402(5)
C1-C2	1.419(5)
C1-C35	1.509(7)
C1-C35'	1.514(10)
C2-C3	1.419(5)

C2-C19	1.426(5)
C3-C4	1.382(5)
C4-C17	1.429(5)
C4-C5	1.473(5)
C5-C6	1.401(6)
C5-C10	1.407(5)
C6-C7	1.377(6)
C7-C8	1.383(6)
C8-C9	1.368(6)
C9-C10	1.412(6)
C10-C11	1.474(6)
C11-C12	1.395(5)
C11-C16	1.411(5)
C12-C13	1.383(6)
C13-C14	1.384(6)
C14-C15	1.373(6)
C15-C16	1.410(5)
C16-C17	1.468(5)
C17-C18	1.390(5)
C18-C19	1.413(5)
C19-C20	1.426(5)
C20-C21	1.391(5)
C20-C51'	1.510(9)
C20-C51	1.515(8)
C21-C34	1.442(5)
C21-C22	1.486(5)
C22-C23	1.404(6)
C22-C27	1.408(5)
C23-C24	1.369(6)
C24-C25	1.376(6)
C25-C26	1.376(6)
C26-C27	1.402(5)
C27-C28	1.474(5)
C28-C33	1.398(5)
C28-C29	1.403(5)
C29-C30	1.378(6)
C30-C31	1.388(5)
C31-C32	1.382(5)

C32-C33	1.407(5)
C33-C34	1.469(5)
C35-C36	1.33(4)
C35-C44	1.39(3)
C36-C37	1.41(2)
C37-C38	1.379(16)
C38-C39	1.44(2)
C38-C45	1.524(7)
C39-C40	1.429(19)
C39-C44	1.44(2)
C40-C41	1.380(18)
C41-C42	1.41(2)
C42-C43	1.36(3)
C43-C44	1.42(4)
C45-C46	1.535(7)
C46-C47"	1.531(10)
C47-C48	1.574(8)
C48-C49	1.498(8)
C49-C50	1.552(9)
C47"-C48"	1.513(10)
C48"-C49"	1.520(10)
C49"-C50"	1.553(10)
C49"-C50"#1	1.83(2)
C50"-C49"#1	1.83(2)
C50"-C50"#1	2.00(4)
C35'-C36'	1.46(8)
C35'-C44'	1.52(6)
C36'-C37'	1.42(4)
C37'-C38'	1.34(3)
C38'-C39'	1.39(4)
C38'-C45'	1.518(10)
C39'-C40'	1.40(4)
C39'-C44'	1.42(4)
C40'-C41'	1.32(3)
C41'-C42'	1.45(3)
C42'-C43'	1.37(5)
C43'-C44'	1.42(6)
C45'-C46'	1.533(9)

C46'-C47'	1.539(9)
C47'-C48'	1.538(9)
C48'-C49'	1.607(9)
C49'-C50'	1.565(10)
C51-C52	1.400(15)
C51-C60	1.452(15)
C52-C53	1.398(17)
C53-C54	1.376(13)
C54-C55	1.437(12)
C54-C61	1.540(8)
C55-C56	1.417(12)
C55-C60	1.421(14)
C56-C57	1.343(13)
C57-C58	1.379(13)
C58-C59	1.389(15)
C59-C60	1.401(13)
C61-C62	1.533(8)
C62-C63	1.520(8)
C63-C64	1.530(8)
C64-C65	1.538(8)
C65-C66	1.531(9)
C51'-C52'	1.30(3)
C51'-C60'	1.42(2)
C52'-C53'	1.47(3)
C53'-C54'	1.366(19)
C54'-C55'	1.440(18)
C54'-C61'	1.528(11)
C55'-C56'	1.38(2)
C55'-C60'	1.40(2)
C56'-C57'	1.37(2)
C57'-C58'	1.41(2)
C58'-C59'	1.356(19)
C59'-C60'	1.435(19)
C61'-C62'	1.542(11)
C62'-C63'	1.542(11)
C63'-C64'	1.543(11)
C64'-C65'	1.542(11)
C65'-C66'	1.540(11)

C61"-C62"	1.543(10)
C62"-C63"	1.542(10)
C63"-C64"	1.544(10)
C64"-C65"	1.539(10)
C65"-C66"	1.538(10)
Cl1S-C1S	1.793(11)
Cl2S-C1S	1.777(10)
C1S-Cl3S	1.776(10)

Angles----------

C34-C1-C2	118.9(3)
C34-C1-C35	119.8(16)
C2-C1-C35	120.8(15)
C34-C1-C35'	119(3)
C2-C1-C35'	122(3)
C1-C2-C3	121.7(3)
C1-C2-C19	119.6(3)
C3-C2-C19	118.5(3)
C4-C3-C2	122.6(4)
C3-C4-C17	118.9(3)
C3-C4-C5	121.2(4)
C17-C4-C5	119.8(3)
C6-C5-C10	118.6(4)
C6-C5-C4	121.7(3)
C10-C5-C4	119.7(3)
C7-C6-C5	122.3(4)
C6-C7-C8	119.1(4)
C9-C8-C7	120.1(4)
C8-C9-C10	122.0(4)
C5-C10-C9	118.0(4)
C5-C10-C11	120.4(3)
C9-C10-C11	121.4(4)
C12-C11-C16	119.4(4)
C12-C11-C10	120.7(4)
C16-C11-C10	119.8(3)
C13-C12-C11	120.7(4)
C12-C13-C14	120.5(4)
C15-C14-C13	119.4(4)

C14-C15-C16	121.8(4)
C15-C16-C11	118.0(3)
C15-C16-C17	121.8(3)
C11-C16-C17	120.1(3)
C18-C17-C4	118.4(3)
C18-C17-C16	121.9(3)
C4-C17-C16	119.6(3)
C17-C18-C19	123.4(4)
C18-C19-C2	117.5(3)
C18-C19-C20	122.9(3)
C2-C19-C20	119.6(3)
C21-C20-C19	119.5(3)
C21-C20-C51'	123.0(14)
C19-C20-C51'	117.5(14)
C21-C20-C51	118.7(9)
C19-C20-C51	120.8(10)
C20-C21-C34	118.8(3)
C20-C21-C22	125.1(3)
C34-C21-C22	115.8(3)
C23-C22-C27	117.1(3)
C23-C22-C21	122.4(3)
C27-C22-C21	119.8(3)
C24-C23-C22	122.3(4)
C23-C24-C25	120.4(4)
C26-C25-C24	119.2(4)
C25-C26-C27	121.3(4)
C26-C27-C22	119.7(4)
C26-C27-C28	121.2(4)
C22-C27-C28	119.2(3)
C33-C28-C29	120.0(4)
C33-C28-C27	118.4(3)
C29-C28-C27	121.6(3)
C30-C29-C28	120.6(4)
C29-C30-C31	119.9(4)
C32-C31-C30	119.9(4)
C31-C32-C33	121.3(4)
C28-C33-C32	118.2(3)
C28-C33-C34	120.0(3)

C32-C33-C34	121.4(3)
C1-C34-C21	119.5(3)
C1-C34-C33	123.1(3)
C21-C34-C33	117.3(3)
C36-C35-C44	123.2(12)
C36-C35-C1	115(2)
C44-C35-C1	122(2)
C35-C36-C37	120.3(15)
C38-C37-C36	121.5(14)
C37-C38-C39	117.7(10)
C37-C38-C45	120.3(10)
C39-C38-C45	122.0(10)
C40-C39-C44	117.5(15)
C40-C39-C38	122.5(13)
C44-C39-C38	120.0(13)
C41-C40-C39	122.4(13)
C40-C41-C42	119.6(12)
C43-C42-C41	119.2(18)
C42-C43-C44	124(2)
C35-C44-C43	125.2(18)
C35-C44-C39	117.2(17)
C43-C44-C39	117.6(16)
C38-C45-C46	112.3(6)
C47"-C46-C45	116.3(9)
C49-C48-C47	113.2(7)
C48-C49-C50	113.2(8)
C48"-C47"-C46	114.5(9)
C47"-C48"-C49"	112.8(9)
C48"-C49"-C50"	109.2(9)
C48"-C49"-C50"#1	163.7(15)
C50"-C49"-C50"#1	71.9(13)
C49"-C50"-C49"#1	108.1(13)
C49"-C50"-C50"#1	60.5(9)
C49"#1-C50"-C50"#1	47.6(8)
C36'-C35'-C1	119(4)
C36'-C35'-C44'	111(2)
C1-C35'-C44'	130(5)
C37'-C36'-C35'	123(3)

C38'-C37'-C36'	122(3)
C37'-C38'-C39'	120(2)
C37'-C38'-C45'	117(2)
C39'-C38'-C45'	123(2)
C38'-C39'-C40'	121(2)
C38'-C39'-C44'	121(3)
C40'-C39'-C44'	118(3)
C41'-C40'-C39'	122(2)
C40'-C41'-C42'	120(2)
C43'-C42'-C41'	121(3)
C42'-C43'-C44'	117(4)
C39'-C44'-C43'	122(3)
C39'-C44'-C35'	122(3)
C43'-C44'-C35'	116(3)
C38'-C45'-C46'	114.2(14)
C45'-C46'-C47'	112.1(8)
C48'-C47'-C46'	111.6(8)
C47'-C48'-C49'	107.1(8)
C50'-C49'-C48'	102.9(8)
C52-C51-C60	115.4(9)
C52-C51-C20	122.1(10)
C60-C51-C20	122.4(10)
C53-C52-C51	123.8(10)
C54-C53-C52	120.6(8)
C53-C54-C55	119.6(7)
C53-C54-C61	119.6(8)
C55-C54-C61	120.8(9)
C56-C55-C60	118.9(9)
C56-C55-C54	122.0(9)
C60-C55-C54	119.0(8)
C57-C56-C55	120.6(9)
C56-C57-C58	121.5(10)
C57-C58-C59	119.8(9)
C58-C59-C60	120.7(9)
C59-C60-C55	118.4(9)
C59-C60-C51	119.9(9)
C55-C60-C51	121.5(8)
C62-C61-C54	112.2(6)

C63-C62-C61	110.0(8)
C62-C63-C64	119.9(9)
C63-C64-C65	107.4(9)
C66-C65-C64	101.0(9)
C52'-C51'-C60'	123.7(14)
C52'-C51'-C20	112.7(16)
C60'-C51'-C20	123.6(14)
C51'-C52'-C53'	118.1(15)
C54'-C53'-C52'	120.8(13)
C53'-C54'-C55'	119.7(11)
C53'-C54'-C61'	112(3)
C55'-C54'-C61'	128(2)
C56'-C55'-C60'	121.6(14)
C56'-C55'-C54'	120.3(13)
C60'-C55'-C54'	118.1(12)
C57'-C56'-C55'	119.6(14)
C56'-C57'-C58'	120.0(13)
C59'-C58'-C57'	121.5(12)
C58'-C59'-C60'	119.2(13)
C55'-C60'-C51'	119.4(14)
C55'-C60'-C59'	118.1(15)
C51'-C60'-C59'	122.5(14)
C54'-C61'-C62'	126(3)
C63'-C62'-C61'	128(5)
C62'-C63'-C64'	91(3)
C65'-C64'-C63'	131(6)
C66'-C65'-C64'	137(7)
C63"-C62"-C61"	121.0(15)
C62"-C63"-C64"	127.6(15)
C65"-C64"-C63"	116.6(16)
C66"-C65"-C64"	131(2)
Cl3S-C1S-Cl2S	105.2(10)
Cl3S-C1S-Cl1S	112.3(10)
Cl2S-C1S-Cl1S	107.5(10)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1, -y+1, -z+2

Table 9. Torsion angles [°] for **2b**.

C34-C1-C2-C3	-176.3(3)
C35-C1-C2-C3	11.9(16)
C35'-C1-C2-C3	7(3)
C34-C1-C2-C19	-1.8(5)
C35-C1-C2-C19	-173.7(15)
C35'-C1-C2-C19	-178(3)
C1-C2-C3-C4	166.0(4)
C19-C2-C3-C4	-8.5(5)
C2-C3-C4-C17	2.1(6)
C2-C3-C4-C5	-175.2(3)
C3-C4-C5-C6	1.3(6)
C17-C4-C5-C6	-176.0(4)
C3-C4-C5-C10	-179.3(4)
C17-C4-C5-C10	3.4(5)
C10-C5-C6-C7	1.3(6)
C4-C5-C6-C7	-179.3(4)
C5-C6-C7-C8	-1.1(7)
C6-C7-C8-C9	0.4(8)
C7-C8-C9-C10	0.1(7)
C6-C5-C10-C9	-0.7(6)
C4-C5-C10-C9	179.9(4)
C6-C5-C10-C11	174.4(4)
C4-C5-C10-C11	-5.0(6)
C8-C9-C10-C5	0.1(6)
C8-C9-C10-C11	-175.0(4)
C5-C10-C11-C12	-176.3(4)
C9-C10-C11-C12	-1.3(6)
C5-C10-C11-C16	0.7(6)
C9-C10-C11-C16	175.6(4)
C16-C11-C12-C13	-3.4(7)
C10-C11-C12-C13	173.6(4)
C11-C12-C13-C14	0.3(8)
C12-C13-C14-C15	1.9(8)
C13-C14-C15-C16	-0.9(7)
C14-C15-C16-C11	-2.2(6)
C14-C15-C16-C17	179.8(4)

C12-C11-C16-C15	4.2(6)
C10-C11-C16-C15	-172.7(4)
C12-C11-C16-C17	-177.7(4)
C10-C11-C16-C17	5.3(5)
C3-C4-C17-C18	4.5(5)
C5-C4-C17-C18	-178.2(3)
C3-C4-C17-C16	-174.8(3)
C5-C4-C17-C16	2.5(5)
C15-C16-C17-C18	-8.2(6)
C11-C16-C17-C18	173.9(3)
C15-C16-C17-C4	171.1(4)
C11-C16-C17-C4	-6.9(5)
C4-C17-C18-C19	-4.7(6)
C16-C17-C18-C19	174.6(3)
C17-C18-C19-C2	-1.7(6)
C17-C18-C19-C20	178.7(4)
C1-C2-C19-C18	-166.5(3)
C3-C2-C19-C18	8.1(5)
C1-C2-C19-C20	13.1(5)
C3-C2-C19-C20	-172.3(3)
C18-C19-C20-C21	173.3(3)
C2-C19-C20-C21	-6.3(5)
C18-C19-C20-C51'	-6.7(12)
C2-C19-C20-C51'	173.6(11)
C18-C19-C20-C51	5.0(9)
C2-C19-C20-C51	-174.7(7)
C19-C20-C21-C34	-11.3(5)
C51'-C20-C21-C34	168.8(11)
C51-C20-C21-C34	157.3(8)
C19-C20-C21-C22	162.7(4)
C51'-C20-C21-C22	-17.2(12)
C51-C20-C21-C22	-28.7(9)
C20-C21-C22-C23	-20.0(6)
C34-C21-C22-C23	154.2(4)
C20-C21-C22-C27	170.2(4)
C34-C21-C22-C27	-15.7(5)
C27-C22-C23-C24	0.4(7)
C21-C22-C23-C24	-169.7(4)

C22-C23-C24-C25	1.0(8)
C23-C24-C25-C26	-1.5(9)
C24-C25-C26-C27	0.5(8)
C25-C26-C27-C22	0.9(7)
C25-C26-C27-C28	-178.6(4)
C23-C22-C27-C26	-1.3(6)
C21-C22-C27-C26	169.1(4)
C23-C22-C27-C28	178.1(4)
C21-C22-C27-C28	-11.5(5)
C26-C27-C28-C33	-159.0(4)
C22-C27-C28-C33	21.6(5)
C26-C27-C28-C29	22.9(6)
C22-C27-C28-C29	-156.5(4)
C33-C28-C29-C30	0.1(5)
C27-C28-C29-C30	178.1(3)
C28-C29-C30-C31	-1.4(5)
C29-C30-C31-C32	1.0(5)
C30-C31-C32-C33	0.7(5)
C29-C28-C33-C32	1.6(5)
C27-C28-C33-C32	-176.5(3)
C29-C28-C33-C34	174.3(3)
C27-C28-C33-C34	-3.9(5)
C31-C32-C33-C28	-2.0(5)
C31-C32-C33-C34	-174.6(3)
C2-C1-C34-C21	-15.9(5)
C35-C1-C34-C21	156.0(15)
C35'-C1-C34-C21	161(3)
C2-C1-C34-C33	159.1(3)
C35-C1-C34-C33	-29.0(15)
C35'-C1-C34-C33	-24(3)
C20-C21-C34-C1	22.7(5)
C22-C21-C34-C1	-151.8(3)
C20-C21-C34-C33	-152.6(3)
C22-C21-C34-C33	32.9(5)
C28-C33-C34-C1	161.2(3)
C32-C33-C34-C1	-26.3(5)
C28-C33-C34-C21	-23.6(5)
C32-C33-C34-C21	148.8(3)

C34-C1-C35-C36	-57(3)
C2-C1-C35-C36	115(3)
C35'-C1-C35-C36	-130(65)
C34-C1-C35-C44	120(3)
C2-C1-C35-C44	-68(3)
C35'-C1-C35-C44	47(61)
C44-C35-C36-C37	3(4)
C1-C35-C36-C37	-180.0(19)
C35-C36-C37-C38	-2(3)
C36-C37-C38-C39	0.6(19)
C36-C37-C38-C45	-178.2(14)
C37-C38-C39-C40	178.2(11)
C45-C38-C39-C40	-3.0(16)
C37-C38-C39-C44	0.3(18)
C45-C38-C39-C44	179.0(12)
C44-C39-C40-C41	-1.1(17)
C38-C39-C40-C41	-179.1(11)
C39-C40-C41-C42	0.6(15)
C40-C41-C42-C43	-1.1(19)
C41-C42-C43-C44	2(3)
C36-C35-C44-C43	178(3)
C1-C35-C44-C43	2(4)
C36-C35-C44-C39	-3(4)
C1-C35-C44-C39	-179(2)
C42-C43-C44-C35	177(2)
C42-C43-C44-C39	-3(3)
C40-C39-C44-C35	-177(2)
C38-C39-C44-C35	1(3)
C40-C39-C44-C43	2(2)
C38-C39-C44-C43	180.0(16)
C37-C38-C45-C46	98.0(10)
C39-C38-C45-C46	-80.7(12)
C38-C45-C46-C47"	175.7(10)
C47-C48-C49-C50	165.1(11)
C45-C46-C47"-C48"	-31.4(17)
C46-C47"-C48"-C49"	-79.0(18)
C47"-C48"-C49"-C50"	-173.5(13)
C47"-C48"-C49"-C50"#1	95(5)

C48"-C49"-C50"-C49"#1	-162.8(17)
C50"#1-C49"-C50"-C49"#1	0.003(2)
C48"-C49"-C50"-C50"#1	-162.8(17)
C34-C1-C35'-C36'	-64(6)
C2-C1-C35'-C36'	112(5)
C35-C1-C35'-C36'	44(59)
C34-C1-C35'-C44'	119(6)
C2-C1-C35'-C44'	-64(7)
C35-C1-C35'-C44'	-132(67)
C1-C35'-C36'-C37'	174(4)
C44'-C35'-C36'-C37'	-9(7)
C35'-C36'-C37'-C38'	6(6)
C36'-C37'-C38'-C39'	1(4)
C36'-C37'-C38'-C45'	-175(3)
C37'-C38'-C39'-C40'	180(2)
C45'-C38'-C39'-C40'	-5(4)
C37'-C38'-C39'-C44'	-3(4)
C45'-C38'-C39'-C44'	173(3)
C38'-C39'-C40'-C41'	177(2)
C44'-C39'-C40'-C41'	0(3)
C39'-C40'-C41'-C42'	-2(3)
C40'-C41'-C42'-C43'	1(3)
C41'-C42'-C43'-C44'	2(4)
C38'-C39'-C44'-C43'	-174(3)
C40'-C39'-C44'-C43'	4(5)
C38'-C39'-C44'-C35'	-1(5)
C40'-C39'-C44'-C35'	176(4)
C42'-C43'-C44'-C39'	-4(5)
C42'-C43'-C44'-C35'	-177(4)
C36'-C35'-C44'-C39'	7(7)
C1-C35'-C44'-C39'	-176(5)
C36'-C35'-C44'-C43'	-180(4)
C1-C35'-C44'-C43'	-3(8)
C37'-C38'-C45'-C46'	-97(2)
C39'-C38'-C45'-C46'	87(3)
C38'-C45'-C46'-C47'	-179.6(16)
C45'-C46'-C47'-C48'	-169.8(14)
C46'-C47'-C48'-C49'	-169.9(12)

C47'-C48'-C49'-C50'	82.9(17)
C21-C20-C51-C52	-58(2)
C19-C20-C51-C52	110.7(17)
C51'-C20-C51-C52	-174(14)
C21-C20-C51-C60	120.5(16)
C19-C20-C51-C60	-71(2)
C51'-C20-C51-C60	4(11)
C60-C51-C52-C53	-3(2)
C20-C51-C52-C53	174.8(16)
C51-C52-C53-C54	3(2)
C52-C53-C54-C55	0.0(15)
C52-C53-C54-C61	177.3(10)
C53-C54-C55-C56	-178.3(8)
C61-C54-C55-C56	4.4(12)
C53-C54-C55-C60	-2.4(13)
C61-C54-C55-C60	-179.7(9)
C60-C55-C56-C57	0.0(13)
C54-C55-C56-C57	176.0(8)
C55-C56-C57-C58	-2.2(13)
C56-C57-C58-C59	2.4(14)
C57-C58-C59-C60	-0.4(15)
C58-C59-C60-C55	-1.6(16)
C58-C59-C60-C51	-177.9(14)
C56-C55-C60-C59	1.8(14)
C54-C55-C60-C59	-174.2(10)
C56-C55-C60-C51	178.0(13)
C54-C55-C60-C51	2.0(17)
C52-C51-C60-C59	176.9(15)
C20-C51-C60-C59	-1(2)
C52-C51-C60-C55	1(2)
C20-C51-C60-C55	-177.4(14)
C53-C54-C61-C62	-94.7(10)
C55-C54-C61-C62	82.6(11)
C54-C61-C62-C63	-179.3(8)
C61-C62-C63-C64	-79.7(14)
C62-C63-C64-C65	-157.6(11)
C63-C64-C65-C66	-170.7(12)
C21-C20-C51'-C52'	-63(3)

C19-C20-C51'-C52'	117(2)
C51-C20-C51'-C52'	7(11)
C21-C20-C51'-C60'	116(2)
C19-C20-C51'-C60'	-64(3)
C51-C20-C51'-C60'	-174(15)
C60'-C51'-C52'-C53'	5(4)
C20-C51'-C52'-C53'	-176(2)
C51'-C52'-C53'-C54'	-2(3)
C52'-C53'-C54'-C55'	0(2)
C52'-C53'-C54'-C61'	-172(3)
C53'-C54'-C55'-C56'	-177.1(14)
C61'-C54'-C55'-C56'	-7(3)
C53'-C54'-C55'-C60'	0(2)
C61'-C54'-C55'-C60'	171(3)
C60'-C55'-C56'-C57'	0(2)
C54'-C55'-C56'-C57'	176.9(13)
C55'-C56'-C57'-C58'	2(2)
C56'-C57'-C58'-C59'	-3(2)
C57'-C58'-C59'-C60'	1(2)
C56'-C55'-C60'-C51'	179(2)
C54'-C55'-C60'-C51'	2(3)
C56'-C55'-C60'-C59'	-2(2)
C54'-C55'-C60'-C59'	-178.7(15)
C52'-C51'-C60'-C55'	-5(4)
C20-C51'-C60'-C55'	176(2)
C52'-C51'-C60'-C59'	176(3)
C20-C51'-C60'-C59'	-3(4)
C58'-C59'-C60'-C55'	1(2)
C58'-C59'-C60'-C51'	-180(2)
C53'-C54'-C61'-C62'	-50(7)
C55'-C54'-C61'-C62'	139(5)
C54'-C61'-C62'-C63'	-122(6)
C61'-C62'-C63'-C64'	-135(7)
C62'-C63'-C64'-C65'	-178(9)
C63'-C64'-C65'-C66'	55(14)
C61"-C62"-C63"-C64"	106(3)
C62"-C63"-C64"-C65"	162(2)
C63"-C64"-C65"-C66"	-88(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1, -y+1, -z+2

*2.4. 9,20-Bis(4-dodecylnaphthalen-1-yl)tetrabenzo[a,c,j,l]tetracene (**2c**)*

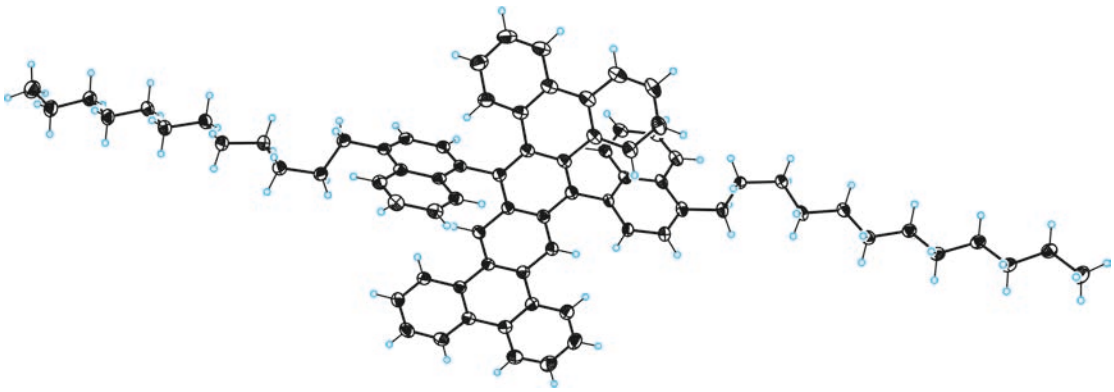

Table 10. Crystal data and structure refinement for **2c**.

Identification code	RD393_0m	
Empirical formula	C78 H81.40	
Formula weight	1018.83	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.6054(2) Å	a= 72.252(2) °.
	b = 18.7609(6) Å	b = 84.027(2) °.
	c = 21.2252(8) Å	g = 87.900(2) °.
Volume	2868.67(16) $Å^3$	
Z	2	
Density (calculated)	1.180 Mg/m^3	
Absorption coefficient	0.066 mm^{-1}	
F(000)	1099	
Crystal size	0.06 x 0.01 x 0.001 mm^3	
Theta range for data collection	1.14 to 29.91 °.	
Index ranges	-10 <=h<=10 ,-26 <=k<=26 ,-29 <=l<=29	
Reflections collected	25427	

Independent reflections	15305 [R(int) = 0.0232]
Completeness to theta =29.91 °	92.1%
Absorption correction	Empirical
Max. and min. transmission	0.9999 and 0.9960
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	15305 / 852 / 1103
Goodness-of-fit on F^2	1.013
Final R indices [I>2sigma(I)]	R1 = 0.0603 , wR2 = 0.1406
R indices (all data)	R1 = 0.1053 , wR2 = 0.1644
Largest diff. peak and hole	0.355 and -0.295 e.Å^{-3}

Table 11. Bond lengths [Å] and angles [°] for **2c**.

Bond lengths----	
C1-C34	1.414(2)
C1-C2	1.414(2)
C1-C35	1.489(3)
C1-C35'	1.510(5)
C2-C15	1.433(2)
C2-C3	1.486(2)
C3-C4	1.403(2)
C3-C8	1.422(2)
C4-C5	1.379(2)
C5-C6	1.392(3)
C6-C7	1.363(3)
C7-C8	1.405(2)
C8-C9	1.462(2)
C9-C14	1.400(2)
C9-C10	1.413(2)
C10-C11	1.373(3)
C11-C12	1.380(3)
C12-C13	1.378(2)
C13-C14	1.410(2)
C14-C15	1.476(2)
C15-C16	1.406(2)
C16-C17	1.408(2)
C16-C57'	1.471(7)
C16-C57	1.503(3)

C17-C34	1.400(2)
C17-C18	1.468(2)
C18-C19	1.457(2)
C19-C32	1.382(2)
C19-C20	1.454(2)
C20-C21	1.412(2)
C20-C25	1.415(2)
C21-C22	1.375(2)
C22-C23	1.387(3)
C23-C24	1.368(3)
C24-C25	1.413(2)
C25-C26	1.454(2)
C26-C27	1.412(2)
C26-C31	1.418(2)
C27-C28	1.368(2)
C28-C29	1.393(2)
C29-C30	1.377(2)
C30-C31	1.408(2)
C31-C32	1.4581(19)
C32-C33	1.464(2)
C33-C34	1.479(2)
C35-C44	1.372(3)
C35-C36	1.426(3)
C36-C37	1.413(3)
C36-C41	1.432(3)
C37-C38	1.381(3)
C38-C39	1.399(4)
C39-C40	1.368(4)
C40-C41	1.421(3)
C41-C42	1.430(3)
C42-C43	1.369(3)
C42-C45	1.512(3)
C43-C44	1.411(3)
C45-C46	1.535(3)
C46-C47	1.521(3)
C47-C48	1.529(4)
C48-C49	1.527(4)
C49-C50	1.523(4)

C50-C51	1.526(4)
C51-C52	1.515(4)
C52-C53	1.521(4)
C53-C54	1.518(4)
C54-C55	1.520(5)
C55-C56	1.524(5)
C35'-C44'	1.372(4)
C35'-C36'	1.426(4)
C36'-C37'	1.413(5)
C36'-C41'	1.431(4)
C37'-C38'	1.380(4)
C38'-C39'	1.393(5)
C39'-C40'	1.362(5)
C40'-C41'	1.421(5)
C41'-C42'	1.429(5)
C42'-C43'	1.368(5)
C42'-C45'	1.516(6)
C43'-C44'	1.412(5)
C45'-C46'	1.498(6)
C46'-C47'	1.541(6)
C47'-C48'	1.512(7)
C48'-C49'	1.521(8)
C49'-C50'	1.503(7)
C50'-C51'	1.509(8)
C51'-C52'	1.505(8)
C52'-C53'	1.506(8)
C53'-C54'	1.508(8)
C54'-C55'	1.504(9)
C55'-C56'	1.507(9)
C57-C66	1.372(3)
C57-C58	1.431(2)
C58-C59	1.414(3)
C58-C63	1.427(3)
C59-C60	1.370(3)
C60-C61	1.402(4)
C61-C62	1.367(4)
C62-C63	1.432(3)
C63-C64	1.431(3)

C64-C65	1.373(3)
C64-C67	1.517(3)
C65-C66	1.407(3)
C67-C68	1.553(3)
C68-C69	1.525(3)
C69-C70	1.527(3)
C70-C71	1.537(3)
C71-C72	1.521(3)
C72-C73	1.531(3)
C73-C74	1.528(3)
C74-C75	1.525(3)
C75-C76	1.521(3)
C76-C77	1.527(4)
C77-C78	1.524(4)
C57'-C66'	1.369(4)
C57'-C58'	1.428(4)
C58'-C59'	1.411(5)
C58'-C63'	1.427(4)
C59'-C60'	1.367(5)
C60'-C61'	1.399(5)
C61'-C62'	1.366(5)
C62'-C63'	1.433(4)
C63'-C64'	1.428(5)
C64'-C65'	1.371(5)
C64'-C67'	1.502(7)
C65'-C66'	1.408(5)
C67'-C68'	1.469(7)
C68'-C69'	1.525(7)
C69'-C70'	1.509(8)
C70'-C71'	1.516(9)
C71'-C72'	1.525(9)
C72'-C73'	1.507(9)
C73'-C74'	1.517(9)
C74'-C75'	1.509(9)
C75'-C76'	1.508(9)
C76'-C77'	1.521(9)
C77'-C78'	1.521(9)

Angles----------

C34-C1-C2	120.47(14)
C34-C1-C35	116.6(4)
C2-C1-C35	122.8(4)
C34-C1-C35'	112.8(10)
C2-C1-C35'	126.7(10)
C35-C1-C35'	6.5(8)
C1-C2-C15	118.43(14)
C1-C2-C3	123.36(14)
C15-C2-C3	117.92(13)
C4-C3-C8	116.72(15)
C4-C3-C2	124.40(14)
C8-C3-C2	118.85(15)
C5-C4-C3	122.64(16)
C4-C5-C6	119.50(19)
C7-C6-C5	119.31(17)
C6-C7-C8	122.10(16)
C7-C8-C3	118.95(17)
C7-C8-C9	120.63(15)
C3-C8-C9	119.82(14)
C14-C9-C10	118.40(16)
C14-C9-C8	119.06(14)
C10-C9-C8	121.98(16)
C11-C10-C9	121.34(17)
C10-C11-C12	119.86(16)
C13-C12-C11	119.90(17)
C12-C13-C14	121.20(16)
C9-C14-C13	118.40(14)
C9-C14-C15	119.13(15)
C13-C14-C15	122.46(15)
C16-C15-C2	120.16(13)
C16-C15-C14	120.74(14)
C2-C15-C14	119.00(14)
C15-C16-C17	120.24(14)
C15-C16-C57'	119.7(8)
C17-C16-C57'	119.9(9)
C15-C16-C57	121.4(3)
C17-C16-C57	118.2(3)

C57'-C16-C57	2.4(6)
C34-C17-C16	119.84(14)
C34-C17-C18	120.69(13)
C16-C17-C18	119.45(14)
C19-C18-C17	118.88(14)
C32-C19-C20	120.65(13)
C32-C19-C18	121.07(14)
C20-C19-C18	118.27(14)
C21-C20-C25	118.57(15)
C21-C20-C19	121.47(14)
C25-C20-C19	119.96(14)
C22-C21-C20	121.40(16)
C21-C22-C23	119.84(17)
C24-C23-C22	120.28(17)
C23-C24-C25	121.52(16)
C24-C25-C20	118.38(16)
C24-C25-C26	122.05(14)
C20-C25-C26	119.54(14)
C27-C26-C31	118.56(15)
C27-C26-C25	121.63(15)
C31-C26-C25	119.77(13)
C28-C27-C26	121.40(16)
C27-C28-C29	120.18(15)
C30-C29-C28	119.95(16)
C29-C30-C31	121.26(15)
C30-C31-C26	118.64(13)
C30-C31-C32	121.55(14)
C26-C31-C32	119.81(14)
C19-C32-C31	120.14(14)
C19-C32-C33	120.73(13)
C31-C32-C33	119.12(13)
C32-C33-C34	118.90(14)
C17-C34-C1	120.38(13)
C17-C34-C33	119.69(14)
C1-C34-C33	119.75(14)
C44-C35-C36	119.3(2)
C44-C35-C1	119.9(2)
C36-C35-C1	120.8(2)

C37-C36-C35	121.2(2)
C37-C36-C41	119.2(2)
C35-C36-C41	119.6(2)
C38-C37-C36	121.2(3)
C37-C38-C39	119.5(2)
C40-C39-C38	120.9(2)
C39-C40-C41	121.4(2)
C40-C41-C42	122.7(2)
C40-C41-C36	117.8(2)
C42-C41-C36	119.6(2)
C43-C42-C41	118.6(2)
C43-C42-C45	120.8(2)
C41-C42-C45	120.6(2)
C42-C43-C44	122.0(2)
C35-C44-C43	120.9(2)
C42-C45-C46	112.58(19)
C47-C46-C45	113.75(19)
C46-C47-C48	114.5(2)
C49-C48-C47	112.0(2)
C50-C49-C48	114.6(3)
C49-C50-C51	112.3(3)
C52-C51-C50	115.4(3)
C51-C52-C53	112.9(3)
C54-C53-C52	115.5(3)
C53-C54-C55	113.3(3)
C54-C55-C56	114.4(4)
C44'-C35'-C36'	118.8(4)
C44'-C35'-C1	121.9(5)
C36'-C35'-C1	119.0(4)
C37'-C36'-C35'	120.7(4)
C37'-C36'-C41'	119.2(4)
C35'-C36'-C41'	120.0(4)
C38'-C37'-C36'	120.5(5)
C37'-C38'-C39'	120.2(5)
C40'-C39'-C38'	120.9(5)
C39'-C40'-C41'	121.2(5)
C40'-C41'-C42'	122.6(5)
C40'-C41'-C36'	118.0(4)

C42'-C41'-C36'	119.4(4)
C43'-C42'-C41'	118.4(4)
C43'-C42'-C45'	123.3(4)
C41'-C42'-C45'	118.2(4)
C42'-C43'-C44'	122.3(4)
C35'-C44'-C43'	120.9(4)
C46'-C45'-C42'	115.8(5)
C45'-C46'-C47'	111.7(5)
C48'-C47'-C46'	111.7(5)
C47'-C48'-C49'	112.8(6)
C50'-C49'-C48'	113.6(6)
C49'-C50'-C51'	114.4(7)
C52'-C51'-C50'	113.7(8)
C51'-C52'-C53'	113.6(8)
C52'-C53'-C54'	114.1(8)
C55'-C54'-C53'	112.8(8)
C54'-C55'-C56'	113.6(9)
C66-C57-C58	118.4(2)
C66-C57-C16	120.5(2)
C58-C57-C16	121.0(2)
C59-C58-C63	119.0(2)
C59-C58-C57	121.7(2)
C63-C58-C57	119.3(2)
C60-C59-C58	121.6(2)
C59-C60-C61	119.9(2)
C62-C61-C60	120.3(2)
C61-C62-C63	121.6(2)
C58-C63-C64	119.84(19)
C58-C63-C62	117.6(2)
C64-C63-C62	122.6(2)
C65-C64-C63	118.4(2)
C65-C64-C67	119.9(2)
C63-C64-C67	121.6(2)
C64-C65-C66	121.3(2)
C57-C66-C65	121.6(2)
C64-C67-C68	110.8(2)
C69-C68-C67	114.07(19)
C68-C69-C70	115.6(2)

C69-C70-C71	111.6(2)
C72-C71-C70	116.3(2)
C71-C72-C73	112.3(2)
C74-C73-C72	115.7(2)
C75-C74-C73	112.6(2)
C76-C75-C74	114.9(2)
C75-C76-C77	113.3(2)
C78-C77-C76	113.5(3)
C66'-C57'-C58'	119.4(5)
C66'-C57'-C16	123.0(6)
C58'-C57'-C16	117.4(6)
C59'-C58'-C63'	118.9(4)
C59'-C58'-C57'	121.8(5)
C63'-C58'-C57'	119.2(4)
C60'-C59'-C58'	121.7(5)
C59'-C60'-C61'	119.5(5)
C62'-C61'-C60'	120.9(5)
C61'-C62'-C63'	121.0(5)
C58'-C63'-C64'	119.0(4)
C58'-C63'-C62'	117.6(4)
C64'-C63'-C62'	123.4(5)
C65'-C64'-C63'	119.4(5)
C65'-C64'-C67'	120.9(6)
C63'-C64'-C67'	119.5(6)
C64'-C65'-C66'	120.7(5)
C57'-C66'-C65'	121.1(5)
C68'-C67'-C64'	115.4(6)
C67'-C68'-C69'	113.1(6)
C70'-C69'-C68'	111.1(6)
C69'-C70'-C71'	111.2(7)
C70'-C71'-C72'	111.2(8)
C73'-C72'-C71'	111.4(8)
C72'-C73'-C74'	113.0(8)
C75'-C74'-C73'	111.1(8)
C76'-C75'-C74'	113.2(9)
C75'-C76'-C77'	111.5(9)
C76'-C77'-C78'	110.6(9)

Table 12. Torsion angles [°] for **2c**.

C34-C1-C2-C15	-1.3(2)
C35-C1-C2-C15	-177.72(17)
C35'-C1-C2-C15	175.9(3)
C34-C1-C2-C3	172.44(13)
C35-C1-C2-C3	-4.0(2)
C35'-C1-C2-C3	-10.4(4)
C1-C2-C3-C4	17.3(2)
C15-C2-C3-C4	-168.99(14)
C1-C2-C3-C8	-160.61(13)
C15-C2-C3-C8	13.1(2)
C8-C3-C4-C5	6.9(2)
C2-C3-C4-C5	-171.02(15)
C3-C4-C5-C6	0.9(3)
C4-C5-C6-C7	-5.9(3)
C5-C6-C7-C8	2.9(3)
C6-C7-C8-C3	5.0(2)
C6-C7-C8-C9	-166.12(15)
C4-C3-C8-C7	-9.6(2)
C2-C3-C8-C7	168.41(14)
C4-C3-C8-C9	161.59(14)
C2-C3-C8-C9	-20.4(2)
C7-C8-C9-C14	175.72(15)
C3-C8-C9-C14	4.7(2)
C7-C8-C9-C10	4.4(2)
C3-C8-C9-C10	-166.63(14)
C14-C9-C10-C11	-5.7(2)
C8-C9-C10-C11	165.64(15)
C9-C10-C11-C12	-2.3(3)
C10-C11-C12-C13	5.0(3)
C11-C12-C13-C14	0.3(3)
C10-C9-C14-C13	10.8(2)
C8-C9-C14-C13	-160.84(14)
C10-C9-C14-C15	-170.45(14)
C8-C9-C14-C15	17.9(2)
C12-C13-C14-C9	-8.3(2)
C12-C13-C14-C15	172.95(15)

C1-C2-C15-C16	6.8(2)
C3-C2-C15-C16	-167.25(13)
C1-C2-C15-C14	-176.88(12)
C3-C2-C15-C14	9.05(19)
C9-C14-C15-C16	151.31(14)
C13-C14-C15-C16	-30.0(2)
C9-C14-C15-C2	-25.0(2)
C13-C14-C15-C2	153.77(15)
C2-C15-C16-C17	-7.7(2)
C14-C15-C16-C17	176.03(13)
C2-C15-C16-C57'	166.5(6)
C14-C15-C16-C57'	-9.7(6)
C2-C15-C16-C57	168.4(2)
C14-C15-C16-C57	-7.8(3)
C15-C16-C17-C34	3.0(2)
C57'-C16-C17-C34	-171.3(5)
C57-C16-C17-C34	-173.3(2)
C15-C16-C17-C18	-178.51(14)
C57'-C16-C17-C18	7.2(5)
C57-C16-C17-C18	5.2(3)
C34-C17-C18-C19	-0.8(2)
C16-C17-C18-C19	-179.23(13)
C17-C18-C19-C32	2.0(2)
C17-C18-C19-C20	-177.59(14)
C32-C19-C20-C21	179.34(14)
C18-C19-C20-C21	-1.1(2)
C32-C19-C20-C25	0.2(2)
C18-C19-C20-C25	179.77(14)
C25-C20-C21-C22	-0.2(2)
C19-C20-C21-C22	-179.34(16)
C20-C21-C22-C23	-0.8(3)
C21-C22-C23-C24	0.9(3)
C22-C23-C24-C25	0.1(3)
C23-C24-C25-C20	-1.1(3)
C23-C24-C25-C26	176.94(17)
C21-C20-C25-C24	1.1(2)
C19-C20-C25-C24	-179.74(15)
C21-C20-C25-C26	-176.93(14)

C19-C20-C25-C26	2.2(2)
C24-C25-C26-C27	-1.8(2)
C20-C25-C26-C27	176.17(14)
C24-C25-C26-C31	-179.44(15)
C20-C25-C26-C31	-1.5(2)
C31-C26-C27-C28	0.4(2)
C25-C26-C27-C28	-177.28(15)
C26-C27-C28-C29	-0.7(3)
C27-C28-C29-C30	0.9(3)
C28-C29-C30-C31	-0.8(2)
C29-C30-C31-C26	0.4(2)
C29-C30-C31-C32	179.52(14)
C27-C26-C31-C30	-0.2(2)
C25-C26-C31-C30	177.46(13)
C27-C26-C31-C32	-179.34(13)
C25-C26-C31-C32	-1.6(2)
C20-C19-C32-C31	-3.4(2)
C18-C19-C32-C31	177.11(13)
C20-C19-C32-C33	177.90(13)
C18-C19-C32-C33	-1.6(2)
C30-C31-C32-C19	-174.99(14)
C26-C31-C32-C19	4.1(2)
C30-C31-C32-C33	3.8(2)
C26-C31-C32-C33	-177.16(14)
C19-C32-C33-C34	0.1(2)
C31-C32-C33-C34	-178.61(13)
C16-C17-C34-C1	2.6(2)
C18-C17-C34-C1	-175.89(13)
C16-C17-C34-C33	177.78(13)
C18-C17-C34-C33	-0.7(2)
C2-C1-C34-C17	-3.4(2)
C35-C1-C34-C17	173.24(16)
C35'-C1-C34-C17	179.1(3)
C2-C1-C34-C33	-178.59(13)
C35-C1-C34-C33	-1.9(2)
C35'-C1-C34-C33	3.9(3)
C32-C33-C34-C17	1.0(2)
C32-C33-C34-C1	176.25(13)

C34-C1-C35-C44	-91.3(6)
C2-C1-C35-C44	85.3(6)
C35'-C1-C35-C44	-146(10)
C34-C1-C35-C36	87.4(6)
C2-C1-C35-C36	-96.0(6)
C35'-C1-C35-C36	32(8)
C44-C35-C36-C37	-179.0(6)
C1-C35-C36-C37	2.3(9)
C44-C35-C36-C41	-0.8(9)
C1-C35-C36-C41	-179.5(5)
C35-C36-C37-C38	179.7(5)
C41-C36-C37-C38	1.5(7)
C36-C37-C38-C39	-0.9(5)
C37-C38-C39-C40	-0.3(4)
C38-C39-C40-C41	0.9(4)
C39-C40-C41-C42	-179.4(3)
C39-C40-C41-C36	-0.3(4)
C37-C36-C41-C40	-0.9(6)
C35-C36-C41-C40	-179.1(5)
C37-C36-C41-C42	178.3(4)
C35-C36-C41-C42	0.1(7)
C40-C41-C42-C43	179.9(2)
C36-C41-C42-C43	0.8(4)
C40-C41-C42-C45	-2.8(4)
C36-C41-C42-C45	178.2(3)
C41-C42-C43-C44	-0.9(3)
C45-C42-C43-C44	-178.3(2)
C36-C35-C44-C43	0.7(8)
C1-C35-C44-C43	179.4(4)
C42-C43-C44-C35	0.1(5)
C43-C42-C45-C46	102.5(3)
C41-C42-C45-C46	-74.8(3)
C42-C45-C46-C47	171.5(2)
C45-C46-C47-C48	72.6(3)
C46-C47-C48-C49	169.7(3)
C47-C48-C49-C50	-176.2(3)
C48-C49-C50-C51	169.8(3)
C49-C50-C51-C52	-177.0(4)

C50-C51-C52-C53	178.4(4)
C51-C52-C53-C54	179.1(5)
C52-C53-C54-C55	178.1(5)
C53-C54-C55-C56	176.9(7)
C34-C1-C35'-C44'	-83.3(18)
C2-C1-C35'-C44'	99.4(18)
C35-C1-C35'-C44'	44(7)
C34-C1-C35'-C36'	91.4(18)
C2-C1-C35'-C36'	-85.9(18)
C35-C1-C35'-C36'	-141(11)
C44'-C35'-C36'-C37'	-179.5(16)
C1-C35'-C36'-C37'	6(3)
C44'-C35'-C36'-C41'	-3(3)
C1-C35'-C36'-C41'	-177.6(14)
C35'-C36'-C37'-C38'	-179.8(15)
C41'-C36'-C37'-C38'	3.5(19)
C36'-C37'-C38'-C39'	-2.9(16)
C37'-C38'-C39'-C40'	1.5(13)
C38'-C39'-C40'-C41'	-0.6(13)
C39'-C40'-C41'-C42'	179.7(8)
C39'-C40'-C41'-C36'	1.2(14)
C37'-C36'-C41'-C40'	-2.6(18)
C35'-C36'-C41'-C40'	-179.3(15)
C37'-C36'-C41'-C42'	178.9(11)
C35'-C36'-C41'-C42'	2(2)
C40'-C41'-C42'-C43'	179.8(7)
C36'-C41'-C42'-C43'	-1.8(13)
C40'-C41'-C42'-C45'	-1.3(11)
C36'-C41'-C42'-C45'	177.2(9)
C41'-C42'-C43'-C44'	2.1(10)
C45'-C42'-C43'-C44'	-176.8(6)
C36'-C35'-C44'-C43'	3(2)
C1-C35'-C44'-C43'	177.8(13)
C42'-C43'-C44'-C35'	-2.9(15)
C43'-C42'-C45'-C46'	-2.6(9)
C41'-C42'-C45'-C46'	178.5(6)
C42'-C45'-C46'-C47'	176.6(6)
C45'-C46'-C47'-C48'	177.4(6)

C46'-C47'-C48'-C49'	175.2(8)
C47'-C48'-C49'-C50'	177.0(9)
C48'-C49'-C50'-C51'	176.4(10)
C49'-C50'-C51'-C52'	179.1(12)
C50'-C51'-C52'-C53'	178.5(13)
C51'-C52'-C53'-C54'	-179.3(14)
C52'-C53'-C54'-C55'	178.2(14)
C53'-C54'-C55'-C56'	179.7(18)
C15-C16-C57-C66	114.4(5)
C17-C16-C57-C66	-69.3(6)
C57'-C16-C57-C66	158(26)
C15-C16-C57-C58	-62.8(6)
C17-C16-C57-C58	113.4(5)
C57'-C16-C57-C58	-20(25)
C66-C57-C58-C59	170.1(6)
C16-C57-C58-C59	-12.5(9)
C66-C57-C58-C63	-9.6(8)
C16-C57-C58-C63	167.7(4)
C63-C58-C59-C60	1.0(8)
C57-C58-C59-C60	-178.7(5)
C58-C59-C60-C61	-1.8(7)
C59-C60-C61-C62	0.5(5)
C60-C61-C62-C63	1.6(5)
C59-C58-C63-C64	-178.3(4)
C57-C58-C63-C64	1.4(7)
C59-C58-C63-C62	0.9(6)
C57-C58-C63-C62	-179.3(5)
C61-C62-C63-C58	-2.2(5)
C61-C62-C63-C64	177.0(3)
C58-C63-C64-C65	7.5(5)
C62-C63-C64-C65	-171.7(3)
C58-C63-C64-C67	-167.3(4)
C62-C63-C64-C67	13.5(5)
C63-C64-C65-C66	-8.5(5)
C67-C64-C65-C66	166.5(3)
C58-C57-C66-C65	9.0(8)
C16-C57-C66-C65	-168.3(4)
C64-C65-C66-C57	0.1(7)

C65-C64-C67-C68	-97.2(3)
C63-C64-C67-C68	77.6(3)
C64-C67-C68-C69	-179.5(2)
C67-C68-C69-C70	-75.9(3)
C68-C69-C70-C71	178.8(3)
C69-C70-C71-C72	171.6(3)
C70-C71-C72-C73	-176.7(3)
C71-C72-C73-C74	171.5(3)
C72-C73-C74-C75	-172.8(3)
C73-C74-C75-C76	-179.0(3)
C74-C75-C76-C77	-176.7(4)
C75-C76-C77-C78	-177.9(4)
C15-C16-C57'-C66'	108.6(17)
C17-C16-C57'-C66'	-77(2)
C57-C16-C57'-C66'	-29(24)
C15-C16-C57'-C58'	-65.1(19)
C17-C16-C57'-C58'	109.2(16)
C57-C16-C57'-C58'	157(27)
C66'-C57'-C58'-C59'	177.0(18)
C16-C57'-C58'-C59'	-9(3)
C66'-C57'-C58'-C63'	-6(3)
C16-C57'-C58'-C63'	167.9(15)
C63'-C58'-C59'-C60'	7(3)
C57'-C58'-C59'-C60'	-176.4(18)
C58'-C59'-C60'-C61'	-4(2)
C59'-C60'-C61'-C62'	-1.8(17)
C60'-C61'-C62'-C63'	4.3(17)
C59'-C58'-C63'-C64'	173.8(15)
C57'-C58'-C63'-C64'	-3(3)
C59'-C58'-C63'-C62'	-4(2)
C57'-C58'-C63'-C62'	178.9(17)
C61'-C62'-C63'-C58'	-1(2)
C61'-C62'-C63'-C64'	-179.0(13)
C58'-C63'-C64'-C65'	11(2)
C62'-C63'-C64'-C65'	-171.5(13)
C58'-C63'-C64'-C67'	-164.8(14)
C62'-C63'-C64'-C67'	13(2)
C63'-C64'-C65'-C66'	-9(2)

C67'-C64'-C65'-C66'	166.3(13)
C58'-C57'-C66'-C65'	8(3)
C16-C57'-C66'-C65'	-165.7(15)
C64'-C65'-C66'-C57'	0(2)
C65'-C64'-C67'-C68'	-16.5(17)
C63'-C64'-C67'-C68'	158.9(12)
C64'-C67'-C68'-C69'	-174.4(10)
C67'-C68'-C69'-C70'	-170.5(11)
C68'-C69'-C70'-C71'	179.5(13)
C69'-C70'-C71'-C72'	-177.4(15)
C70'-C71'-C72'-C73'	178.6(16)
C71'-C72'-C73'-C74'	178.3(17)
C72'-C73'-C74'-C75'	-177.4(18)
C73'-C74'-C75'-C76'	178.6(19)
C74'-C75'-C76'-C77'	-175(2)
C75'-C76'-C77'-C78'	-168(2)

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*2.5. 9,20-Di(phenanthren-9-yl)tetrabenzo[a,c,j,l]tetracene (**2d**)*

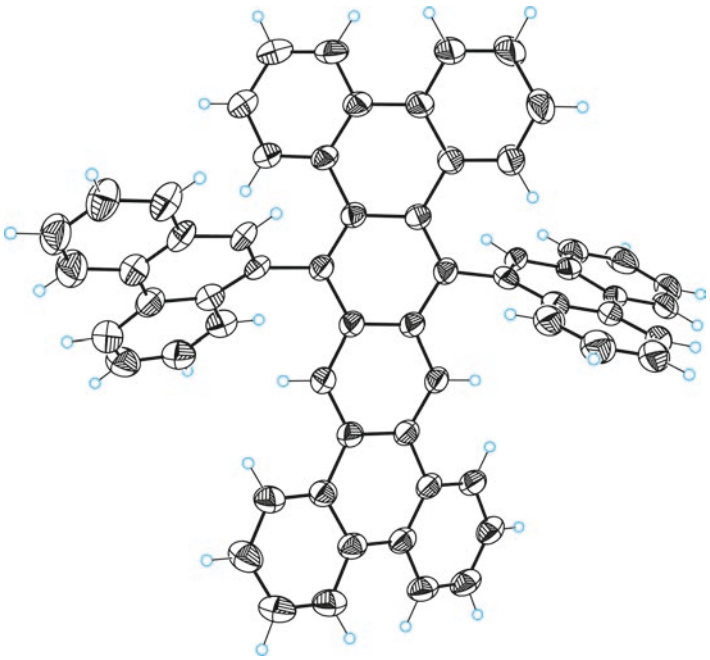

Table 13. Crystal data and structure refinement for ***2d***.

Identification code	mo_RD566_0m
Empirical formula	C62 H36
Formula weight	780.91

Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.1459(4)Å	a= 66.7820(10)°.
	b = 14.0677(6)Å	b = 77.518(2)°.
	c = 15.4819(7)Å	g = 85.704(2)°.
Volume	1982.63(15) $Å^3$	
Z	2	
Density (calculated)	1.308 Mg/m^3	
Absorption coefficient	0.074 mm^{-1}	
F(000)	816	
Crystal size	0.30 x 0.10 x 0.02 mm^3	
Theta range for data collection	1.575 to 25.998°.	
Index ranges	-11<=h<=12,-16<=k<=17,-19<=l<=19	
Reflections collected	22068	
Independent reflections	7717[R(int) = 0.0255]	
Completeness to theta =25.998°	99.0%	
Absorption correction	Empirical	
Max. and min. transmission	0.998 and 0.919	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7717/ 948/ 811	
Goodness-of-fit on F^2	1.036	
Final R indices [I>2sigma(I)]	R1 = 0.0538, wR2 = 0.1433	
R indices (all data)	R1 = 0.0763, wR2 = 0.1594	
Largest diff. peak and hole	0.332 and -0.267 $e.Å^{-3}$	

Table 14. Bond lengths [Å] and angles [°] for ***2d***.

Bond lengths----	
C1-C7	1.411(3)
C1-C2	1.424(3)
C1-C6	1.425(3)
C2-C22	1.413(3)
C2-C3	1.420(3)
C3-C4	1.390(3)
C3-C35	1.461(7)

C3-C35'	1.545(10)
C4-C5	1.443(3)
C4-C23	1.480(3)
C5-C6	1.395(3)
C5-C34	1.476(3)
C6-C49	1.498(8)
C6-C49'	1.504(11)
C7-C8	1.384(3)
C8-C21	1.426(3)
C8-C9	1.470(3)
C9-C10	1.397(3)
C9-C14	1.411(3)
C10-C11	1.374(3)
C11-C12	1.378(3)
C12-C13	1.372(3)
C13-C14	1.402(3)
C14-C15	1.468(3)
C15-C20	1.400(3)
C15-C16	1.407(3)
C16-C17	1.371(3)
C17-C18	1.373(3)
C18-C19	1.378(3)
C19-C20	1.402(3)
C20-C21	1.471(3)
C21-C22	1.377(3)
C23-C24	1.402(3)
C23-C28	1.411(3)
C24-C25	1.380(3)
C25-C26	1.379(4)
C26-C27	1.374(4)
C27-C28	1.400(3)
C28-C29	1.461(3)
C29-C30	1.402(3)
C29-C34	1.408(3)
C30-C31	1.366(3)
C31-C32	1.391(3)
C32-C33	1.370(3)
C33-C34	1.402(3)

C35-C48	1.353(5)
C35-C36	1.453(5)
C36-C37	1.409(6)
C36-C41	1.422(6)
C37-C38	1.375(6)
C38-C39	1.387(7)
C39-C40	1.380(7)
C40-C41	1.417(6)
C41-C42	1.441(7)
C42-C43	1.414(5)
C42-C47	1.422(6)
C43-C44	1.345(8)
C44-C45	1.427(8)
C45-C46	1.386(6)
C46-C47	1.404(6)
C47-C48	1.433(5)
C35'-C48'	1.353(6)
C35'-C36'	1.451(6)
C36'-C37'	1.405(7)
C36'-C41'	1.421(7)
C37'-C38'	1.368(7)
C38'-C39'	1.399(8)
C39'-C40'	1.374(8)
C40'-C41'	1.423(8)
C41'-C42'	1.441(7)
C42'-C43'	1.416(6)
C42'-C47'	1.418(7)
C43'-C44'	1.364(9)
C44'-C45'	1.437(10)
C45'-C46'	1.387(8)
C46'-C47'	1.407(7)
C47'-C48'	1.433(7)
C49-C62	1.375(5)
C49-C50	1.440(5)
C50-C51	1.399(5)
C50-C55	1.427(6)
C51-C52	1.390(6)
C52-C53	1.374(6)

C53-C54	1.380(6)
C54-C55	1.412(5)
C55-C56	1.455(5)
C56-C57	1.410(5)
C56-C61	1.414(5)
C57-C58	1.377(6)
C58-C59	1.383(6)
C59-C60	1.361(5)
C60-C61	1.399(5)
C61-C62	1.429(6)
C49'-C62'	1.372(6)
C49'-C50'	1.445(6)
C50'-C51'	1.404(6)
C50'-C55'	1.428(6)
C51'-C52'	1.392(6)
C52'-C53'	1.381(7)
C53'-C54'	1.379(7)
C54'-C55'	1.414(6)
C55'-C56'	1.460(6)
C56'-C57'	1.416(7)
C56'-C61'	1.418(7)
C57'-C58'	1.387(8)
C58'-C59'	1.380(8)
C59'-C60'	1.363(7)
C60'-C61'	1.397(7)
C61'-C62'	1.426(7)

Angles----------

C7-C1-C2	117.80(17)
C7-C1-C6	122.96(17)
C2-C1-C6	119.22(17)
C22-C2-C3	122.28(17)
C22-C2-C1	118.02(17)
C3-C2-C1	119.68(17)
C4-C3-C2	119.73(17)
C4-C3-C35	125.1(6)
C2-C3-C35	115.0(6)
C4-C3-C35'	122.5(8)

C2-C3-C35'	117.7(8)
C3-C4-C5	118.89(17)
C3-C4-C23	123.93(17)
C5-C4-C23	116.97(16)
C6-C5-C4	119.54(17)
C6-C5-C34	123.25(17)
C4-C5-C34	117.12(17)
C5-C6-C1	119.21(17)
C5-C6-C49	122.6(8)
C1-C6-C49	117.8(8)
C5-C6-C49'	119.6(11)
C1-C6-C49'	120.8(12)
C8-C7-C1	122.91(18)
C7-C8-C21	118.27(18)
C7-C8-C9	122.36(18)
C21-C8-C9	119.31(17)
C10-C9-C14	118.69(18)
C10-C9-C8	121.88(18)
C14-C9-C8	119.30(18)
C11-C10-C9	121.8(2)
C10-C11-C12	119.6(2)
C13-C12-C11	120.0(2)
C12-C13-C14	121.8(2)
C13-C14-C9	118.1(2)
C13-C14-C15	122.03(18)
C9-C14-C15	119.88(18)
C20-C15-C16	118.32(19)
C20-C15-C14	120.25(17)
C16-C15-C14	121.40(19)
C17-C16-C15	121.4(2)
C16-C17-C18	120.29(19)
C17-C18-C19	119.7(2)
C18-C19-C20	121.2(2)
C15-C20-C19	119.04(18)
C15-C20-C21	119.31(18)
C19-C20-C21	121.55(18)
C22-C21-C8	118.80(17)
C22-C21-C20	121.79(18)

C8-C21-C20	119.40(17)
C21-C22-C2	122.72(18)
C24-C23-C28	117.96(18)
C24-C23-C4	121.60(19)
C28-C23-C4	119.85(18)
C25-C24-C23	121.8(2)
C26-C25-C24	119.9(2)
C27-C26-C25	119.7(2)
C26-C27-C28	121.6(2)
C27-C28-C23	119.0(2)
C27-C28-C29	121.5(2)
C23-C28-C29	119.41(18)
C30-C29-C34	119.4(2)
C30-C29-C28	121.38(19)
C34-C29-C28	119.20(19)
C31-C30-C29	121.2(2)
C30-C31-C32	119.8(2)
C33-C32-C31	120.0(2)
C32-C33-C34	121.66(19)
C33-C34-C29	117.92(18)
C33-C34-C5	121.57(17)
C29-C34-C5	120.10(18)
C48-C35-C36	119.2(6)
C48-C35-C3	116.5(5)
C36-C35-C3	124.3(5)
C37-C36-C41	119.7(5)
C37-C36-C35	120.7(5)
C41-C36-C35	119.6(5)
C38-C37-C36	121.4(6)
C37-C38-C39	119.5(6)
C40-C39-C38	120.6(5)
C39-C40-C41	121.6(5)
C40-C41-C36	117.2(5)
C40-C41-C42	123.0(5)
C36-C41-C42	119.8(4)
C43-C42-C47	117.7(5)
C43-C42-C41	123.0(5)
C47-C42-C41	119.2(4)

C44-C43-C42	121.4(6)
C43-C44-C45	120.8(5)
C46-C45-C44	119.9(6)
C45-C46-C47	119.0(5)
C46-C47-C42	121.2(5)
C46-C47-C48	119.9(5)
C42-C47-C48	118.9(5)
C35-C48-C47	122.9(6)
C48'-C35'-C36'	120.7(7)
C48'-C35'-C3	122.5(7)
C36'-C35'-C3	115.7(7)
C37'-C36'-C41'	119.6(6)
C37'-C36'-C35'	120.8(6)
C41'-C36'-C35'	119.5(6)
C38'-C37'-C36'	121.6(7)
C37'-C38'-C39'	118.9(7)
C40'-C39'-C38'	121.7(7)
C39'-C40'-C41'	120.1(7)
C36'-C41'-C40'	118.0(6)
C36'-C41'-C42'	118.6(6)
C40'-C41'-C42'	123.3(6)
C43'-C42'-C47'	117.4(6)
C43'-C42'-C41'	121.9(7)
C47'-C42'-C41'	120.7(5)
C44'-C43'-C42'	120.4(7)
C43'-C44'-C45'	122.3(7)
C46'-C45'-C44'	118.0(7)
C45'-C46'-C47'	119.7(7)
C46'-C47'-C42'	122.2(6)
C46'-C47'-C48'	119.0(7)
C42'-C47'-C48'	118.8(5)
C35'-C48'-C47'	121.6(7)
C62-C49-C50	119.7(5)
C62-C49-C6	117.5(5)
C50-C49-C6	122.7(5)
C51-C50-C55	118.5(5)
C51-C50-C49	121.6(5)
C55-C50-C49	119.9(5)

C52-C51-C50	120.7(6)
C53-C52-C51	121.1(6)
C52-C53-C54	119.8(6)
C53-C54-C55	120.9(6)
C54-C55-C50	118.9(5)
C54-C55-C56	122.3(5)
C50-C55-C56	118.8(5)
C57-C56-C61	117.5(5)
C57-C56-C55	122.5(5)
C61-C56-C55	120.0(5)
C58-C57-C56	120.9(5)
C57-C58-C59	121.0(5)
C60-C59-C58	119.3(5)
C59-C60-C61	121.6(5)
C60-C61-C56	119.7(5)
C60-C61-C62	121.1(5)
C56-C61-C62	119.2(5)
C49-C62-C61	122.0(6)
C62'-C49'-C50'	119.3(7)
C62'-C49'-C6	116.4(7)
C50'-C49'-C6	124.0(8)
C51'-C50'-C55'	119.7(6)
C51'-C50'-C49'	120.8(6)
C55'-C50'-C49'	119.4(6)
C52'-C51'-C50'	121.2(7)
C53'-C52'-C51'	119.2(7)
C54'-C53'-C52'	120.7(7)
C53'-C54'-C55'	122.0(6)
C54'-C55'-C50'	116.9(6)
C54'-C55'-C56'	123.2(6)
C50'-C55'-C56'	119.9(6)
C57'-C56'-C61'	116.8(6)
C57'-C56'-C55'	124.3(6)
C61'-C56'-C55'	118.7(6)
C58'-C57'-C56'	120.4(7)
C59'-C58'-C57'	121.4(7)
C60'-C59'-C58'	119.7(8)
C59'-C60'-C61'	120.7(8)

C60'-C61'-C56'	121.0(7)
C60'-C61'-C62'	119.6(7)
C56'-C61'-C62'	119.3(7)
C49'-C62'-C61'	122.6(8)

Table 15. Torsion angles [°] for ***2d***.

C7-C1-C2-C22	10.7(3)
C6-C1-C2-C22	-167.73(18)
C7-C1-C2-C3	-167.73(19)
C6-C1-C2-C3	13.9(3)
C22-C2-C3-C4	175.33(19)
C1-C2-C3-C4	-6.4(3)
C22-C2-C3-C35	0.1(4)
C1-C2-C3-C35	178.4(4)
C22-C2-C3-C35'	-2.6(5)
C1-C2-C3-C35'	175.7(5)
C2-C3-C4-C5	-11.0(3)
C35-C3-C4-C5	163.7(4)
C35'-C3-C4-C5	166.9(5)
C2-C3-C4-C23	163.57(19)
C35-C3-C4-C23	-21.7(5)
C35'-C3-C4-C23	-18.6(6)
C3-C4-C5-C6	21.3(3)
C23-C4-C5-C6	-153.65(19)
C3-C4-C5-C34	-155.36(18)
C23-C4-C5-C34	29.7(3)
C4-C5-C6-C1	-13.7(3)
C34-C5-C6-C1	162.71(18)
C4-C5-C6-C49	158.4(7)
C34-C5-C6-C49	-25.2(7)
C4-C5-C6-C49'	159.4(8)
C34-C5-C6-C49'	-24.2(9)
C7-C1-C6-C5	178.03(19)
C2-C1-C6-C5	-3.7(3)
C7-C1-C6-C49	5.6(6)
C2-C1-C6-C49	-176.1(6)
C7-C1-C6-C49'	5.0(8)

C2-C1-C6-C49'	-176.7(7)
C2-C1-C7-C8	-6.7(3)
C6-C1-C7-C8	171.64(19)
C1-C7-C8-C21	-4.5(3)
C1-C7-C8-C9	172.71(19)
C7-C8-C9-C10	-5.7(3)
C21-C8-C9-C10	171.5(2)
C7-C8-C9-C14	178.42(19)
C21-C8-C9-C14	-4.4(3)
C14-C9-C10-C11	1.4(3)
C8-C9-C10-C11	-174.5(2)
C9-C10-C11-C12	2.0(4)
C10-C11-C12-C13	-3.0(4)
C11-C12-C13-C14	0.7(4)
C12-C13-C14-C9	2.6(3)
C12-C13-C14-C15	-175.3(2)
C10-C9-C14-C13	-3.6(3)
C8-C9-C14-C13	172.46(19)
C10-C9-C14-C15	174.37(19)
C8-C9-C14-C15	-9.6(3)
C13-C14-C15-C20	-169.6(2)
C9-C14-C15-C20	12.6(3)
C13-C14-C15-C16	12.2(3)
C9-C14-C15-C16	-165.6(2)
C20-C15-C16-C17	-0.7(3)
C14-C15-C16-C17	177.6(2)
C15-C16-C17-C18	0.6(3)
C16-C17-C18-C19	-0.5(3)
C17-C18-C19-C20	0.5(3)
C16-C15-C20-C19	0.7(3)
C14-C15-C20-C19	-177.59(18)
C16-C15-C20-C21	176.93(18)
C14-C15-C20-C21	-1.3(3)
C18-C19-C20-C15	-0.6(3)
C18-C19-C20-C21	-176.76(19)
C7-C8-C21-C22	11.5(3)
C9-C8-C21-C22	-165.80(18)
C7-C8-C21-C20	-167.14(18)

C9-C8-C21-C20	15.6(3)
C15-C20-C21-C22	168.71(19)
C19-C20-C21-C22	-15.1(3)
C15-C20-C21-C8	-12.7(3)
C19-C20-C21-C8	163.44(19)
C8-C21-C22-C2	-7.5(3)
C20-C21-C22-C2	171.13(19)
C3-C2-C22-C21	174.56(19)
C1-C2-C22-C21	-3.8(3)
C3-C4-C23-C24	-21.5(3)
C5-C4-C23-C24	153.1(2)
C3-C4-C23-C28	167.5(2)
C5-C4-C23-C28	-17.9(3)
C28-C23-C24-C25	-0.5(4)
C4-C23-C24-C25	-171.6(2)
C23-C24-C25-C26	-0.7(5)
C24-C25-C26-C27	1.1(5)
C25-C26-C27-C28	-0.4(5)
C26-C27-C28-C23	-0.8(4)
C26-C27-C28-C29	177.9(3)
C24-C23-C28-C27	1.2(3)
C4-C23-C28-C27	172.5(2)
C24-C23-C28-C29	-177.6(2)
C4-C23-C28-C29	-6.2(3)
C27-C28-C29-C30	19.9(3)
C23-C28-C29-C30	-161.4(2)
C27-C28-C29-C34	-160.5(2)
C23-C28-C29-C34	18.3(3)
C34-C29-C30-C31	1.5(3)
C28-C29-C30-C31	-178.8(2)
C29-C30-C31-C32	-2.1(3)
C30-C31-C32-C33	0.1(3)
C31-C32-C33-C34	2.6(3)
C32-C33-C34-C29	-3.1(3)
C32-C33-C34-C5	-175.81(19)
C30-C29-C34-C33	1.1(3)
C28-C29-C34-C33	-178.58(18)
C30-C29-C34-C5	173.89(18)

C28-C29-C34-C5	-5.8(3)
C6-C5-C34-C33	-22.3(3)
C4-C5-C34-C33	154.18(19)
C6-C5-C34-C29	165.17(19)
C4-C5-C34-C29	-18.3(3)
C4-C3-C35-C48	-69.3(14)
C2-C3-C35-C48	105.6(12)
C35'-C3-C35-C48	-116(14)
C4-C3-C35-C36	111.7(14)
C2-C3-C35-C36	-73.4(16)
C35'-C3-C35-C36	65(12)
C48-C35-C36-C37	173.6(15)
C3-C35-C36-C37	-7(2)
C48-C35-C36-C41	-5(2)
C3-C35-C36-C41	174.0(13)
C41-C36-C37-C38	0(2)
C35-C36-C37-C38	-178.7(14)
C36-C37-C38-C39	-0.1(16)
C37-C38-C39-C40	-0.2(11)
C38-C39-C40-C41	0.7(11)
C39-C40-C41-C36	-0.8(14)
C39-C40-C41-C42	178.5(9)
C37-C36-C41-C40	1(2)
C35-C36-C41-C40	179.2(13)
C37-C36-C41-C42	-178.8(13)
C35-C36-C41-C42	0(2)
C40-C41-C42-C43	2.7(14)
C36-C41-C42-C43	-178.1(11)
C40-C41-C42-C47	-175.1(8)
C36-C41-C42-C47	4.2(15)
C47-C42-C43-C44	1.1(10)
C41-C42-C43-C44	-176.7(8)
C42-C43-C44-C45	-0.5(10)
C43-C44-C45-C46	-1.2(9)
C44-C45-C46-C47	2.3(8)
C45-C46-C47-C42	-1.7(10)
C45-C46-C47-C48	179.3(8)
C43-C42-C47-C46	0.1(11)

C41-C42-C47-C46	178.0(8)
C43-C42-C47-C48	179.0(9)
C41-C42-C47-C48	-3.1(13)
C36-C35-C48-C47	6(2)
C3-C35-C48-C47	-172.8(11)
C46-C47-C48-C35	176.7(12)
C42-C47-C48-C35	-2.3(18)
C4-C3-C35'-C48'	-79(2)
C2-C3-C35'-C48'	99.2(18)
C35-C3-C35'-C48'	57(12)
C4-C3-C35'-C36'	112.8(17)
C2-C3-C35'-C36'	-69.4(19)
C35-C3-C35'-C36'	-112(14)
C48'-C35'-C36'-C37'	178(2)
C3-C35'-C36'-C37'	-13(3)
C48'-C35'-C36'-C41'	1(3)
C3-C35'-C36'-C41'	169.9(17)
C41'-C36'-C37'-C38'	1(3)
C35'-C36'-C37'-C38'	-176(2)
C36'-C37'-C38'-C39'	-1(2)
C37'-C38'-C39'-C40'	1.7(16)
C38'-C39'-C40'-C41'	-2.2(16)
C37'-C36'-C41'-C40'	-1(3)
C35'-C36'-C41'-C40'	175.8(19)
C37'-C36'-C41'-C42'	-177.9(19)
C35'-C36'-C41'-C42'	-1(3)
C39'-C40'-C41'-C36'	2(2)
C39'-C40'-C41'-C42'	178.5(13)
C36'-C41'-C42'-C43'	180.0(16)
C40'-C41'-C42'-C43'	3(2)
C36'-C41'-C42'-C47'	1(2)
C40'-C41'-C42'-C47'	-175.3(12)
C47'-C42'-C43'-C44'	-0.3(14)
C41'-C42'-C43'-C44'	-178.9(11)
C42'-C43'-C44'-C45'	0.2(13)
C43'-C44'-C45'-C46'	0.9(13)
C44'-C45'-C46'-C47'	-1.9(13)
C45'-C46'-C47'-C42'	1.9(14)

C45'-C46'-C47'-C48'	-178.5(12)
C43'-C42'-C47'-C46'	-0.8(16)
C41'-C42'-C47'-C46'	177.8(12)
C43'-C42'-C47'-C48'	179.6(12)
C41'-C42'-C47'-C48'	-1.7(19)
C36'-C35'-C48'-C47'	-1(3)
C3-C35'-C48'-C47'	-169.4(15)
C46'-C47'-C48'-C35'	-177.8(16)
C42'-C47'-C48'-C35'	2(2)
C5-C6-C49-C62	-55(2)
C1-C6-C49-C62	116.7(16)
C49'-C6-C49-C62	-72(16)
C5-C6-C49-C50	124.3(16)
C1-C6-C49-C50	-63(2)
C49'-C6-C49-C50	108(18)
C62-C49-C50-C51	176(2)
C6-C49-C50-C51	-4(3)
C62-C49-C50-C55	-8(3)
C6-C49-C50-C55	172.3(15)
C55-C50-C51-C52	-2(3)
C49-C50-C51-C52	174.6(18)
C50-C51-C52-C53	0(2)
C51-C52-C53-C54	0.7(16)
C52-C53-C54-C55	0.7(13)
C53-C54-C55-C50	-2.5(16)
C53-C54-C55-C56	176.5(9)
C51-C50-C55-C54	3(2)
C49-C50-C55-C54	-173.4(15)
C51-C50-C55-C56	-176.1(15)
C49-C50-C55-C56	8(2)
C54-C55-C56-C57	-3.7(16)
C50-C55-C56-C57	175.3(13)
C54-C55-C56-C61	177.8(12)
C50-C55-C56-C61	-3.2(18)
C61-C56-C57-C58	-0.2(14)
C55-C56-C57-C58	-178.8(9)
C56-C57-C58-C59	-0.5(11)
C57-C58-C59-C60	0.4(12)

C58-C59-C60-C61	0.4(18)
C59-C60-C61-C56	-1(2)
C59-C60-C61-C62	179.2(16)
C57-C56-C61-C60	0.9(19)
C55-C56-C61-C60	179.5(13)
C57-C56-C61-C62	-179.4(14)
C55-C56-C61-C62	-1(2)
C50-C49-C62-C61	4(3)
C6-C49-C62-C61	-176.2(15)
C60-C61-C62-C49	-179.9(18)
C56-C61-C62-C49	0(3)
C5-C6-C49'-C62'	-62(3)
C1-C6-C49'-C62'	111(2)
C49-C6-C49'-C62'	102(18)
C5-C6-C49'-C50'	124(2)
C1-C6-C49'-C50'	-63(3)
C49-C6-C49'-C50'	-71(16)
C62'-C49'-C50'-C51'	179(3)
C6-C49'-C50'-C51'	-8(4)
C62'-C49'-C50'-C55'	3(4)
C6-C49'-C50'-C55'	176(2)
C55'-C50'-C51'-C52'	-5(3)
C49'-C50'-C51'-C52'	179(2)
C50'-C51'-C52'-C53'	2(3)
C51'-C52'-C53'-C54'	2(2)
C52'-C53'-C54'-C55'	-1.6(18)
C53'-C54'-C55'-C50'	-2(2)
C53'-C54'-C55'-C56'	177.6(14)
C51'-C50'-C55'-C54'	6(3)
C49'-C50'-C55'-C54'	-178(2)
C51'-C50'-C55'-C56'	-174(2)
C49'-C50'-C55'-C56'	2(3)
C54'-C55'-C56'-C57'	-5(2)
C50'-C55'-C56'-C57'	174.7(18)
C54'-C55'-C56'-C61'	179.4(18)
C50'-C55'-C56'-C61'	-1(3)
C61'-C56'-C57'-C58'	-1(2)
C55'-C56'-C57'-C58'	-176.4(14)

C56'-C57'-C58'-C59'	-1.3(19)
C57'-C58'-C59'-C60'	1(2)
C58'-C59'-C60'-C61'	0(3)
C59'-C60'-C61'-C56'	-3(3)
C59'-C60'-C61'-C62'	-179(2)
C57'-C56'-C61'-C60'	3(3)
C55'-C56'-C61'-C60'	178(2)
C57'-C56'-C61'-C62'	180(2)
C55'-C56'-C61'-C62'	-5(3)
C50'-C49'-C62'-C61'	-9(4)
C6-C49'-C62'-C61'	177(2)
C60'-C61'-C62'-C49'	-173(3)
C56'-C61'-C62'-C49'	10(4)

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*2.6. 10,19-Dihexyltetrabenzo[a,fg,ij,o]benzo[5,6]tetrapheno[8,9,10,11-rst]pentaphene (**8**)*

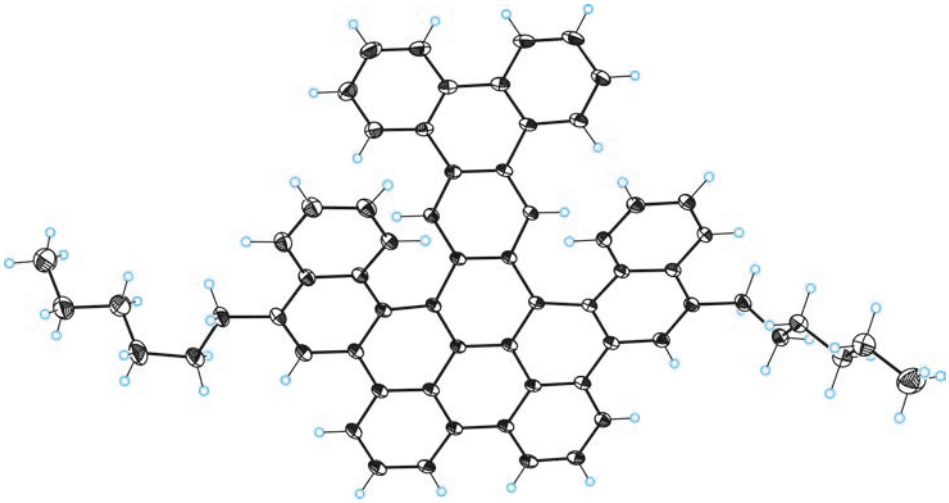

Table 16. Crystal data and structure refinement for **8**.

Identification code	mo_RD471_0m	
Empirical formula	C68 H54 Cl4	
Formula weight	1012.91	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 47.051(2)Å	a= 90°.

	b = 9.3095(5)Å b = 125.063(2)°.
	c = 27.9099(13)Å g = 90°.
Volume	10006.6(9) $Å^3$
Z	8
Density (calculated)	1.345 Mg/m^3
Absorption coefficient	0.282 mm^{-1}
F(000)	4240
Crystal size	0.03 x 0.005 x 0.002 mm^3
Theta range for data collection	1.783 to 29.461°.
Index ranges	-64<=h<=64,-12<=k<=12,-34<=l<=38
Reflections collected	83017
Independent reflections	13669[R(int) = 0.0394]
Completeness to theta =29.461°	98.4%
Absorption correction	Empirical
Max. and min. transmission	0.999 and 0.914
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	13669/ 197/ 727
Goodness-of-fit on F^2	1.014
Final R indices [I>2sigma(I)]	R1 = 0.0677, wR2 = 0.1859
R indices (all data)	R1 = 0.0915, wR2 = 0.2041
Largest diff. peak and hole	0.978 and -0.862 $e.Å^{-3}$

Table 17. Bond lengths [Å] and angles [°] for **8**.

Bond lengths----	
C1-C2	1.363(3)
C1-C10	1.424(3)
C2-C3	1.442(3)
C2-C55	1.501(3)
C3-C8	1.414(3)
C3-C4	1.417(3)
C4-C5	1.372(3)
C5-C6	1.398(3)
C6-C7	1.373(3)
C7-C8	1.421(3)
C8-C9	1.456(3)
C9-C10	1.402(3)

C9-C18	1.445(3)
C10-C11	1.450(3)
C11-C12	1.407(3)
C11-C16	1.422(3)
C12-C13	1.378(3)
C13-C14	1.383(3)
C14-C15	1.398(3)
C15-C16	1.420(3)
C15-C40	1.462(3)
C16-C17	1.438(2)
C17-C18	1.403(3)
C17-C38	1.438(3)
C18-C19	1.449(3)
C19-C20	1.407(3)
C19-C36	1.416(3)
C20-C21	1.389(3)
C21-C34	1.424(3)
C21-C22	1.471(3)
C22-C23	1.406(3)
C22-C27	1.413(3)
C23-C24	1.374(3)
C24-C25	1.393(4)
C25-C26	1.376(4)
C26-C27	1.406(3)
C27-C28	1.468(3)
C28-C33	1.408(3)
C28-C29	1.411(3)
C29-C30	1.372(4)
C30-C31	1.394(3)
C31-C32	1.380(3)
C32-C33	1.411(3)
C33-C34	1.468(3)
C34-C35	1.391(3)
C35-C36	1.412(3)
C36-C37	1.450(3)
C37-C38	1.406(2)
C37-C46	1.452(3)
C38-C39	1.437(3)

C39-C44	1.417(3)
C39-C40	1.425(2)
C40-C41	1.399(3)
C41-C42	1.385(3)
C42-C43	1.380(3)
C43-C44	1.407(3)
C44-C45	1.455(3)
C45-C46	1.402(3)
C45-C54	1.421(3)
C46-C47	1.452(3)
C47-C48	1.422(3)
C47-C52	1.423(3)
C48-C49	1.375(3)
C49-C50	1.400(3)
C50-C51	1.371(3)
C51-C52	1.417(3)
C52-C53	1.440(3)
C53-C54	1.367(3)
C53-C61	1.517(3)
C55-C56	1.520(3)
C56-C57	1.515(4)
C57-C58	1.502(4)
C57-C58'	1.556(5)
C58-C59	1.526(4)
C59-C60	1.527(4)
C58'-C59'	1.550(5)
C59'-C60'	1.540(5)
C61-C62	1.532(3)
C62-C63	1.521(3)
C63-C64	1.526(3)
C64-C65	1.517(4)
C65-C66	1.531(4)
C1S-C2S	1.478(6)
C1S-Cl1S	1.718(5)
C1S-Cl2S	1.762(4)
C2S-Cl3S	1.780(4)
C2S-Cl4S	1.825(5)
C1S'-C2S'	1.470(7)

C1S'-Cl1'	1.704(6)
C1S'-Cl2'	1.758(6)
C2S'-Cl3'	1.771(6)
C2S'-Cl4'	1.829(6)

Angles----------

C2-C1-C10	123.36(18)
C1-C2-C3	117.86(19)
C1-C2-C55	122.29(18)
C3-C2-C55	119.79(19)
C8-C3-C4	119.03(18)
C8-C3-C2	119.98(18)
C4-C3-C2	120.81(19)
C5-C4-C3	121.1(2)
C4-C5-C6	120.0(2)
C7-C6-C5	120.11(19)
C6-C7-C8	121.4(2)
C3-C8-C7	118.05(18)
C3-C8-C9	119.94(17)
C7-C8-C9	121.70(18)
C10-C9-C18	119.02(18)
C10-C9-C8	117.45(18)
C18-C9-C8	123.39(17)
C9-C10-C1	119.37(18)
C9-C10-C11	119.93(18)
C1-C10-C11	120.71(17)
C12-C11-C16	118.81(18)
C12-C11-C10	121.77(19)
C16-C11-C10	119.36(17)
C13-C12-C11	120.5(2)
C12-C13-C14	120.74(19)
C13-C14-C15	121.30(19)
C14-C15-C16	118.40(19)
C14-C15-C40	121.72(18)
C16-C15-C40	119.85(17)
C15-C16-C11	120.19(17)
C15-C16-C17	120.05(18)
C11-C16-C17	119.53(17)

C18-C17-C16	119.76(18)
C18-C17-C38	120.19(16)
C16-C17-C38	120.03(17)
C17-C18-C9	119.46(17)
C17-C18-C19	116.34(18)
C9-C18-C19	123.77(17)
C20-C19-C36	118.38(17)
C20-C19-C18	121.33(18)
C36-C19-C18	119.69(17)
C21-C20-C19	123.16(19)
C20-C21-C34	118.41(18)
C20-C21-C22	121.94(19)
C34-C21-C22	119.59(17)
C23-C22-C27	118.48(19)
C23-C22-C21	121.55(19)
C27-C22-C21	119.96(19)
C24-C23-C22	121.6(2)
C23-C24-C25	120.1(2)
C26-C25-C24	119.3(2)
C25-C26-C27	121.9(2)
C26-C27-C22	118.6(2)
C26-C27-C28	121.4(2)
C22-C27-C28	120.05(19)
C33-C28-C29	118.4(2)
C33-C28-C27	120.05(18)
C29-C28-C27	121.5(2)
C30-C29-C28	121.6(2)
C29-C30-C31	120.2(2)
C32-C31-C30	119.4(2)
C31-C32-C33	121.4(2)
C28-C33-C32	118.97(18)
C28-C33-C34	120.13(19)
C32-C33-C34	120.84(18)
C35-C34-C21	118.70(17)
C35-C34-C33	121.58(18)
C21-C34-C33	119.71(18)
C34-C35-C36	122.75(19)
C35-C36-C19	118.34(18)

C35-C36-C37	121.46(18)
C19-C36-C37	119.67(17)
C38-C37-C36	116.32(18)
C38-C37-C46	119.08(17)
C36-C37-C46	124.01(16)
C37-C38-C39	119.74(18)
C37-C38-C17	120.23(17)
C39-C38-C17	120.01(16)
C44-C39-C40	120.15(17)
C44-C39-C38	119.66(17)
C40-C39-C38	119.98(18)
C41-C40-C39	118.25(19)
C41-C40-C15	121.92(17)
C39-C40-C15	119.80(17)
C42-C41-C40	121.40(18)
C43-C42-C41	120.67(19)
C42-C43-C44	120.4(2)
C43-C44-C39	119.11(17)
C43-C44-C45	121.42(19)
C39-C44-C45	119.37(17)
C46-C45-C54	118.90(17)
C46-C45-C44	119.71(18)
C54-C45-C44	121.39(18)
C45-C46-C47	117.72(18)
C45-C46-C37	118.76(17)
C47-C46-C37	123.49(17)
C48-C47-C52	117.95(17)
C48-C47-C46	121.66(18)
C52-C47-C46	120.24(17)
C49-C48-C47	121.38(19)
C48-C49-C50	120.0(2)
C51-C50-C49	120.35(18)
C50-C51-C52	121.0(2)
C51-C52-C47	119.07(18)
C51-C52-C53	121.52(19)
C47-C52-C53	119.39(17)
C54-C53-C52	117.95(19)
C54-C53-C61	119.02(19)

C52-C53-C61	123.02(18)
C53-C54-C45	123.76(19)
C2-C55-C56	116.15(19)
C57-C56-C55	113.4(2)
C58-C57-C56	115.0(3)
C56-C57-C58'	109.3(6)
C57-C58-C59	110.7(3)
C58-C59-C60	111.3(3)
C59'-C58'-C57	136.4(13)
C60'-C59'-C58'	112.2(12)
C53-C61-C62	114.87(19)
C63-C62-C61	115.73(19)
C62-C63-C64	112.6(2)
C65-C64-C63	113.7(2)
C64-C65-C66	112.3(2)
C2S-C1S-Cl1S	109.8(4)
C2S-C1S-Cl2S	112.5(3)
Cl1S-C1S-Cl2S	110.9(3)
C1S-C2S-Cl3S	113.9(3)
C1S-C2S-Cl4S	108.2(3)
Cl3S-C2S-Cl4S	110.1(2)
C2S'-C1S'-Cl1'	113.7(5)
C2S'-C1S'-Cl2'	114.6(5)
Cl1'-C1S'-Cl2'	110.9(5)
C1S'-C2S'-Cl3'	115.3(5)
C1S'-C2S'-Cl4'	109.4(5)
Cl3'-C2S'-Cl4'	107.7(4)

Table 18. Torsion angles [°] for **8**.

C10-C1-C2-C3	-7.9(3)
C10-C1-C2-C55	174.7(2)
C1-C2-C3-C8	6.6(3)
C55-C2-C3-C8	-176.0(2)
C1-C2-C3-C4	-168.4(2)
C55-C2-C3-C4	9.0(3)
C8-C3-C4-C5	-4.2(3)
C2-C3-C4-C5	170.9(2)

C3-C4-C5-C6	-0.8(4)
C4-C5-C6-C7	3.9(4)
C5-C6-C7-C8	-1.9(3)
C4-C3-C8-C7	6.0(3)
C2-C3-C8-C7	-169.10(19)
C4-C3-C8-C9	179.86(19)
C2-C3-C8-C9	4.7(3)
C6-C7-C8-C3	-3.1(3)
C6-C7-C8-C9	-176.8(2)
C3-C8-C9-C10	-14.9(3)
C7-C8-C9-C10	158.66(19)
C3-C8-C9-C18	169.31(19)
C7-C8-C9-C18	-17.1(3)
C18-C9-C10-C1	-170.20(18)
C8-C9-C10-C1	13.8(3)
C18-C9-C10-C11	10.2(3)
C8-C9-C10-C11	-165.71(18)
C2-C1-C10-C9	-2.6(3)
C2-C1-C10-C11	177.0(2)
C9-C10-C11-C12	-178.9(2)
C1-C10-C11-C12	1.6(3)
C9-C10-C11-C16	4.0(3)
C1-C10-C11-C16	-175.58(19)
C16-C11-C12-C13	0.1(3)
C10-C11-C12-C13	-177.1(2)
C11-C12-C13-C14	0.3(4)
C12-C13-C14-C15	-0.4(4)
C13-C14-C15-C16	0.1(3)
C13-C14-C15-C40	-178.0(2)
C14-C15-C16-C11	0.3(3)
C40-C15-C16-C11	178.40(18)
C14-C15-C16-C17	-174.11(19)
C40-C15-C16-C17	4.0(3)
C12-C11-C16-C15	-0.4(3)
C10-C11-C16-C15	176.84(18)
C12-C11-C16-C17	174.05(19)
C10-C11-C16-C17	-8.7(3)
C15-C16-C17-C18	173.44(18)

C11-C16-C17-C18	-1.0(3)
C15-C16-C17-C38	-5.2(3)
C11-C16-C17-C38	-179.65(18)
C16-C17-C18-C9	15.4(3)
C38-C17-C18-C9	-165.99(18)
C16-C17-C18-C19	-157.36(18)
C38-C17-C18-C19	21.3(3)
C10-C9-C18-C17	-20.1(3)
C8-C9-C18-C17	155.62(19)
C10-C9-C18-C19	152.09(19)
C8-C9-C18-C19	-32.2(3)
C17-C18-C19-C20	147.98(19)
C9-C18-C19-C20	-24.4(3)
C17-C18-C19-C36	-23.0(3)
C9-C18-C19-C36	164.60(18)
C36-C19-C20-C21	-3.1(3)
C18-C19-C20-C21	-174.18(18)
C19-C20-C21-C34	-0.8(3)
C19-C20-C21-C22	176.21(19)
C20-C21-C22-C23	-0.6(3)
C34-C21-C22-C23	176.4(2)
C20-C21-C22-C27	-178.99(19)
C34-C21-C22-C27	-2.0(3)
C27-C22-C23-C24	1.3(3)
C21-C22-C23-C24	-177.1(2)
C22-C23-C24-C25	-0.2(4)
C23-C24-C25-C26	-0.4(4)
C24-C25-C26-C27	-0.2(4)
C25-C26-C27-C22	1.3(4)
C25-C26-C27-C28	-177.9(2)
C23-C22-C27-C26	-1.8(3)
C21-C22-C27-C26	176.6(2)
C23-C22-C27-C28	177.5(2)
C21-C22-C27-C28	-4.1(3)
C26-C27-C28-C33	-175.6(2)
C22-C27-C28-C33	5.1(3)
C26-C27-C28-C29	5.6(3)
C22-C27-C28-C29	-173.7(2)

C33-C28-C29-C30	-0.1(3)
C27-C28-C29-C30	178.7(2)
C28-C29-C30-C31	-0.7(4)
C29-C30-C31-C32	0.1(4)
C30-C31-C32-C33	1.3(3)
C29-C28-C33-C32	1.5(3)
C27-C28-C33-C32	-177.37(19)
C29-C28-C33-C34	178.8(2)
C27-C28-C33-C34	0.0(3)
C31-C32-C33-C28	-2.1(3)
C31-C32-C33-C34	-179.4(2)
C20-C21-C34-C35	5.0(3)
C22-C21-C34-C35	-172.09(18)
C20-C21-C34-C33	-175.84(18)
C22-C21-C34-C33	7.1(3)
C28-C33-C34-C35	173.07(19)
C32-C33-C34-C35	-9.6(3)
C28-C33-C34-C21	-6.1(3)
C32-C33-C34-C21	171.19(19)
C21-C34-C35-C36	-5.5(3)
C33-C34-C35-C36	175.35(18)
C34-C35-C36-C19	1.6(3)
C34-C35-C36-C37	173.24(18)
C20-C19-C36-C35	2.7(3)
C18-C19-C36-C35	173.92(17)
C20-C19-C36-C37	-169.13(18)
C18-C19-C36-C37	2.1(3)
C35-C36-C37-C38	-150.97(19)
C19-C36-C37-C38	20.6(3)
C35-C36-C37-C46	20.1(3)
C19-C36-C37-C46	-168.41(18)
C36-C37-C38-C39	155.93(18)
C46-C37-C38-C39	-15.6(3)
C36-C37-C38-C17	-22.5(3)
C46-C37-C38-C17	165.96(18)
C18-C17-C38-C37	1.6(3)
C16-C17-C38-C37	-179.82(18)
C18-C17-C38-C39	-176.91(18)

C16-C17-C38-C39	1.7(3)
C37-C38-C39-C44	-0.8(3)
C17-C38-C39-C44	177.68(18)
C37-C38-C39-C40	-175.51(18)
C17-C38-C39-C40	3.0(3)
C44-C39-C40-C41	-0.8(3)
C38-C39-C40-C41	173.92(18)
C44-C39-C40-C15	-178.85(18)
C38-C39-C40-C15	-4.2(3)
C14-C15-C40-C41	0.7(3)
C16-C15-C40-C41	-177.31(19)
C14-C15-C40-C39	178.7(2)
C16-C15-C40-C39	0.7(3)
C39-C40-C41-C42	0.0(3)
C15-C40-C41-C42	178.00(19)
C40-C41-C42-C43	0.3(3)
C41-C42-C43-C44	0.3(3)
C42-C43-C44-C39	-1.1(3)
C42-C43-C44-C45	175.14(19)
C40-C39-C44-C43	1.3(3)
C38-C39-C44-C43	-173.38(18)
C40-C39-C44-C45	-174.98(18)
C38-C39-C44-C45	10.3(3)
C43-C44-C45-C46	-179.47(19)
C39-C44-C45-C46	-3.2(3)
C43-C44-C45-C54	0.7(3)
C39-C44-C45-C54	176.93(19)
C54-C45-C46-C47	-15.0(3)
C44-C45-C46-C47	165.21(18)
C54-C45-C46-C37	166.85(18)
C44-C45-C46-C37	-13.0(3)
C38-C37-C46-C45	22.5(3)
C36-C37-C46-C45	-148.26(19)
C38-C37-C46-C47	-155.53(19)
C36-C37-C46-C47	33.7(3)
C45-C46-C47-C48	-161.25(19)
C37-C46-C47-C48	16.8(3)
C45-C46-C47-C52	14.2(3)

C37-C46-C47-C52	-167.66(18)
C52-C47-C48-C49	4.9(3)
C46-C47-C48-C49	-179.5(2)
C47-C48-C49-C50	-0.7(3)
C48-C49-C50-C51	-2.5(3)
C49-C50-C51-C52	1.4(3)
C50-C51-C52-C47	2.9(3)
C50-C51-C52-C53	-175.5(2)
C48-C47-C52-C51	-5.9(3)
C46-C47-C52-C51	178.47(19)
C48-C47-C52-C53	172.52(19)
C46-C47-C52-C53	-3.1(3)
C51-C52-C53-C54	171.2(2)
C47-C52-C53-C54	-7.1(3)
C51-C52-C53-C61	-7.9(3)
C47-C52-C53-C61	173.71(19)
C52-C53-C54-C45	6.5(3)
C61-C53-C54-C45	-174.3(2)
C46-C45-C54-C53	4.8(3)
C44-C45-C54-C53	-175.3(2)
C1-C2-C55-C56	-5.3(3)
C3-C2-C55-C56	177.4(2)
C2-C55-C56-C57	-174.2(2)
C55-C56-C57-C58	61.9(4)
C55-C56-C57-C58'	80.7(7)
C56-C57-C58-C59	171.2(3)
C58'-C57-C58-C59	96(2)
C57-C58-C59-C60	177.3(4)
C58-C57-C58'-C59'	-62.4(19)
C56-C57-C58'-C59'	-174.2(15)
C57-C58'-C59'-C60'	63(2)
C54-C53-C61-C62	-82.0(3)
C52-C53-C61-C62	97.2(2)
C53-C61-C62-C63	-72.4(2)
C61-C62-C63-C64	-173.42(19)
C62-C63-C64-C65	179.8(2)
C63-C64-C65-C66	-178.6(2)
Cl1S-C1S-C2S-Cl3S	-65.3(4)

Cl2S-C1S-C2S-Cl3S	58.7(4)
Cl1S-C1S-C2S-Cl4S	171.9(3)
Cl2S-C1S-C2S-Cl4S	-64.1(4)
Cl1'-C1S'-C2S'-Cl3'	65.9(8)
Cl2'-C1S'-C2S'-Cl3'	-165.1(5)
Cl1'-C1S'-C2S'-Cl4'	-55.6(7)
Cl2'-C1S'-C2S'-Cl4'	73.4(6)

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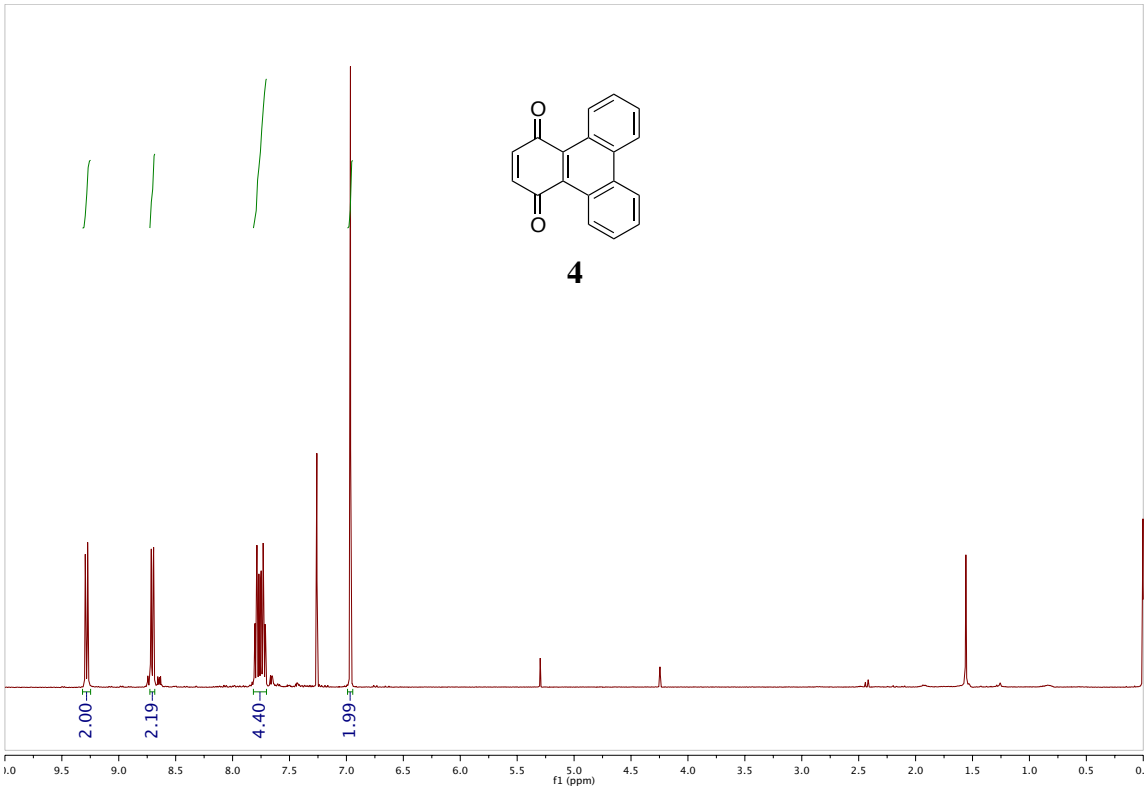
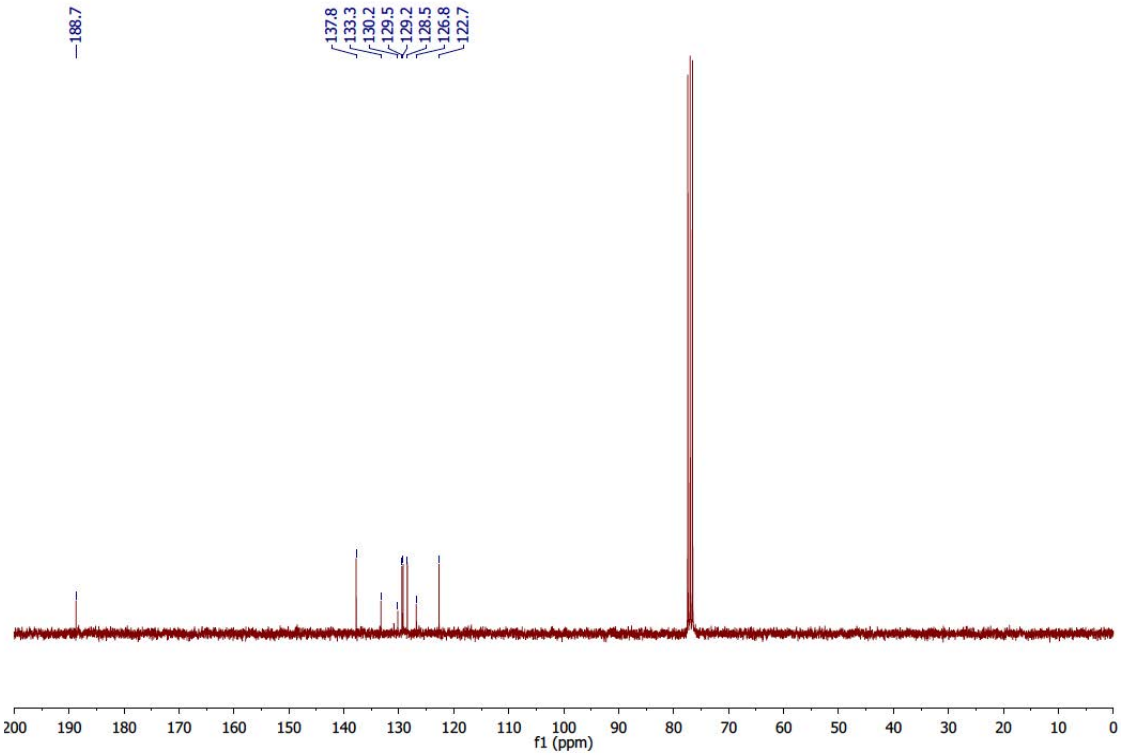
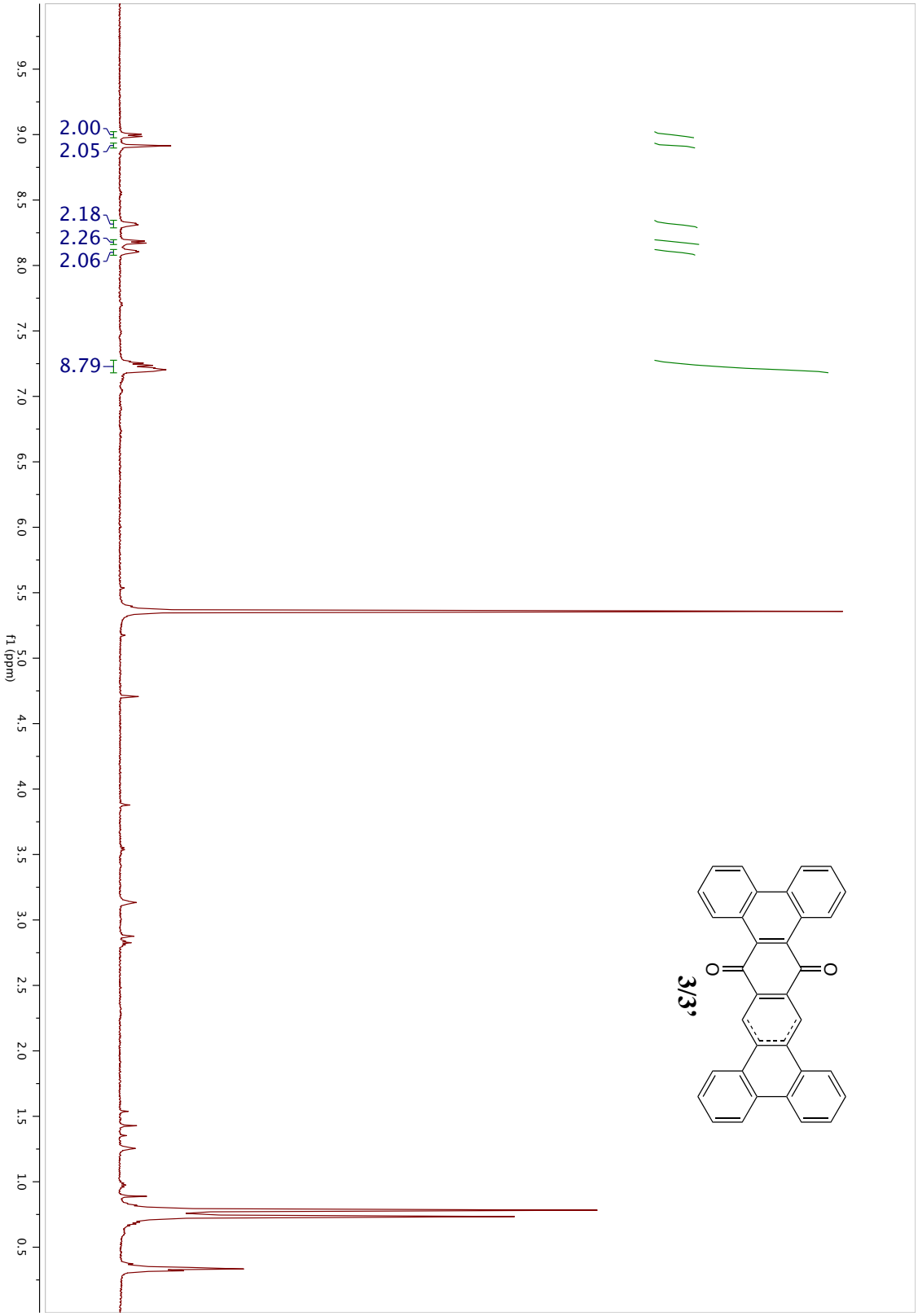
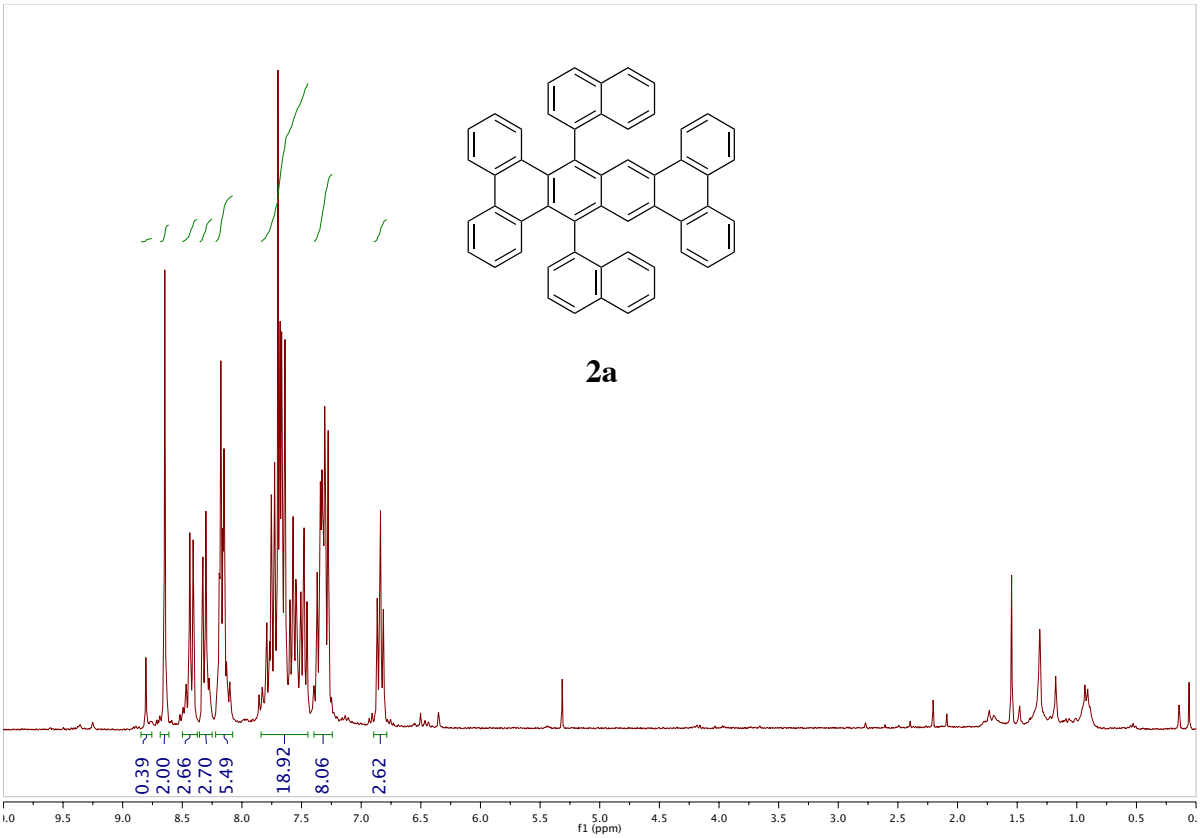
3. ^{1}H-NMR and ^{13}C-NMR Spectra



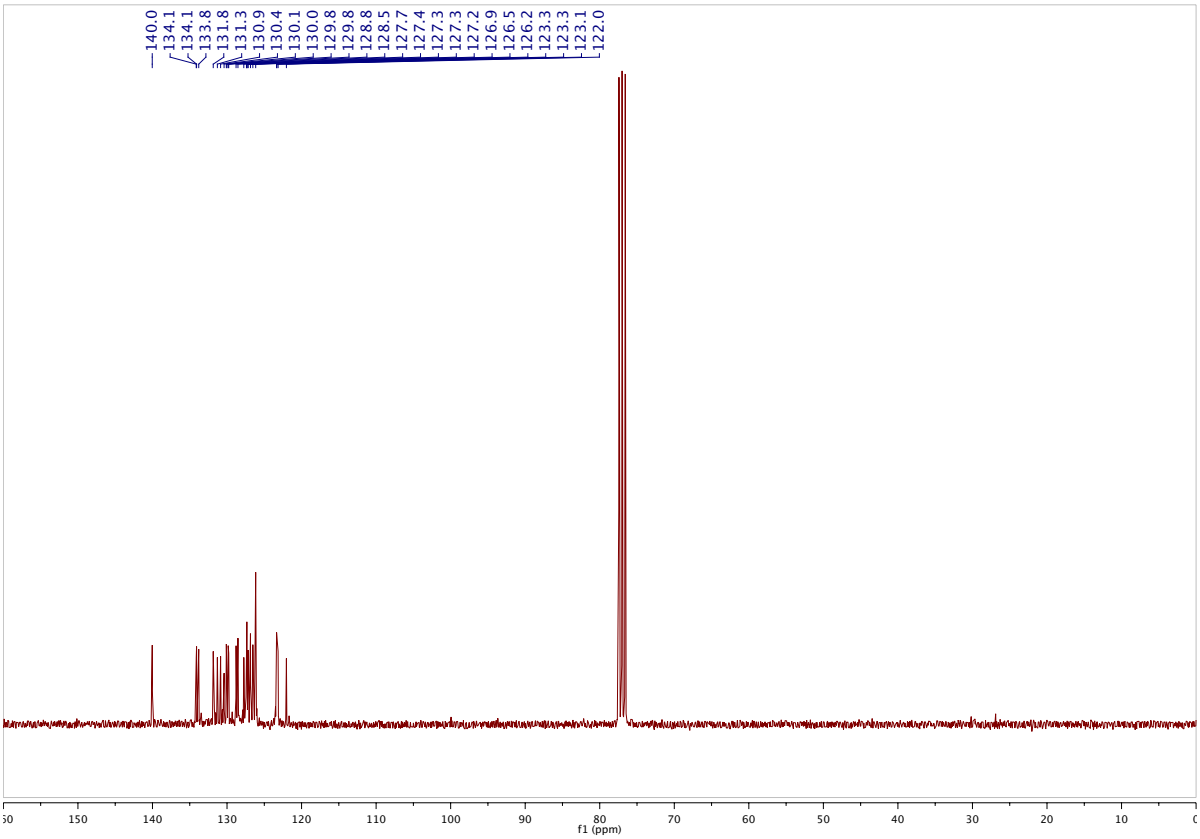
4

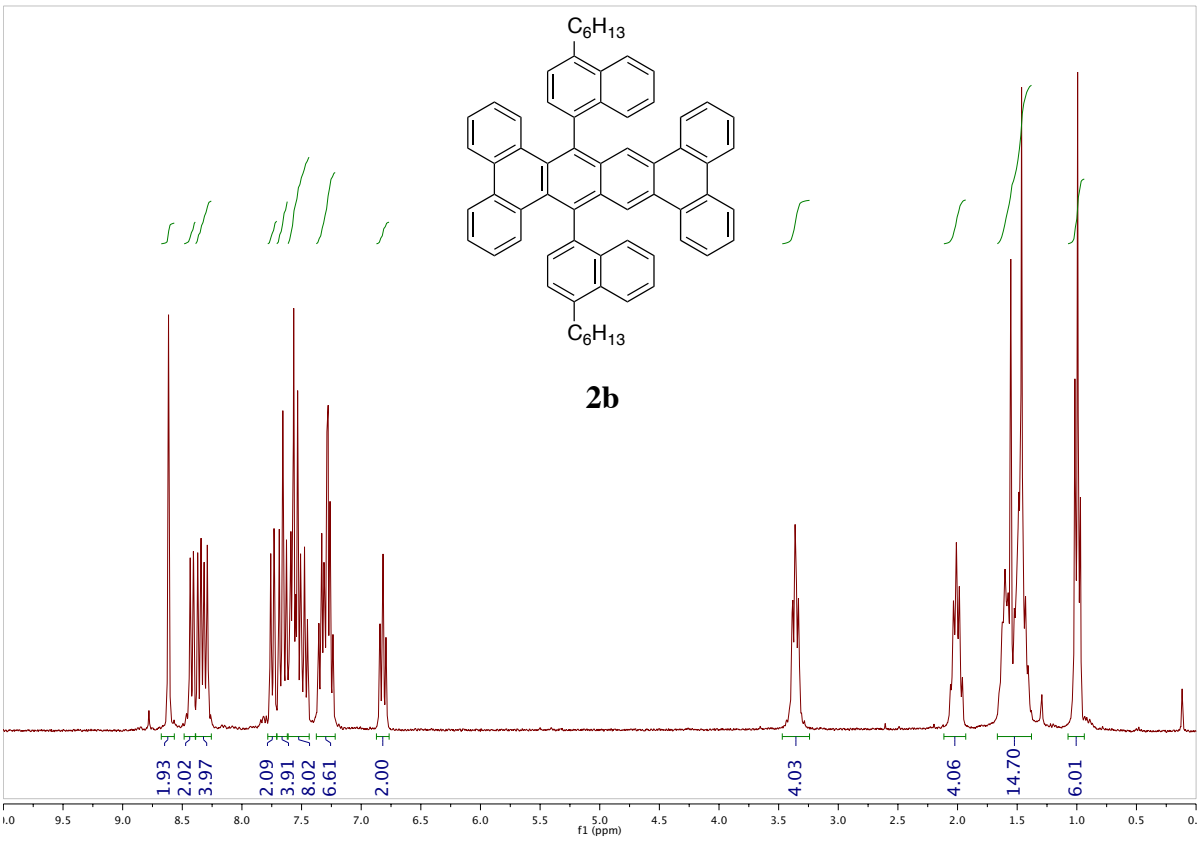



2.00
2.05
2.18
2.26
2.06
8.79
f1 (ppm)
3/3'

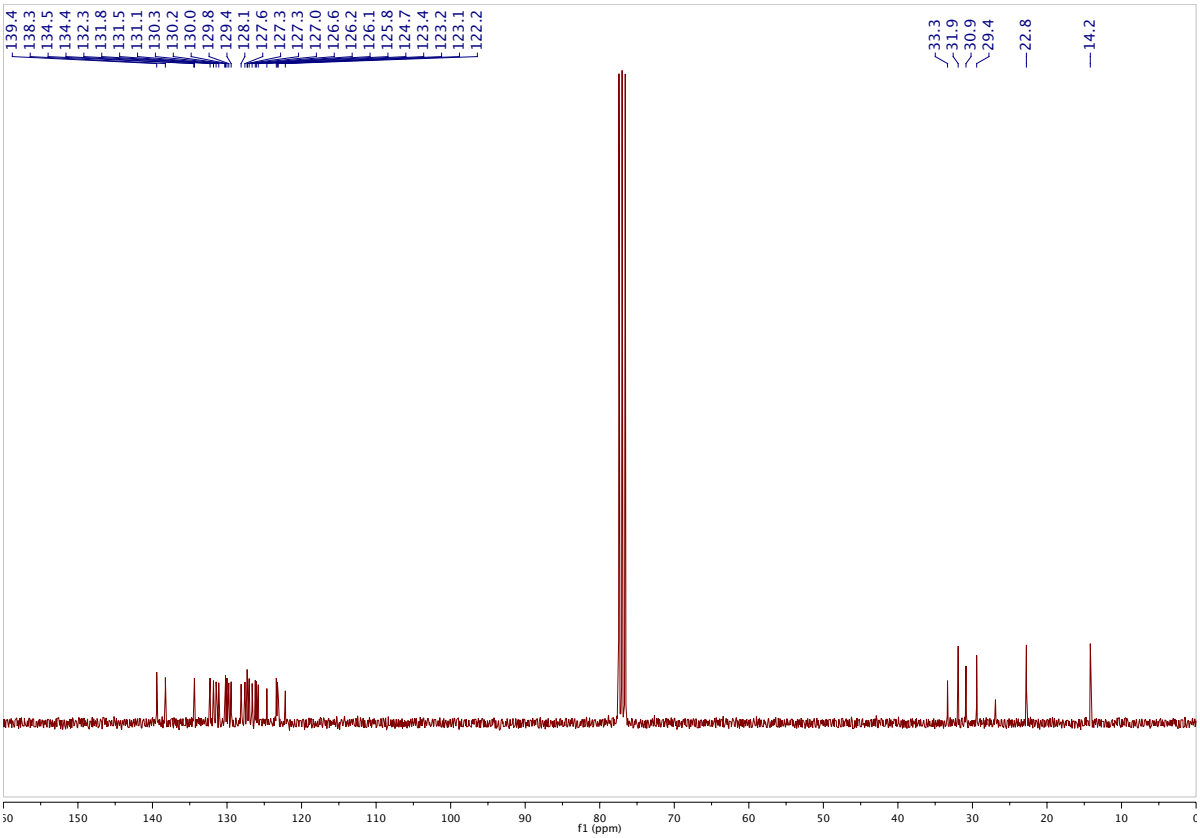

0.39
2.00
2.66
2.70
5.49
18.92
8.06
2.62
f1 (ppm)

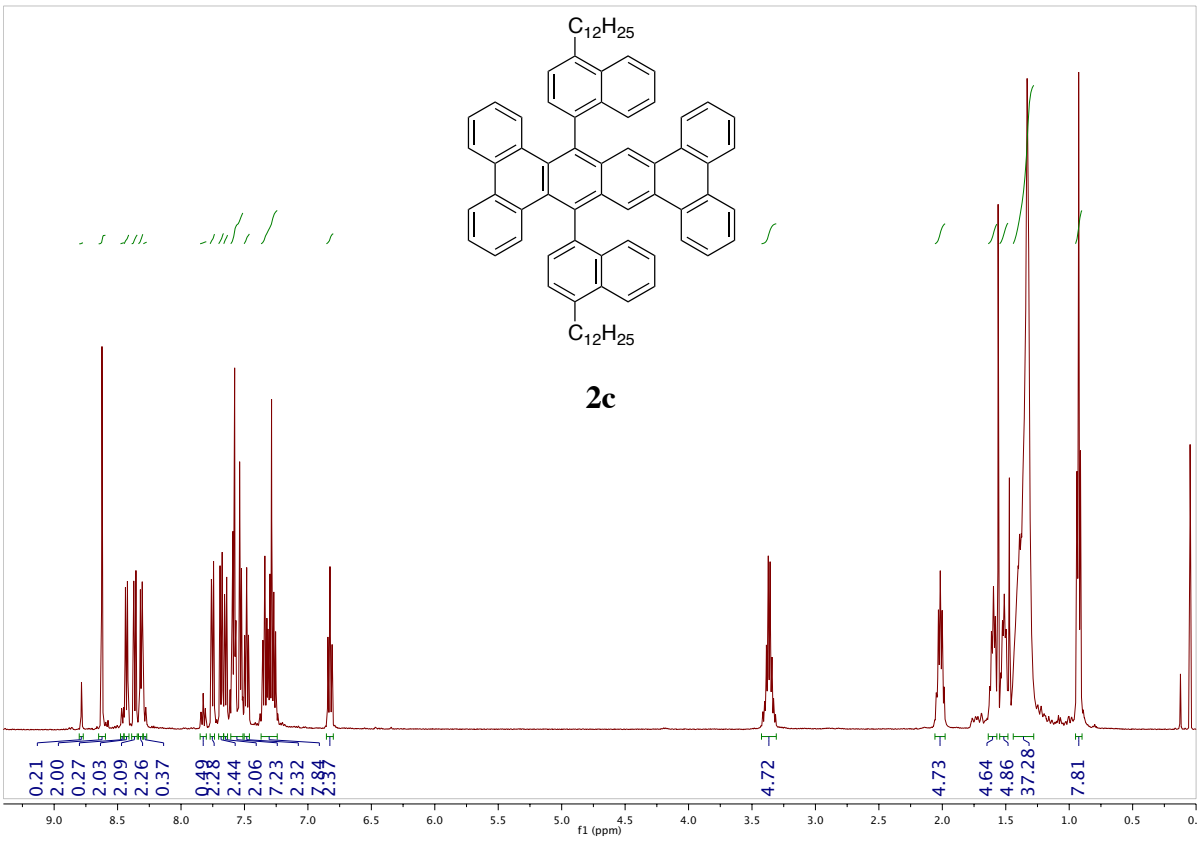
2a


140.0
134.1
134.1
133.8
131.8
131.3
130.9
130.4
130.1
130.0
129.8
129.8
128.8
128.5
127.7
127.4
127.3
127.3
127.2
126.9
126.5
126.2
123.3
123.3
123.1
122.0
f1 (ppm)

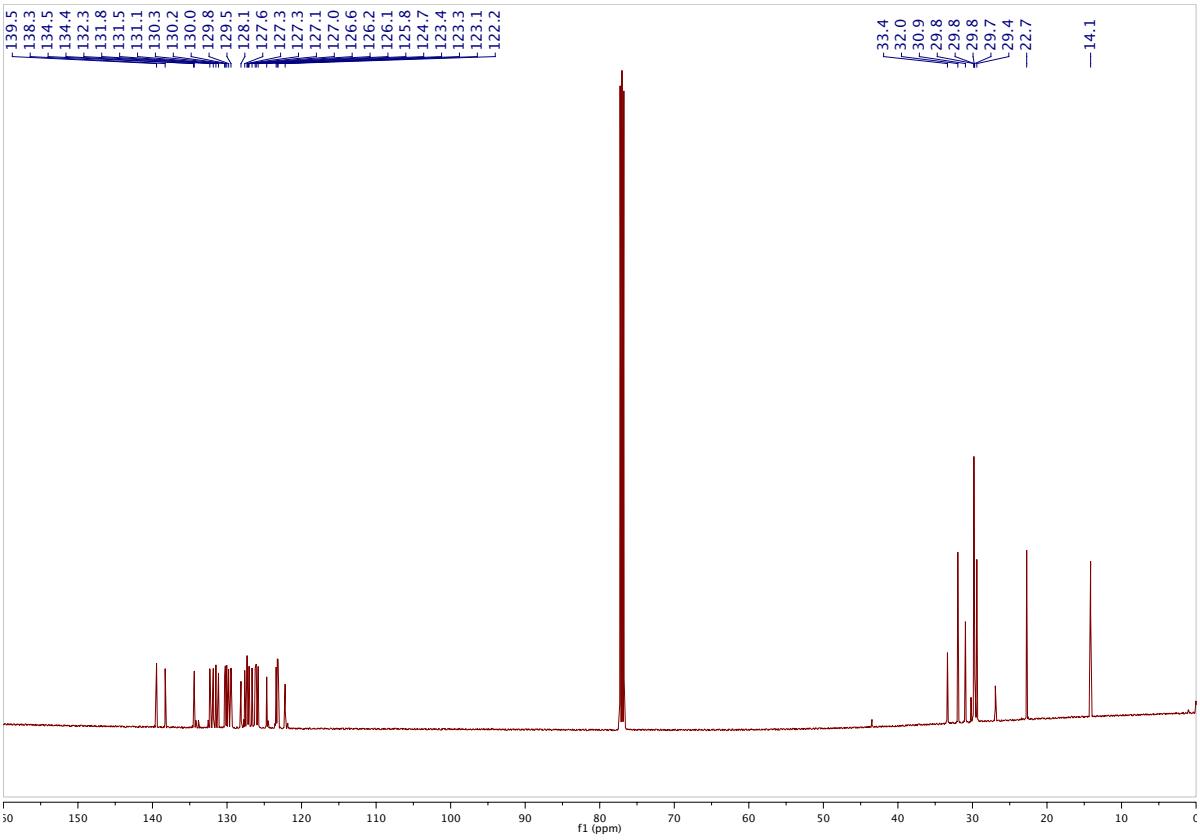

C6H13
C6H13
1.93
2.02
3.97
2.09
3.91
8.02
6.61
2.00
4.03
4.06
14.70
6.01
f1 (ppm)

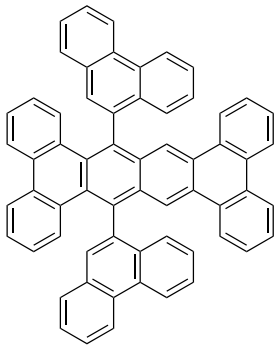
2b


139.4
138.3
134.5
134.4
132.3
131.8
131.5
131.1
130.3
130.2
130.0
129.8
129.4
128.1
127.6
127.3
127.3
127.0
126.6
126.2
126.1
125.8
124.7
123.4
123.2
123.1
122.2
33.3
31.9
30.9
29.4
22.8
14.2
f1 (ppm)


C12H25
C12H25
0.21
2.00
0.27
2.03
2.09
2.26
0.37
2.44
2.06
7.23
2.32
4.72
4.73
4.64
4.86
37.28
7.81
f1 (ppm)

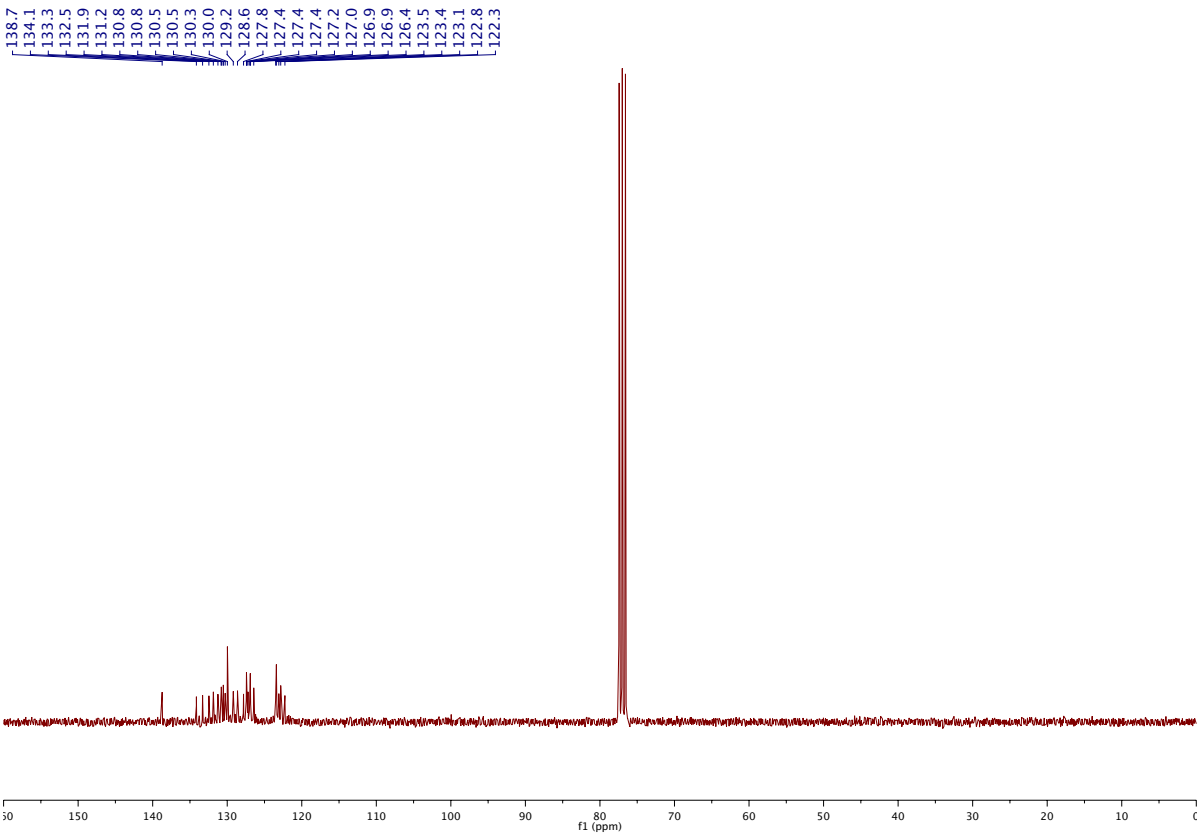
2c

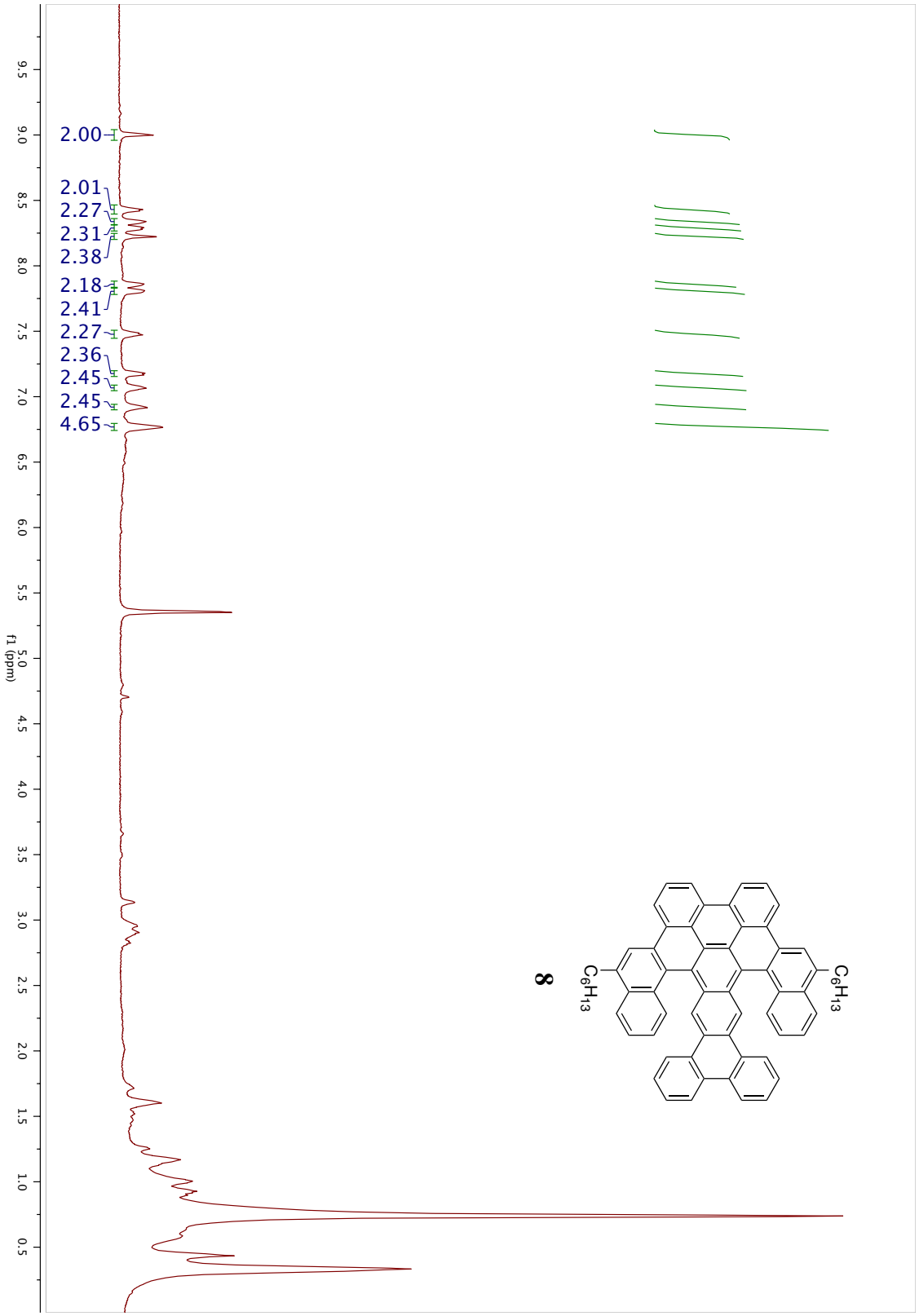

139.5
138.3
134.5
134.4
132.3
131.8
131.5
131.1
130.3
130.2
130.0
129.8
129.5
128.1
127.6
127.3
127.3
127.1
127.0
126.6
126.2
126.1
125.8
124.7
123.4
123.3
123.1
122.2
33.4
32.0
30.9
29.8
29.8
29.8
29.7
29.4
22.7
14.1
f1 (ppm)



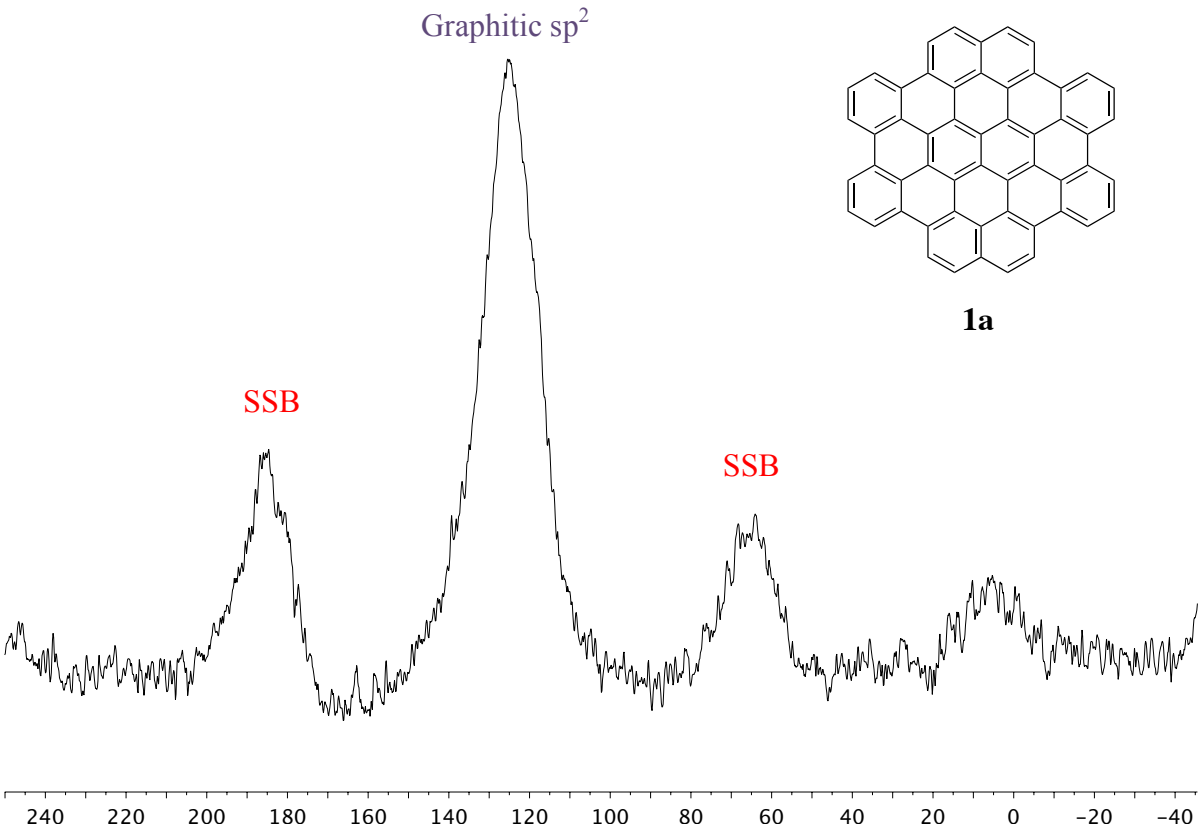
2d

2.05
2.42
2.10
2.00
2.02
1.98
8.34
2.54
2.57
2.16
4.28
2.55
2.34
2.14
f1 (ppm)

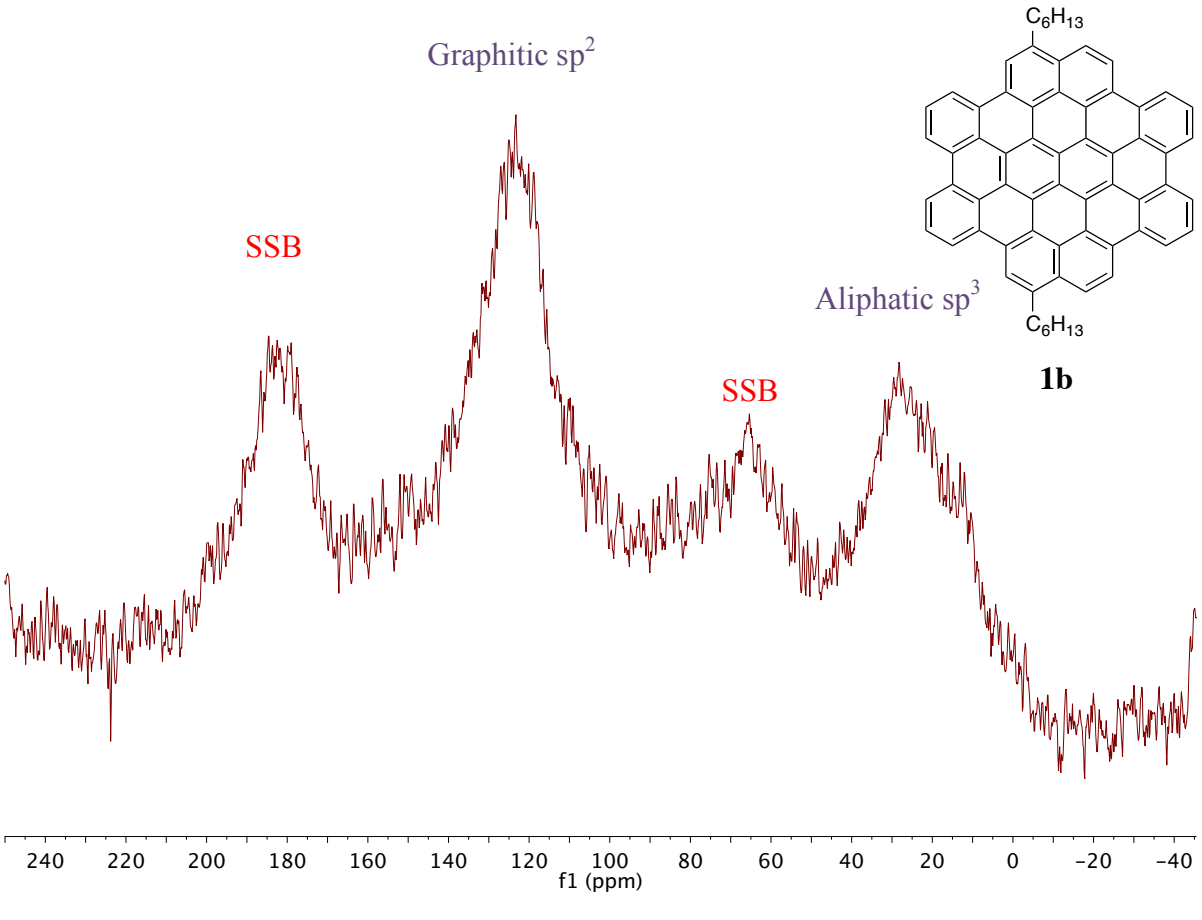

138.7
134.1
133.3
132.5
131.9
131.2
130.8
130.8
130.5
130.5
130.3
130.0
129.2
128.6
127.8
127.4
127.4
127.4
127.2
127.0
126.9
126.9
126.4
123.5
123.4
123.1
122.8
122.3
f1 (ppm)


2.00
2.01
2.27
2.31
2.38
2.18
2.41
2.27
2.36
2.45
2.45
4.65
f1 (ppm)
8
C6H13
C6H13

SS-NMR

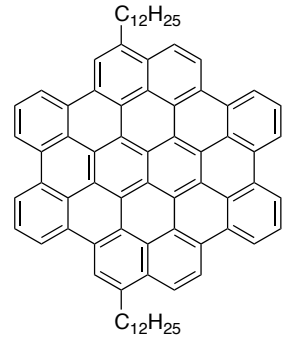

Graphitic sp2
SSB
SSB
240
220
200
180
160
140
120
100
80
60
40
20
0
-20
-40

1a


Graphitic sp2
SSB
SSB
Aliphatic sp3
240
220
200
180
160
140
120
100
80
60
40
20
0
-20
-40
f1 (ppm)

C6H13
C6H13

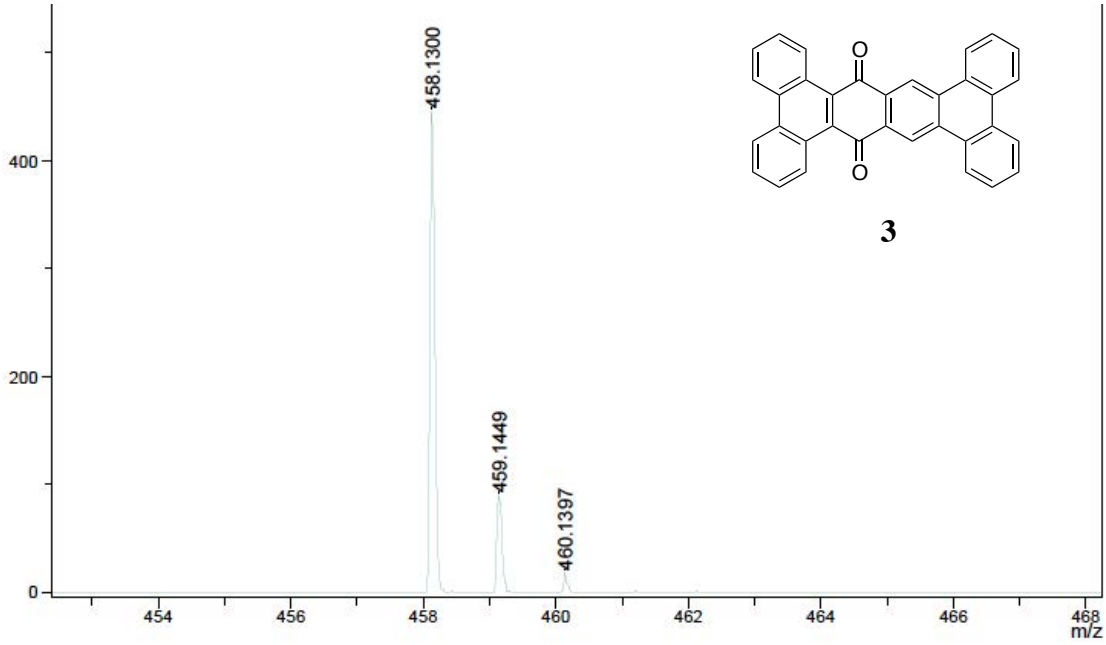
1b


C12H25
C12H25

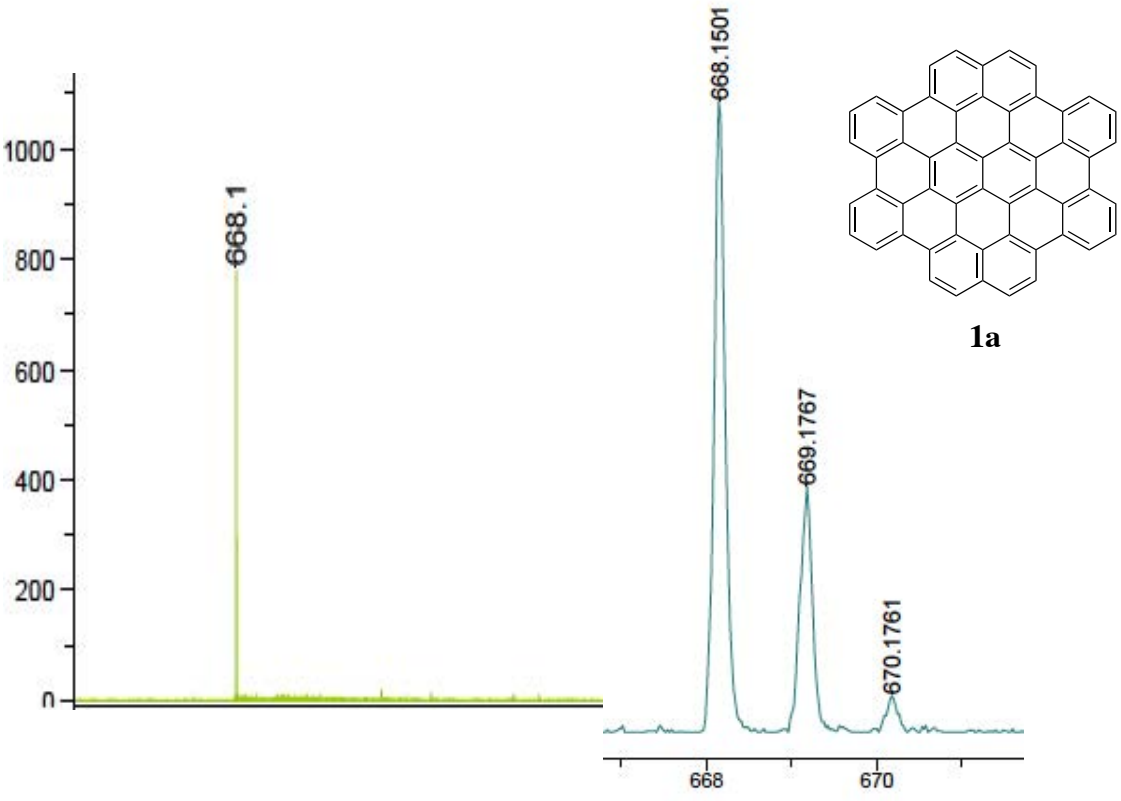
1c

Aliphatic sp3
Graphitic sp2
SSB
240
220
200
180
160
140
120
100
80
60
40
20
0
-20
-40
f1 (ppm)

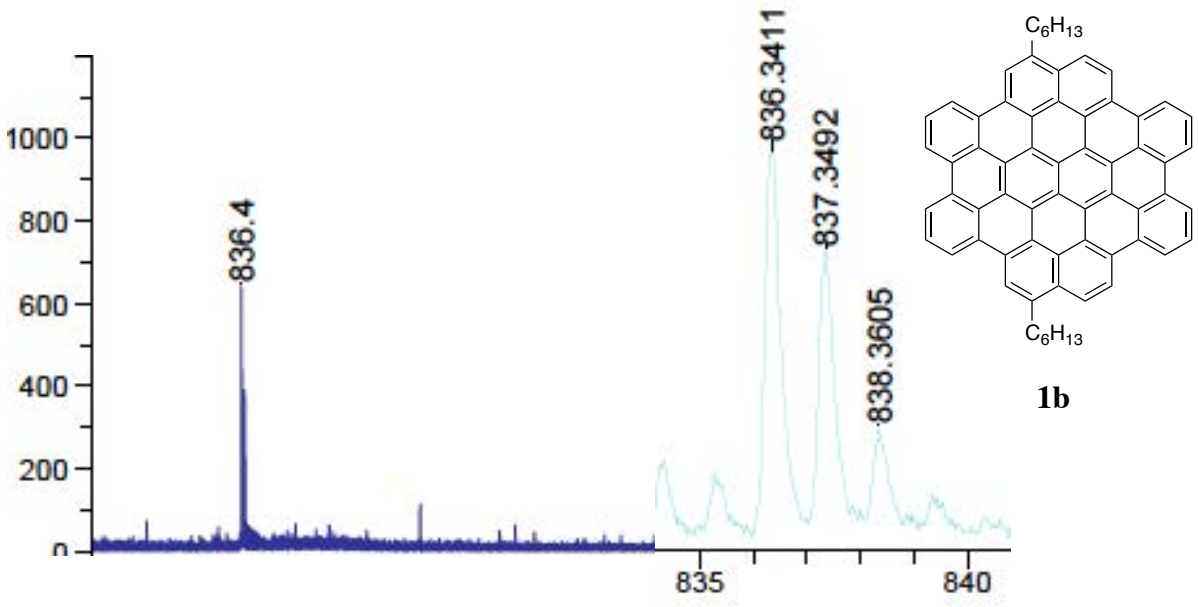
4. Mass Spectra



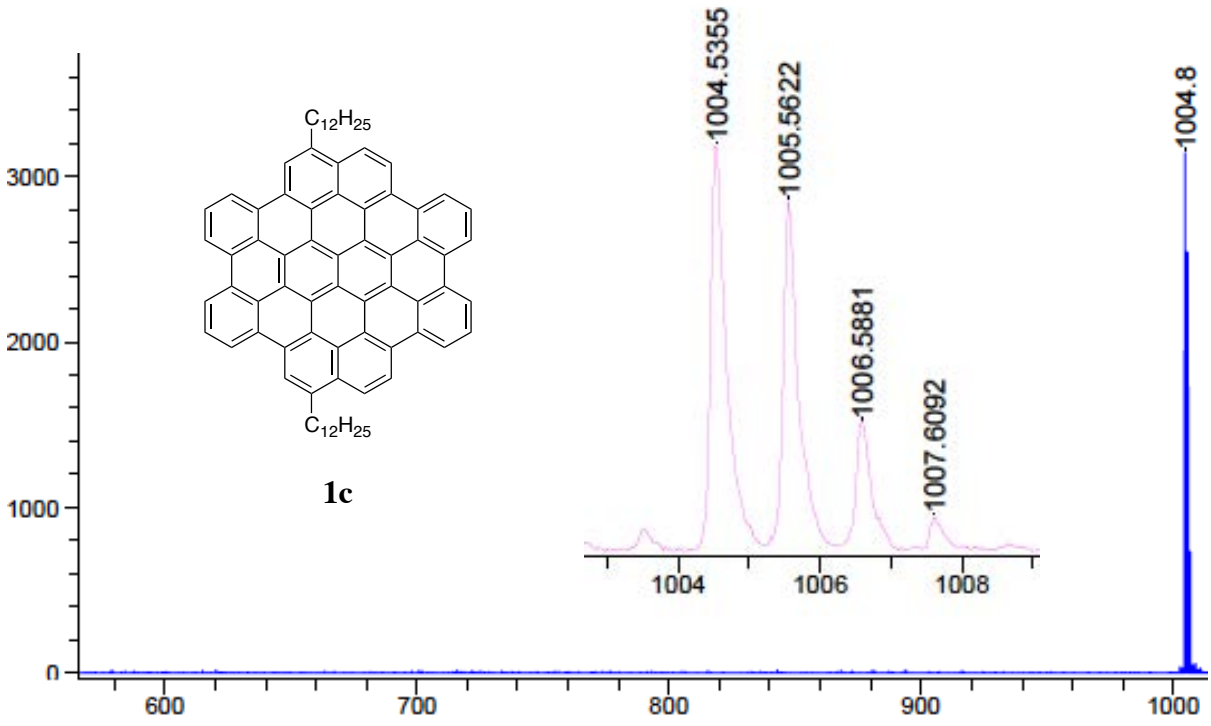
3



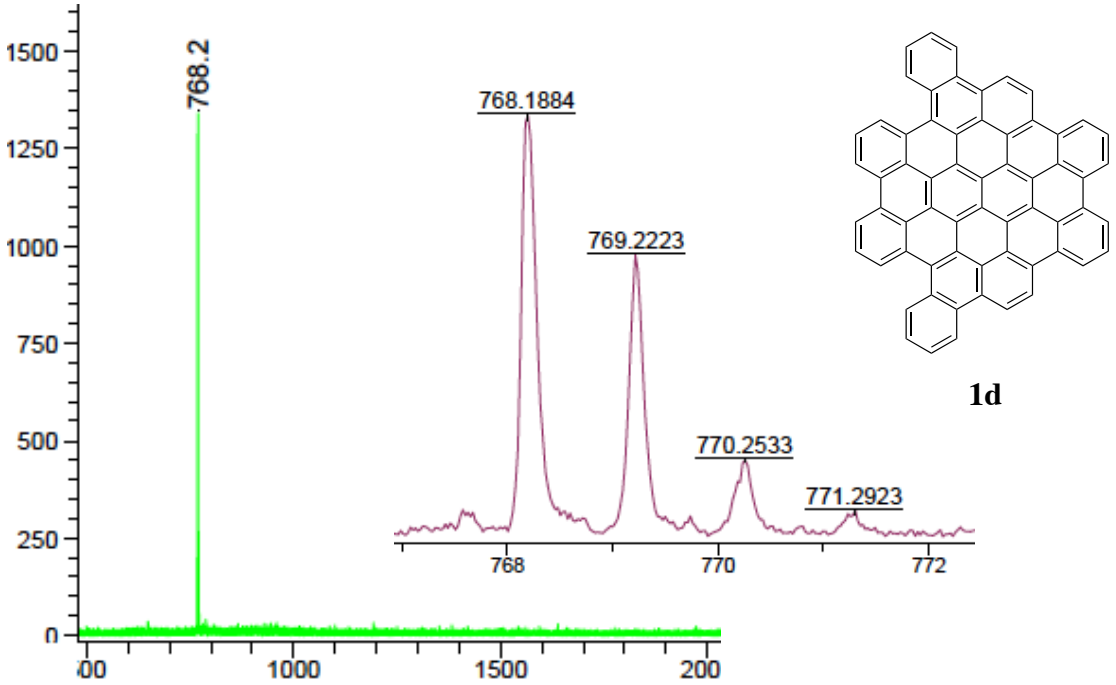
1a


836.4
836.3411
837.3492
838.3605
1000
800
600
400
200
0
835
840
C6H13
C6H13

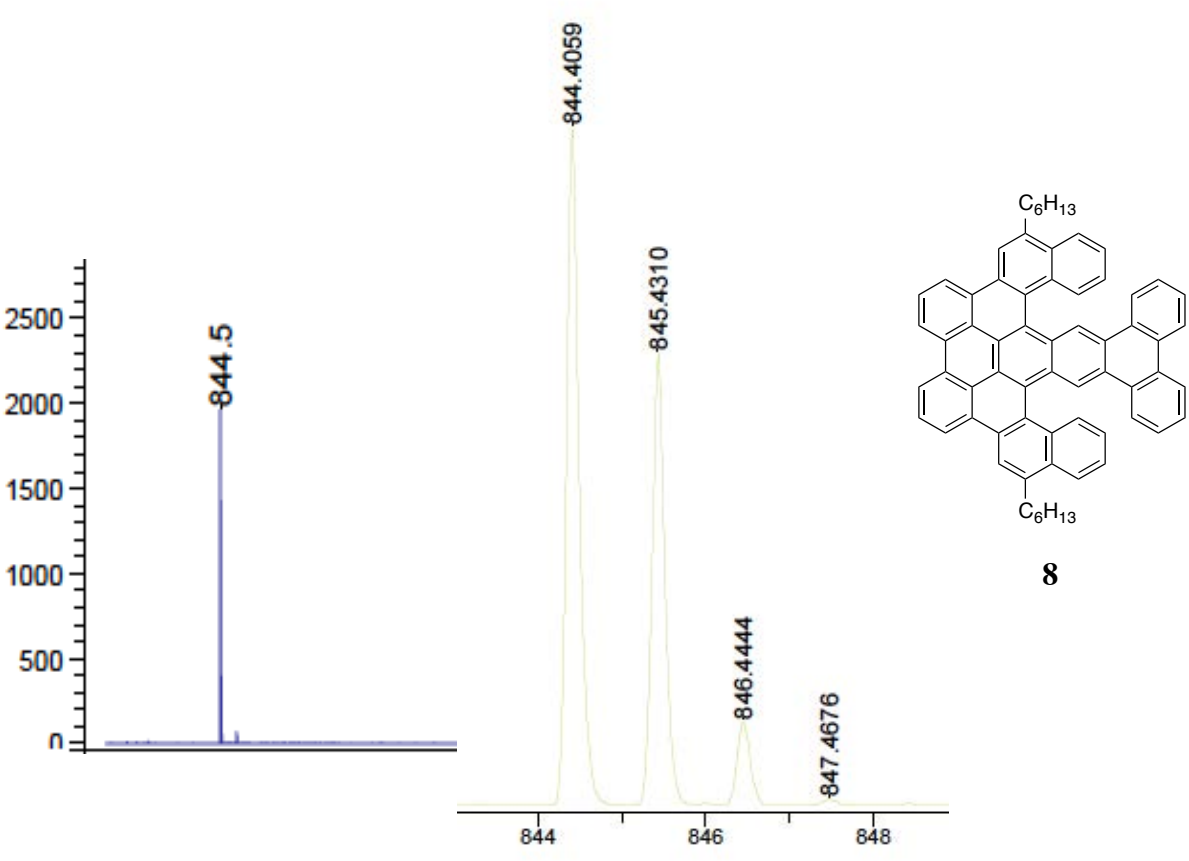
1b


1004.5355
1005.5622
1006.5881
1007.6092
1004.8
3000
2000
1000
0
600
700
800
900
1000
1004
1006
1008
C12H25
C12H25

1c


768.2
768.1884
769.2223
770.2533
771.2923
768
770
772

1d


844.5
844.4059
845.4310
846.4444
847.4676
844
846
848
C6H13
C6H13

8

5. STM Studies and ESQC Calculations

The synthesized molecules of **1a** were deposited via sublimation on a gold Au(111) monocrystal substrate to be imaged and identified using a low temperature ultra-high vacuum scanning tunneling microscope (LT-UHV-STM).

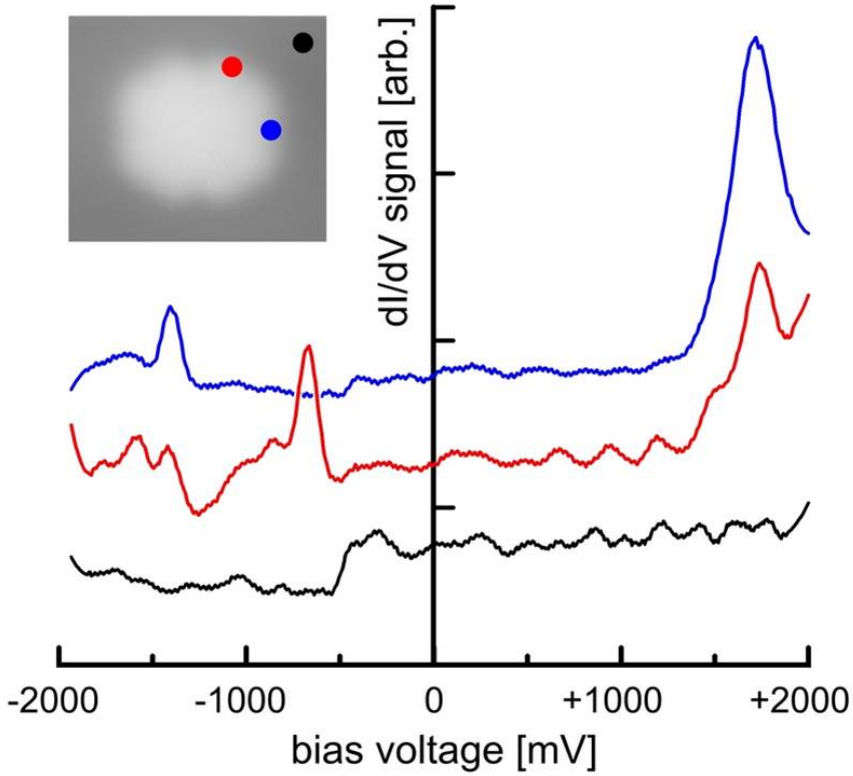


Figure S1: LT-UHV-STM dI/dV characteristic spectra recorded on a single molecule of **1a**, at places on the molecule indicated by red and blue solid dots. The spectra taken from **1a** zigzag edges show only one peak that corresponds to the molecule ground state (HOMO), while the spectra taken on the armchair edges show two peaks that correspond to the molecule's HOMO-1 and first excited state (LUMO). The spectrum in black taken from the Au(111) bare metal shows the characteristic resonance corresponding to the Au(111) surface state demonstrating that the STM tip was in conditions to be used to acquire dI/dV spectra.

Figure S1 shows a typical constant current STM image obtained in our experiments after the molecules sublimation on the Au(111) substrate. Single molecules of **1a** could be identified on the substrate terraces. dI/dV tunneling spectra were taken by positioning the STM tip over a single molecule of **1a** to track and measure the low laying electronic states characteristics of this compound. Although spectra were taken at different locations covering the whole molecule only spectra taken from the molecule edge's presented tunneling resonances, while spectra from the molecule center are featureless. The spectra from armchair edges show two distinctive resonances, one at each voltage polarity. Spectra from zigzag edges show only one resonance.

For those experiments, the Au(111) surface was intentionally selected to analyze the synthesized molecules because it has been already demonstrated that planar polyaromatic molecules like pentacene, coronene and others are physiadsorbed upon deposition on Au(111). Due to their adsorption state, the weak electronic coupling in between the molecules and Au(111) surface precludes the intermixing of molecular electronic states and the metal substrate states hence facilitating the identification of molecular electronic states whose spatial electronic distribution can be imaged in real space using the dI/dV mapping technique.

Molecules **1a** were imaged using a constant height dI/dV imaging mode to map the spatial distribution of the molecule's electronic states at -0.750 and 1.650 V, i.e. at the bias voltages corresponding to the two resonances nearest to the substrate's Fermi level. Characteristic STM topographic images taken concurrently with the dI/dV maps show slightly different features reflecting the fact that at these polarities, occupied and unoccupied states with various symmetries are captured during the imaging process. That is clearly visualized in the corresponding dI/dV maps: at -0.750 V the molecule's differential conductance map is made of four peripheral lobes, while the dI/dV map taken at 1.650 V shows six outer lobes. In both dI/dV maps intramolecular features are absent.

The ESQC calculated dI/dV STM images were calculated at the energies corresponding to the two resonances in the tunneling electron transmission of the tunnel junction, corresponding to electronic states nearest to the substrate's Fermi level. The calculations include all the elements of a tunneling junction made of the gold substrate, metal tip and one single molecule of **1a** trapped within the junction. These two resonances correspond respectively to the Highest Occupied and Lowest Unoccupied Molecular Orbitals, i.e. HOMO AND LUMO, in this mono-electronic approximation. The calculated and experimental images show identical nodal features enabling the molecule's identification indicating that effectively the synthesized and deposited molecules are tetrabenzocircumpyrene **1a**. Therefore, the experimental dI/dV maps and the resonances they arise from correspond to **1a** HOMO and LUMO.

6. Structures Optimized by DFT Calculations

Calculations were carried out with DFT using the B3LYP functional as implemented in Gaussian 09.[3] The 6-31G(d) basis set[4] was used for all atoms. Frequency calculations were performed to characterize the stationary points as minima.

*6.1. Tetrabenzocircumpyrene (**1a**)*

Element	X	Y	Z
C	4.95889600	0.73232400	0.00042800
C	3.71771600	1.43765100	0.00020900
C	2.47052600	0.71644700	0.00009800
C	2.47052600	-0.71645000	0.00007900
C	3.71771600	-1.43765400	0.00023000
C	4.95889600	-0.73232600	0.00051300
C	1.24313800	1.42209300	-0.00001200
C	1.24313700	-1.42209500	-0.00003600
C	-0.00003800	-0.71222300	-0.00002600
C	-0.00003800	0.71222300	-0.00002300
C	-1.24314900	1.42210500	-0.00006900
C	-2.47050500	0.71641500	0.00002300
C	-2.47050600	-0.71641400	0.00006900
C	-1.24315000	-1.42210400	-0.00002200
C	-3.71777300	-1.43759800	0.00031100

[3] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, K. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian 09, revision 02; Gaussian, Inc.: Wallingford, CT, 2009.

[4] (a) M. M. Francl, W. J. Pietro, W. J. Hehre, J. S. Binkley, M. S. Gordon, D. J. Defrees, J. A. Pople, *J. Chem. Phys.* **1982**, *77*, 3654–3665. (b) W. J. Hehre, R. Ditchfield, J. A. Pople, *J. Chem. Phys.* **1972**, *56*, 2257–2261.

C	-4.95900100	-0.73236800	0.00059100
C	-3.71777300	1.43760000	0.00000000
C	-4.95900100	0.73237100	0.00017800
C	6.15332000	-1.46021700	0.00086600
C	6.15147200	-2.85180800	0.00093500
H	7.09329800	-3.39349600	0.00128300
C	4.95465100	-3.54495200	0.00057400
H	4.98522000	-4.62699000	0.00070700
C	3.72124500	-2.86546900	0.00015800
C	6.15332100	1.46021500	0.00053600
C	6.15147200	2.85180600	0.00047100
H	7.09329800	3.39349500	0.00057800
C	4.95465100	3.54495000	0.00027000
H	4.98521800	4.62698800	0.00025400
C	3.72124600	2.86546600	0.00011200
C	-3.72119100	-2.86537300	0.00039200
C	-4.95444300	-3.54508900	0.00106200
H	-4.98475100	-4.62714100	0.00134700
C	-6.15134500	-2.85209700	0.00154400
H	-7.09309300	-3.39391600	0.00215100
C	-3.72119000	2.86537500	-0.00024900
C	-4.95444100	3.54509200	-0.00039000
H	-4.98475000	4.62714400	-0.00056000
C	-6.15333300	1.46050500	-0.00008400
C	-6.15134400	2.85210100	-0.00035300
H	-7.09309200	3.39392000	-0.00053900
H	7.10837300	-0.94994000	0.00113900
H	7.10837300	0.94993800	0.00066700
H	-7.10843800	0.95037300	-0.00014800
C	2.41911300	5.00470000	-0.00039100
C	1.23356300	5.68647600	-0.00057200

C	-0.00006100	4.99274900	-0.00050300
C	-0.00000400	3.56982700	-0.00028700
C	1.24326900	2.86285200	-0.00013000
C	2.46077300	3.58363500	-0.00013600
H	-1.22481500	6.77363400	-0.00084900
H	3.33956600	5.57455000	-0.00047800
C	-1.23368900	5.68656600	-0.00066700
C	-1.24324400	2.86289300	-0.00022500
C	-2.46075200	3.58355500	-0.00035900
C	-2.41916200	5.00454100	-0.00059600
H	-3.33965600	5.57440600	-0.00073200
C	2.46077100	-3.58363800	-0.00030100
C	1.24326700	-2.86285400	-0.00024900
C	-0.00000700	-3.56982700	-0.00044300
C	-0.00006600	-4.99275000	-0.00085200
C	1.23355700	-5.68647800	-0.00111200
C	2.41910800	-5.00470300	-0.00083000
C	-1.24324600	-2.86289300	-0.00019600
C	-1.23369400	-5.68656500	-0.00105700
H	3.33956000	-5.57455500	-0.00110100
C	-2.41916700	-5.00453900	-0.00070400
C	-2.46075500	-3.58355300	-0.00016100
H	-1.22482100	-6.77363300	-0.00149900
H	-3.33966100	-5.57440300	-0.00095600
C	-6.15333400	-1.46050200	0.00127100
H	-7.10843900	-0.95036900	0.00170500
H	1.22446700	6.77362500	-0.00077400
H	1.22446000	-6.77362700	-0.00153400

6.2. Hexabenzocoronene (HBC)

Element	X	Y	Z
C	5.13582800	0.06366500	-0.00017700
C	3.77460800	0.40259300	-0.00006100
C	3.34263000	1.79857000	-0.00002500
C	4.27483400	2.84678100	-0.00013200
C	2.80014000	-0.63674000	0.00004900
C	1.95157600	2.10631200	0.00012900
C	0.96751700	1.04430600	0.00010200
C	1.38831200	-0.31571300	0.00007900
C	0.42062100	-1.36016700	0.00007100
C	-0.96760100	-1.04445100	-0.00005500
C	-1.38846300	0.31578100	-0.00009800
C	-0.42083900	1.36009700	0.00003800
C	-2.80028200	0.63685500	-0.00043000
C	-3.77477200	-0.40262500	-0.00080700
C	-1.95162800	-2.10648800	-0.00009500
C	-3.34278400	-1.79863600	-0.00036400
C	3.86545600	4.17153700	-0.00010300
C	5.54609400	-1.26083000	-0.00019600
C	-3.22957200	1.99539500	-0.00053500
C	-4.60377800	2.27798200	-0.00138200
H	-4.95456800	3.30206100	-0.00173800
C	-5.54632100	1.26079500	-0.00196700
H	-6.60579100	1.50144900	-0.00270400
C	-1.53865200	-3.47008200	0.00016200
C	-2.51341900	-4.47906200	0.00024400
H	-2.22509400	-5.52248900	0.00042900
C	-4.27503700	-2.84664400	-0.00017100

C	-3.86566800	-4.17163000	0.00012600
H	-4.60423200	-4.96846600	0.00026900
H	-5.33723300	-2.63777100	-0.00017700
C	2.62333400	-4.41539500	0.00051200
C	2.23616500	-3.06726800	0.00026900
C	3.22954500	-1.99518200	0.00008800
C	4.60347700	-2.27789300	-0.00005000
H	2.00239000	-6.47088800	0.00085900
C	1.68116100	-5.43300800	0.00066000
C	0.84865100	-2.74323900	0.00020200
C	-0.11348100	-3.79417700	0.00031800
C	0.32897400	-5.12541400	0.00055600
H	-0.38230700	-5.94147600	0.00067400
C	2.51321400	4.47882100	0.00015100
C	1.53874900	3.46988900	0.00029100
C	0.11360300	3.79407300	0.00055900
C	-0.32829700	5.12529500	0.00115000
C	-0.84868800	2.74322600	0.00022300
C	-1.68049700	5.43321200	0.00135200
C	-2.62284200	4.41587200	0.00084100
C	-2.23612000	3.06741900	0.00017800
H	-2.00120400	6.47125300	0.00191600
H	-3.67068300	4.68738100	0.00109000
C	-5.13592400	-0.06388800	-0.00162800
H	-5.89474000	-0.83598600	-0.00214100
H	3.67128300	-4.68672200	0.00061200
H	4.95437700	-3.30197600	-0.00007500
H	6.60542300	-1.50188800	-0.00031300
H	5.89464700	0.83570100	-0.00027000
H	5.33699600	2.63796300	-0.00030500
H	4.60366800	4.96862900	-0.00025700

H	2.22497100	5.52229800	0.00014500
H	0.38315500	5.94125400	0.00156000