Electronic Supplementary Information (ESI)

Preparation of a Large-sized Highly Flexible Carbon Nanohoop

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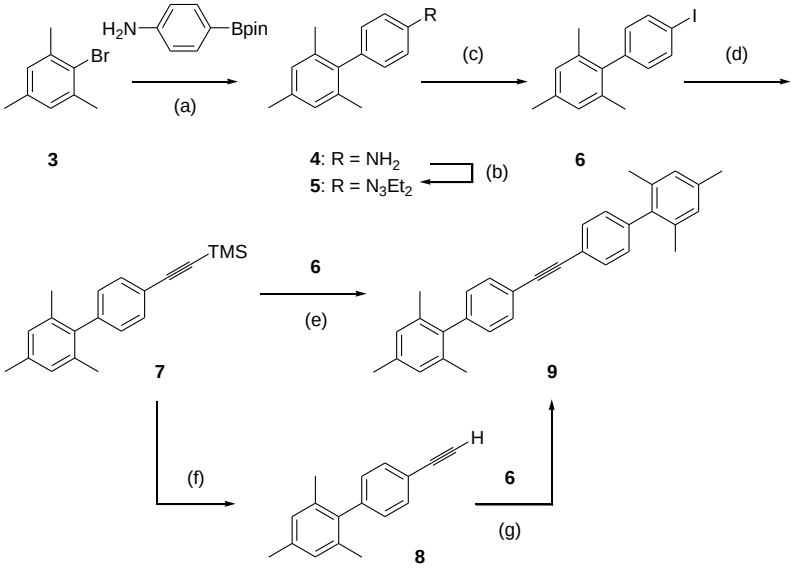
Contents

(1) Sample Preparation

Synthesis of Bis(4-mesitylphenyl)acetylene (9):

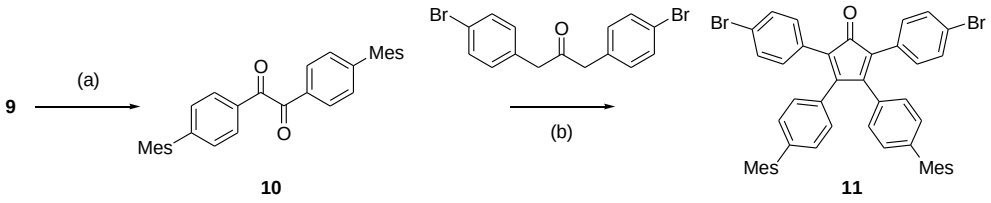
Mesityl bromide (**3**) was reacted with 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)aniline by Pd-catalyzed Suzuki–Miyaura cross-coupling reaction to yield 4-mesitylaniline (**4**) in quantitative yield. The amino group in the product **4** was transformed to iodo function to serve for the Sonogashira cross-coupling reaction via triazene **5** in 85% yield in the two-step protocol. Thus, bis(4-mesitylphenyl)acetylene (**9**) was prepared by the sila-Sonogashira cross-coupling reaction of the iodide **6** with (4-mesitylphenylethynyl)trimethylsilane (**7**), which was prepared by the Sonogashira cross-coupling reaction of **6** with trimethylsilylacetylene, in the presence of tetrabutylammonium fluoride (TBAF) in 89% yield (Scheme S-1). Under these conditions homocoupling products as an undesirable by-product were not detected even in the crude product mixture by the NMR analysis. Bis(4-mesitylphenyl)acetylene (**9**) was also obtained by the cross-coupling reaction of **6** with 1-ethynyl-4-mesitylbenzene prepared by the desilylation of **7** under the Sonogashira cross-coupling conditions in 76% yield.



Scheme S-1. An efficient preparation of bis(mesitylphenyl)acetylene (**9**). Reagents and conditions: (a) $Pd(PPh_3)_4$, 2M K_2CO_3, 1,4-dioxane, reflux, 17 h, quant.; (b) 1) conc. HCl, $NaNO_2$ aq., THF, −20 °C, 10 min, 2) Et_2NH, K_2CO_3, THF, water, −20 °C, 10 min, 89%; (c) CH_3I, 120 ºC [in a sealed tube], 19 h, 96%; (d) trimethylsilylacetylene, $Pd(PPh_3)_4$, CuI, Et_3N, THF, 80 °C [in a sealed tube], 3 h, 99%; (e) $Pd(PPh_3)_4$, CuI, Et_3N, THF, TBAF, reflux, 2 h, 89%; (f) THF, methanol, K_2CO_3, RT, 2 h, quant.; (g) $Pd(PPh_3)_4$, CuI, Et_3N, THF, reflux, 2 h, 76%.

Synthesis of Cyclopentadienone Derivative 11:

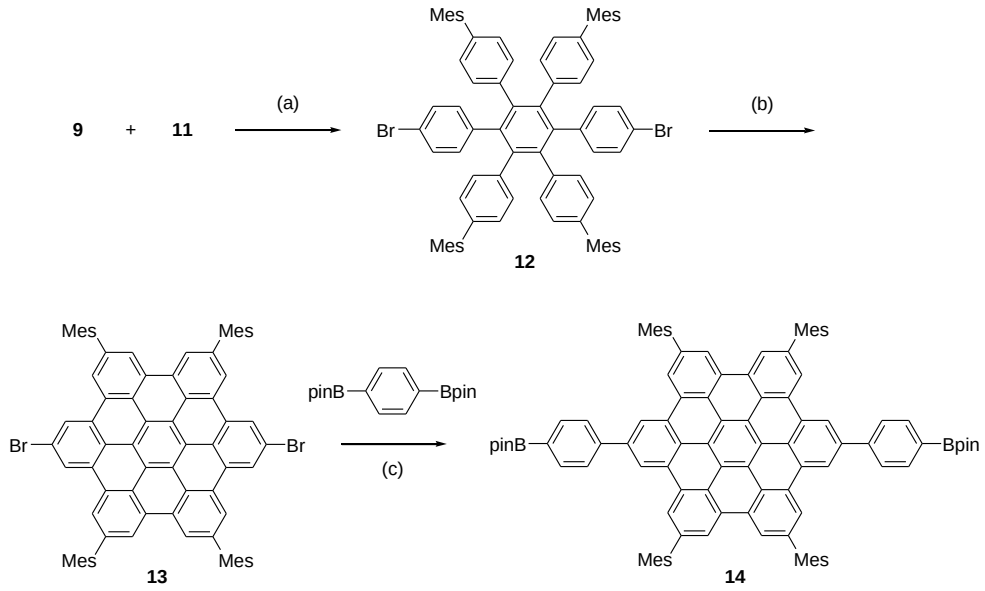
Cyclopentadienone derivative **11** was prepared by the Knoevenagel condensation of 1,3-bis(4-bromophenyl)acetone with 1,2-bis(4-mesitylphenyl)ethane-1,2-dione (**10**), which was prepared by the iodine oxidation of the tolan derivative **9** in DMSO, in the presence of tetrabutylammonium hydroxide (TBAH) in *t*-BuOH in 95% yield (Scheme S-2). The Knoevenagel condensation was much improved by using TBAH in *t*-BuOH.



Scheme S-2. Preparation of cyclopentadienone derivative **11**. Reagents and conditions: (a) I_2, DMSO, 155 °C, 15 h, 84%; (b) TBAH, *t*-BuOH, 80 °C, 1 h, 95%.

Synthesis of 1,4-Bis(4-bromophenyl)-2,3,5,6-tetrakis(4-mesitylphenyl)benzene (12):

Diles–Alder reaction of the tolan derivative **9** with the cyclopentadienone derivative **11** was accomplished by heating in diphenyl ether at 200–220 °C to afford hexaphenylbenzene derivative **12** in 91% yield (Scheme S-3). The yield of the product depended on the loadings of the cyclopentadienone derivative **11** and the reaction period (Table S-1). High yield was obtained by five-fold excess of cyclopentadienone derivative **11**. Prolonged heating showed a trend to decrease the yield due to the decomposition of the product under the reaction conditions. The highest yield was obtained by the reaction for 7 h with five-fold excess of the cyclopentadienone derivative **11**.



Scheme S-3. Preparation of HBC derivative **14**. Reagents and conditions: (a) diphenyl ether, 200–220 °C, 7 h, 91%; (b) DDQ, TfOH, CH_2Cl_2, RT, 1 h, 98%; (c) $Pd(PPh_3)_4$, Ag_2CO_3, 1,4-dioxane, 90 °C, 4 h, 46%.

Table S-1. Optimization of the Diels–Alder Reaction of **9** with **11**

Entry	Compound **11**	Time / h	Yield / %
1	2.7 eq.	6	67
2	2.7 eq.	7	79
3	2.7 eq.	8	77
4	2.7 eq.	9	73
5	1.3 eq.	10	77
6	5.0 eq.	7	91

Synthesis of 2,11-Dibromo-5,8,14,17-tetramesitylhexabenzo[*bc*,*ef*,*hi*,*kl*,*no*,*qr*]coronene (13):
Hexaphenylbenzene derivative **12** was effectively transformed into HBC derivative **13** by the cyclodehydrogenation reaction with 2,3-dichloro-5,6-dicyano-*p*-benzoquinone (DDQ) in the presence of trifluoromethanesulfonic acid in dry dichloromethane (Table S-2). By using $FeCl_3$ in nitromethane as an oxidizing reagent caused a contamination of the small amount of chlorinated product even if the continuous Ar bubbling throughout the reaction to prevent the chlorination reaction. Thus, the HBC derivative **13** was obtained in high yield in pure form by the reaction at room temperature with DDQ in the presence of trifluoromethanesulfonic acid in dry dichloromethane.

Table S-2. Optimization of the Cyclodehydrogenation Reaction of **12**

Entry	Temperature / °C	Oxidant / eq.	Yield / %
1	R.T.	$FeCl_3$ / 12×3.1	15
2	R.T.	$FeCl_3$ / 12×5.3	53
3	30	$FeCl_3$ / 12×5.8	89
4	R.T.	$FeCl_3$ / 12×7.8	68
5	0	DDQ / 12×5.8	33
6	R.T.	DDQ / 12×5.8	98

Synthesis of 2,11-Bis(4-borylphenyl)-5,8,14,17-tetramesitylhexabenzo[*bc*,*ef*,*hi*,*kl*,*no*,*qr*]-coronene (14):

The two pinacolatoboryl groups, which were required to the Pt-mediated cycloorigomerization, were introduced to the HBC derivative **13** by selective Suzuki–Miyaura cross-coupling reaction with 1,4-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzene. The reaction was optimized by solvent, temperature, and reaction period. The results on the examination were summarized in Table S-3. When the reaction was carried out according to those of the reported conditions,[S-1] the yield of the desired product **14** was not improved by changing the reaction period and temperature (entries 1–3). Changing the base or Pd catalyst did not afford satisfactory results (entries 4 and 5). Elevating the reaction temperature by changing the solvent as toluene the reaction was completed in shorter period, but the yield was not increase under these conditions (entries 6–8). The yield was improved by setting the reaction temperature in 1,4-dioxane. By changing the solvent into 1,4-dioxane the highest yield was obtained in 46% yield at 90 °C for 4 h (entry 10). The reaction under both higher and lower temperatures in the same solvent decrease the product yield (entries 9 and 11).

Table S-3. Optimization of the Selective Suzuki–Miyaura Cross-coupling Reaction of **13** with 1,4-Bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzene

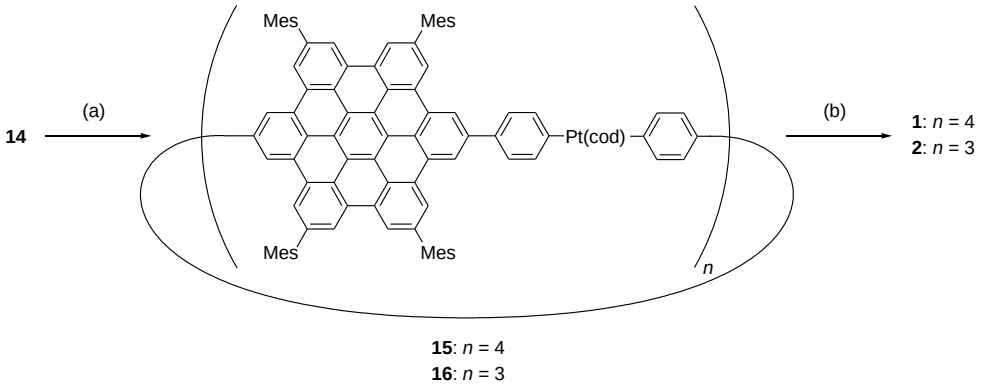
Entry	Solvent	Catalyst	Base	Temperature / °C	Time / h	Yield / %
1	THF	$Pd(PPh_3)_4$	Ag_2CO_3	50	24	24
2	THF	$Pd(PPh_3)_4$	Ag_2CO_3	65	12	26
3	THF	$Pd(PPh_3)_4$	Ag_2CO_3	65	24	32
4	THF	$Pd(PPh_3)_4$	CH_3COONa	65	24	—
5	THF	$Pd[P(t\text{-}Bu)_3]_2$	Ag_2CO_3	65	24	—
6	toluene	$Pd(PPh_3)_4$	Ag_2CO_3	80	3	20
7	toluene	$Pd(PPh_3)_4$	Ag_2CO_3	80	6	23
8	toluene	$Pd(PPh_3)_4$	Ag_2CO_3	80	12	11
9	1,4-dioxane	$Pd(PPh_3)_4$	Ag_2CO_3	65	24	17
10	1,4-dioxane	$Pd(PPh_3)_4$	Ag_2CO_3	90	4	46
11	1,4-dioxane	$Pd(PPh_3)_4$	Ag_2CO_3	120	3	37

Synthesis of [4]Cyclo(2,5,11,14-tetramesityl-8,17-diphenylhexabenzo[*bc*,*ef*,*hi*,*kl*,*no*,*qr*]-coronene) (1):

The preparation of **1** was examined by the reductive elimination of the square-shaped tetranuclear planer Pt complex **15** under the several reaction conditions. The total synthetic procedure by reductive elimination of the Pt metal via square-shaped tetranuclear Pt-complex **15** is illustrated in Scheme S-4. Table S-4 summarized the reaction conditions examined for the optimization. Without isolating the square-shaped tetranuclear Pt-complex **15**, final nanohoop **1** was obtained after the reductive elimination step in toluene at 100 °C in 10% yield by the two-step reaction. The yield of the product was slightly improved by changing the reaction conditions from in toluene at 100 °C to in *o*-DCB at 180 °C (18%).

The low yield of the product **1** was attributed to the formation of linear oligomers from dimer to pentamer or much higher oligomeric products, in which the terminal 4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl groups were replaced by hydrogen atoms and a very small amount of cyclic trimer **2** under the reaction conditions characterized by MALDI-TOF MS measurements. Figure S-1 represents the gel permeation chromatography (GPC) analysis of the crude mixture of the products. Peak assignment of the products in the GPC analysis was represented on the second cycles, which was characterized by MALDI-TOF MS measurements. The cyclic tetramer **1** and trimer **2** was eluted as a shoulder peak of the linear trimer and dimer, respectively, on the GPC. Most of the by-products were removed by the column chromatography on silica gel with

hexane/chloroform (1:3). The pure cyclic products **1** and **2** was obtained by the repeated column chromatography on silica gel with hexane/toluene/CS_2 (10:10:1) and GPC with chloroform. Thus, we have obtained the cyclic tetramer **1** in 18% yield, along with a very small amount of cyclic trimer **2** in pure form.



Scheme S-4. Preparation of a large sized highly flexible carbon nanohoop **1**. Reagents and conditions: (a) $PtCl_2$(cod), CsF, THF, reflux, 24 h; (b) PPh_3, *o*-dichlorobenzene, reflux, 24 h, 18% (2 steps).

Table S-4. Reductive elimination of the square-shaped tetranuclear Pt-complex **13**

Entry	solvent	Temperature / °C	Yield / %
1	toluene	100	10
2	*o*-DCB	180	18

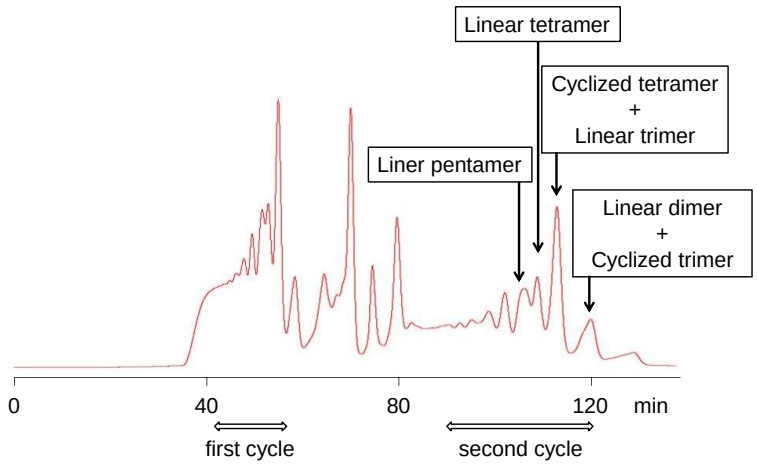
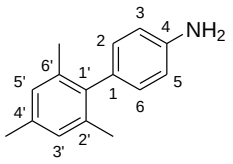


Figure S-1. GPC analysis of the Pt-mediated macrocyclization products (eluent: $CHCl_3$).

(2) Experimental Details for the Reported Compounds

General: Melting points were determined on a Yanagimoto micro melting point apparatus MP-S3 and are uncorrected. Mass spectra were obtained with a Bruker Daltonics autoflex III TOF/TOF instrument under MALDI-TOF conditions. IR and UV spectra were measured on a Varian 670-IR and a JASCO V-670 spectrophotometers, respectively. Fluorescence spectra were collected with a Hitachi F-4500 fluorescence spectrophotometer using an excitation wavelength equal to the absorption maximum. Absorption and fluorescence spectra were performed in a spectrophotometric cell with a 1 cm path length. ^{1}H NMR (^{13}C NMR) spectra were recorded on a JEOL ECA500 or a JEOL ECZ500R spectrometer at 500 MHz (125 MHz). ^{1}H NMR chemical shifts in $CDCl_3$ are reported in parts per million (ppm) downfield from tetramethylsilane. ^{13}C NMR chemical shifts in $CDCl_3$ are referred by the solvent signals as 77.0 ppm. ^{1}H NMR (^{13}C NMR) chemical shifts in $(CDCl_2)_2$ are referred by the solvent signals as 5.90 ppm and 74.2 ppm, respectively. The peak assignment of ^{1}H and ^{13}C NMR spectra reported was accomplished by HH COSY, DEPT, HMQC, and HMBC experiments. The numbering scheme of the products is represented on the structures. The voltammetry measurements were carried out in *o*-dichlorobenzene containing *n*-Bu_4NClO_4 (0.1 M) as a supporting electrolyte utilizing Pt working and auxiliary electrodes, and a reference electrode formed from $Ag/AgNO_3$ (0.01 M) in acetonitrile containing *n*-Bu_4NClO_4 (0.1 M) at the scan rate of 100 mV s^{-1}. The internal reference Fc/Fc^{+} discharges at +0.26 V under these conditions. Elemental analyses were performed at the Instrumental Analysis Center of Hirosaki University.

4-Mesitylaniline (4):[S-2]



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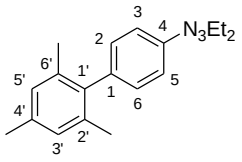
To a degassed solution of mesityl bromide (**3**) (4.10 g, 20.6 mmol), 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)aniline (4.97 g, 22.7 mmol), and 2M K_2CO_3 solution (31 mL) in 1,4-dioxane (35 mL) was added $Pd(PPh_3)_4$ (241 mg, 0.209 mmol). The resulting mixture was refluxed for 17 h under an Ar atmosphere. The reaction mixture was poured into brine and extracted with toluene. The organic layer was washed with brine, dried over $MgSO_4$, and concentrated under reduced pressure. The residue was purified by column chromatography on Al_2O_3 with hexane/dichloromethane (1:3) to afford 4-mesitylaniline (**4**) (4.33 g, 100%). Colorless crystals; mp 124.4–125.3 °C (H_2O/methanol); ^{1}H NMR (500 MHz, $CDCl_3$): δ_H = 6.923 (s, 2H, 3',5'-H), 6.915 (d, 2H, *J* = 8.3 Hz, 2,6-H), 6.74 (d, 2H, *J* = 8.3 Hz, 3,5-H), 3.67 (br s, 2H, 4-NH_2), 2.32 (s, 3H, 4'-Me), 2.02 (s, 6H, 2',6'-Me); ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 144.7 (C-4), 139.0 (C-1'), 136.5 (C-2',6'), 136.1 (C-4'), 131.2 (C-1), 130.1 (C-2,6), 127.9 (C-3',5'), 115.1 (C-3,5), 21.0 (4'-Me), 20.8 (2',6'-Me); HRMS (dithranol + CF_3CO_2Ag): calcd for $C_{15}H_{17}N + Ag^+$ 318.0406, found 318.0381.

4-Mesitylphenyl-3,3'-diethyltriazene (5):



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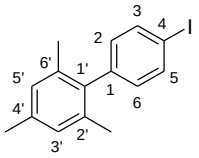
To a solution of 4-mesitylaniline (**4**) (4.19 g, 19.8 mmol) in tetrahydrofuran (100 mL) was added hydrochloric acid (6.4 mL, 77 mmol) and a solution of sodium nitrite (2.07 g, 30.0 mmol) in water (5 mL), successively, at −20 °C. The mixture was stirred at the same temperature for 10 min. The resulting mixture was added dropwise at −20 °C to a mixture of diethylamine (20.5 mL, 198 mmol) and potassium carbonate (13.7 g, 99.1 mmol) in tetrahydrofuran (30 mL) and water (20 mL) and stirred at −20 °C for 10 min. The reaction mixture was poured into water and extracted with dichloromethane. The organic layer was washed with water, dried over $MgSO_4$, and concentrated under reduced pressure. The residue was purified by column chromatography on Al_2O_3 with dichloromethane/hexane (1:20 to 1:5) to afford 4-mesitylphenyl-3,3'-diethyltriazene (**5**) (5.19 g, 89%). Yellow oil; IR (neat): ν_{max} = 2973 (s), 2933 (s), 2871 (m), 1612 (w), 1569 (w), 1507 (m), 1467 (s), 1452 (s), 1435 (s), 1396 (s), 1372 (s), 1349 (s), 1303 (m), 1236 (s), 1199 (s), 1160 (m), 1108 (s), 1094 (s), 1028 (w), 1004 (m), 949 (w), 891 (w), 843 (s), 811 (w), 765 (w), 747 (w), 591 (m), 578 (w), 558 (m), 527 (w), 507 (w) cm^{-1}; UV–vis (CH_2Cl_2): λ_{max} = 229 (log ε 4.12), 238 sh (3.96), 285 sh (4.17), 291 (4.20), 299 (4.19), 320 (4.21) nm; ^1H NMR (500 MHz, $CDCl_3$): δ_H = 7.47 (d, 2H, *J* = 8.4 Hz, 3,5-H), 7.10 (d, 2H, *J* = 8.4 Hz, 2,6-H), 6.94 (s, 2H, 3',5'-H), 3.78 (q, 4H, *J* = 7.1 Hz, 4-N_3Et_2), 2.33 (s, 3H, 4'-Me), 2.03 (s, 6H, 2',6'-Me), 1.29 (t, 6H, *J* = 7.1 Hz, 4-N_3Et_2); ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 149.7 (C-4), 139.0 (C-1'), 137.8 (C-1), 136.3 (C-4'), 136.2 (C-2',6'), 129.8 (C-2,6), 128.0 (C-3',5'), 120.3 (C-3,5), 21.0 (4'-Me), 20.8 (2',6'-Me); HRMS (dithranol): calcd for $C_{19}H_{25}N_3 + H^+$ 296.2121, found 296.2105.

1-Iodo-4-mesitylbenzene (6):[S-3]



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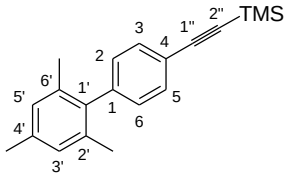
A solution of 4-mesitylphenyl-3,3'-diethyltriazene (**5**) (4.67 g, 15.8 mmol) in iodomethane (21 mL) was stirred at 120 °C for 19 h in a sealed tube. The reaction mixture was poured into 30% $NaHSO_3$ aq. and extracted with dichloromethane. The organic layer was washed with 30% $NaHSO_3$ aq., dried over $MgSO_4$, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel with dichloromethane/hexane (1:4) to afford 1-iodo-4-mesitylbenzene (**6**) (4.90 g, 96%). Colorless crystals; mp 86.2–86.9 °C (methanol); ^{1}H NMR (500 MHz, $CDCl_3$) δ_H = 7.74 (d, 2H, *J* = 8.3 Hz, 3,5-H), 6.93 (s, 2H, 3',5'-H), 6.89 (d, 2H, *J* = 8.3 Hz, 2,6-H), 2.32 (s, 3H, 4'-Me), 1.99 (s, 6H, 2',6'-Me); ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 140.6 (C-1), 137.7 (C-1'), 137.5 (C-3,5), 136.9 (C-4'), 135.7 (C-2',6'), 131.4 (C-2,6), 128.1 (C-3',5'), 92.1 (C-4), 21.0 (4'-Me), 20.7 (2',6'-Me). This compound could not be ionized by the MALDI-TOF conditions even though the measurements was carried out with silver trifluoroacetate as an auxiliary agent.

(4-Mesitylphenylethynyl)trimethylsilane (7):



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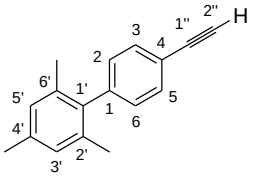
To a degassed solution of 1-iodo-4-mesitylbenzene (**6**) (2.55 g, 7.91 mmol), CuI (29.5 mg, 0.155 mmol), $Pd(PPh_3)_4$ (91.2 mg, 0.0789 mmol), and triethylamine (10 mL) in tetrahydrofuran (15 mL) was added trimethylsilylacethylene (1.7 mL, 12 mmol). The resulting mixture was stirred at 80 °C for 3 h under an Ar atmosphere in a sealed tube. The reaction mixture was poured into a 5% NH_4Cl solution and extracted with dichloromethane. The organic layer was washed with a 5% NH_4Cl solution, dried over $MgSO_4$, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel with hexane and on silica gel with dichloromethane/hexane (1:20) to afford (4-mesitylphenylethynyl)trimethylsilane (**7**) (2.29 g, 99%). Colorless crystals; mp 99.3–100.4 °C (methanol); IR (KBr disk): ν_{max} = 3089 (m), 3027 (m), 3000 (m), 2961 (s), 2919 (m), 2856 (m), 2159 (s, C≡C), 1612 (m), 1572 (w), 1508 (m), 1476 (m), 1448 (m), 1412 (w), 1400 (m), 1374 (m), 1324 (w), 1251 (s), 1221 (m), 1101 (m), 1029 (w), 1012 (w), 1010 (m), 950 (w), 864 (s), 846 (s), 838 (s), 758 (s), 693 (m), 627 (m), 587 (m), 579 (w), 549 (w), 532 (m) cm^{-1}; UV–vis (CH_2Cl_2): λ_{max} = 223 (log ε 3.96), 244 sh (4.05), 254 (4.23), 265 (4.27), 278 sh (3.93) nm; ^1H NMR (500 MHz, $CDCl_3$): δ_H = 7.52 (d, 2H, *J* = 8.3 Hz, 3,5-H), 7.08 (d, 2H, *J* = 8.3 Hz, 2,6-H), 6.93 (s, 2H, 3',5'-H), 2.32 (s, 3H, 4'-Me), 1.97 (s, 6H, 2',6'-Me), 0.27 (s, 9H, TMS); ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 141.6 (C-1), 138.3 (C-1'), 136.8 (C-4'), 135.7 (C-2',6'), 132.1 (C-3,5), 129.3 (C-2,6), 128.1 (C-3',5'), 121.2 (C-4), 105.1 (C-1''), 94.0 (C-2''), 21.0 (4'-Me), 20.6 (2',6'-Me), −0.02 (TMS); HRMS (dithranol + CF_3CO_2Ag): calcd for $C_{20}H_{24}Si + 2Ag^+ - TMS^+$ 432.9270, found 432.9280. Anal. Calcd for $C_{20}H_{24}Si$ (292.4901): C, 82.13; H, 8.27. Found: C, 81.96; H, 8.46.

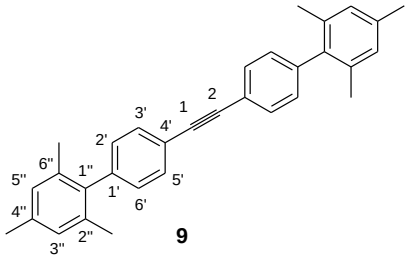
1-Ethynyl-4-mesitylbenzene (8):



8

To a solution of (4-mesitylphenylethynyl)trimethylsilane (**7**) (760 mg, 2.60 mmol) in tetrahydrofuran (10 mL) and methanol (10 mL) was added potassium carbonate (1.14 g, 8.25 mmol). The resulting mixture was stirred at room temperature for 2 h under an Ar atmosphere. The reaction mixture was poured into water and extracted with diethyl ether. The organic layer was subsequently washed with water and brine, dried over $MgSO_4$, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel with dichloromethane/hexane (1:6) to afford 1-ethynyl-4-mesitylbenzene (**8**) (572 mg, 100%). Pale yellow crystals; mp 35.3–36.0 °C (methanol); IR (KBr disk): ν_{max} = 3306 (s, C≡C-H), 3283 (s, C≡C-H), 3124 (w), 3028 (w), 2970 (m), 2942 (m), 2919 (s), 2856 (m), 2735 (w), 2107 (w, C≡C), 1927 (w), 1731 (w), 1690 (w), 1680 (w), 1612 (m), 1571 (w), 1513 (m), 1477 (s), 1464 (m), 1440 (m), 1395 (m), 1378 (m), 1342 (w), 1250 (m), 1215 (w), 1200 (w), 1181 (w), 1170 (w), 1150 (w), 1101 (m), 1031 (w), 1004 (m), 959 (w), 952 (w), 852 (m), 840 (s), 746 (w), 672 (m), 631 (m), 588 (m), 581 (w), 529 (w), 517 (w) cm^{-1}; UV–vis (CH_2Cl_2): λ_{max} = 233 sh (log ε 4.21), 242 (4.26), 251 (4.27), 278 sh (3.64) nm; ^1H NMR (500 MHz, $CDCl_3$): δ_H = 7.55 (d, 2H, *J* = 8.2 Hz, 3,5-H), 7.11 (d, 2H, *J* = 8.2 Hz, 2,6-H), 6.94 (s, 2H, 3',5'-H), 3.09 (s, 1H, 4-C≡CH), 2.33 (s, 3H, 4'-Me), 1.99 (s, 6H, 2',6'-Me); ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 141.9 (C-1), 138.2 (C-1'), 136.9 (C-4'), 135.7 (C-2',6'), 132.2 (C-3,5), 129.4 (C-2,6), 128.1 (C-3',5'), 120.3 (C-4), 83.7 (C-1''), 77.0 (C-2''), 21.0 (4'-Me), 20.6 (2',6'-Me); HRMS (dithranol + CF_3CO_2Ag): calcd for $C_{17}H_{16} - H^+ + 2Ag^+$ 432.9270, found 432.9253. Anal. Calcd for $C_{17}H_{16}$ (220.3089): C, 92.68; H, 7.32. Found: C, 92.33; H, 7.11.

Bis(4-mesitylphenyl)acetylene (9):[S-4]



9

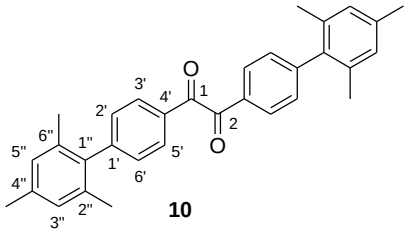
Reaction of 6 with 7: To a degassed solution of 1-iodo-4-mesitylbenzene (**6**) (3.73 g, 11.6 mmol), CuI (50.3 mg, 0.264 mmol), $Pd(PPh_3)_4$ (141 mg, 0.122 mmol), and triethylamine (25 mL), and TBAF (1 M in tetrahydrofuran, 17 mL, 17 mmol) in tetrahydrofuran (50 mL) was added dropwise at the refluxing temperature for 2 h (4-mesitylphenylethynyl)trimethylsilane (**7**) (3.43 g, 11.7 mmol) in tetrahydrofuran (20 mL) divided into five portions. The resulting mixture was stirred at the same temperature for 30 min under an Ar atmosphere. The reaction mixture was poured into a 5% NH_4Cl solution and extracted with dichloromethane. The organic layer was washed with a 5% NH_4Cl solution, dried over $MgSO_4$, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel with hot hexane/toluene (1:2) and recrystallization from hexane to afford **9** (4.28 g, 89%).

Reaction of 6 with 8: To a degassed solution of 1-iodo-4-mesitylbenzene (**6**) (152 mg, 0.472 mmol), CuI (8.9 mg, 0.047 mmol), $Pd(PPh_3)_4$ (28.2 mg, 0.0244 mmol), and triethylamine (5 mL) in tetrahydrofuran (10 mL) was added dropwise at the refluxing temperature for 1.5 h 1-ethynyl-4-mesitylbenzene (**8**) (108 mg, 0.490 mmol) in tetrahydrofuran (5 mL) divided into five portions. The resulting mixture was stirred at the same temperature for 30 min under an Ar atmosphere. The reaction mixture was poured into a 5% NH_4Cl solution and extracted with dichloromethane. The organic layer was washed with a 5% NH_4Cl solution, dried over $MgSO_4$, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel with dichloromethane/hexane (1:1) and GPC with chloroform to afford **9** (148 mg, 76%).

9: Colorless crystals (lit. beige solid); mp 250.2–250.9 °C (ethanol) (lit. mp 246 °C); IR (KBr disk): ν_{max} = 3071 (w), 3025 (m), 2980 (m), 2958 (m), 2914 (s), 2855 (m), 1612 (m), 1570 (w), 1518 (s), 1477 (s), 1442 (m), 1396 (m), 1377 (m), 1309 (w), 1270 (w), 1177 (w), 1100 (m), 1039 (m), 1004 (s), 947 (w), 882 (w), 850 (s), 837 (s), 746 (w), 587 (m), 570 (m), 523 (w), 408 (w) cm^{-1}; UV–vis (CH_2Cl_2) λ_{max} = 229 (log ε 4.40), 278 (4.47), 292 (4.59), 300 (4.56), 308 (4.52) nm; ^1H NMR (500 MHz, $CDCl_3$): δ_H = 7.60 (d, 4H, *J* = 8.3 Hz, 3',5'-H), 7.14 (d, 4H, *J* = 8.3, 2',6'-H), 6.95 (s, 4H, 3'',5''-H), 2.34 (s, 6H, 4''-Me), 2.02 (s, 12H, 2'',6''-Me); ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 141.3 (C-1'), 138.4 (C-1''), 136.8 (C-4''), 135.8 (C-2'',6''), 131.7 (C-3',5'), 129.5 (C-2',6'), 128.1 (C-3'',5''), 121.5 (s), 89.3 (C-1,2), 21.0 (4''-Me), 20.7 (2'',6''-Me); HRMS (dithranol +

CF_3CO_2Ag): calcd for $C_{32}H_{30}$ + Ag^+ 521.1393, found 521.1381. Anal. Calcd for $C_{32}H_{30}$ (414.5806): C, 92.71; H, 7.29. Found: C, 92.33; H, 7.45.

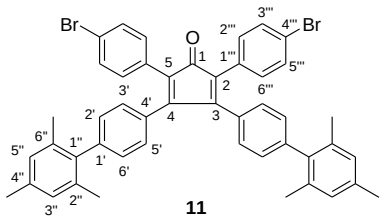
1,2-Bis(4-mesitylphenyl)ethane-1,2-dione (10):[S-4]



10

A solution of bis(4-mesitylphenyl)acetylene (**9**) (1.55 g, 3.74 mmol) and iodine (527 mg, 2.08 mmol) in dimethyl sulfoxide (25 mL) was stirred at 155 °C for 15 h under an Ar atmosphere. The reaction mixture was poured into a 10% $Na_2S_2O_3$ solution and extracted with dichloromethane. The organic layer was subsequently washed with a 10% $Na_2S_2O_3$ solution and a 5% NH_4Cl solution, dried over $MgSO_4$, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel with dichloromethane/hexane (1:1) and recrystallization from dichloromethane/methanol to afford 1,2-bis(4-mesitylphenyl)ethane-1,2-dione (**10**) (1.41 g, 84%). Pale yellow crystals (lit. yellow solid); mp 188.0–188.9 °C (ethanol) (lit. mp 182 °C); IR (KBr disk): ν_{max} = 3110 (w), 2971 (s), 2956 (s), 2918 (s), 2858 (s), 1673 (s, C=O), 1602 (s), 1559 (s), 1512 (m), 1477 (s), 1442 (s), 1401 (s), 1379 (s), 1317 (s), 1296 (s), 1281 (s), 1244 (m), 1212 (s), 1173 (s), 1107 (m), 1034 (m), 1004 (s), 998 (w), 960 (w), 949 (w), 888 (s), 850 (s), 838 (s), 778 (s), 743 (m), 720 (m), 696 (s), 632 (m), 598 (m), 577 (s), 516 (m), 484 (w), 462 (w), 418 (w) cm^{-1}; UV–vis (CH_2Cl_2): λ_{max} = 228 (log ε 4.27), 264 (4.26), 290 (4.21) nm; ^1H NMR (500 MHz, $CDCl_3$): δ_H = 8.09 (d, 4H, *J* = 8.5 Hz, 3',5'-H), 7.33 (d, 4H, *J* = 8.5 Hz, 2',6'-H), 6.96 (s, 4H, 3'',5''-H), 2.34 (s, 6H, 4''-Me), 2.00 (s, 12H, 2'',6''-Me); ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 194.2 (C-1,2), 148.7 (C-1'), 137.6 (C-1''), 137.4 (C-4''), 135.3 (C-2'',6''), 131.4 (C-4'), 130.25 (C-2',6'), 130.21 (C-3',5'), 128.3 (C-3'',5''), 21.0 (4''-Me), 20.7 (2'',6''-Me); HRMS (dithranol + CF_3CO_2Ag): calcd for $C_{32}H_{30}O_2 + Ag^+$ 553.1291, found 553.1274. Anal. Calcd for $C_{32}H_{30}O_2$ (446.5794): C, 86.06; H, 6.77. Found: C, 85.87; H, 6.61.

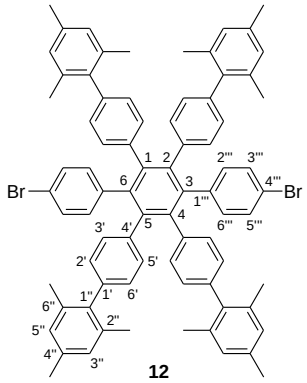
2,3-Bis(4-bromophenyl)-4,5-bis(4-mesitylphenyl)cyclopentadienone (11):[S-4]



11

TBAH (10% in methanol, 1.0 mL, 0.32 mmol) was added to a stirred mixture of 1,2-bis(4-mesitylphenyl)ethane-1,2-dione (**10**) (249 mg, 0.558 mmol) and 1,3-bis(4-bromophenyl)acetone (215 mg, 0.584 mmol) in 2-methyl-2-propanol (2.5 mL) at 80 °C. The resulting mixture was stirred at the same temperature for 1 h under an Ar atmosphere. The reaction mixture was poured into brine and extracted with dichloromethane. The organic layer was washed with brine, dried over $MgSO_4$, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel with dichloromethane/hexane (1:1) to afford 2,3-bis(4-bromophenyl)-4,5-bis(4-mesitylphenyl)cyclopentadienone (**11**) (411 mg, 95%). Wine red crystals (lit. purple solid); mp 264.0–264.9 °C (ethanol) (lit. mp 235 °C); IR (KBr disk): ν_{max} = 3044 (w), 2979 (m), 2948 (m), 2917 (m), 2858 (w), 1711 (s, C=O), 1612 (m), 1587 (m), 1487 (m), 1397 (m), 1357 (m), 1316 (m), 1298 (m), 1185 (w), 1120 (m), 1102 (m), 1073 (s), 1009 (s), 968 (w), 851 (s), 840 (m), 813 (m), 777 (m), 744 (m), 611 (w), 591 (w), 573 (w), 552 (w), 521 (w), 507 (w), 495 (w) cm^{-1}; UV–vis (CH_2Cl_2): λ_{max} = 228 (log ε 4.66), 274 (4.63), 362 (4.06), 462 (3.17), 522 (3.25) nm; ^1H NMR (500 MHz, $CDCl_3$): δ_H = 7.40 (d, 4H, *J* = 8.6 Hz, 2’’’,6’’’-H or 3’’’,5’’’-H), 7.22 (d, 4H, *J* = 8.6 Hz, 2’’’,6’’’-H or 3’’’,5’’’-H), 6.99 (s, 8H, 2’,6’-H and 3’,5’-H), 6.94 (s, 4H, 3’’,5’’-H), 2.32 (s, 6H, 4’’-Me), 1.95 (s, 12H, 2’’,6’’-Me) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 199.7 (C=O), 155.2 (s), 141.8 (s), 138.2 (C-1’’), 136.9 (C-4’’), 135.6 (C-2’’,6’’), 131.6 (C-2’’’,6’’’ or C-3’’’,5’’’), 131.3 (C-2’’’,6’’’ or C-3’’’,5’’’), 131.1 (s), 129.5 (s), 129.19 (C-2’,6’ or C-3’,5’), 129.18 (C-2’,6’ or C-3’,5’), 128.1 (C-3’’,5’’), 123.9 (s), 122.0 (s), 21.0 (4’’-Me), 20.4 (2’’,6’’-Me) ppm; HRMS (dithranol + CF_3CO_2Ag): calcd for $C_{47}H_{38}OBr_2 + Ag^+$ 883.0335, found 883.0342. Anal. Calcd for $C_{47}H_{38}Br_2O$ (778.6120): C, 72.50; H, 4.92. Found: C, 72.53; H, 4.94.

1,4-Bis(4-bromophenyl)-2,3,5,6-tetrakis(4-mesitylphenyl)benzene (12):[S-4]

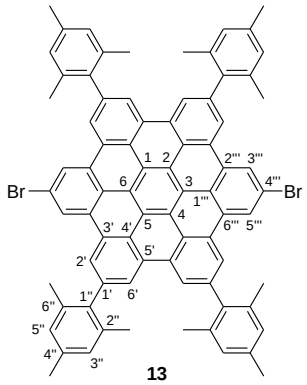


12

Bis(4-mesitylphenyl)acetylene (**9**) (89.6 mg, 0.216 mmol) and 2,3-bis(4-bromophenyl)-4,5-bis(4-mesitylphenyl)cyclopentadienone (**11**) (253 mg, 0.325 mmol) was mixed by the concentration after dissolving the mixture into appropriate amount of tetrahydrofuran. After the addition of diphenylether (200 μL) and tetrahydrofuran (100 μL) in the well-combined mixture, the combined mixture was stirred at 200–220 ℃ for 7 h under an Ar atmosphere. The precipitated crystals were purified by rinsing with dichloromethane to afford **12** (228 mg, 91%). Colorless crystals (lit. white solid); mp >300 °C (1,1,2,2-tetrachloroethane/ethanol) (lit. mp >300 °C); IR (KBr disk): ν_{max} = 3020 (s), 3000 (s), 2975 (s), 2954 (s), 2918 (s), 2857 (s), 1613 (m), 1589 (m), 1569 (m), 1518 (m), 1491 (s), 1479 (s), 1443 (s), 1394 (s), 1376 (m), 1298 (w), 1271 (w), 1257 (w), 1182 (w), 1165 (w), 1140 (m), 1104 (m), 1072 (s), 1014 (s), 1006 (s), 947 (w), 869 (m), 849 (s), 836 (s), 811 (m), 791 (m), 777 (s), 744 (m), 726 (m), 719 (m), 698 (w), 671 (w), 645 (w), 638 (m), 627 (w), 622 (m), 592 (m), 574 (m), 539 (m), 508 (w), 478 (w), 468 (w) cm^{-1}; UV–vis (CH_2Cl_2): λ_{max} = 228 (log ε 4.84), 257 (4.73), 285 sh (4.43) nm; ^{1}H NMR (500 MHz, $CDCl_3$): δ_H = 7.01 (d, 4H, *J* = 8.5 Hz, 2’’’,6’’’-H or 3’’’,5’’’-H), 6.95 (d, 8H, *J* = 8.1 Hz, 2’,6’-H or 3’,5’-H), 6.87 (br s, 4H, 3’’-H or 5’’-H), 6.86 (br s, 4H, 3’’-H or 5’’-H), 6.78 (d, 4H, *J* = 8.5 Hz, 2’’’,6’’’-H or 3’’’,5’’’-H), 6.71 (d, 8H, *J* = 8.1 Hz, 2’,6’-H or 3’,5’-H), 2.29 (s, 12H, 4’’-Me), 1.79 (s, 24H, 2’’,6’’-Me) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 140.3 (C-1,2,4,5, C-1’, or C-4’), 139.8 (C-3,6 or C-1’’’), 138.8 (C-1’’), 138.6 (C-1,2,4,5, C-1’, or C-4’), 138.3 (C-1,2,4,5, C-1’, or C-4’), 136.3 (C-4’’), 136.0 (C-2’’ or C-6’’), 135.6 (C-2’’ or C-6’’), 133.2 (C-2’’’,6’’’ or C-3’’’,5’’’), 131.5 (C-2’,6’ or C-3’,5’), 129.8 (C-2’’’,6’’’ or C-3’’’,5’’’), 127.9 (C-3’’ or C-5’’), 127.8 (C-2’,6’ or C-3’,5’), 127.7 (C-3’’ or C-5’’), 119.4 (C-4’’’), 21.0 (4’’-Me), 20.3 (2’’-Me or 6’’-Me), 20.2 (2’’-Me or 6’’-Me) ppm. C-3,6 or C-1’’’ carbon is not observed because of the low solubility of the sample under the measurement conditions. ^{1}H NMR (500 MHz, $C_2D_2Cl_4$, 80 °C): δ_H = 6.95 (d, 4H, *J* = 8.3 Hz, 2’’’,6’’’-H or 3’’’,5’’’-H), 6.92 (d, 8H, *J* = 7.9 Hz, 2’,6’-H or 3’,5’-H), 6.77 (br s, 8H, 3’’,5’’-H), 6.74 (d, 4H, *J* = 8.3 Hz, 2’’’,6’’’-H or 3’’’,5’’’-H), 6.66 (d, 8H, *J* = 7.9 Hz, 2’,6’-H or 3’,5’-H), 2.22 (s, 12H, 4’’-Me), 1.73 (s, 24H, 2’’,6’’-Me) ppm; ^{13}C NMR (125 MHz, $C_2D_2Cl_4$, 80 °C): δ_C = 140.5

(C-1,2,4,5, C-1', or C-4'), 140.2 (C-3,6 or C-1'''), 140.1 (C-3,6 or C-1'''), 139.2 (C-1''), 138.9 (C-1,2,4,5, C-1', or C-4'), 138.5 (C-1,2,4,5, C-1', or C-4'), 136.2 (C-4''), 133.5 (C-2''',6''' or C-3''',5'''), 131.8 (C-2',6' or C-3',5'), 129.9 (C-2''',6''' or C-3''',5'''), 128.2 (C-3'',5''), 128.0 (C-2',6' or C-3',5'), 119.6 (C-4'''), 21.3 (4''-Me), 20.4 (2'',6''-Me) ppm. C-2'',6'' carbons are observed as broad signals at around 136 ppm under the measurement conditions. HRMS (dithranol + CF_3CO_2Ag): calcd for $C_{78}H_{68}Br_2 + Ag^+$ 1269.2733, found 1269.2736. Anal. Calcd for $C_{78}H_{68}Br_2$ (1165.1825): C, 80.40; H, 5.88. Found: C, 80.34; H, 5.82.

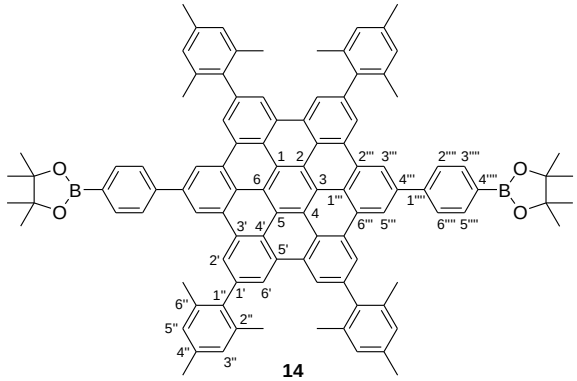
2,11-Dibromo-5,8,14,17-tetramesitylhexabenzo[*bc*,*ef*,*hi*,*kl*,*no*,*qr*]coronene (13):[S-4]



13

DDQ (456 mg, 2.01 mmol) and trifluoromethanesulfonic acid (4.8 mL) was added subsequently to a solution of 1,4-bis(4-bromophenyl)-2,3,5,6-tetrakis(4-mesitylphenyl)benzene (**12**) (355 mg, 0.308 mmol) in dry dichloromethane (178 mL). The resulting mixture was stirred at room temperature for 1 h under an Ar atmosphere. The reaction was quenched by the addition of saturated $NaHCO_3$ solution. The reaction mixture was poured into water and extracted with dichloromethane. The organic layer was washed with water, dried over $MgSO_4$, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel with dichloromethane/hexane (1:3) to afford **13** (346 mg, 98%). Yellow crystals (lit. yellow solid); mp >300 °C (toluene) (lit. mp >300 °C); IR (KBr disk): ν_{max} = 2949 (s), 2917 (s), 2858 (m), 1611 (s), 1597 (s), 1574 (s), 1517 (m), 1485 (s), 1442 (s), 1376 (m), 1367 (m), 1353 (s), 1253 (m), 1213 (m), 1206 (m), 1142 (m), 1077 (w), 1039 (m), 1013 (m), 880 (s), 868 (s), 852 (s), 828 (w), 777 (w), 748 (m), 733 (w), 632 (m), 567 (m), 531 (w) cm^{-1}; UV–vis (CH_2Cl_2): λ_{max} = 229 sh (log ε 5.24), 234 (5.26), 244 (5.21), 271 sh (4.50), 306 sh (4.10), 319 sh (4.27), 333 (4.47), 347 (4.90), 364 (5.28), 375 sh (4.80), 394 (4.83), 407 sh (4.17) nm; ^{1}H NMR (500 MHz, $CDCl_3$): δ_H = 9.29 (s, 4H, 3’’’,5’’’-H), 9.04 (s, 4H, 6’-H), 9.01 (s, 4H, 2’-H), 7.13 (s, 8H, 3’’,5’’-H), 2.45 (s, 12H, 4’’-Me), 2.23 (s, 24H, 2’’-Me) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 140.5 (s), 138.8 (C-1’’), 137.4 (C-4’’), 136.2 (C-2’’), 132.7 (s), 130.9 (s), 129.8 (s), 128.5 (C-3’’,5’’), 125.2 (C-3’’’,5’’’), 124.5 (s), 124.4 (s), 124.2 (C-2’ or C-6’), 123.7 (C-2’ or C-6’), 122.4 (s), 121.3 (s), 121.1 (q), 21.3 (2’’,6’’-Me), 21.2 (4’’-Me) ppm; HRMS (dithranol): calcd for $C_{78}H_{56}Br_2^+$ 1150.2743, found 1150.2723. Anal. Calcd for $C_{78}H_{56}Br_2$ (1153.0872): C, 81.25; H, 4.90. Found: C, 81.22; H, 5.07.

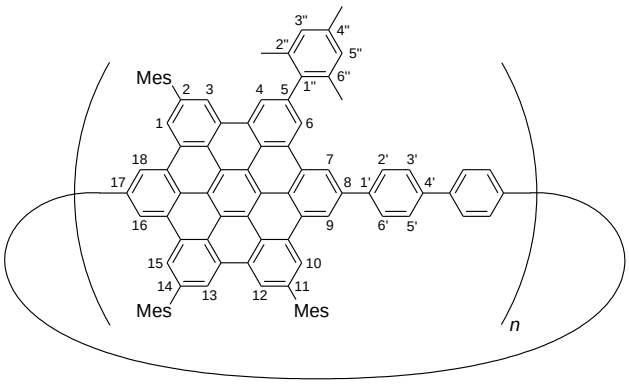
2,11-Bis[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-5,8,14,17-tetramesitylhexabenzo[*bc*,*ef*,*hi*,*kl*,*no*,*qr*]coronene (14):



14

To a degassed mixture of 2,11-dibromo-5,8,14,17-tetramesitylhexabenzo[*bc*,*ef*,*hi*,*kl*,*no*,*qr*]coronene (**13**) (244 mg, 0.212 mmol), 1,4-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzene (593 mg, 1.80 mmol), and silver carbonate (104 mg, 0.377 mmol) in 1,4-dioxane (10 mL) was added $Pd(PPh_3)_4$ (25.8 mg, 0.0223 mmol). The resulting mixture was refluxed for 4 h under an Ar atmosphere. The reaction mixture was poured into brine and extracted with chloroform. The organic layer was washed with brine, dried over $MgSO_4$, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel with dichloromethane/hexane (3:1) and GPC with chloroform to afford **14** (135 mg, 46%). Yellow crystals; mp >300 °C (toluene/ethanol); IR (KBr disk): ν_{max} = 2976 (m), 2922 (m), 2855 (m), 1608 (s), 1577 (m), 1494 (m), 1482 (m), 1445 (m), 1397 (m), 1359 (s), 1319 (m), 1294 (w), 1249 (m), 1219 (w), 1199 (w), 1145 (s), 1096 (s), 1069 (w), 1021 (w), 962 (w), 881 (w), 858 (m), 852 (m), 839 (m), 751 (w), 680 (w), 660 (w) cm^{-1}; UV–vis (CH_2Cl_2): λ_{max} = 233 sh (log ε 5.18), 237 (5.19), 250 sh (5.09), 263 sh (4.97), 306 (4.28), 321 (4.28), 336 (4.52), 351 (4.95), 369 (5.33), 385 sh (4.79), 399 (4.84), 416 (4.38) nm; ^{1}H NMR (500 MHz, $CDCl_3$): δ_H = 9.47 (s, 4H, 3’’’,5’’’-H), 9.20 (s, 4H, 2’-H or 6’-H), 9.04 (s, 4H, 2’-H or 6’-H), 8.09 (d, 4H, *J* = 8.3 Hz, 2’’’’,6’’’’-H or 3’’’’,5’’’’-H), 8.06 (d, 4H, *J* = 8.3 Hz, 2’’’’,6’’’’-H or 3’’’’,5’’’’-H), 7.15 (s, 8H, 3’’,5’’-H), 2.47 (s, 12H, 4’’-Me), 2.26 (s, 24H, 2’’,6’’-Me), 1.42 (s, 24H, B(pin)) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 143.9 (C-1’’’’), 140.0 (s), 139.5 (C-4’’’), 139.2 (C-1’’), 137.4 (C-4’’), 136.4 (C-2’’,6’’), 135.6 (C-2’’’’,6’’’’ or C-3’’’’,5’’’’), 131.2 (s), 131.03 (s), 131.01 (s), 128.5 (C-3’’,5’’), 127.3 (C-2’’’’,6’’’’ or C-3’’’’,5’’’’), 125.2 (s), 124.6 (s), 123.7 (C-2’ or C-6’), 123.5 (C-2’ or C-6’), 121.4 (s), 121.3 (s), 121.2 (C-3’’’,5’’’), 83.9 (s, B(pin)), 24.9 (q, B(pin)), 21.3 (2’’,6’’-Me), 21.2 (4’’-Me) ppm; HRMS (dithranol): calcd for $C_{102}H_{88}B_2O_4^+$ 1396.6936, found 1396.6910. Anal. Calcd for $C_{102}H_{88}B_2O_4$ (1399.4097): C, 87.54; H, 6.34. Found: C, 87.37; H, 6.43.

[4]Cyclo(2,5,11,14-tetramesityl-8,17-diphenylhexabenzo[*bc*,*ef*,*hi*,*kl*,*no*,*qr*]coronene) (1) and [3]Cyclo(2,5,11,14-tetramesityl-8,17-diphenylhexabenzo[*bc*,*ef*,*hi*,*kl*,*no*,*qr*]coronene) (2):



1: *n* = 4
2: *n* = 3

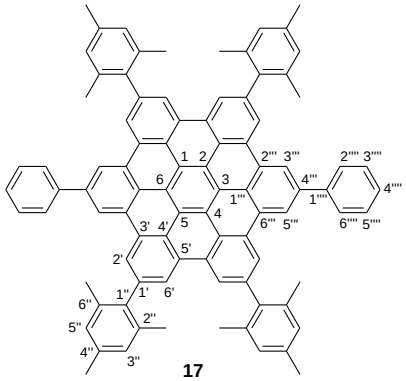
$PtCl_2$(cod) (8.2 mg, 0.022 mmol) and CsF (19.1 mg, 0.126 mmol) was added subsequently to 2,11-bis[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-5,8,14,17-tetramesitylhexabenzo[*bc*,*ef*,*hi*,*kl*,*no*,*qr*]coronene (**14**) (29.1 mg, 0.0208 mmol) in dry tetrahydrofuran (1.1 mL). The resulting mixture was refluxed for 24 h under an Ar atmosphere. The reaction mixture was poured into water and extracted with chloroform. The organic layer was washed with water, dried over $MgSO_4$, and concentrated under reduced pressure. The residue was purified by rinsing with methanol and hexane. The crude product was added to a degassed *o*-DCB (1.5 mL) with PPh_3 (15.2 mg, 0.0580 mmol). The mixture was refluxed for 24 h under an Ar atmosphere. The reaction mixture was poured into brine and extracted with dichloromethane. The organic layer was washed with brine, dried over $MgSO_4$, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel with hexane/chloroform (1:3). The pure product was obtained by the repeated column chromatography on silica gel with hexane/toluene/CS_2 (15:10:1) and GPC with chloroform to give cyclic tetramer **1** (4.2 mg, 18%) and a small amount of cyclic trimer **2**.

Cyclic Tetramer 1: Yellow crystals; mp >300 °C (carbon disulfide/hexane); IR (KBr disk): ν_{max} = 3030 (w), 2943 (m), 2918 (m), 2864 (m), 1610 (s), 1579 (w), 1495 (m), 1442 (m), 1385 (s), 1342 (w), 1198 (w), 1034 (w), 1018 (w), 1003 (w), 881 (m), 850 (m), 822 (m), 771 (w), 750 (w), 742 (w), 706 (w), 677 (w), 648 (w), 602 (w) cm^{-1}; UV–vis (CH_2Cl_2): λ_{max} = 230 (log ε 5.73), 240 sh (5.73), 280 sh (5.18), 322 (5.07), 339 sh (5.14), 355 (5.49), 372 (5.85), 389 sh (5.52), 402 (5.35), 426 (5.20) nm; ^{1}H NMR (500 MHz, $CDCl_3$): δ_H = 9.27 (s, 16H, 7,9,16,18-H), 9.05 (s, 16H, 1,6,10,15-H), 8.98 (s, 16H, 3,4,12,13-H), 8.08 (d, 16H, *J* = 8.6 Hz, 2',6'-H), 7.82 (d, 16H, *J* = 8.6 Hz, 3',5'-H), 7.13 (s, 32H, 3'',5''-H), 2.46 (s, 48H, 4''-Me), 2.22 (s, 96H, 2'',6''-Me) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 140.0 (s), 139.6 (C-1'), 139.2 (C-1''), 138.5 (s), 137.3 (C-4''), 136.4 (C-2'',6''), 131.3

(s), 131.2 (s), 130.7 (s), 128.4 (C-3”,5”), 128.1 (C-2’,6’), 127.8 (C-3’,5’), 125.0 (s), 124.5 (s), 123.8 (C-1,6,10,15), 123.4 (C-3,4,12,13), 121.8 (C-7,9,16,18), 120.79 (s), 120.75 (s), 21.3 (2”,6”-Me), 21.2 (4”-Me) ppm; HRMS (dithranol): calcd for $C_{360}H_{256}^{+}$ 4578.0027, found 4578.0067.

Cyclic Trimer 2: Yellow crystals; UV–vis (CH_2Cl_2): λ_{max} = 229 (log ε 5.38), 241 sh (5.36), 278 sh (4.83), 323 sh (4.70), 339 sh (4.80), 357 (5.12), 372 (5.43), 390 sh (5.06), 406 sh (4.82), 428 (4.69) nm; ^{1}H NMR (500 MHz, $CDCl_3$): δ_H = 9.12 (s, 12H, 1,6,10,15-H, 3,4,12,13-H, or 7,9,16,18-H), 8.94 (s, 12H, 1,6,10,15-H, 3,4,12,13-H, or 7,9,16,18-H), 8.93 (s, 12H, 1,6,10,15-H, 3,4,12,13-H, or 7,9,16,18-H), 7.98 (d, 12H, *J* = 8.7 Hz, 2’,6’-H or 3’,5’-H), 7.68 (s, 12H, *J* = 8.7 Hz, 2’,6’-H or 3’,5’-H), 7.13 (s, 12H, 3”-H or 5”-H), 7.11 (s, 12H, 3”-H or 5”-H), 2.46 (s, 36H, 4”-Me), 2.24 (s, 36H, 2”-Me or 6”-Me), 2.15 (s, 36H, 2”-Me or 6”-Me) ppm; HRMS (dithranol): calcd for $C_{270}H_{192}^{+}$ 3433.5019, found 3433.5027.

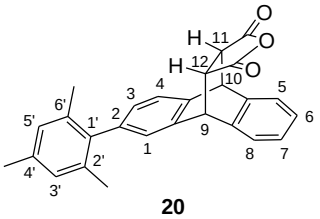
2,5,11,14-Tetramesityl-8,17-diphenylhexabenzo[*bc*,*ef*,*hi*,*kl*,*no*,*qr*]coronene (17):



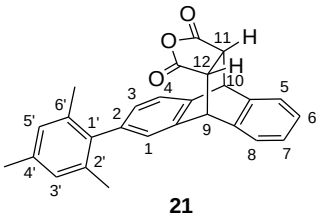
17

To a degassed mixture of 2,11-dibromo-5,8,14,17-tetramesitylhexabenzo[*bc*,*ef*,*hi*,*kl*,*no*,*qr*]coronene (**13**) (96.4 mg, 0.0836 mmol), phenylboronic acid (42.0 mg, 0.344 mmol), and 1M K_2CO_3 solution (0.85 mL) in toluene (1.7 mL) was added $Pd(PPh_3)_4$ (4.8 mg, 4.2 μmol). The resulting mixture was refluxed for 24 h under an Ar atmosphere. The reaction mixture was poured into brine and extracted with dichloromethane. The organic layer was washed with brine, dried over $MgSO_4$, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel with chloroform/hexane (3:1) and GPC with chloroform. The product was further purified by crystallization from chloroform/methanol to afford **17** (71.2 mg, 74%). Yellow crystals; mp >300 °C (toluene/ethanol); IR (KBr disk): ν_{max} = 3066 (w), 2979 (m), 2953 (m), 2918 (m), 2855 (m), 1607 (s), 1576 (m), 1494 (m), 1444 (m), 1383 (m), 1368 (m), 1250 (m), 1198 (w), 1145 (m), 1096 (w), 1071 (w), 1032 (w), 875 (m), 850 (m), 813 (w), 762 (m), 697 (m), 647 (w), 619 (w), 566 (w), 530 (w) cm^{-1}; UV–vis (CH_2Cl_2): λ_{max} = 237 (log ε 5.24), 243 (5.24), 248 sh (5.23), 305 (4.20), 321 (4.28), 335 (4.54), 350 (4.99), 367 (5.37), 376 sh (4.99), 397 (4.90), 412 sh (4.33) nm; ^{1}H NMR (500 MHz, $CDCl_3$): δ_H = 9.45 (s, 4H, 3’’’,5’’’-H), 9.20 (s, 4H, 2’-H or 6’-H), 9.05 (s, 4H, 2’-H or 6’-H), 8.06 (d, 4H, *J* = 8.1 Hz, 2’’’’,6’’’’-H), 7.63 (dd, 4H, *J* = 8.1, 7.4 Hz, 3’’’’,5’’’’-H), 7.50 (t, 2H, *J* = 7.4 Hz, 4’’’’-H), 7.15 (s, 8H, 3’’,5’’-H), 2.46 (s, 12H, 4’’-Me), 2.26 (s, 24H, 2’’,6’’-Me) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 141.4 (C-1’’’’), 140.0 (s), 139.8 (C-4’’’), 139.2 (C-1’’), 137.4 (C-4’’), 136.4 (C-2’’,6’’), 131.2 (s), 131.0 (s), 129.2 (C-3’’’’,5’’’’), 128.4 (C-3’’,5’’), 128.1 (C-2’’’’,6’’’’), 127.9 (C-4’’’’), 125.0 (s), 124.7 (s), 123.6 (C-2’ or C-6’), 123.4 (C-2’ or C-6’), 121.4 (s), 121.3 (s), 121.2 (C-3’’’,5’’’), 21.3 (2’’,6’’-Me), 21.2 (4’’-Me) ppm; HRMS (dithranol): calcd for $C_{90}H_{66}^+$ 1146.5159, found 1146.5165. Anal. Calcd for $C_{90}H_{66}$ (1147.487): C, 94.20; H, 5.80. Found: C, 94.46; H, 5.66.

***anti*-2-Mesityl-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylic anhydride (20) and *syn*-2-Mesityl-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylic anhydride (21):**



20



21

2-Mesitylanthracene (**19**) (86.1 mg, 0.290 mmol) and maleic anhydride (31.1 mg, 0.317 mmol) in toluene (0.5 mL) was refluxed for 12 h under an Ar atmosphere. The solvent was removed under reduced pressure. The residue was purified by GPC with chloroform to afford maleic anhydride adduct major isomer **20** (74.6 mg, 65%) and maleic anhydride adduct minor isomer **21** (21.0 mg, 18%).

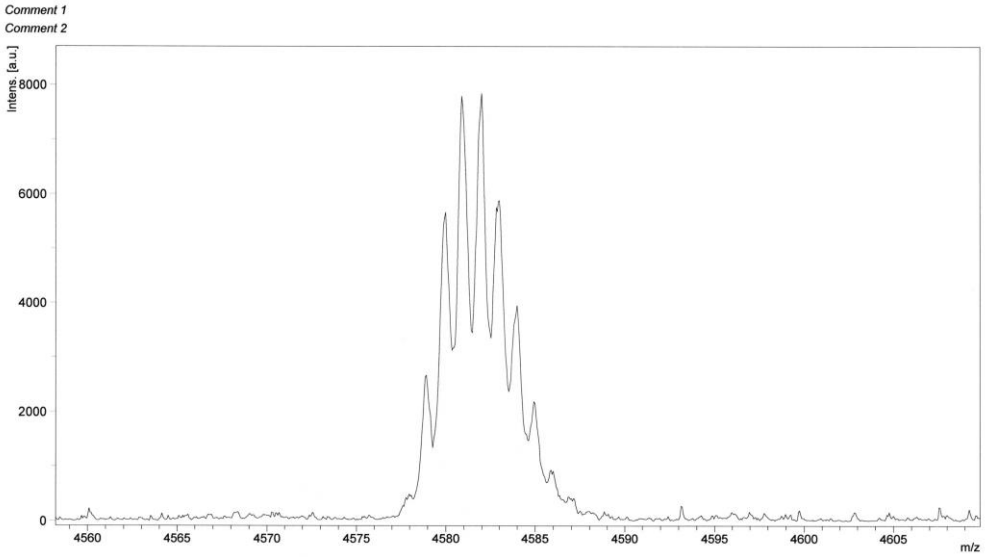
Maleic anhydride adduct major isomer 20: Colorless solid; mp 144.5–145.3 °C (methanol/water); IR (KBr disk): ν_{max} = 3023 (m), 3004 (m), 2951 (s), 2919 (m), 2854 (m), 1750 (s, C=O), 1715 (s, C=O), 1613 (m), 1578 (w), 1470 (s), 1435 (m), 1381 (w), 1346 (m), 1321 (m), 1283 (m), 1205 (s), 1176 (s), 1150 (m), 1122 (m), 1098 (w), 1066 (w), 1026 (m), 966 (w), 919 (w), 905 (w), 882 (w), 850 (m), 830 (w), 806 (w), 761 (m), 670 (w), 641 (w), 622 (w), 599 (w), 574 (w), 531 (w), 479 (w) cm^{-1}; UV–vis (CH_2Cl_2): λ_{max} = 228 (log ε 4.20), 249 sh (3.77), 274 sh (3.16) nm; ^1H NMR (500 MHz, $CDCl_3$): δ_H = 7.45–7.42 (m, 2H, 5,8-H), 7.38 (d, 1H, *J* = 7.6 Hz, 4-H), 7.26–7.24 (m, 2H, 6,7-H), 7.12 (d, 1H, *J* = 1.6 Hz, 1-H), 7.00 (dd, 1H, *J* = 7.6, 1.6 Hz, 3-H), 6.93 (s, 1H, 3'-H or 5'-H), 6.89 (s, 1H, 3'-H or 5'-H), 4.89 (s, 1H, 10-H), 4.83 (s, 1H, 9-H), 3.54 (m, 2H, 11,12-H), 2.31 (s, 3H, 4'-Me), 1.90 (s, 6H, 2',6'-Me); ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 170.6 (C=O), 170.4 (C=O), 140.9 (C-9a), 140.6 (C-8a or C-10a), 140.4 (C-8a or C-10a), 138.14 (C-1' or C-2), 138.07 (C-1' or C-2), 136.8 (C-4'), 136.5 (C-2' or C-6'), 136.1 (C-4a), 135.4 (C-2' or C-6'), 128.6 (C-3), 128.2 (C-3' or C-5'), 127.9 (C-3' or C-5'), 127.20 (C-6 or C-7), 127.16 (C-6 or C-7), 126.2 (C-1), 125.2 (C-4), 124.5 (C-5 or C-8), 124.4 (C-5 or C-8), 48.2 (C-11 or C-12), 48.1 (C-11 or C-12), 45.5 (C-9), 45.4 (C-10), 21.0 (4'-Me), 20.7 (2'-Me or 6'-Me), 20.5 (2'-Me or 6'-Me); HRMS (dithranol + CF_3CO_2Ag): calcd for $C_{27}H_{22}O_3$ + Ag^+ 501.0614, found 501.0634. Anal. Calcd for $C_{27}H_{22}O_3$ (394.4618): C, 82.21; H, 5.62. Found: C, 82.53; H, 5.35.

Maleic anhydride adduct minor isomer 21: Colorless crystals; mp 122.6–123.7 °C (methanol/water); IR (KBr disk): ν_{max} = 3025 (m), 2951 (m), 2918 (m), 2865 (m), 2733 (w), 2627 (w), 1869 (w), 1841 (w), 1779 (m), 1748 (s, C=O), 1718 (s, C=O), 1613 (m), 1575 (w), 1469 (s), 1436 (m), 1378 (m), 1346 (m), 1322 (m), 1290 (m), 1208 (s), 1176 (s), 1125 (m), 1098 (m), 1075 (m), 1032 (w), 968 (w), 935 (m), 904 (w), 850 (m), 841 (m), 823 (w), 801 (w), 778 (w), 752 (m), 706 (w), 671 (w), 591 (w), 534 (w), 510 (w), 477 (w), 442 (w), 410 (w) cm^{-1}; UV–vis (CH_2Cl_2):

λ_{max} = 228 (log ε 4.10), 249 sh (3.64), 276 sh (2.76) nm; ^{1}H NMR (500 MHz, $CDCl_3$): δ_H = 7.42 (d, 1H, *J* = 7.5 Hz, 4-H), 7.39–7.35 (m, 2H, 5,8-H), 7.26–7.24 (m, 2H, 6,7-H), 7.16 (d, 1H, *J* = 1.6 Hz, 1-H), 6.96 (dd, 1H, *J* = 7.5, 1.6 Hz, 3-H), 6.94 (s, 1H, 3'-H or 5'-H), 6.91 (s, 1H, 3'-H or 5'-H), 4.88 (d, 1H, *J* = 3.4 Hz, 10-H), 4.82 (d, 1H, *J* = 3.4 Hz, 9-H), 3.62 (dd, 1H, *J* = 9.2, 3.4 Hz, 11-H), 3.57 (dd, 1H, *J* = 9.2, 3.4 Hz, 12-H), 2.32 (s, 3H, 4'-Me), 2.01 (s, 3H, 2'-Me or 6'-Me), 1.87 (s, 3H, 2'-Me or 6'-Me); ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 170.49 (C=O), 170.47 (C=O), 140.6 (C-9a), 140.2 (C-2), 138.6 (C-4a), 138.23 (C-1', C-8a, or C-10a), 138.15 (C-1', C-8a, or C-10a), 138.1 (C-1', C-8a, or C-10a), 136.8 (C-4'), 136.0 (C-2' or C-6'), 135.8 (C-2' or C-6'), 128.2 (C-3' or C-5'), 128.10 (C-3' or C-5'), 128.05 (C-3), 127.8 (C-6 or C-7), 127.7 (C-6 or C-7), 125.3 (C-5 or C-8), 125.19 (C-1, C-5, or C-8), 125.18 (C-1, C-5, or C-8), 124.3 (C-4), 48.2 (C-11 or C-12), 48.1 (C-11 or C-12), 45.5 (C-9), 45.2 (C-10), 21.0 (4'-Me), 20.9 (2'-Me or 6'-Me), 20.8 (2'-Me or 6'-Me); HRMS (dithranol + CF_3CO_2Ag): calcd for $C_{27}H_{22}O_3 + Ag^+$ 501.0620, found 501.0634. Anal. Calcd for $C_{27}H_{22}O_3$ (394.4618): C, 82.21; H, 5.62. Found: C, 82.41; H, 5.65.

(3) MALDI-TOF MS of Cyclic Tetramer 1 and Cyclic Trimer 2

(a)



(b)

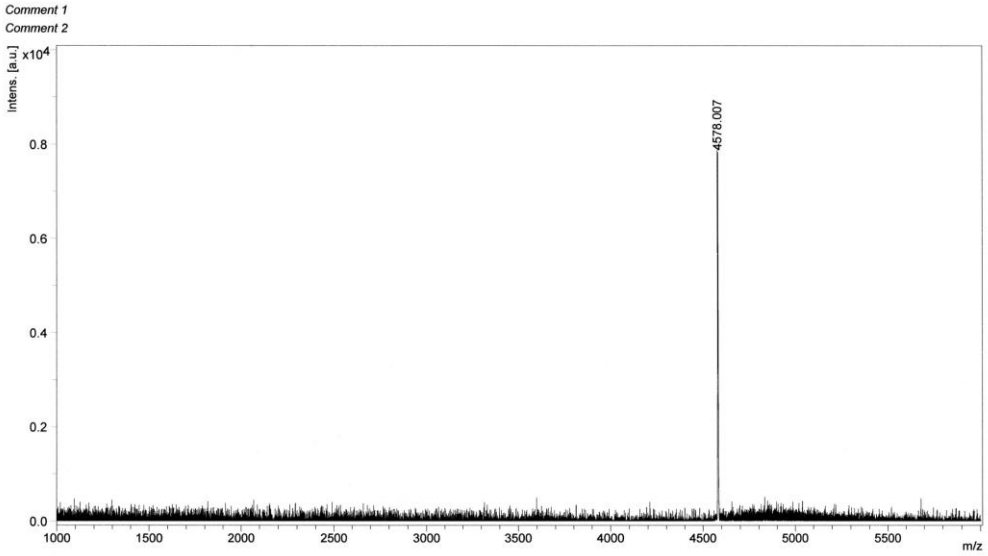
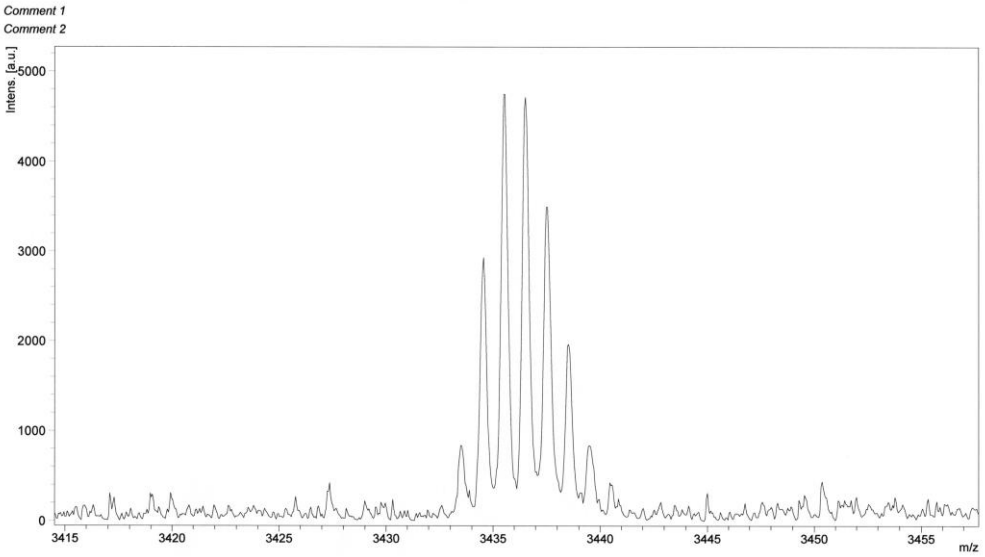


Figure S-2. Representation of (a) the expanded and (b) the full ranged MALDI-TOF MS of cyclic tetramer **1** $[M]^+$.

(a)



(b)

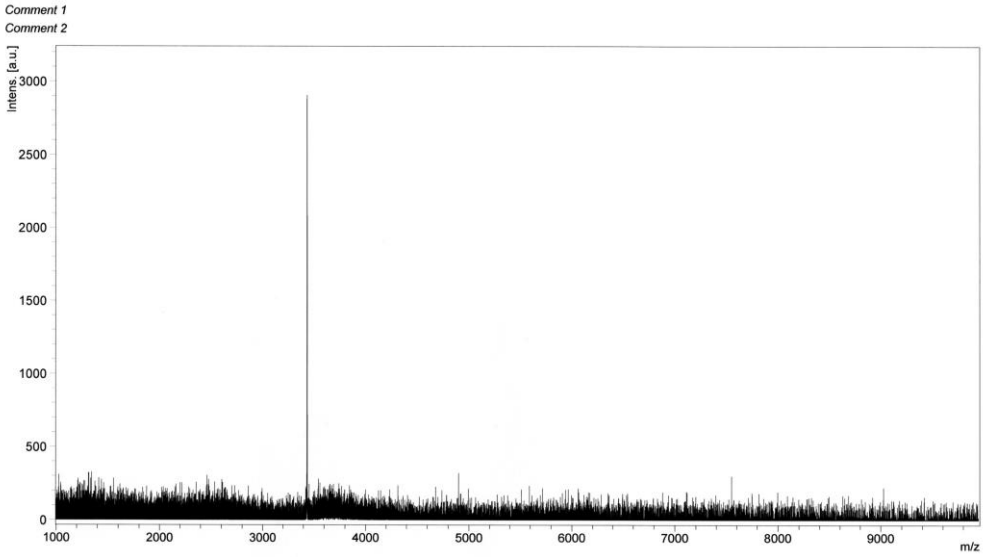


Figure S-3. Representation of (a) the expanded and (b) the full ranged MALDI-TOF MS of cyclic trimer **2** $[M]^+$.

(4) Comparison of UV/Vis Spectra of 1 and 17 and the Normalized Excitation Spectra of 1

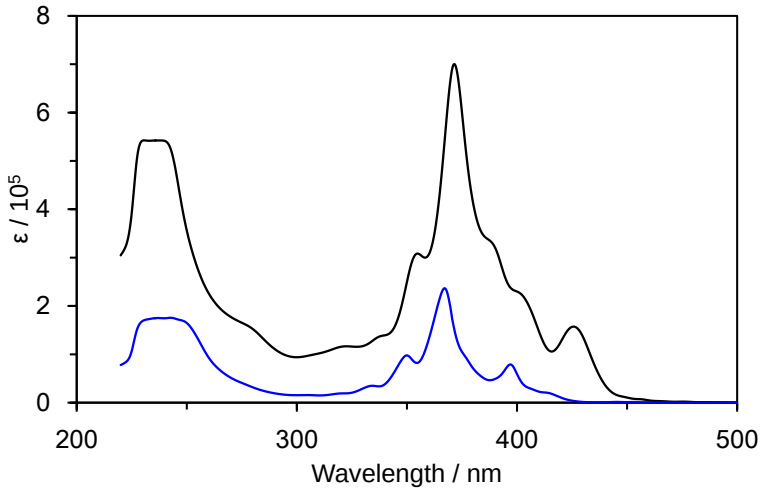


Figure S-4. Comparison of UV/Vis spectra of the cyclic tetramer **1** (2.20×10^{-6} M; black line) and the model PAH derivative **17** (1.19×10^{-5} M; blue line) in dichloromethane.

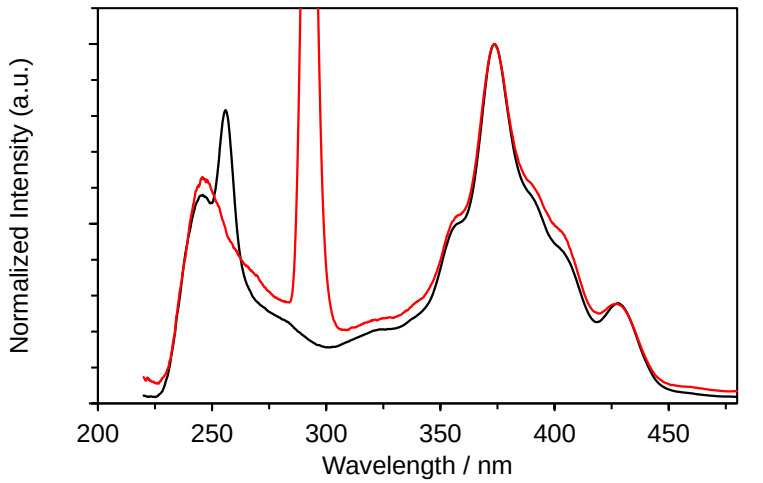
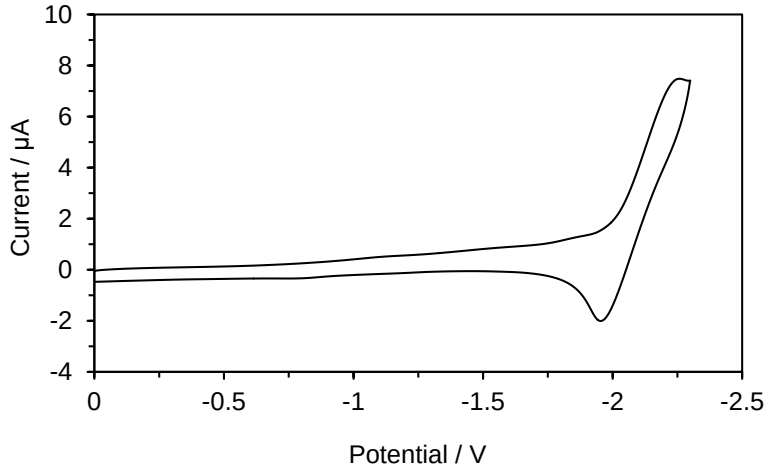


Figure S-5. Normalized excitation spectra of the cyclic trimer **1** (2.40×10^{-6} M) in dichloromethane; λ_{FL} = 508 nm (black line) and λ_{FL} = 580 nm (red line).

(5) Voltammograms of Cyclic Tetramer 1 and the Model HBC Derivative 17

(a)



(b)

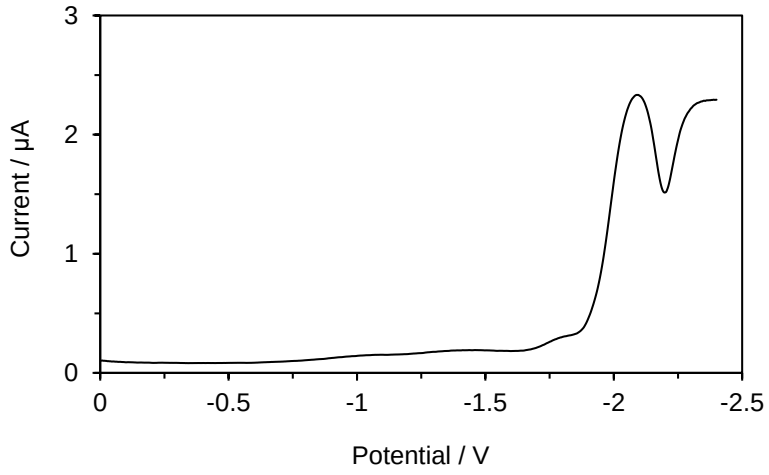
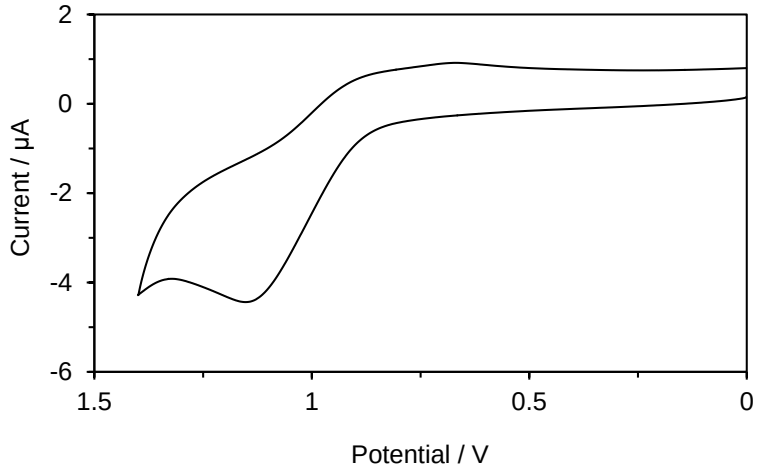


Figure S-6. Reduction wave upon (a) CV and (b) DPV of cyclic tetramer **1** (1 mM) in *o*-dichlorobenzene containing *n*-Bu_4NClO_4 (0.1 M) as a supporting electrolyte.

(a)



(b)

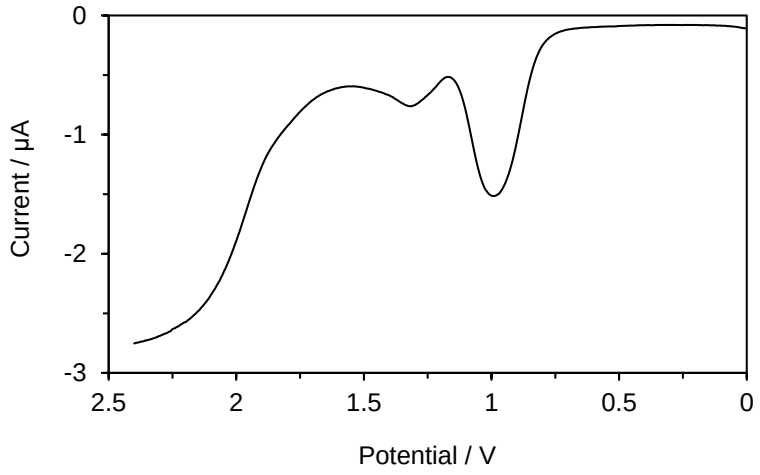
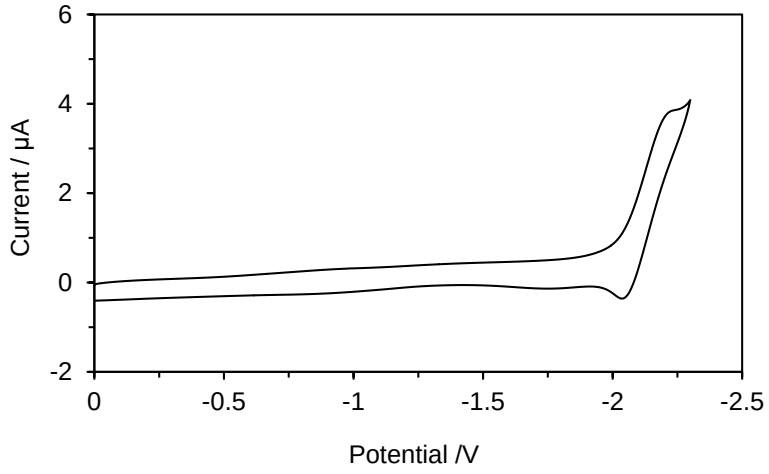


Figure S-7. Oxidation wave upon (a) CV and (b) DPV of cyclic tetramer **1** (1 mM) in *o*-dichlorobenzene containing *n*-Bu_4NClO_4 (0.1 M) as a supporting electrolyte.

(a)



(b)

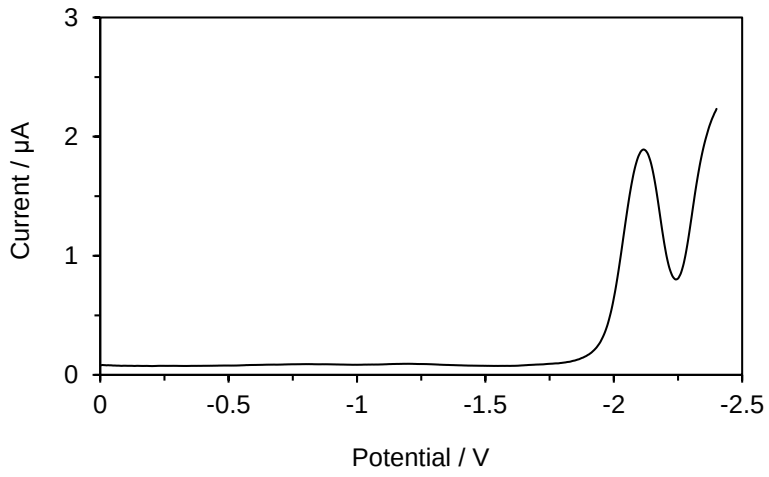
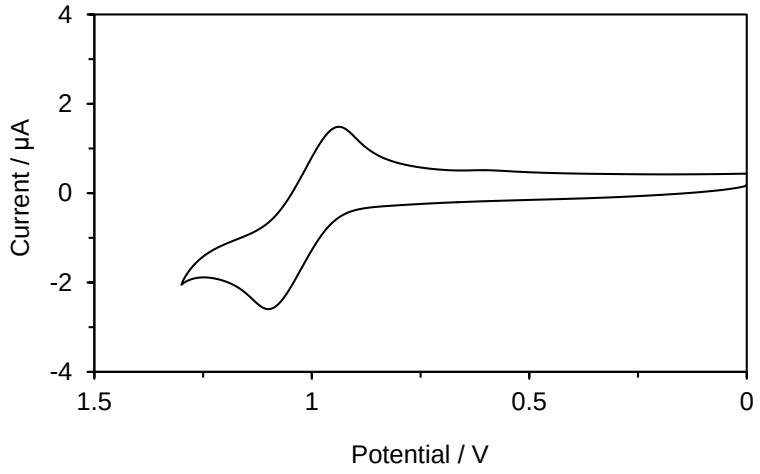


Figure S-8. Reduction wave upon (a) CV and (b) DPV of model PAH derivative **17** (1 mM) in *o*-dichlorobenzene containing *n*-Bu_4NClO_4 (0.1 M) as a supporting electrolyte.

(a)



(b)

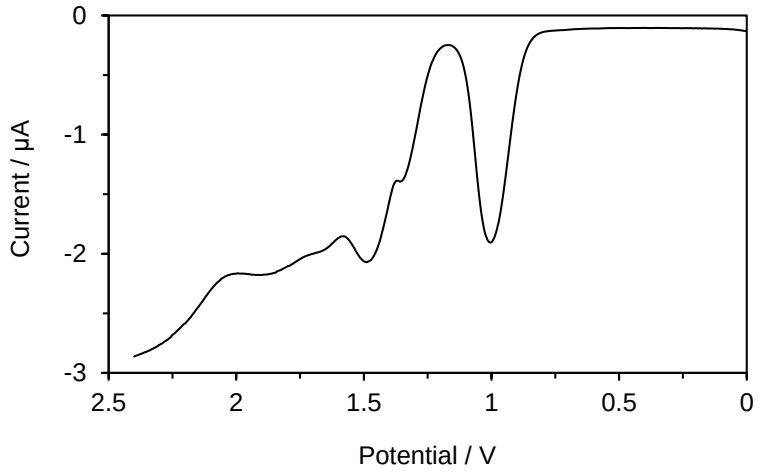


Figure S-9. Oxidation wave upon (a) CV and (b) DPV of model PAH derivative **17** (1 mM) in *o*-dichlorobenzene containing *n*-Bu_4NClO_4 (0.1 M) as a supporting electrolyte.

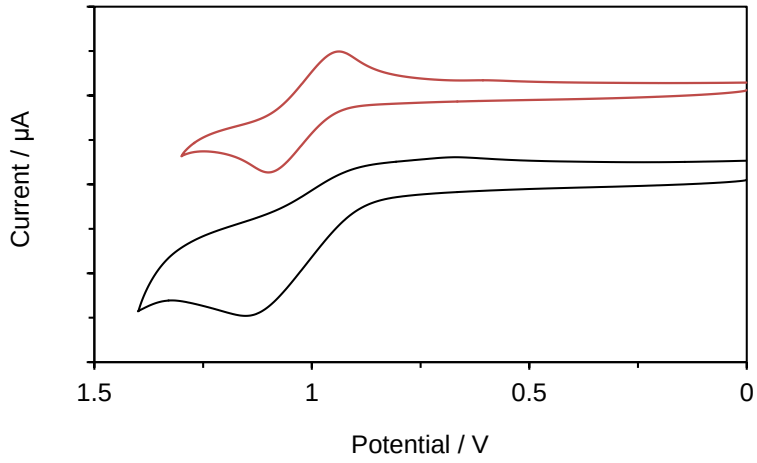


Figure S-10. Comparison of the first oxidation wave of cyclic tetramer **1** (black line) and the model HBC derivative **17** (red line) (1 mM) in *o*-dichlorobenzene containing *n*-Bu_4NClO_4 (0.1 M) as a supporting electrolyte.

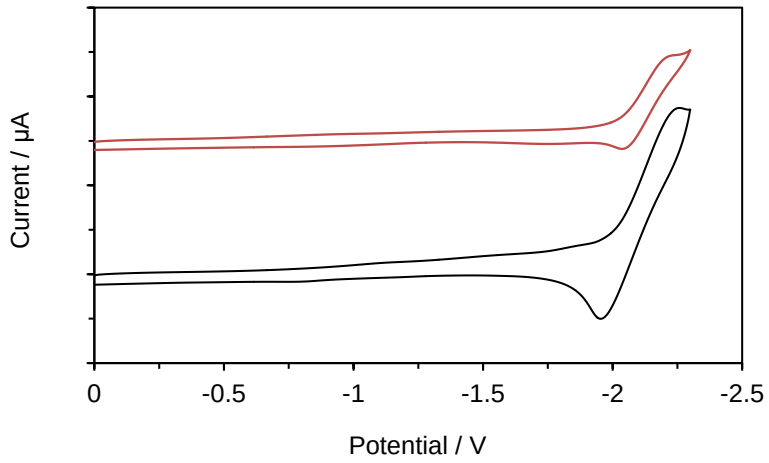


Figure S-11. Comparison of the first reduction wave of cyclic tetramer **1** (black line) and the model HBC derivative **17** (red line) (1 mM) in *o*-dichlorobenzene containing *n*-Bu_4NClO_4 (0.1 M) as a supporting electrolyte.

Table S-5. Redox Potentials[a] of Cyclic Tetramer **1** and Model PAH Derivative **3** Measured by CV and DPV

Sample	E_1^{ox} [V]	E_2^{ox} [V]	E_3^{ox} [V]	E_1^{red} [V]	$E_1^{ox} - E_1^{red}$ [V]
1	(1.12)			−2.11	
DPV[b]	(0.99)	(1.32)		(−2.09)	3.08 V
3	1.02			−2.13	
DPV[b]	(1.00)	(1.36)	(1.49)	(−2.12)	3.12 V

[a] The redox potentials were measured by CV and DPV [V vs $Ag/AgNO_3$, 1 mM in *o*-dichlorobenzene containing *n*-Bu_4NClO_4 (0.1 M), Pt electrode (i.d., 1.6 mm), scan rate 100 mV s^{-1}, and Fc/Fc^+ = 0.25 V]. In the case of irreversible waves, which are given in parentheses, E_{ox} and E_{red} were calculated as E_{pa} (anodic peak potential) – 0.03 V and E_{pc} (cathodic peak potential) + 0.03 V, respectively.

[b] The values are peak potentials measured by DPV.

(6) Temperature Dependency of ^{1}H NMR and Kinetic Data of Cyclic Tetramer 1

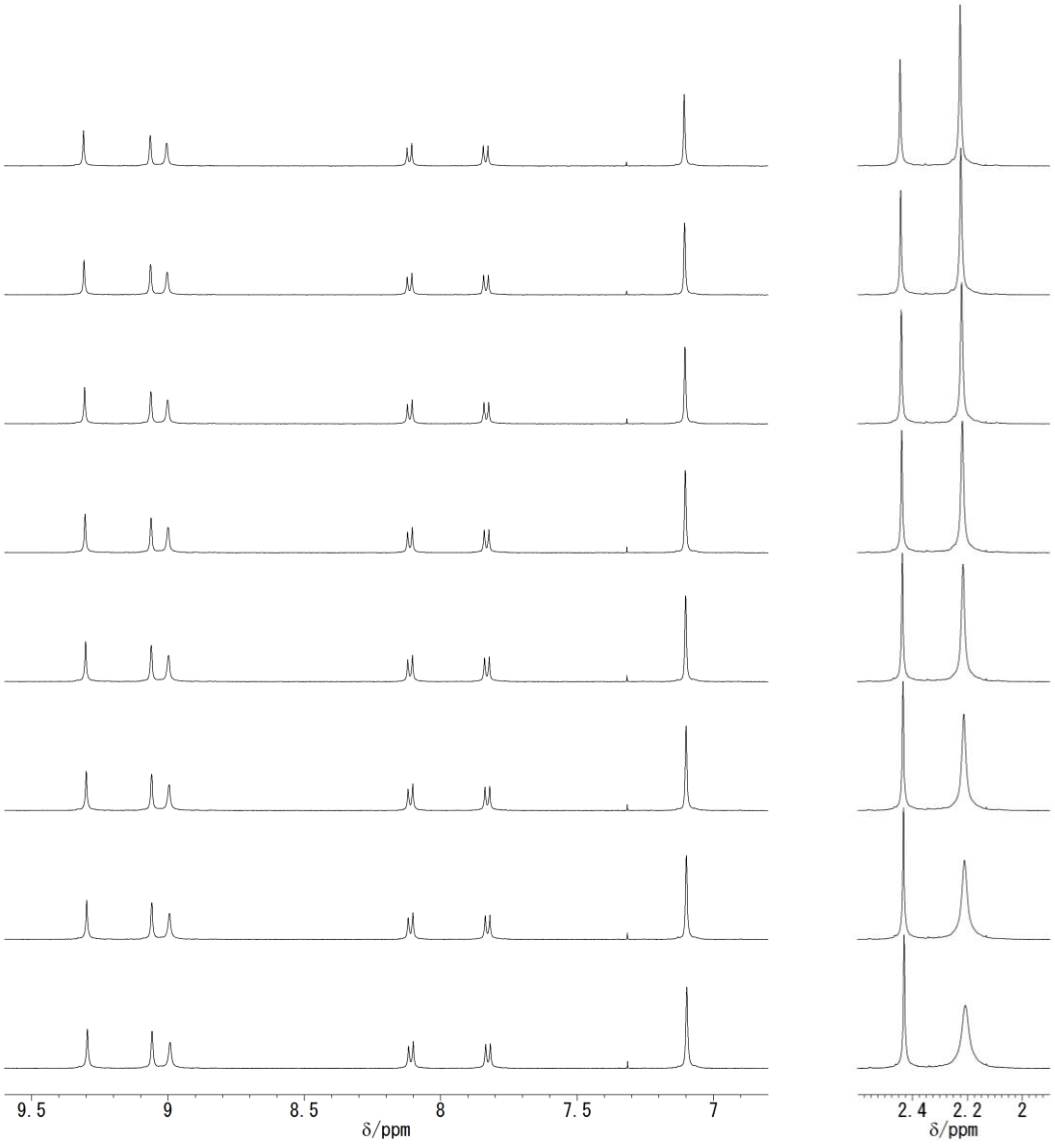


Figure S-12. ^{1}H NMR spectra of cyclic tetramer **1** (500 MHz) in CD_2Cl_2 at various temperatures (25 °C, 20 °C, 15 °C, 10 °C, 5 °C, 0 °C, −5 °C, and −10 °C, respectively, from the top).

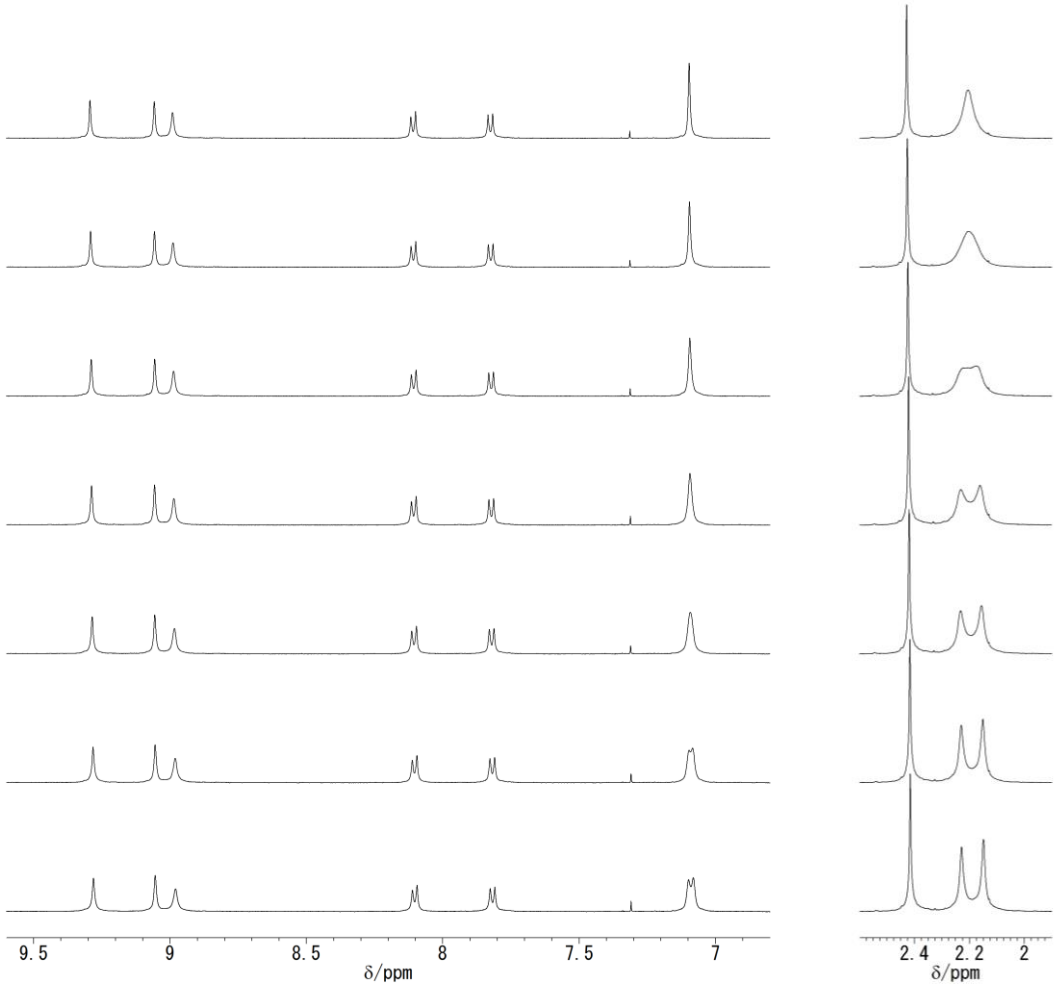


Figure S-13. ^{1}H NMR spectra of cyclic tetramer **1** (500 MHz) in CD_2Cl_2 at various temperatures (−15 °C, −20 °C, −25 °C, −30 °C, −35 °C, −40 °C, and −45 °C, respectively, from the top).

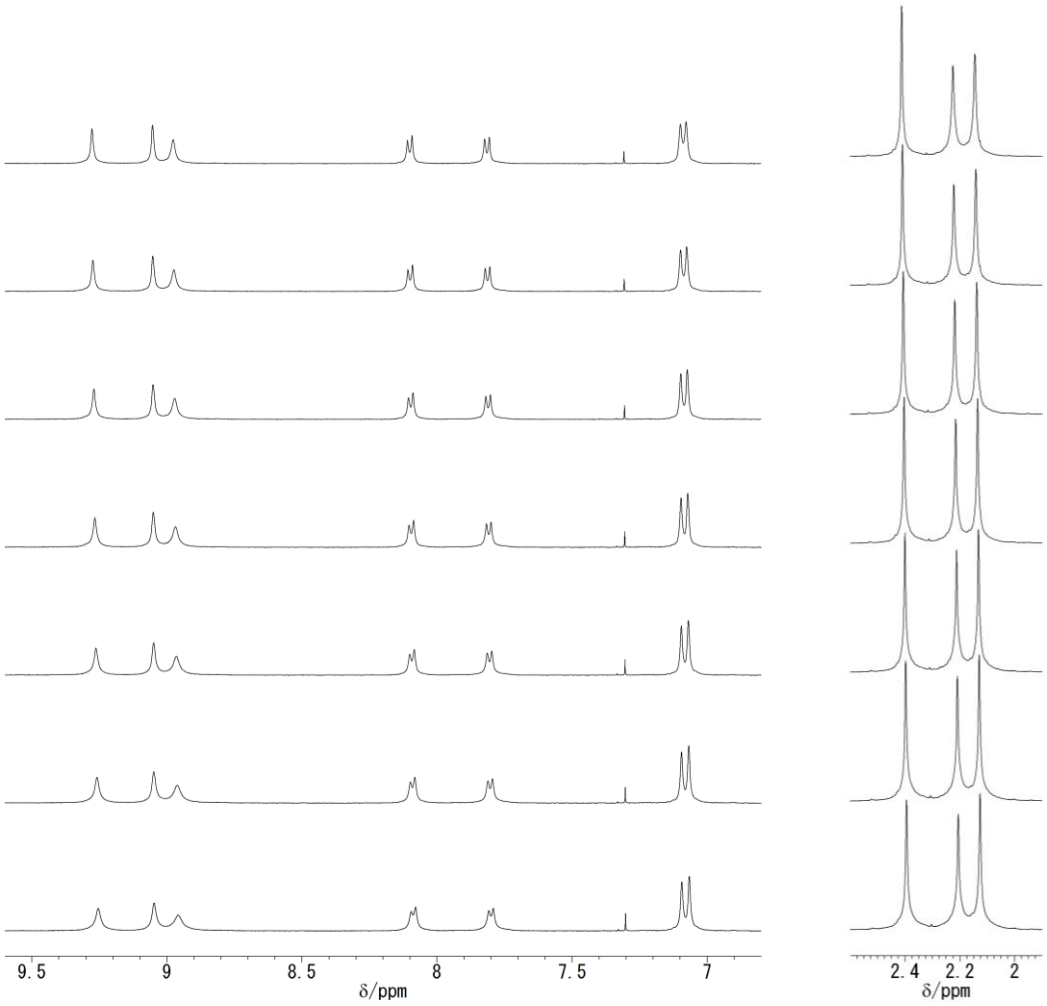


Figure S-14. ^{1}H NMR spectra of cyclic tetramer **1** (500 MHz) in CD_2Cl_2 at various temperatures (−50 °C, −55 °C, −60 °C, −65 °C, −70 °C, −75 °C, and −80 °C, respectively, from the top).

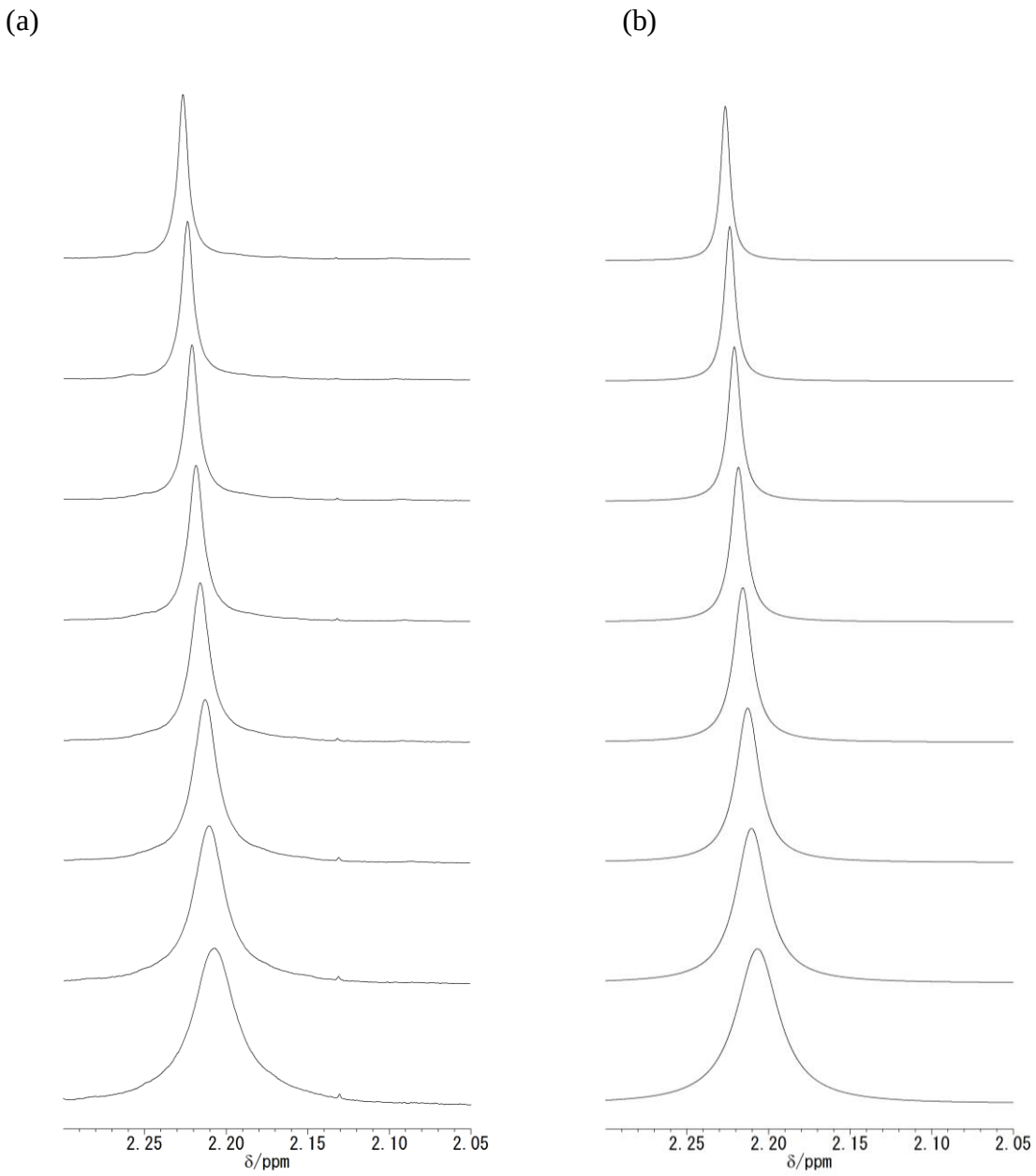


Figure S-15. ^{1}H NMR spectra of cyclic tetramer **1** (500 MHz, (a) observed spectra, (b) calculated spectra of the methyl proton signals at 2,6-positions in the mesityl group) in CD_2Cl_2 at various temperatures (25 °C, 20 °C, 15 °C, 10 °C, 5 °C, 0 °C, −5 °C, and −10 °C, respectively, from the top).

(a) (b)

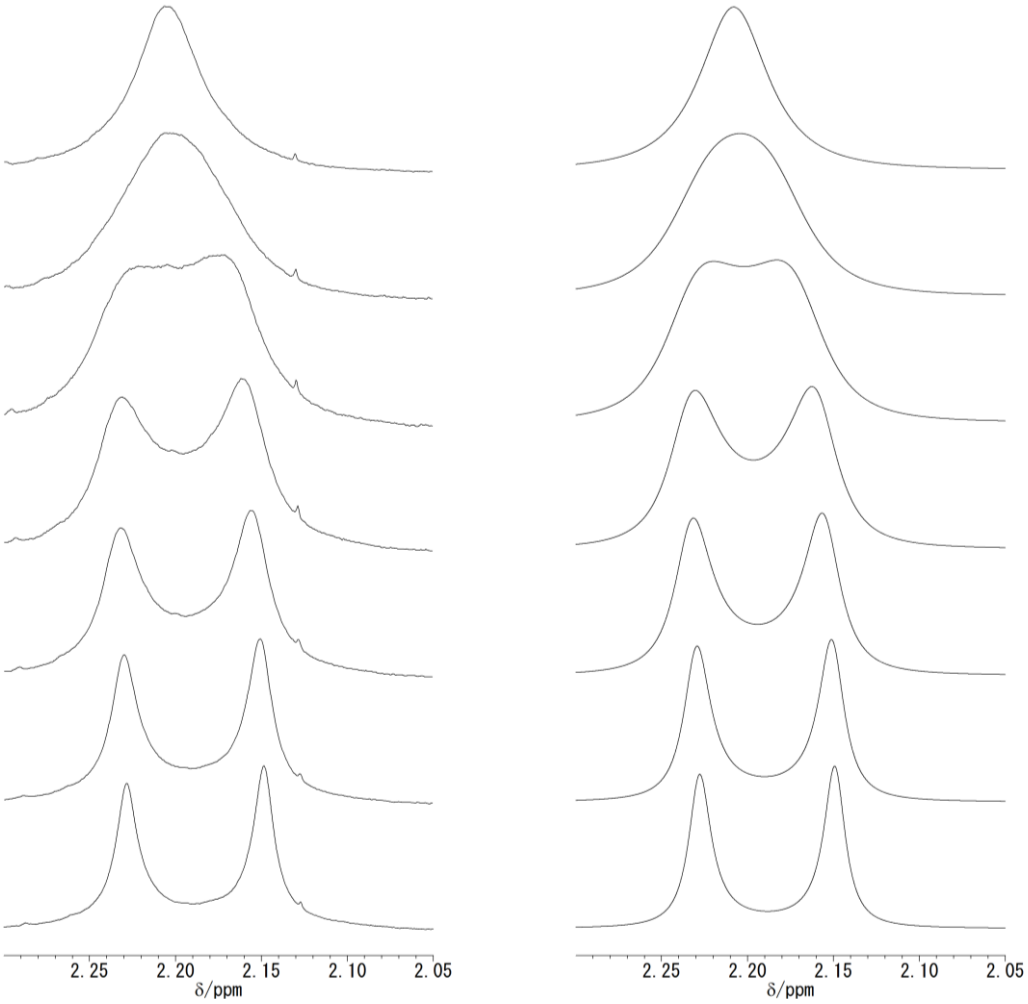


Figure S-16. ^{1}H NMR spectra of cyclic tetramer **1** (500 MHz, (a) observed spectra, (b) calculated spectra of the methyl proton signals at 2,6-positions in the mesityl group) in CD_2Cl_2 at various temperatures (−15 °C, −20 °C, −25 °C, −30 °C, −35 °C, −40 °C, and −45 °C, respectively, from the top).

(a) (b)

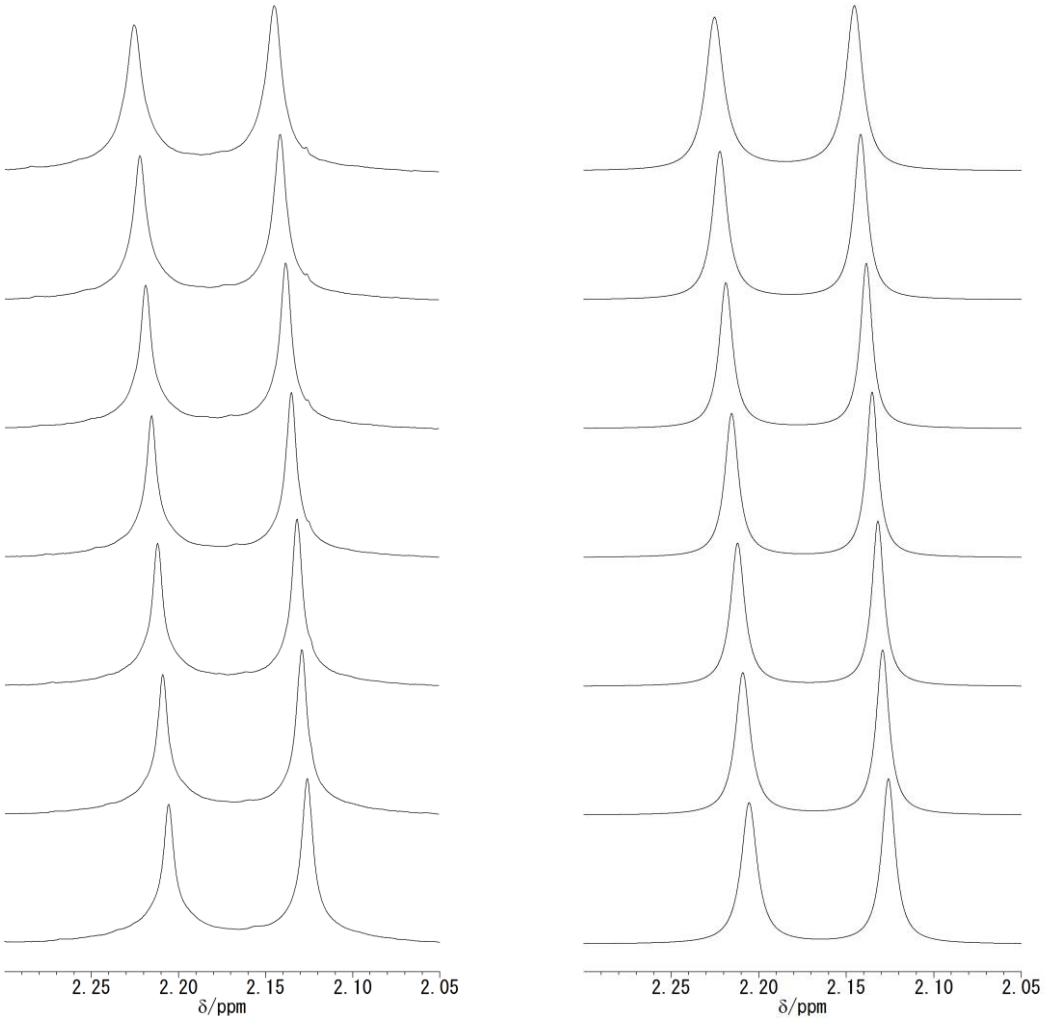


Figure S-17. ^{1}H NMR spectra of cyclic tetramer **1** (500 MHz, (a) observed spectra, (b) calculated spectra of the methyl proton signals at 2,6-positions in the mesityl group) in CD_2Cl_2 at various temperatures (−50 °C, −55 °C, −60 °C, −65 °C, −70 °C, −75 °C, and −80 °C, respectively, from the top).

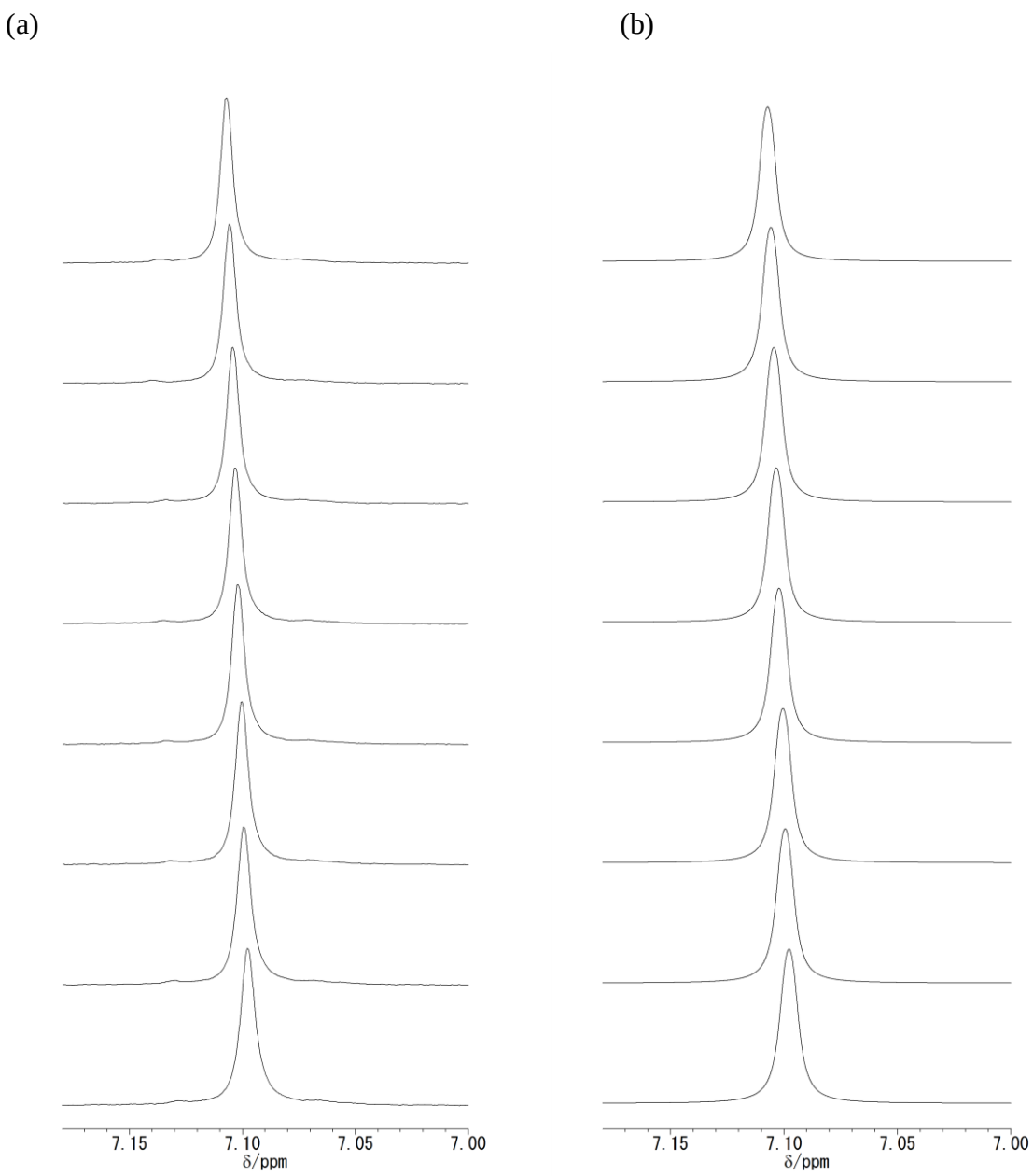


Figure S-18. ^{1}H NMR spectra of cyclic tetramer **1** (500 MHz, (a) observed spectra, (b) calculated spectra of the aromatic proton signals at 3,5-positions in the mesityl group) in CD_2Cl_2 at various temperatures (25 °C, 20 °C, 15 °C, 10 °C, 5 °C, 0 °C, −5 °C, and −10 °C, respectively, from the top).

(a) (b)

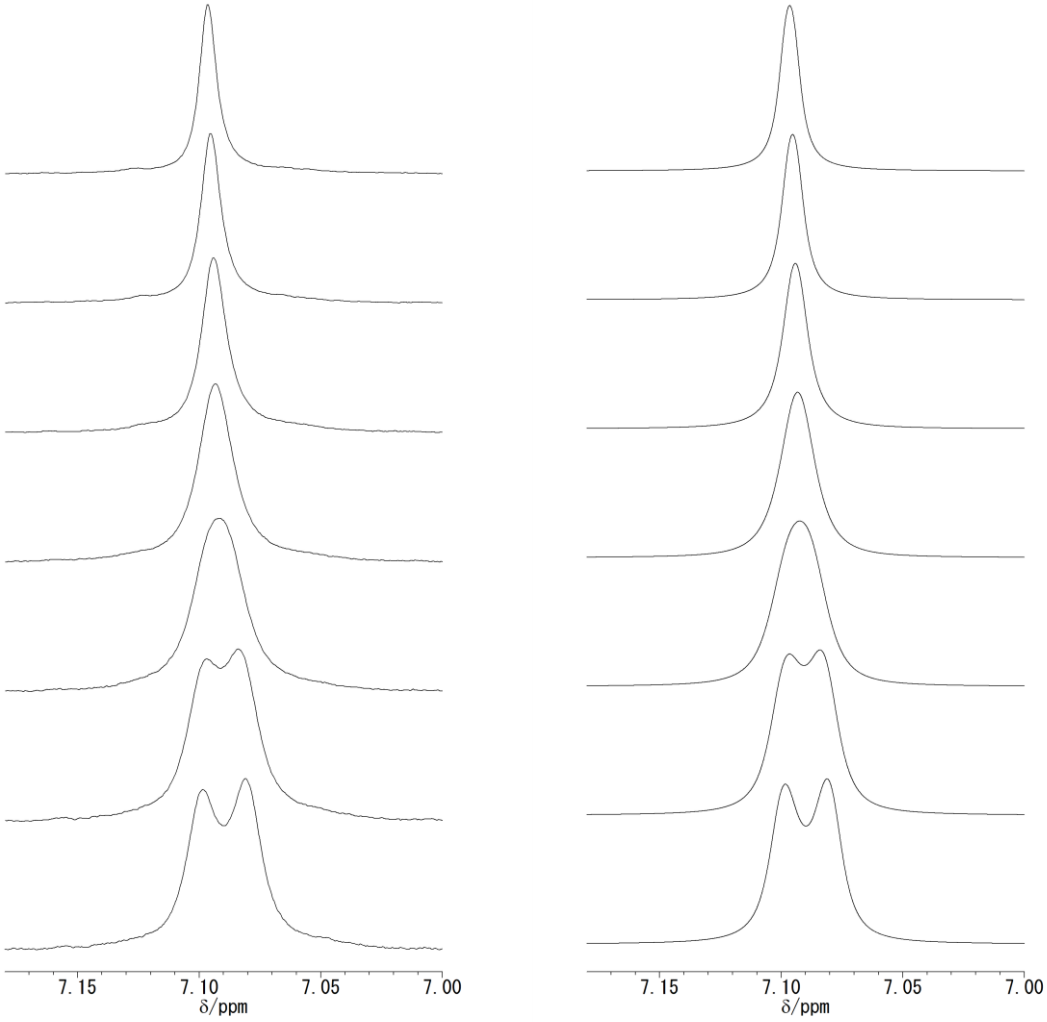


Figure S-19. ^{1}H NMR spectra of cyclic tetramer **1** (500 MHz, (a) observed spectra, (b) calculated spectra of the aromatic proton signals at 3,5-positions in the mesityl group) in CD_2Cl_2 at various temperatures (−15 °C, −20 °C, −25 °C, −30 °C, −35 °C, −40 °C, and −45 °C, respectively, from the top).

(a) (b)

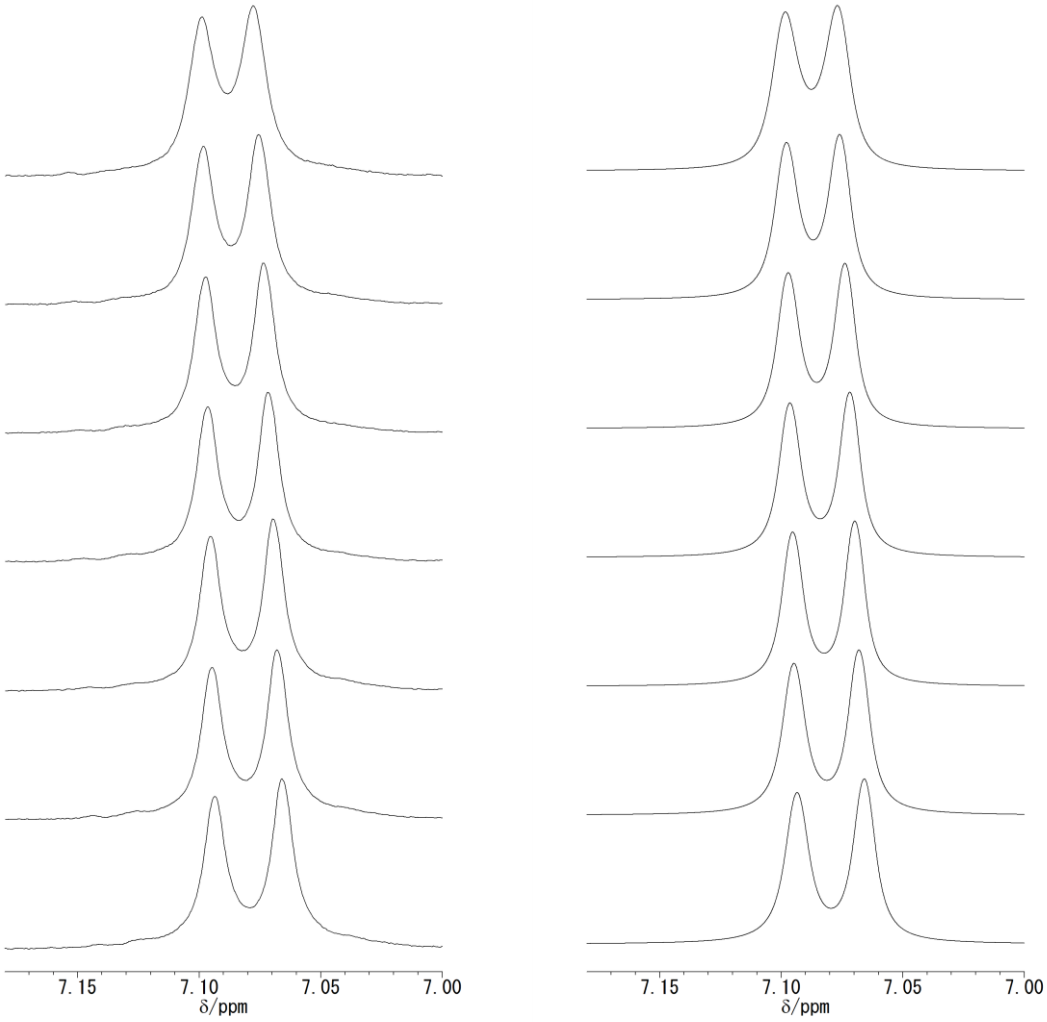


Figure S-20. ^{1}H NMR spectra of cyclic tetramer **1** (500 MHz, (a) observed spectra, (b) calculated spectra of the aromatic proton signals at 3,5-positions in the mesityl group) in CD_2Cl_2 at various temperatures (−15 °C, −20 °C, −25 °C, −30 °C, −35 °C, −40 °C, and −45 °C, respectively, from the top).

Table S-6. Rate Data[a] Determined by Line Shape Analysis for Cyclic Tetramer **1**

Temperature (°C)	Rate Constants (s^{-1}) calcd. by methyl signals	Rate Constants (s^{-1}) calcd. by aromatic signals
-80	1	0
-75	1	0
-70	1	0
-65	1	0.5
-60	1.6	1.5
-55	3.5	2.8
-50	7.5	6
-45	13	8.5
-40	18	12
-35	30	20
-30	45	30
-25	76	55
-20	100	100
-15	150	150
-10	220	200
-5	310	300
0	460	400
5	660	600
10	980	800
15	1500	1100
20	2500	1500
25	4000	2000

[a] The rate data presented by red characters were used to the calculations for the kinetic data.

Table S-7. Kinetic Data Calculated by the Rate Data for Cyclic Tetramer **1**

Sample	$\Delta H^{\neq}$ /kcal mol^{-1}	$\Delta S^{\neq}$ /cal mol^{-1} K^{-1}	$\Delta G^{\neq}_{20}$ /kcal mol^{-1}
1	10.3 ± 0.1	–8.3 ± 0.6	**12.8 ± 0.2**

(7) Temperature Dependency of ^{1}H NMR and Kinetic Data of Cyclic Trimer 2

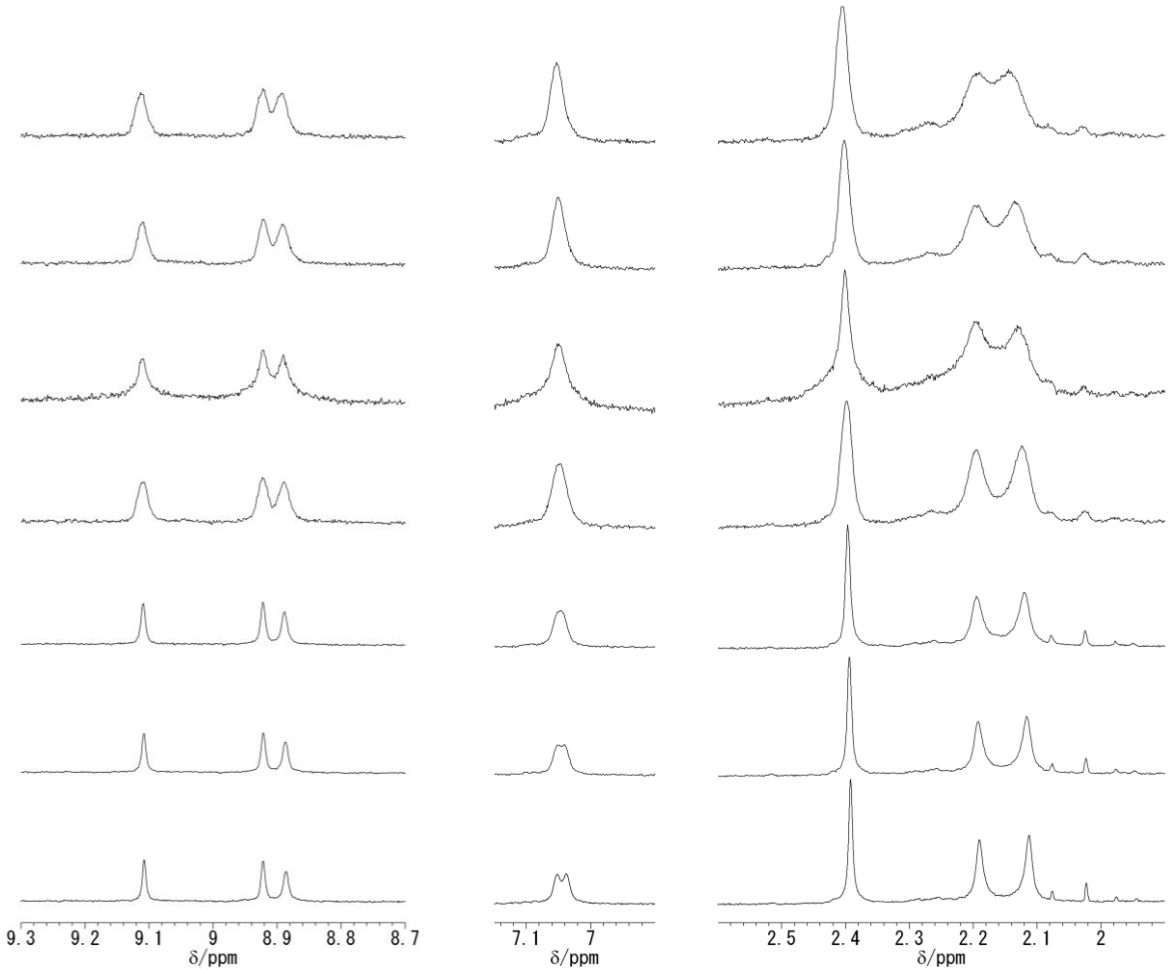


Figure S-21. ^{1}H NMR spectra of cyclic trimer **2** (500 MHz) in $(CDCl_2)_2$ at various temperatures (120 ℃, 115 ℃, 110 ℃, 105 ℃, 100 ℃, 95 ℃, and 90 ℃, respectively, from the top).

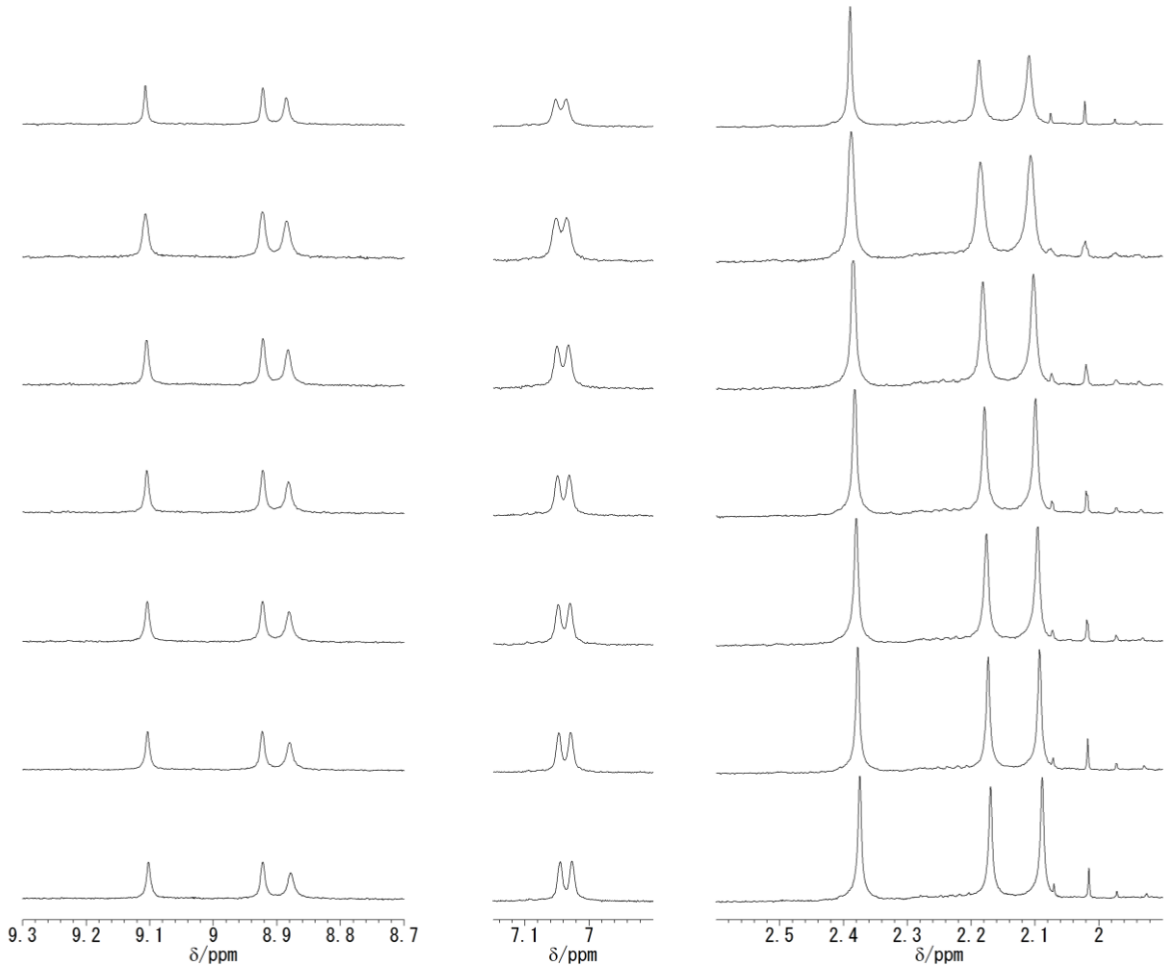


Figure S-22. ^{1}H NMR spectra of cyclic trimer **2** (500 MHz) in $(CDCl_2)_2$ at various temperatures (85 °C, 80 °C, 75 °C, 70 °C, 65 °C, 60 °C, and 55 °C, respectively, from the top).

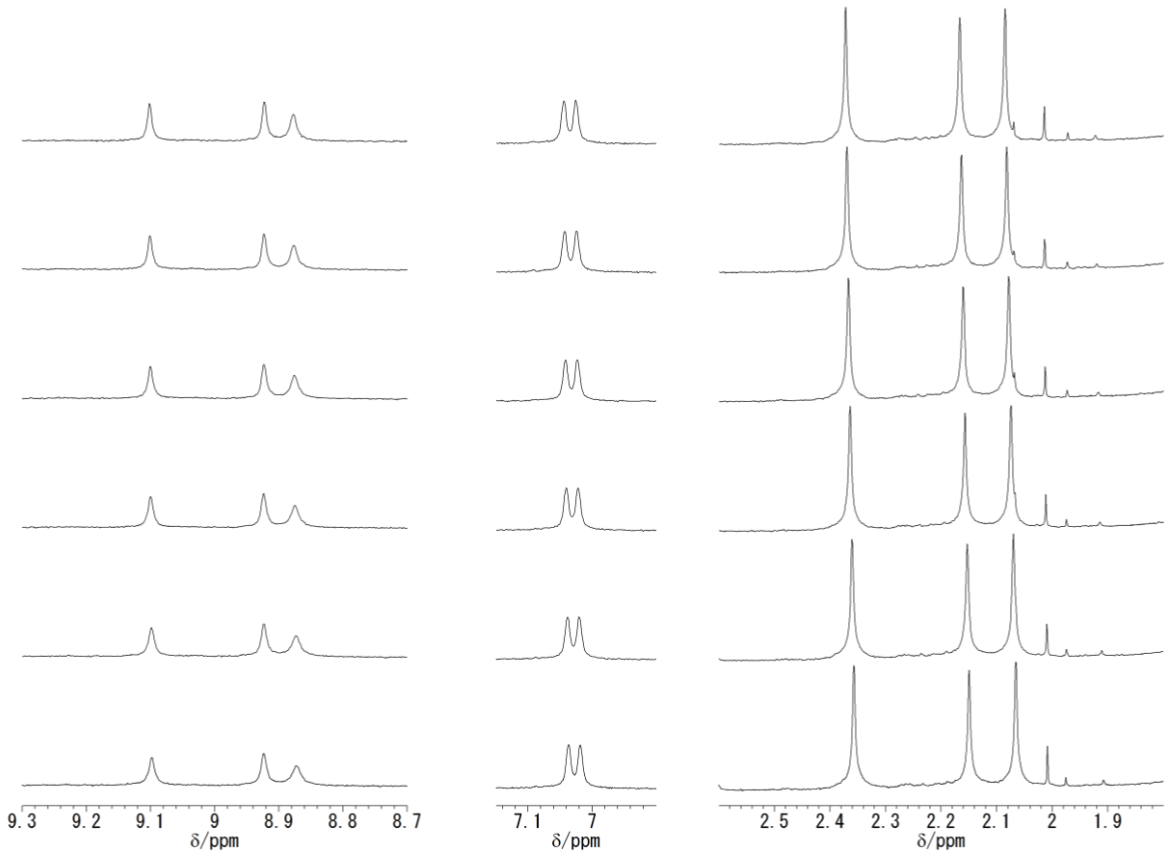


Figure S-23. ^{1}H NMR spectra of cyclic trimer **2** (500 MHz) in $(CDCl_2)_2$ at various temperatures (50 °C, 45 °C, 40 °C, 35 °C, 30 °C, and 25 °C, respectively, from the top).

(a) (b)

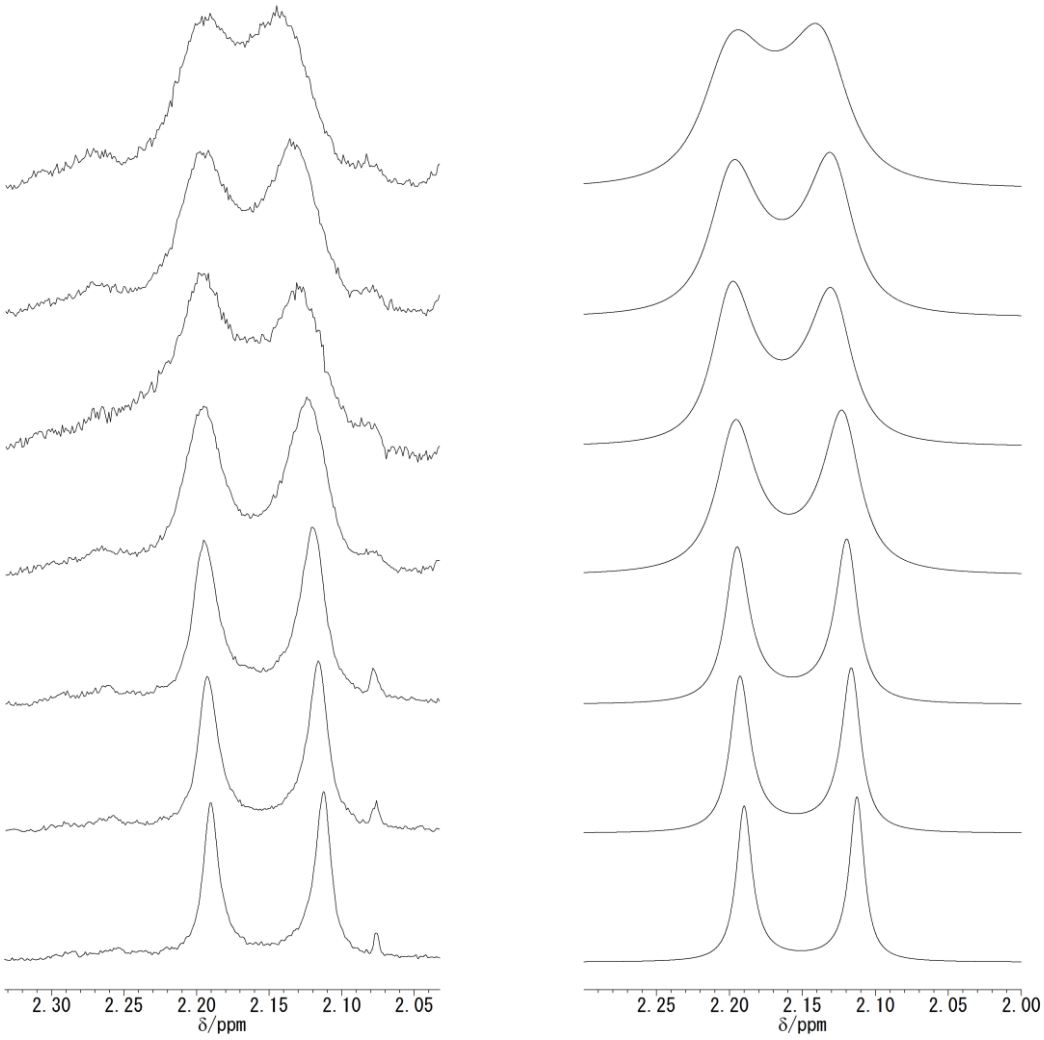


Figure S-24. ^{1}H NMR spectra of cyclic trimer **2** (500 MHz, (a) observed spectra, (b) calculated spectra of the methyl proton signals at 2,6-positions in the mesityl group) in $(CDCl_2)_2$ at various temperatures (120 °C, 115 °C, 110 °C, 105 °C, 100 °C, 95 °C, and 90 °C, respectively, from the top).

(a) (b)

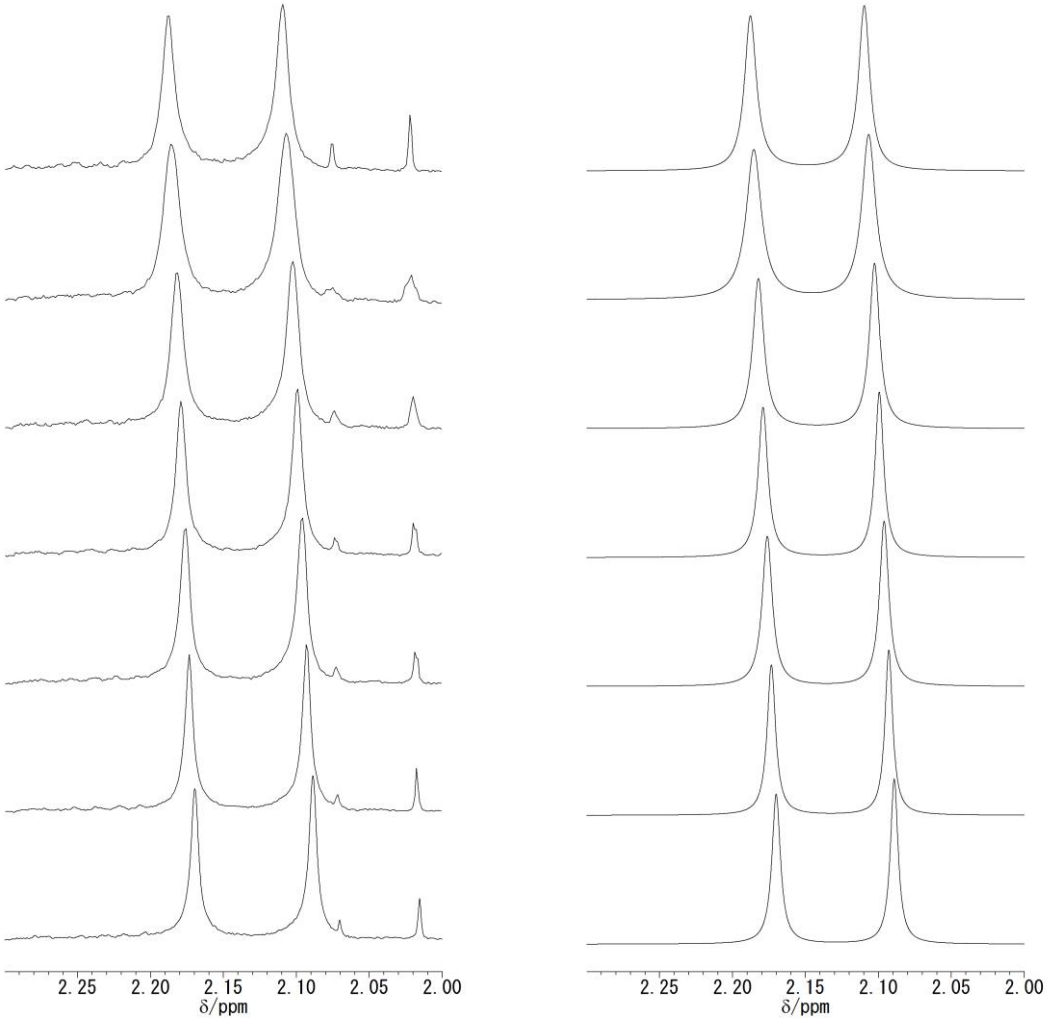


Figure S-25. ^{1}H NMR spectra of cyclic trimer **2** (500 MHz, (a) observed spectra, (b) calculated spectra of the methyl proton signals at 2,6-positions in the mesityl group) in $(CDCl_2)_2$ at various temperatures (85 ℃, 80 ℃, 75 ℃, 70 ℃, 65 ℃, 60 ℃, and 55 ℃, respectively, from the top).

(a) (b)

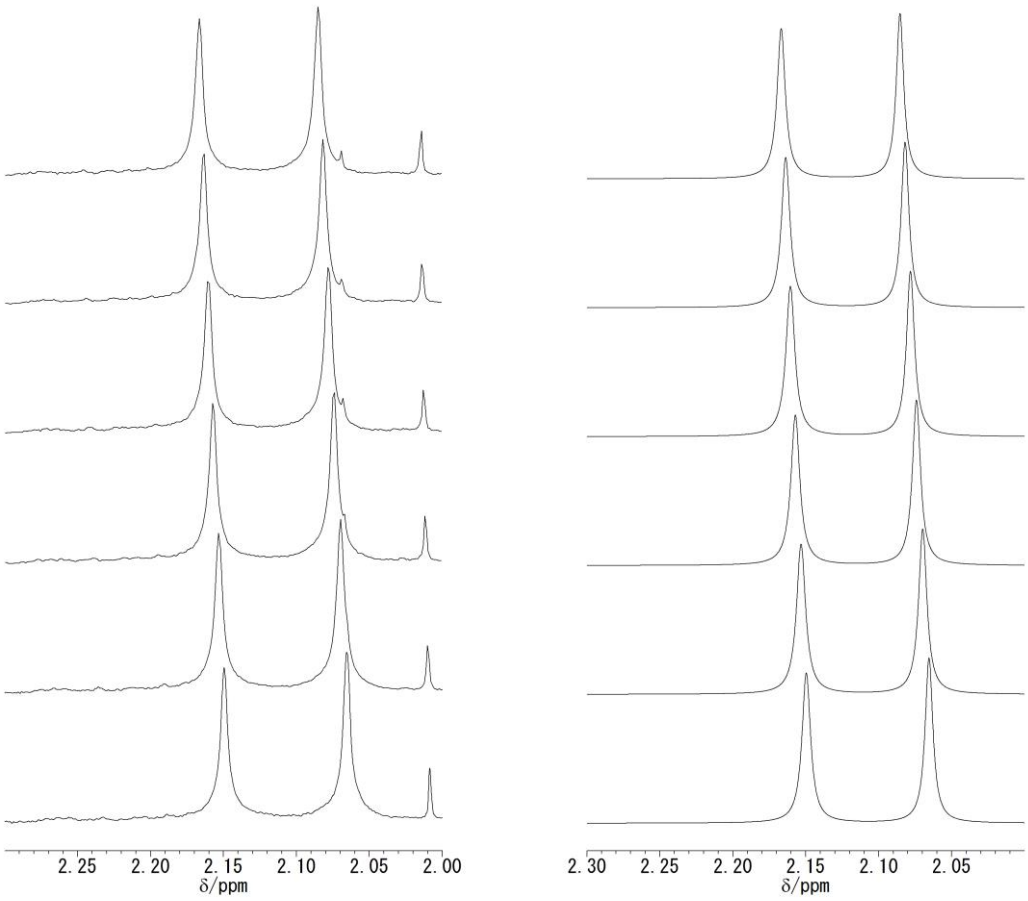


Figure S-26. ^{1}H NMR spectra of cyclic trimer **2** (500 MHz, (a) observed spectra, (b) calculated spectra of the methyl proton signals at 2,6-positions in the mesityl group) in $(CDCl_2)_2$ at various temperatures (50 ℃, 45 ℃, 40 ℃, 35 ℃, 30 ℃, and 25 ℃, respectively, from the top).

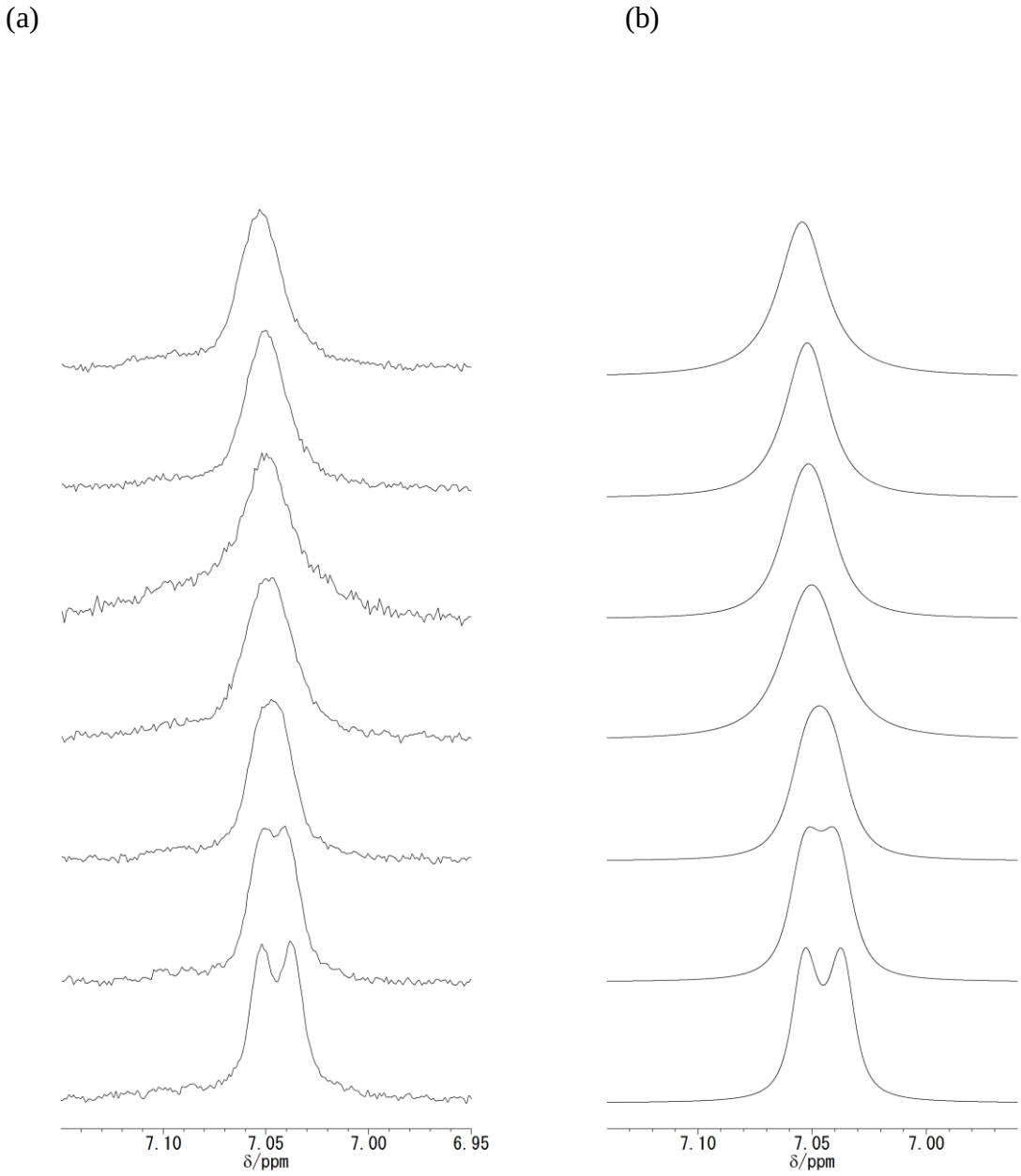


Figure S-27. ^{1}H NMR spectra of cyclic trimer **2** (500 MHz, (a) observed spectra, (b) calculated spectra of the aromatic proton signals at 3,5-positions in the mesityl group) in $(CDCl_2)_2$ at various temperatures (120 °C, 115 °C, 110 °C, 105 °C, 100 °C, 95 °C, and 90 °C, respectively, from the top).

(a) (b)

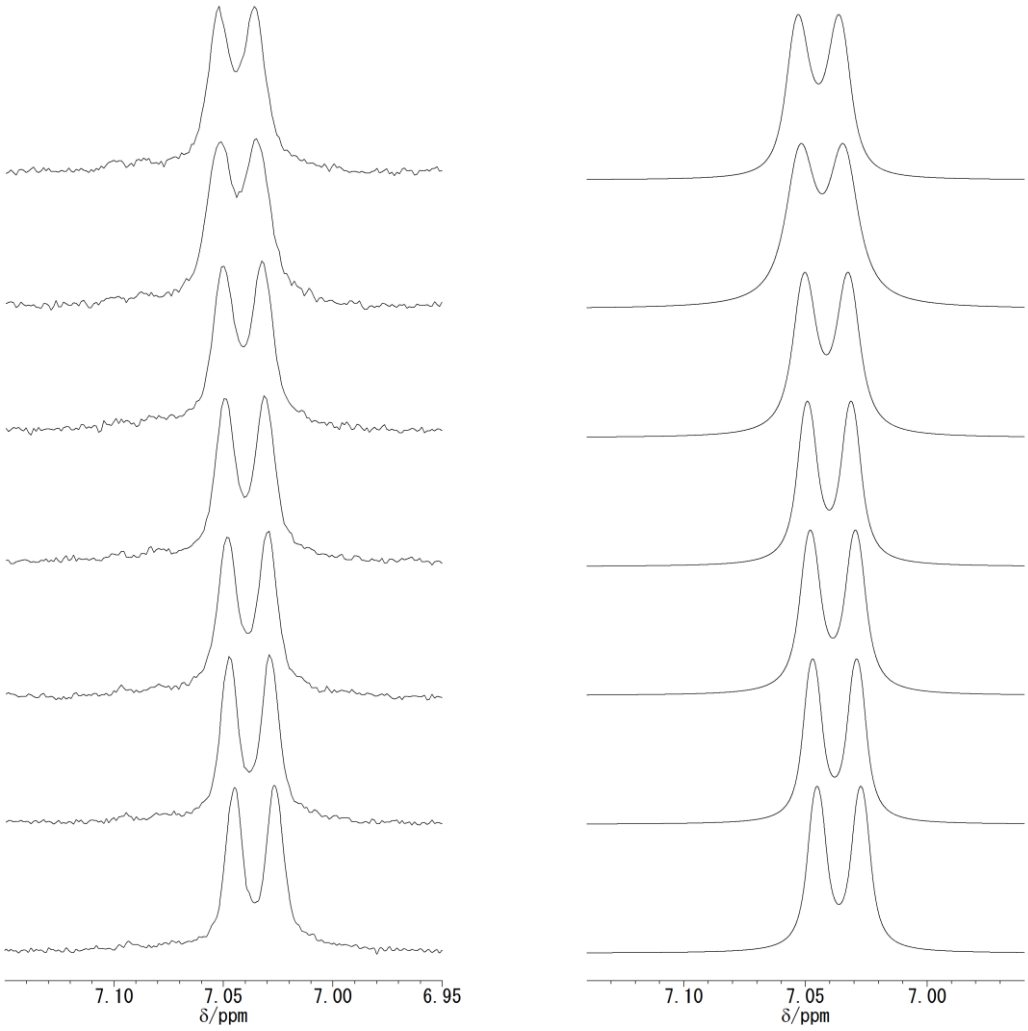


Figure S-28. ^{1}H NMR spectra of cyclic trimer **2** (500 MHz, (a) observed spectra, (b) calculated spectra of the aromatic proton signals at 3,5-positions in the mesityl group) in $(CDCl_2)_2$ at various temperatures (85 ℃, 80 ℃, 75 ℃, 70 ℃, 65 ℃, 60 ℃, and 55 ℃, respectively, from the top).

(a) (b)

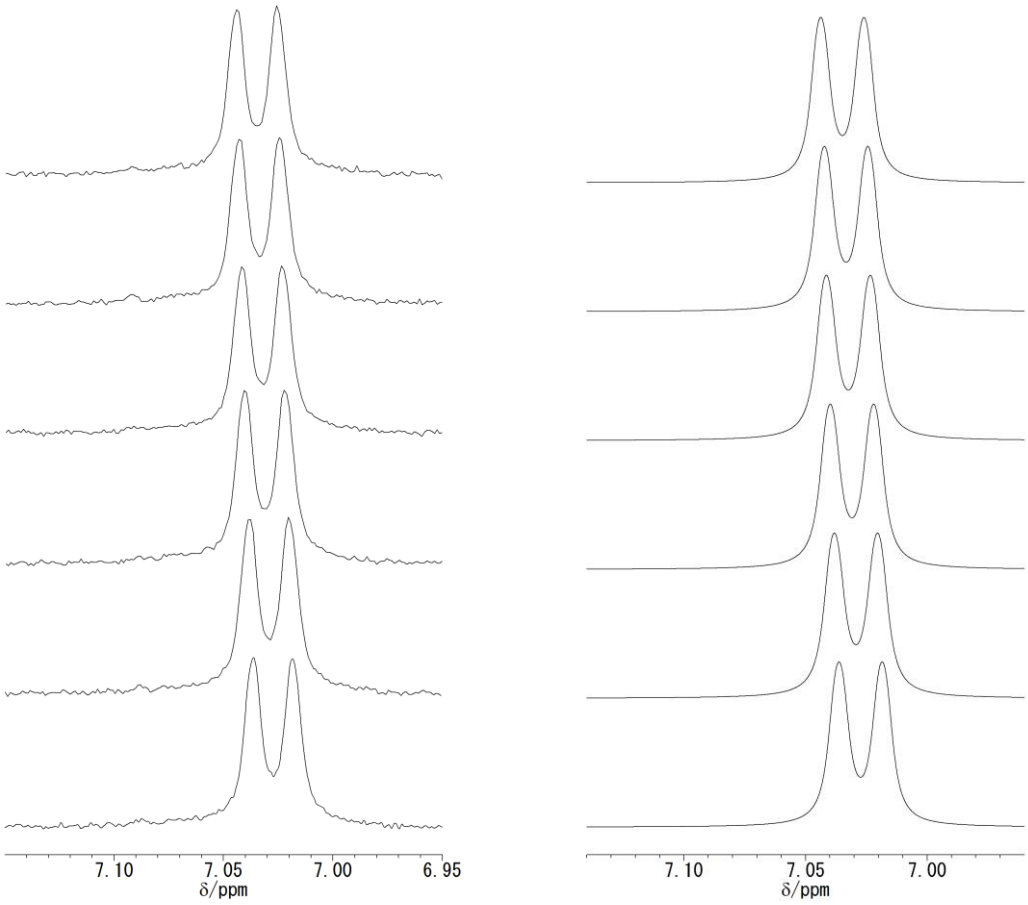


Figure S-29. ^{1}H NMR spectra of cyclic trimer **2** (500 MHz, (a) observed spectra, (b) calculated spectra of the aromatic proton signals at 3,5-positions in the mesityl group) in $(CDCl_2)_2$ at various temperatures (50 ℃, 45 ℃, 40 ℃, 35 ℃, 30 ℃, and 25 ℃, respectively, from the top).

Table S-8. Rate Data[a] Determined by Line Shape Analysis for Cyclic Trimer **2**

Temperature (°C)	Rate Constants (s^{-1}) calcd. by methyl signals	Rate Constants (s^{-1}) calcd. by aromatic signals
25	0	0
30	0	0
35	0	0
40	0	0
45	0	0
50	0	0
55	0	0
60	0	0
65	0	0
70	0	0
75	0	1.5
80	0	2
85	5	5
90	8	7
95	12	12
100	15	18
105	20	23
110	35	23
115	35	35
120	48	50

[a] The rate data presented by red characters were used to the calculations for the kinetic data.

Table S-9. Kinetic Data Calculated by the Rate Data for Cyclic Trimer **2**

Sample	$\Delta H^{\neq}$ /kcal mol^{-1}	$\Delta S^{\neq}$ /cal mol^{-1} K^{-1}	$\Delta G^{\neq}_{20}$ /kcal mol^{-1}
2	16.6 ± 1.1	–9.1 ± 3.0	**19.2 ± 1.4**

(8) Temperature Dependency of ^{1}H NMR and Kinetic Data of Major Isomer 20

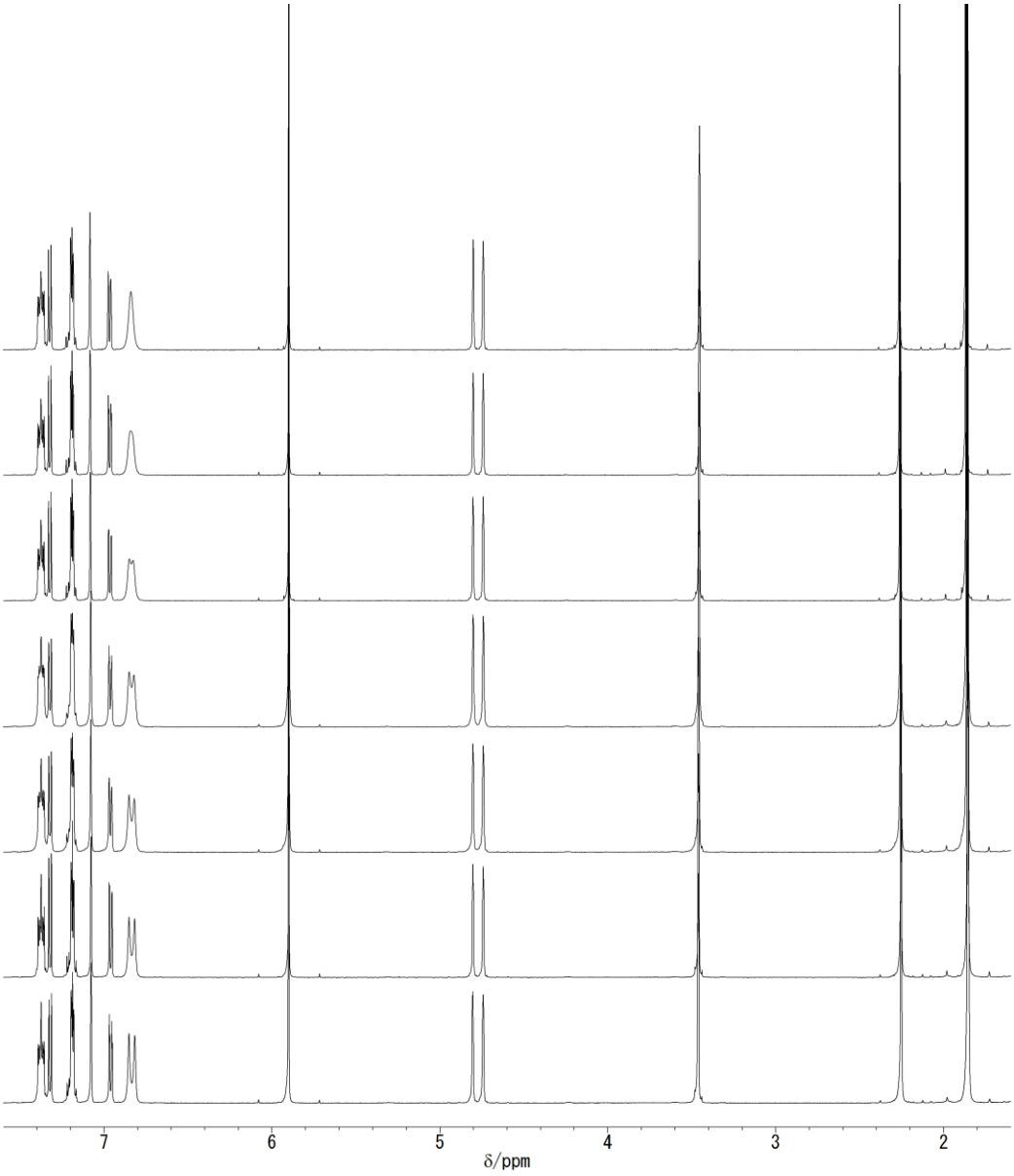


Figure S-30. ^{1}H NMR spectra of *anti*-2-mesityl-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylic anhydride (major isomer **20**) (500 MHz) in $(CDCl_2)_2$ at various temperatures (120 °C, 115 °C, 110 °C, 105 °C, 100 °C, 95 °C, and 90 °C, respectively, from the top).

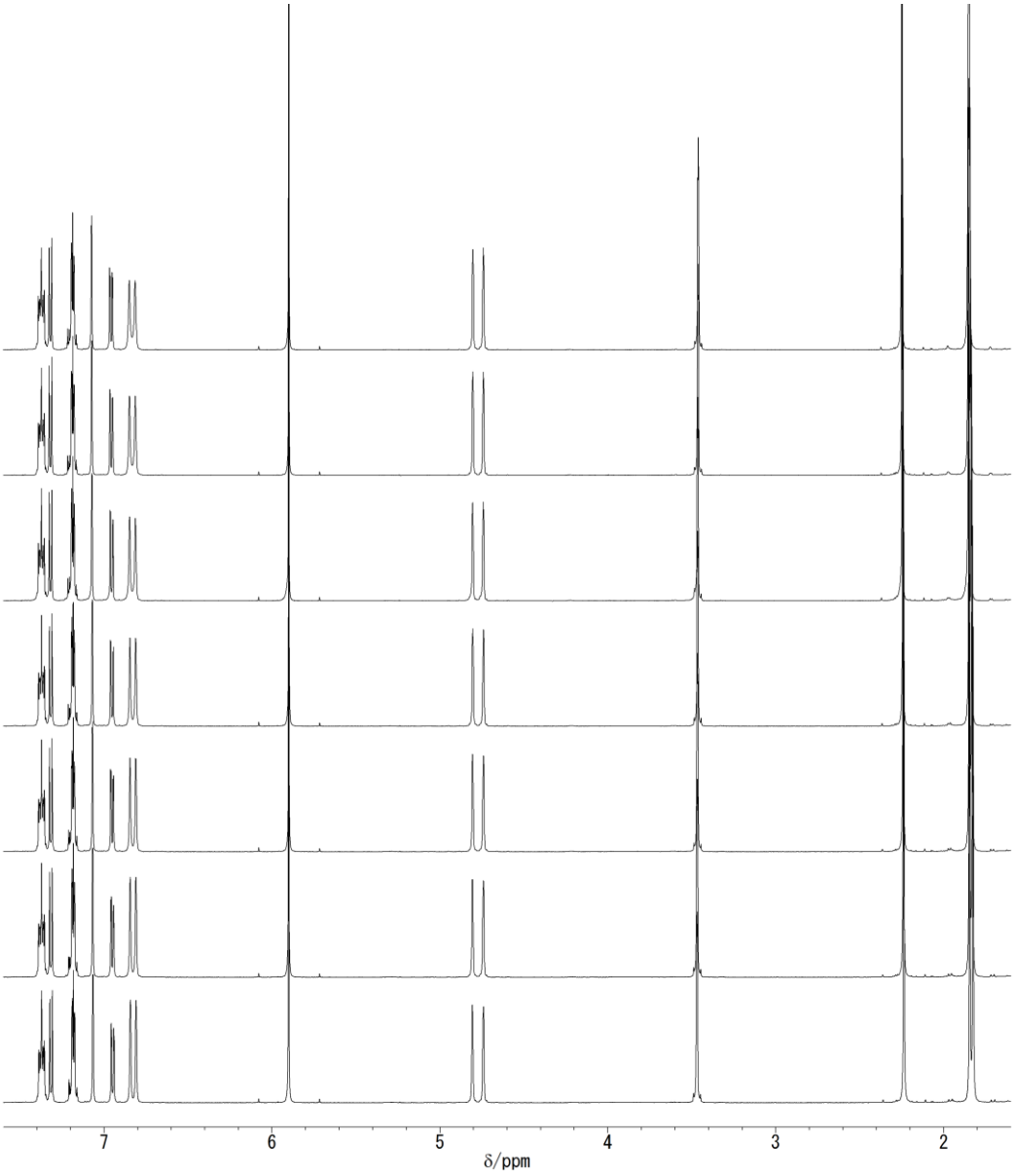


Figure S-31. ^{1}H NMR spectra of *anti*-2-mesityl-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylic anhydride (major isomer **20**) (500 MHz) in $(CDCl_2)_2$ at various temperatures (85 °C, 80 °C, 75 °C, 70 °C, 65 °C, 60 °C, and 55 °C, respectively, from the top).

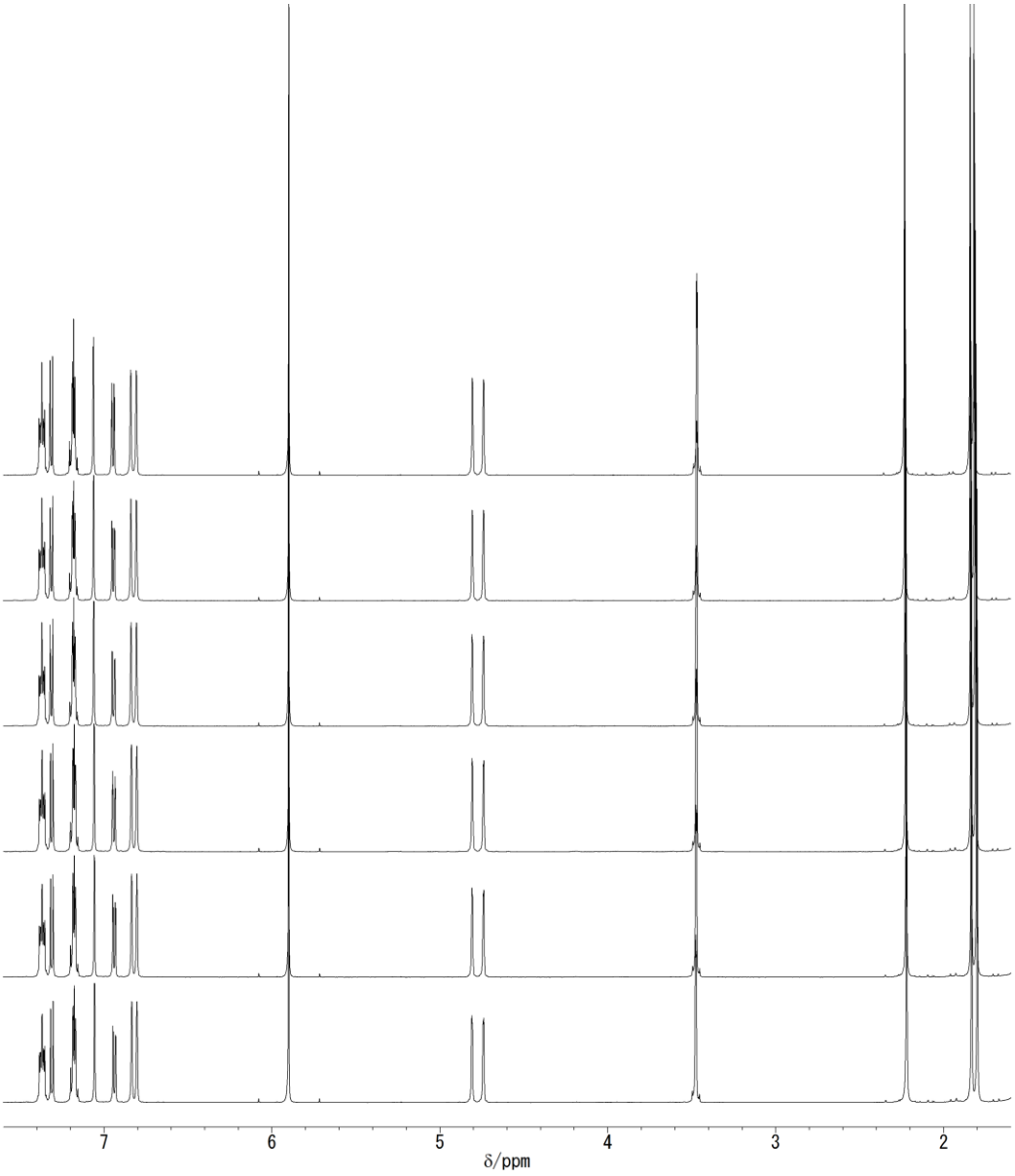


Figure S-32. ^{1}H NMR spectra of *anti*-2-mesityl-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylic anhydride (major isomer **20**) (500 MHz) in $(CDCl_2)_2$ at various temperatures (50 °C, 45 °C, 40 °C, 35 °C, 30 °C, and 25 °C, respectively, from the top).

(a) (b)

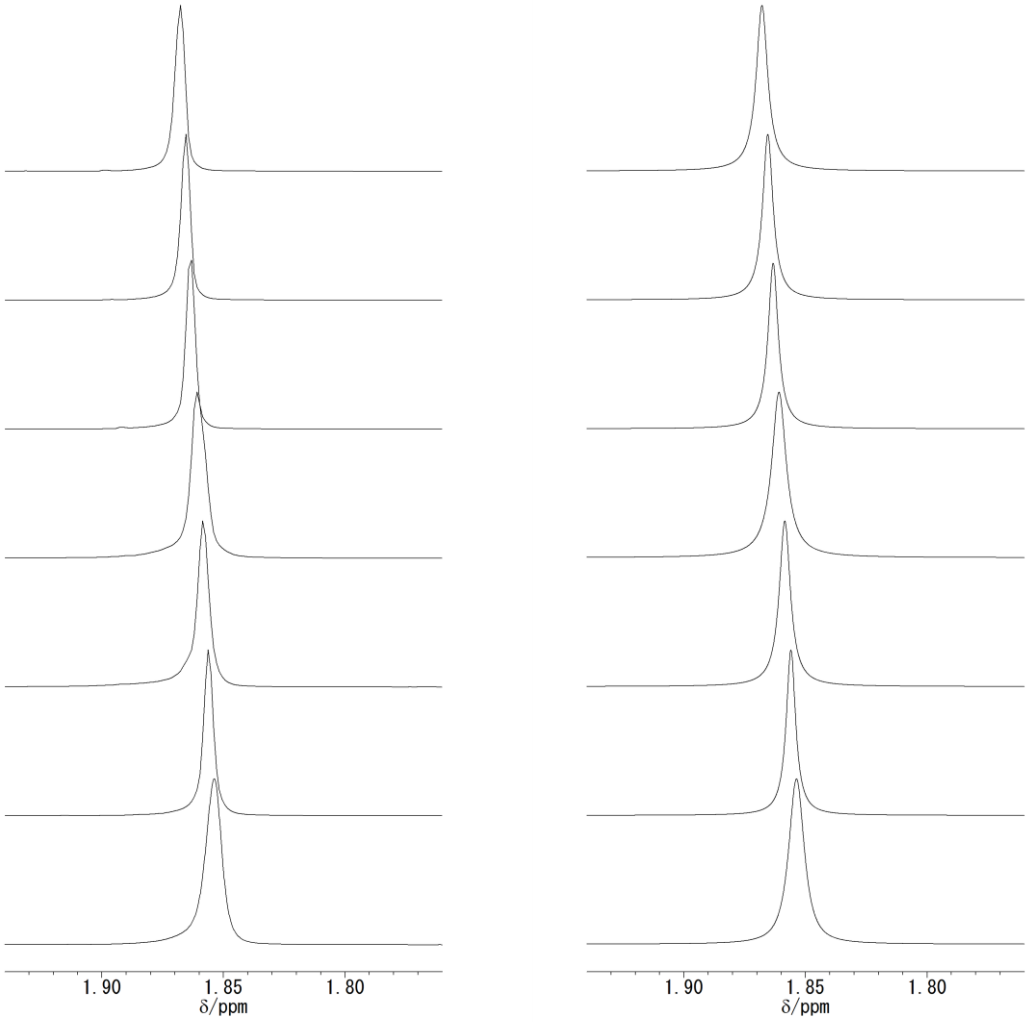


Figure S-33. ^{1}H NMR spectra of *anti*-2-mesityl-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylic anhydride (major isomer **20**) (500 MHz, (a) observed spectra, (b) calculated spectra of the methyl proton signals at 2,6-positions in the mesityl group) in $(CDCl_2)_2$ at various temperatures (120 °C, 115 °C, 110 °C, 105 °C, 100 °C, 95 °C, and 90 °C, respectively, from the top).

(a) (b)

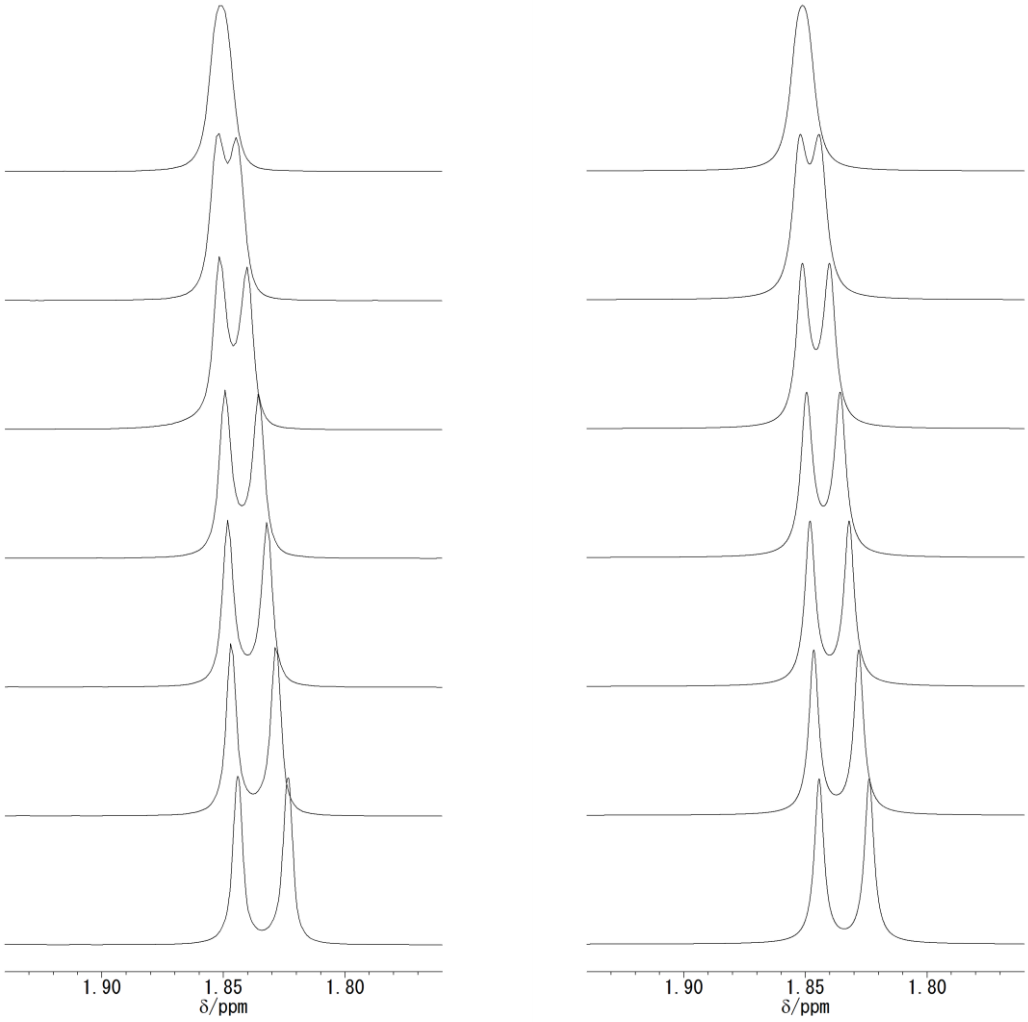


Figure S-34. ^{1}H NMR spectra of *anti*-2-mesityl-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylic anhydride (major isomer **20**) (500 MHz, (a) observed spectra, (b) calculated spectra of the methyl proton signals at 2,6-positions in the mesityl group) in $(CDCl_2)_2$ at various temperatures (85 °C, 80 °C ,75 °C, 70 °C, 65 °C, 60 °C, and 55 °C, respectively, from the top).

(a) (b)

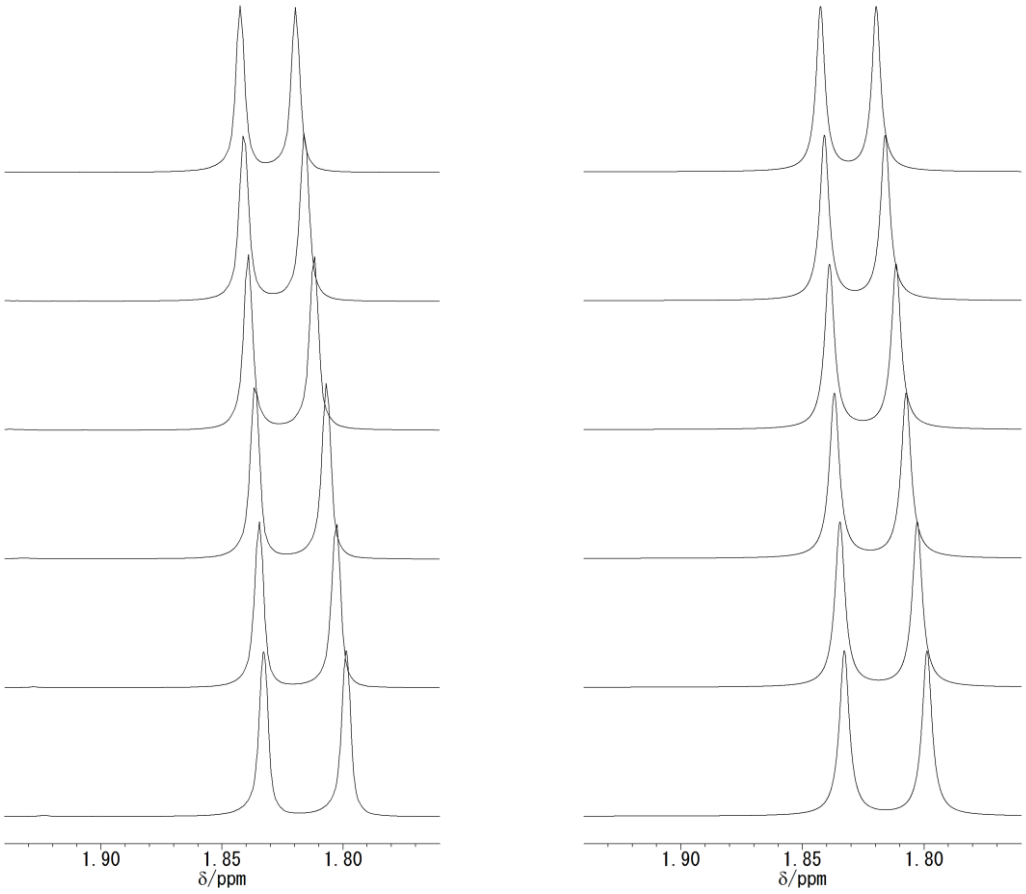


Figure S-35. ^{1}H NMR spectra of *anti*-2-mesityl-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylic anhydride (major isomer **20**) (500 MHz, (a) observed spectra, (b) calculated spectra of the methyl proton signals at 2,6-positions in the mesityl group) in $(CDCl_2)_2$ at various temperatures (50 °C, 45 °C, 40 °C, 35 °C, 30 °C, and 25 °C, respectively, from the top).

(a) (b)

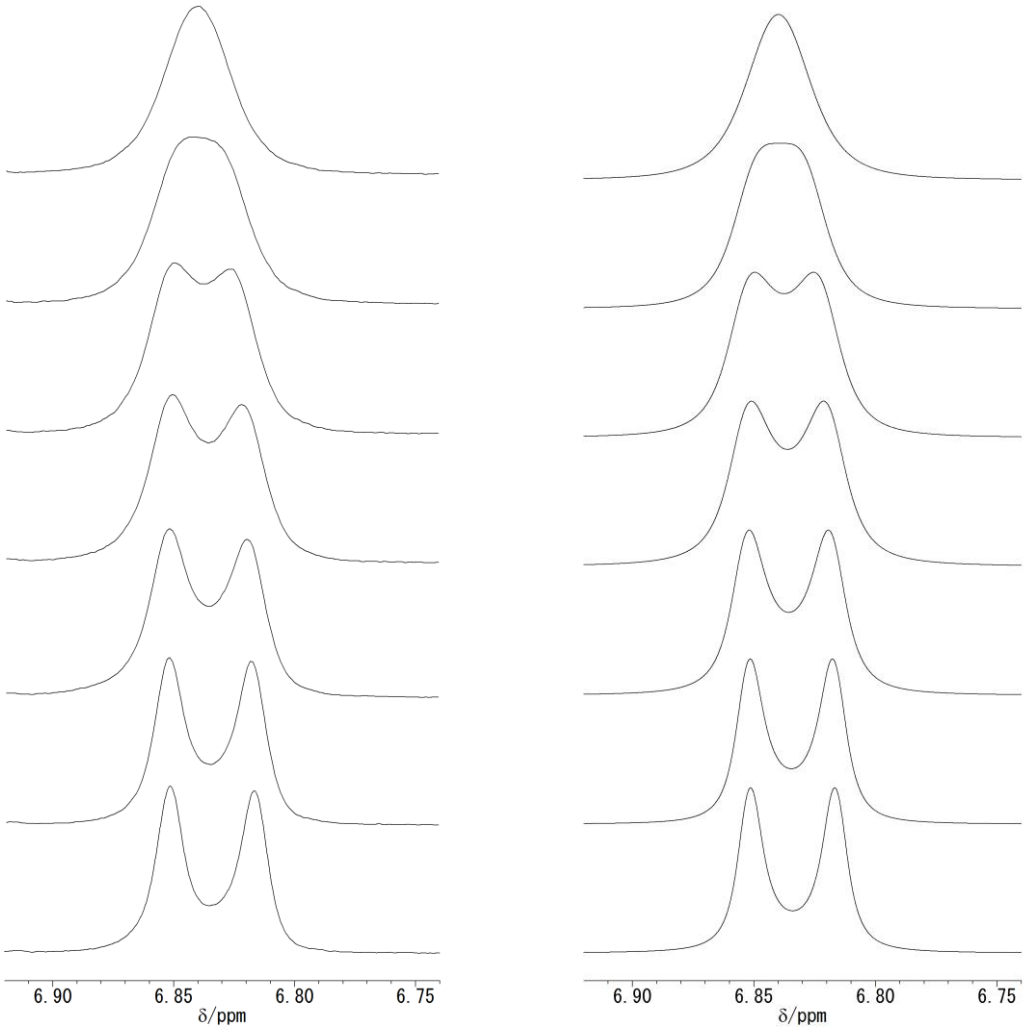


Figure S-36. ^{1}H NMR spectra of *anti*-2-mesityl-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylic anhydride (major isomer **20**) (500 MHz, (a) observed spectra, (b) calculated spectra of the aromatic proton signals at 3,5-positions in the mesityl group) in $(CDCl_2)_2$ at various temperatures (120 °C, 115 °C, 110 °C, 105 °C, 100 °C, 95 °C, and 90 °C, respectively, from the top).

(a) (b)

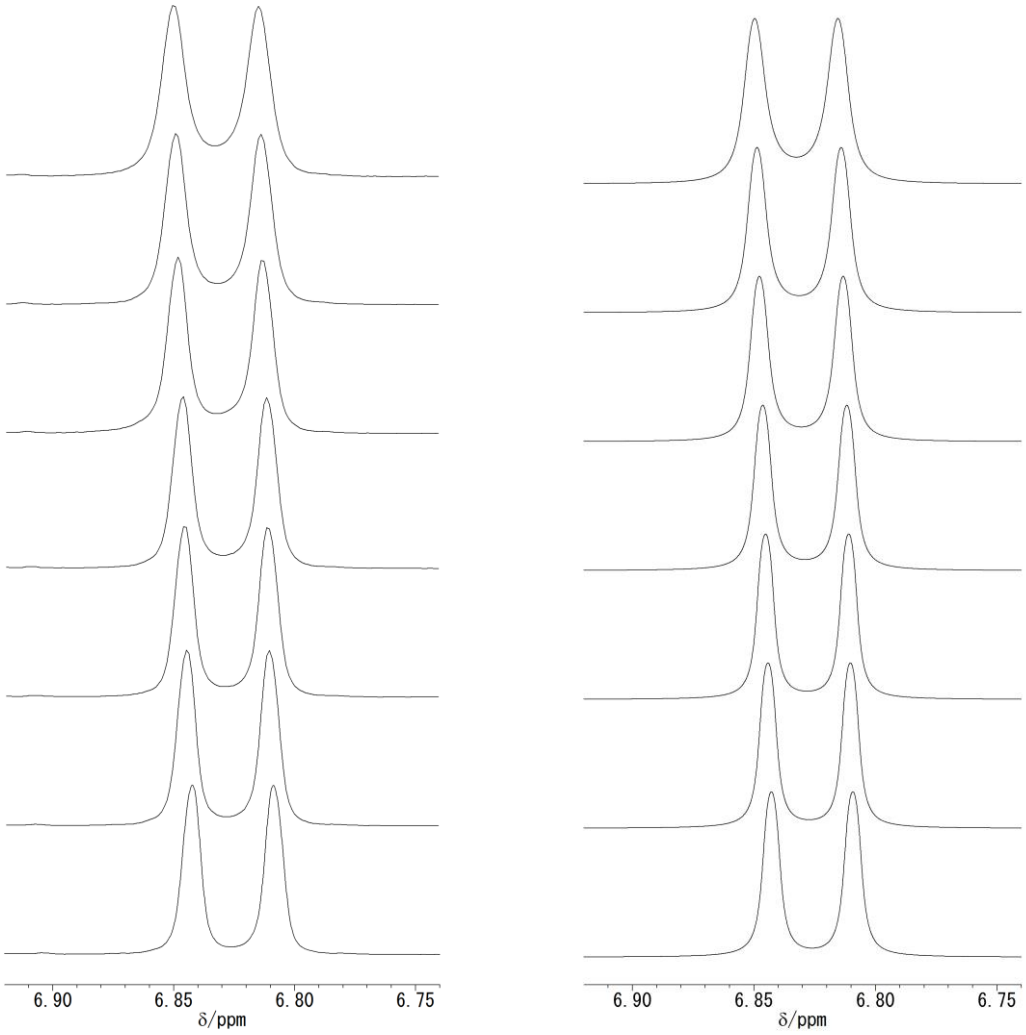


Figure S-37. ^{1}H NMR spectra of *anti*-2-mesityl-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylic anhydride (major isomer **20**) (500 MHz, (a) observed spectra, (b) calculated spectra of the aromatic proton signals at 3,5-positions in the mesityl group) in $(CDCl_2)_2$ at various temperatures (85 °C, 80 °C ,75 °C, 70 °C, 65 °C, 60 °C, and 55 °C, respectively, from the top).

(a) (b)

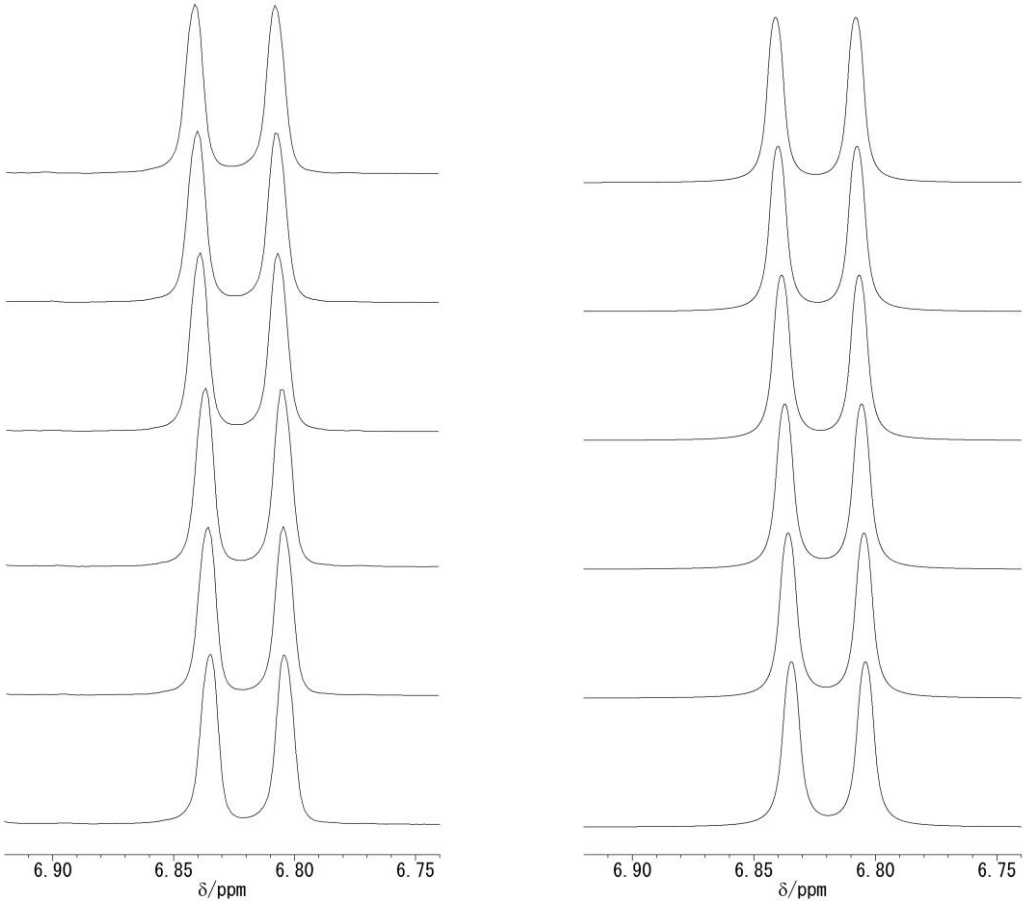


Figure S-38. ^{1}H NMR spectra of *anti*-2-mesityl-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylic anhydride (major isomer **20**) (500 MHz, (a) observed spectra, (b) calculated spectra of the aromatic proton signals at 3,5-positions in the mesityl group) in $(CDCl_2)_2$ at various temperatures (50 °C, 45 °C, 40 °C, 35 °C, 30 °C, and 25 °C, respectively, from the top).

Table S-10. Rate Data[a] Determined by Line Shape Analysis for Major Isomer **20**

Temperature (°C)	Rate Constants (s^{-1}) calcd. by methyl signals	Rate Constants (s^{-1}) calcd. by aromatic signals
25	0	0
30	0	0
35	0	0
40	0	0
45	0	0
50	0	0
55	0	0
60	0.3	0
65	0.9	0
70	1.8	1
75	2.8	2.5
80	4.4	3
85	7	5.5
90	9	8.2
95	20	12
100	30	16
105	40	21
110	50	29
115	60	34
120	70	57

[a] The rate data presented by red characters were used to the calculations for the kinetic data.

Table S-11. Kinetic Data Calculated by the Rate Data for Major Isomer **20**

Sample	$\Delta H^{\neq}$ /kcal mol^{-1}	$\Delta S^{\neq}$ /cal mol^{-1} K^{-1}	$\Delta G^{\neq}_{20}$ /kcal mol^{-1}
20	18.5 ± 1.0	–3.6 ± 1.0	**19.5 ± 1.3**

(9) Temperature Dependency of ^{1}H NMR and Kinetic Data of Minor Isomer 21

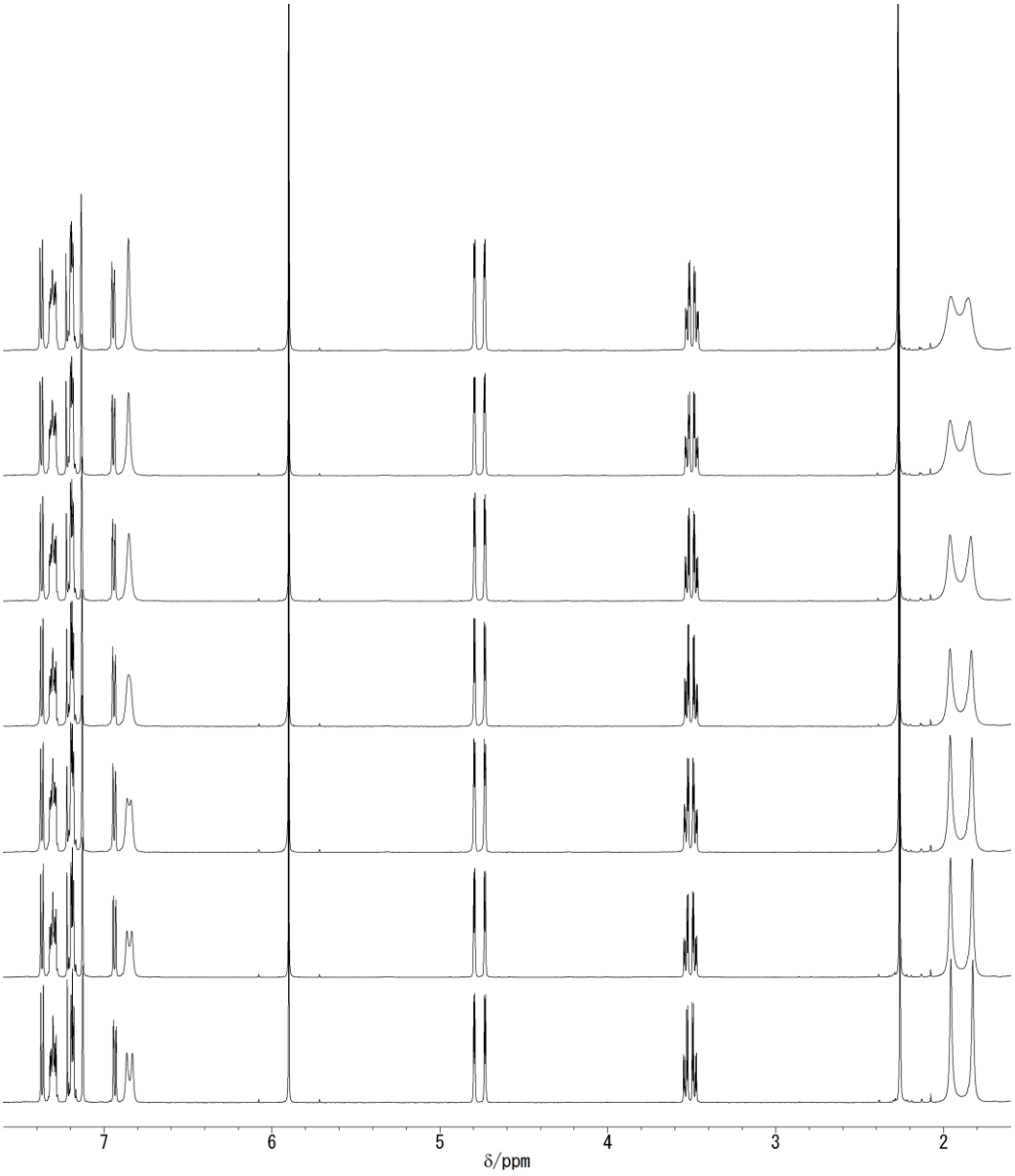


Figure S-39. ^{1}H NMR spectra of *syn*-2-mesityl-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylic anhydride (minor isomer **21**) (500 MHz) in $(CDCl_2)_2$ at various temperatures (120 °C, 115 °C, 110 °C, 105 °C, 100 °C, 95 °C, and 90 °C, respectively, from the top).

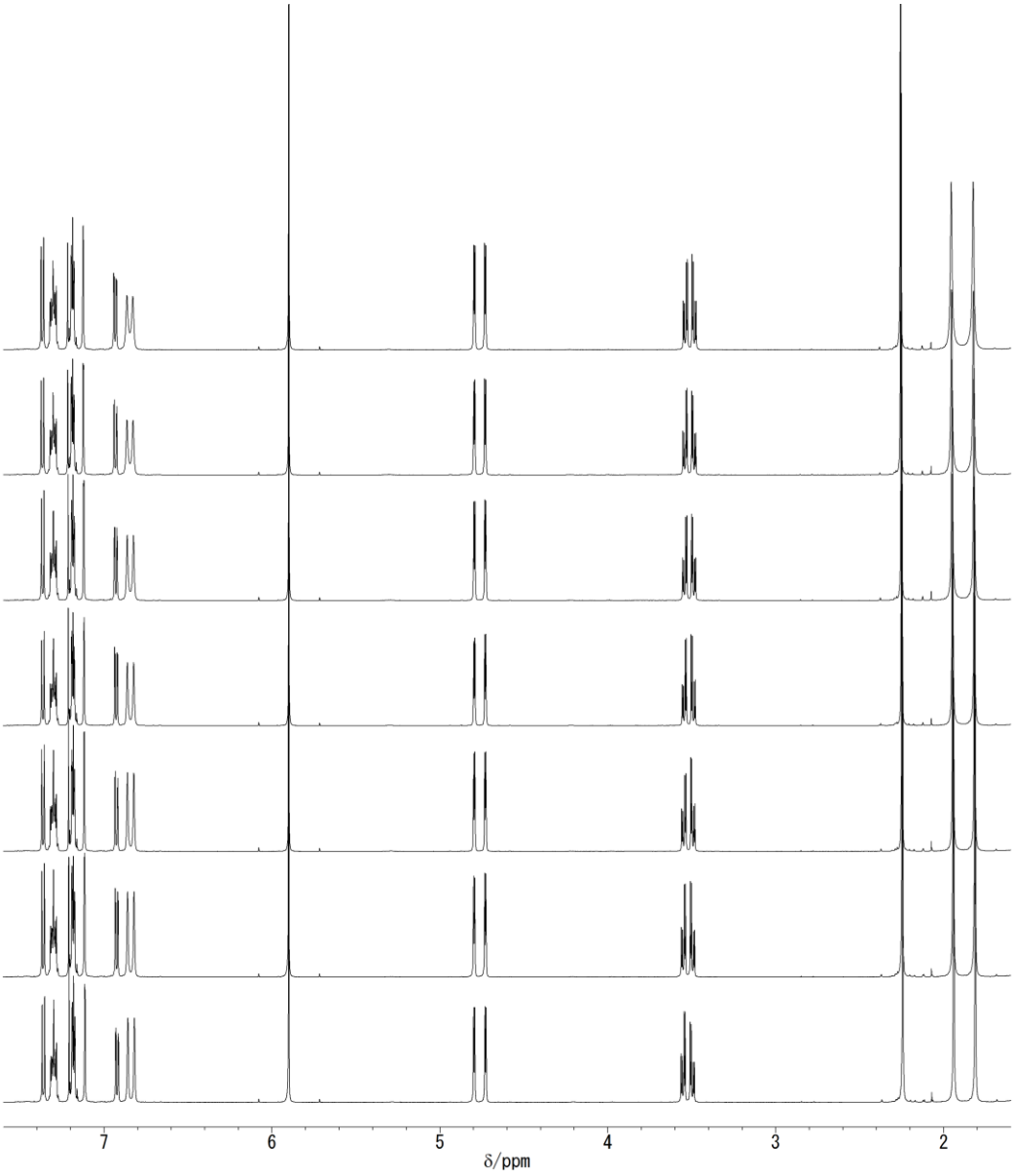


Figure S-40. ^{1}H NMR spectra of *syn*-2-mesityl-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylic anhydride (minor isomer **21**) (500 MHz) in $(CDCl_2)_2$ at various temperatures (85 °C, 80 °C ,75 °C, 70 °C, 65 °C, 60 °C, and 55 °C, respectively, from the top).

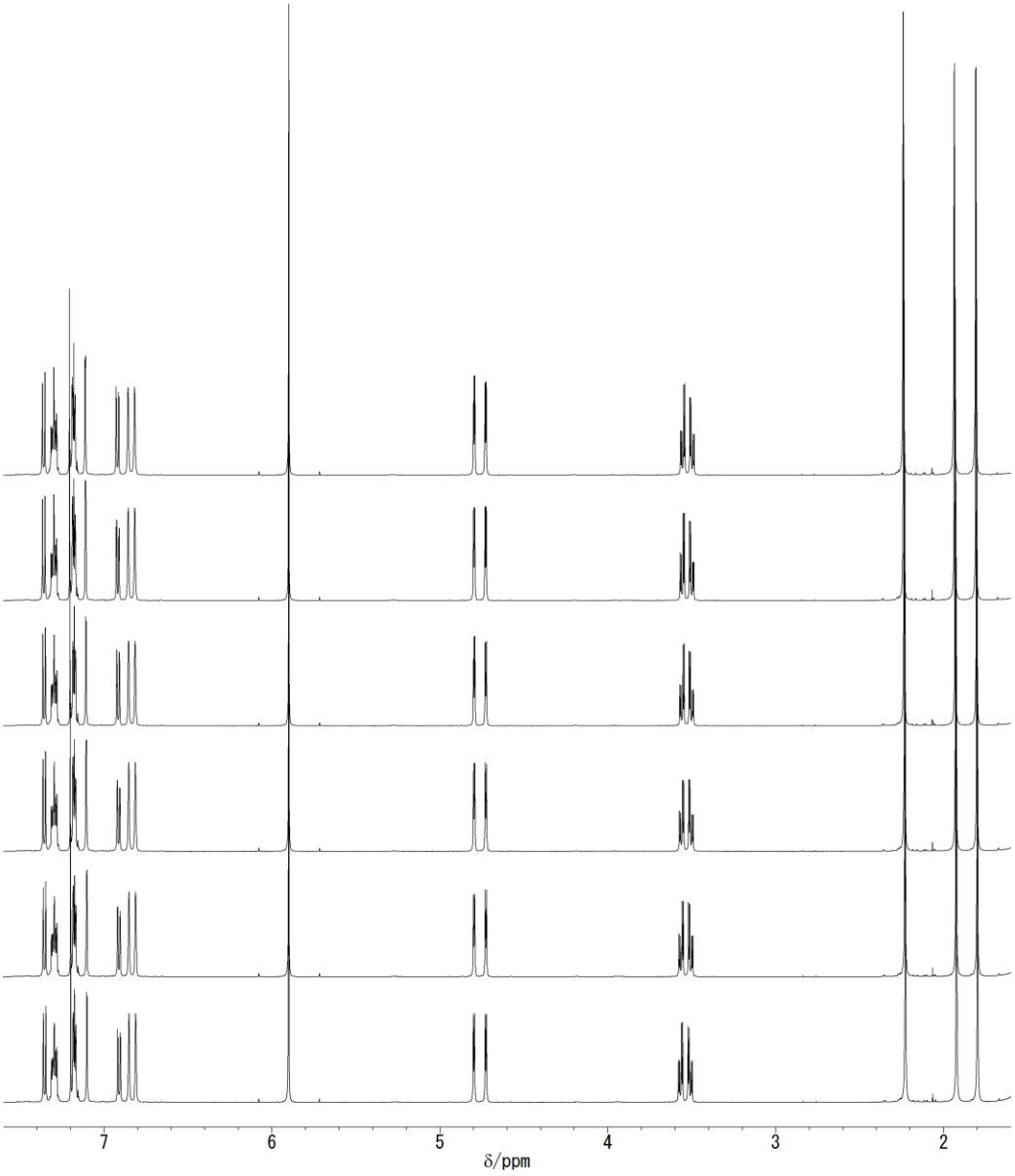


Figure S-41. ^{1}H NMR spectra of *syn*-2-mesityl-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylic anhydride (minor isomer **21**) (500 MHz) in $(CDCl_2)_2$ at various temperatures (50 °C, 45 °C, 40 °C, 35 °C, 30 °C, and 25 °C, respectively, from the top).

(a) (b)

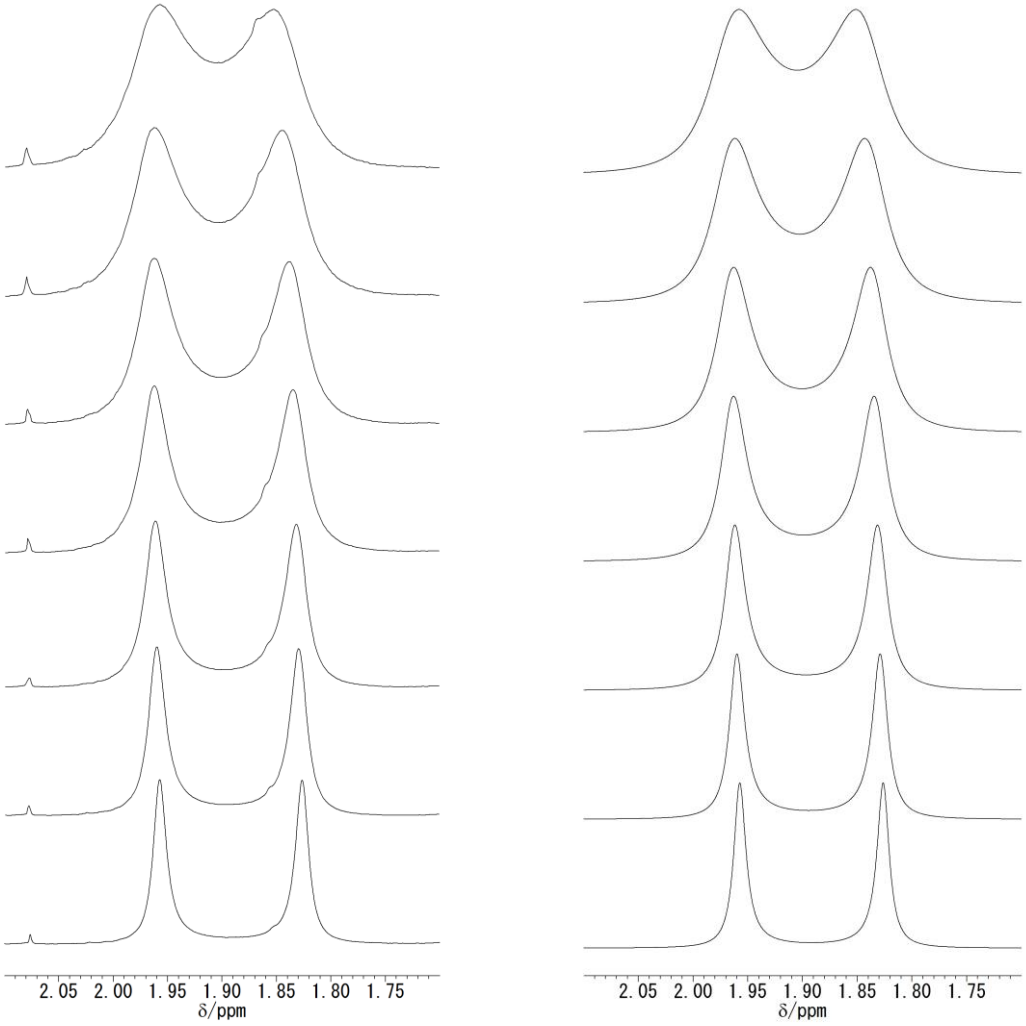


Figure S-42. ^{1}H NMR spectra of *syn*-2-mesityl-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylic anhydride (minor isomer **21**) (500 MHz, (a) observed spectra, (b) calculated spectra of the methyl proton signals at 2,6-positions in the mesityl group) in $(CDCl_2)_2$ at various temperatures (120 °C, 115 °C, 110 °C, 105 °C, 100 °C, 95 °C, and 90 °C, respectively, from the top).

(a) (b)

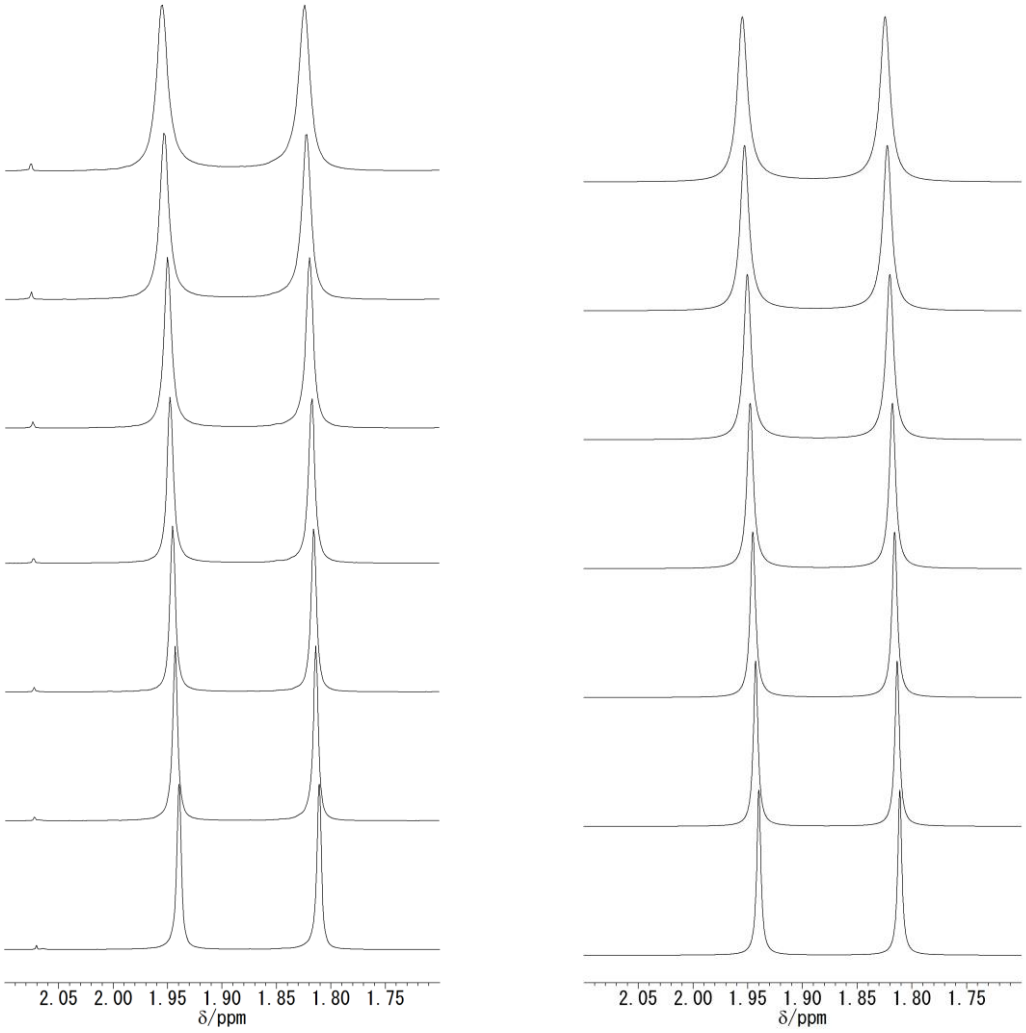


Figure S-43. ^{1}H NMR spectra of *syn*-2-mesityl-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylic anhydride (minor isomer **21**) (500 MHz, (a) observed spectra, (b) calculated spectra of the methyl proton signals at 2,6-positions in the mesityl group) in $(CDCl_2)_2$ at various temperatures (85 °C, 80 °C ,75 °C, 70 °C, 65 °C, 60 °C, and 55 °C, respectively, from the top).

(a) (b)

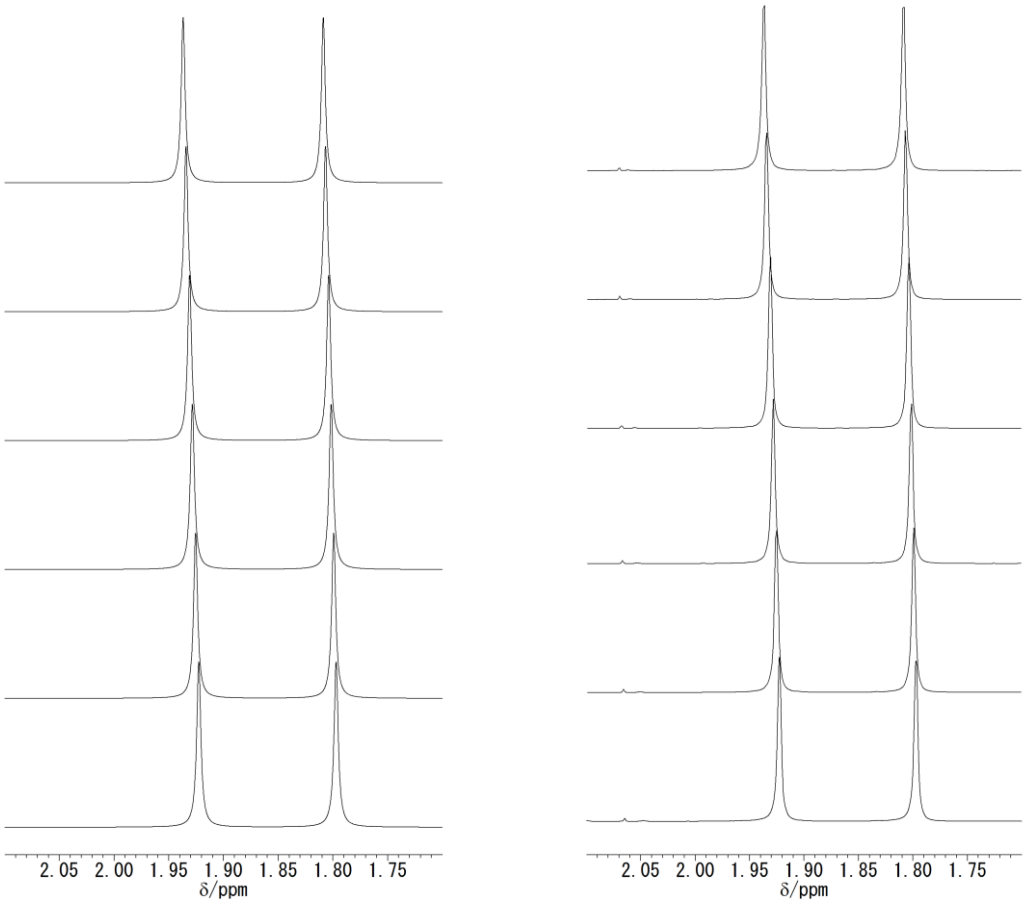


Figure S-44. ^{1}H NMR spectra of *syn*-2-mesityl-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylic anhydride (minor isomer **21**) (500 MHz, (a) observed spectra, (b) calculated spectra of the methyl proton signals at 2,6-positions in the mesityl group) in $(CDCl_2)_2$ at various temperatures (50 °C, 45 °C, 40 °C, 35 °C, 30 °C, and 25 °C, respectively, from the top).

(a) (b)

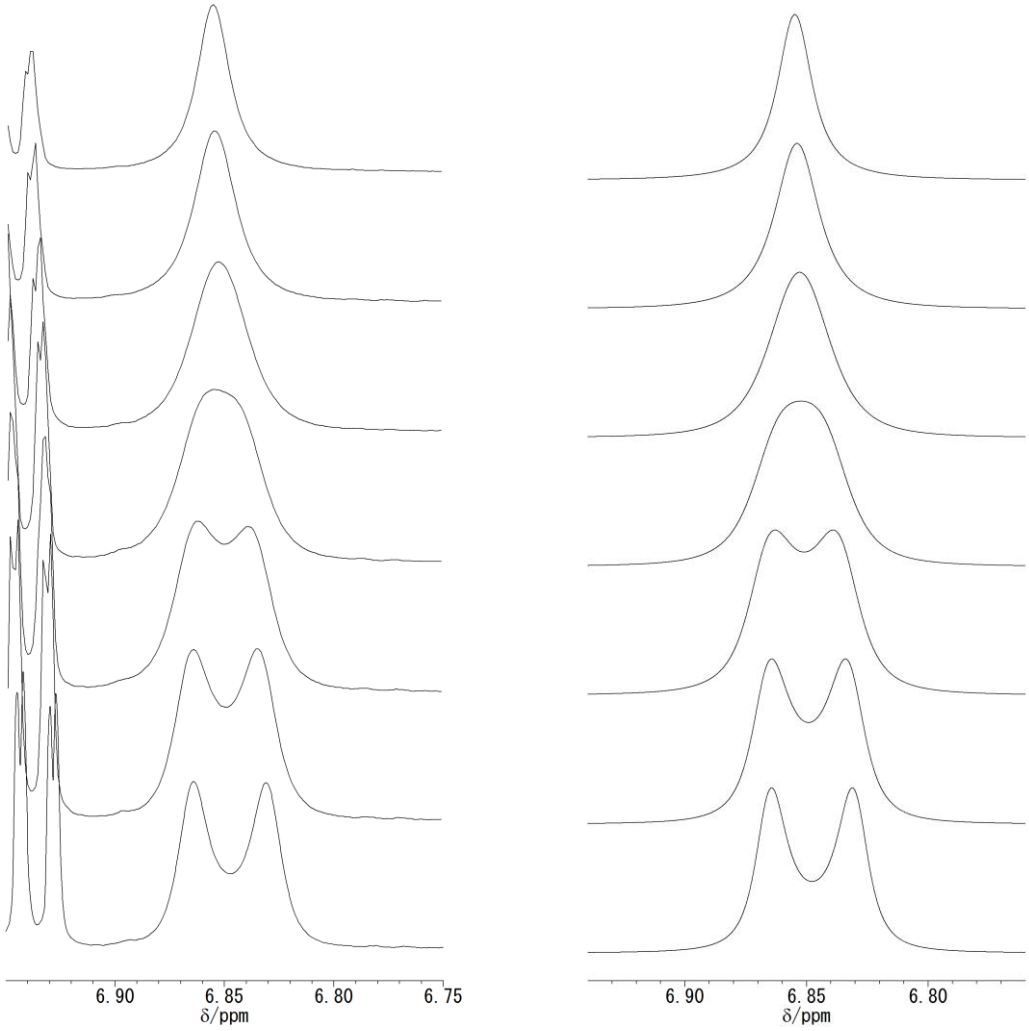


Figure S-45. ^{1}H NMR spectra of *syn*-2-mesityl-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylic anhydride (minor isomer **21**) (500 MHz, (a) observed spectra, (b) calculated spectra of the aromatic proton signals at 3,5-positions in the mesityl group) in $(CDCl_2)_2$ at various temperatures (120 °C, 115 °C, 110 °C, 105 °C, 100 °C, 95 °C, and 90 °C, respectively, from the top).

(a) (b)

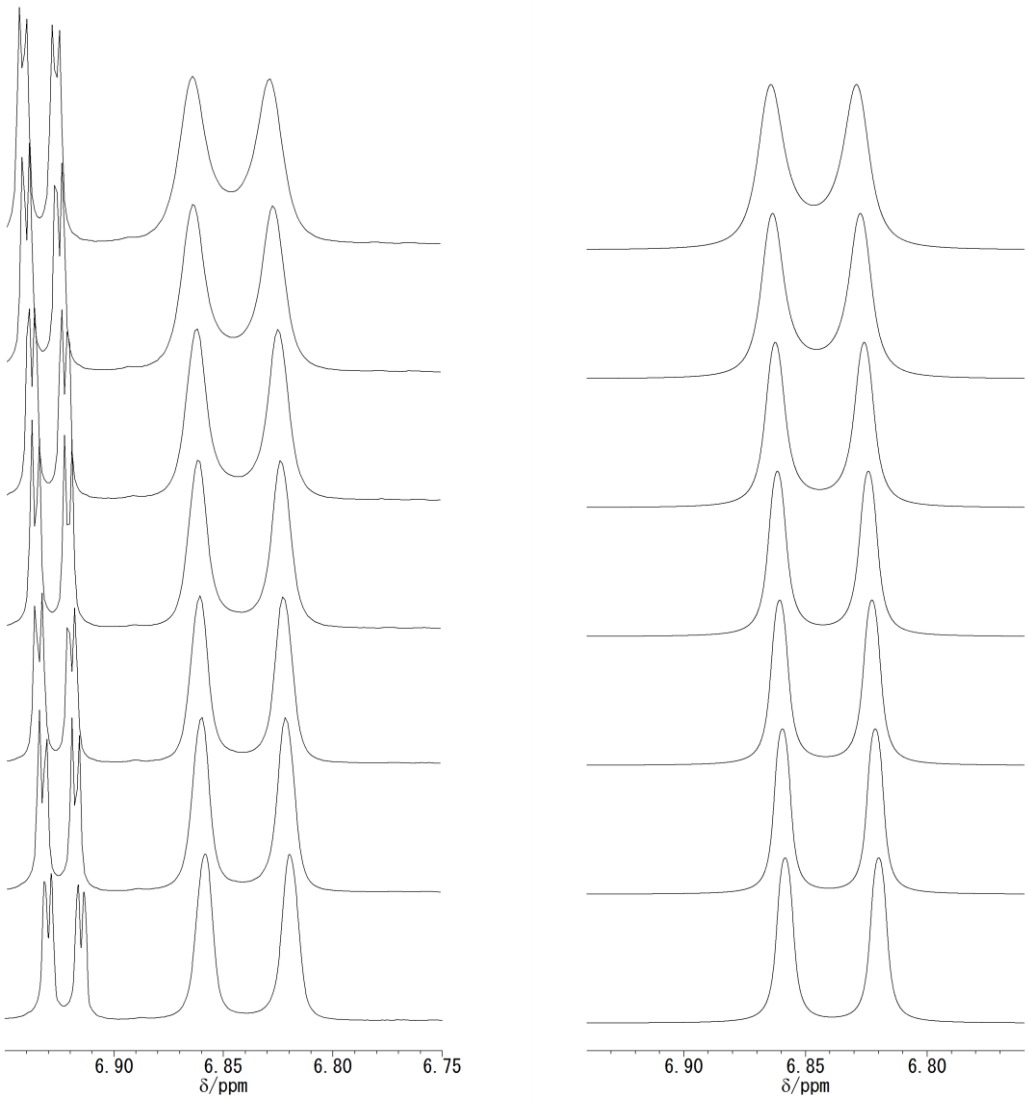


Figure S-46. ^{1}H NMR spectra of *syn*-2-mesityl-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylic anhydride (minor isomer **21**) (500 MHz, (a) observed spectra, (b) calculated spectra of the aromatic proton signals at 3,5-positions in the mesityl group) in $(CDCl_2)_2$ at various temperatures (85 °C, 80 °C ,75 °C, 70 °C, 65 °C, 60 °C, and 55 °C, respectively, from the top).

(a) (b)

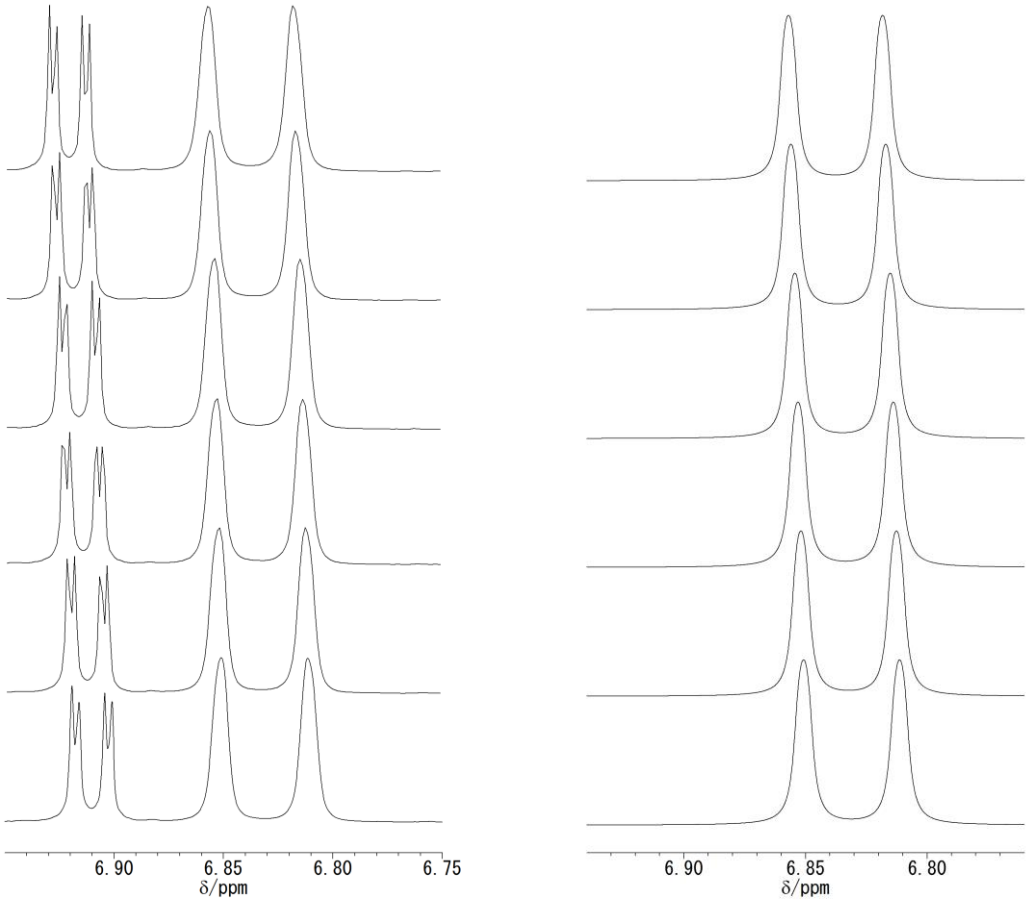


Figure S-47. ^{1}H NMR spectra of *syn*-2-mesityl-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylic anhydride (minor isomer **21**) (500 MHz, (a) observed spectra, (b) calculated spectra of the aromatic proton signals at 3,5-positions in the mesityl group) in $(CDCl_2)_2$ at various temperatures (50 °C, 45 °C, 40 °C, 35 °C, 30 °C, and 25 °C, respectively, from the top).

Table S-12. Rate Data[a] Determined by Line Shape Analysis for Minor Isomer **21**

Temperature (°C)	Rate Constants (s^{-1}) calcd. by methyl signals	Rate Constants (s^{-1}) calcd. by aromatic signals
25	0	0
30	0	0
35	0	0
40	0	0
45	0	0
50	0	0
55	0	0
60	1	0
65	2	1
70	4	2.2
75	6	3.9
80	8	7
85	10	10
90	14	15
95	19	20
100	26	27
105	37	40
110	50	55
115	67	75
120	88	105

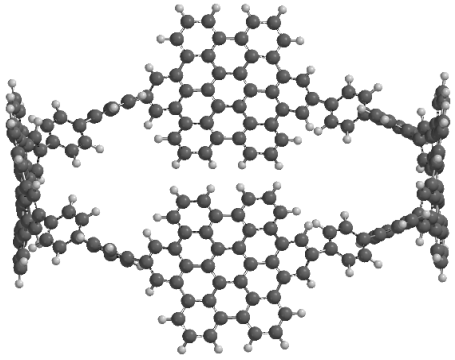
[a] The rate data presented by red characters were used to the calculations for the kinetic data.

Table S-13. Kinetic Data Calculated by the Rate Data for Mainor Isomer **21**

Sample	$\Delta H^{\neq}$ /kcal mol^{-1}	$\Delta S^{\neq}$ /cal mol^{-1} K^{-1}	$\Delta G^{\neq}_{20}$ /kcal mol^{-1}
21	17.5 ± 0.2	–5.5 ± 0.6	**19.1 ± 0.3**

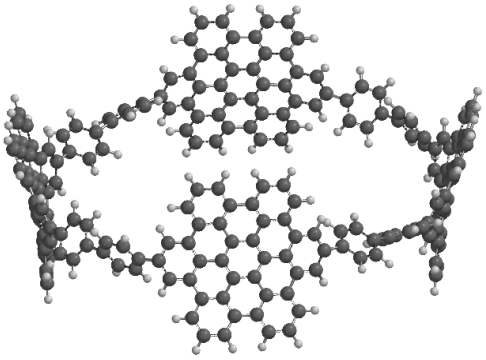
(10) Theoretical Calculations of 1, 2, and the Model HBC Derivative 17

(a) Conformer **A**



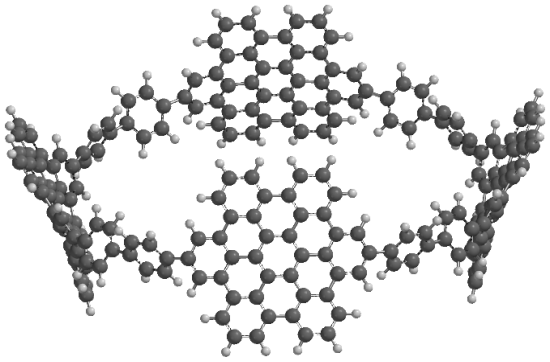
−8190.289026 hartrees (a.u.) (16.3 kJ mol^{-1})

(b) Conformer **B**



−8190.290652 hartrees (a.u.) (12.0 kJ mol^{-1})

(c) Conformer **C**



−8190.295220 hartrees (a.u.) (0.0 kJ mol^{-1})

Figure S-48. Three optimized structure of cyclic tetramer **1** without the mesityl substituents by using ab initio calculations at the HF/3-21G level: (a) Conformer **A**: −8190.289026 hartrees (a.u.) (relative energy: 16.3 kJ mol^{-1}); (b) Conformer **B**: −8190.290652 hartrees (a.u.) (12.0 kJ mol^{-1}); (c) Conformer **C**: −8190.295220 hartrees (a.u.) (0.0 kJ mol^{-1}).

Comparison of the results on the calculations at HF/3-21G and the DFT at B3LYP/6-31G* levels for the cyclic tetramer 1

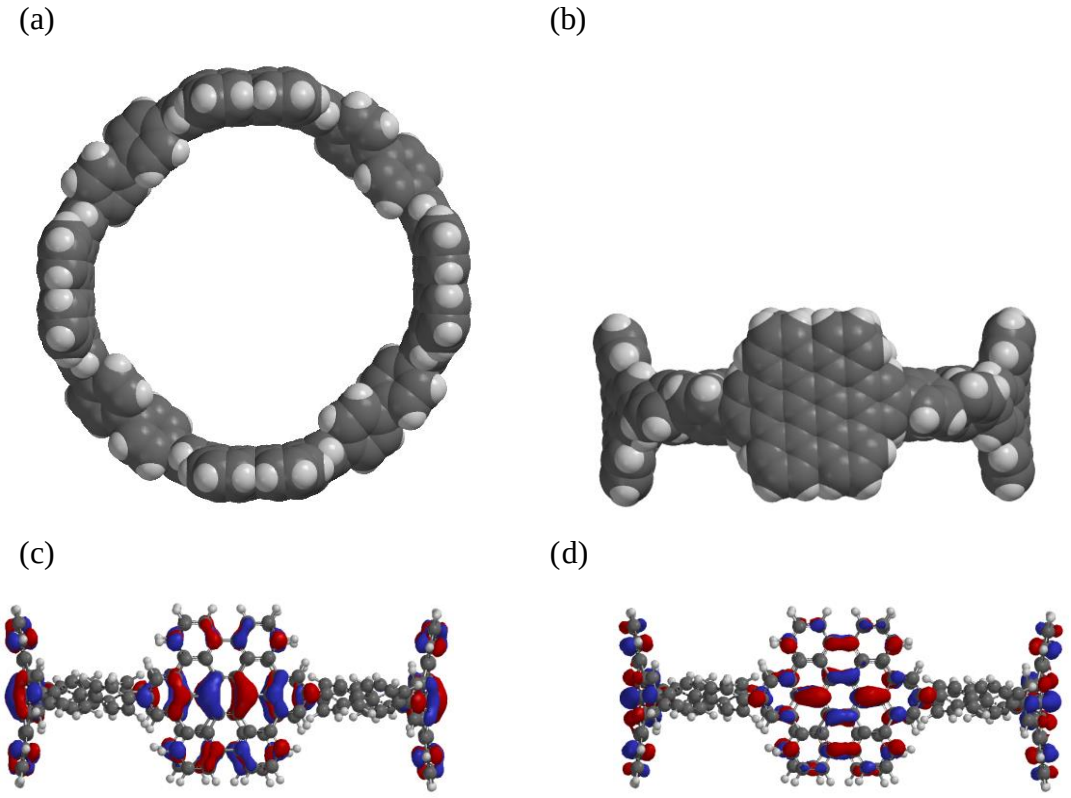


Figure S-49. Optimized structure of cyclic tetramer **1** without the mesityl substituents optimized at the HF/3-21G level: −8190.289025 hartrees (a.u.); (a) top view of the molecular structure; (b) side view of the molecular structure; (c) HOMO of the carbon nanohoop **1** (HOMO −6.88 eV); (d) LUMO of the carbon nanohoop **1** (LUMO 1.30 eV).

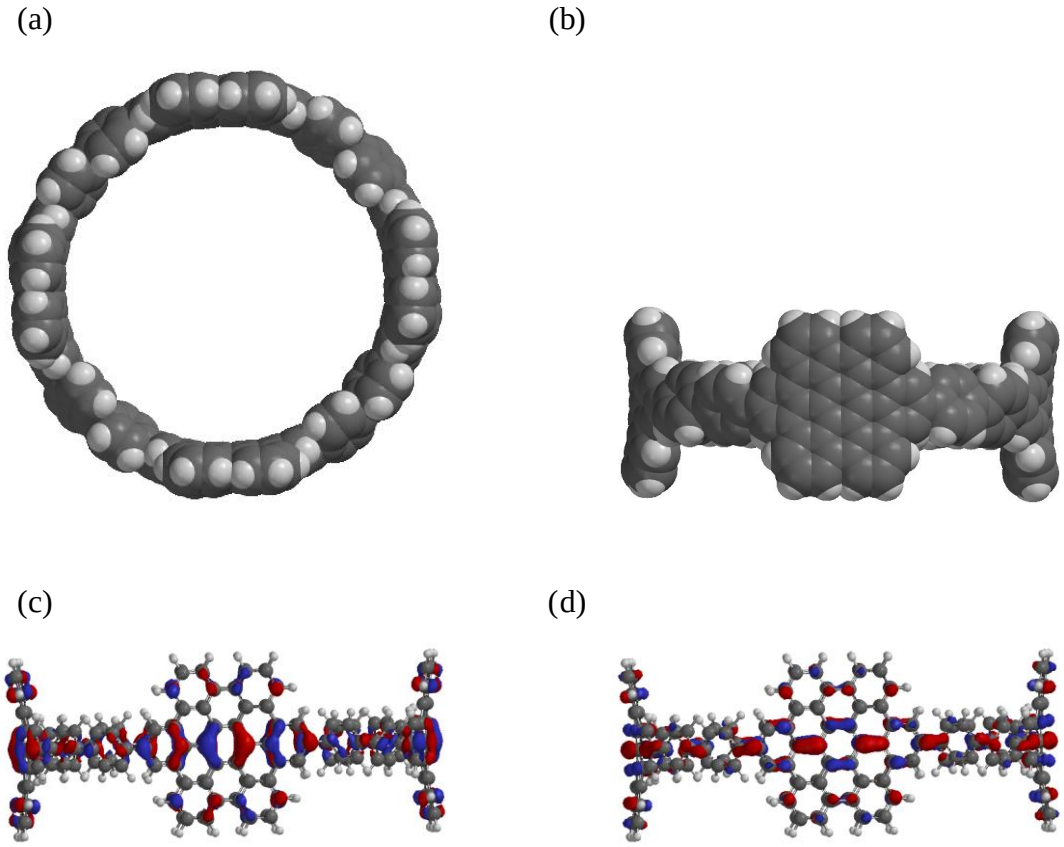
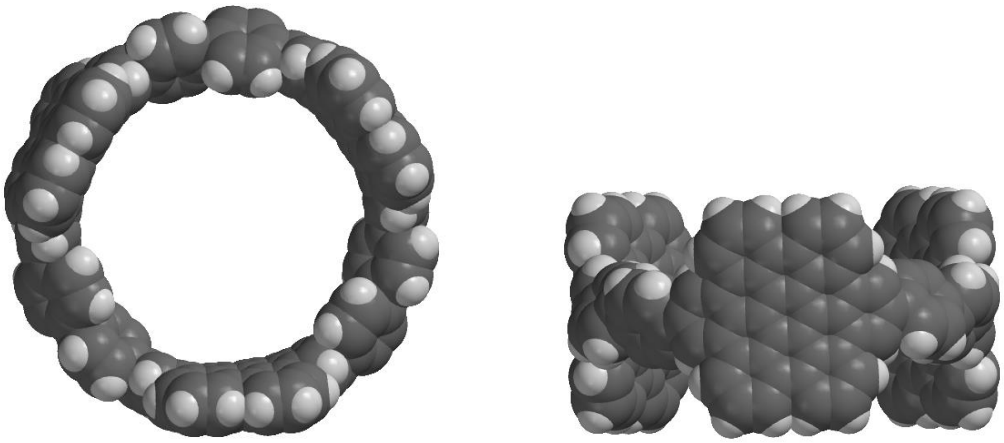


Figure S-50. Optimized structure of cyclic tetramer **1** without the mesityl substituents optimized by DFT calculations at the B3LYP/6-31G* level: −8289.735764 hartrees (a.u.); (a) top view of the molecular structure; (b) side view of the molecular structure; (c) HOMO of the carbon nanohoop **1** (HOMO −5.09 eV); (d) LUMO of the carbon nanohoop **1** (LUMO −1.90 eV).

Comparison of the results on the calculations at HF/3-21G and the DFT at B3LYP/6-31G* levels for the cyclic trimer 2

(a) (b)



(c) (d)

HOMO LUMO

Figure S-51. Optimized structure of cyclic trimer **2** without the mesityl substituents optimized at the HF/3-21G level: −6142.681541 hartrees (a.u.); (a) top view of the molecular structure; (b) side view of the molecular structure; (c) HOMO of the carbon nanohoop **2** (HOMO −6.83 eV); (d) LUMO of the carbon nanohoop **2** (LUMO 1.24 eV).

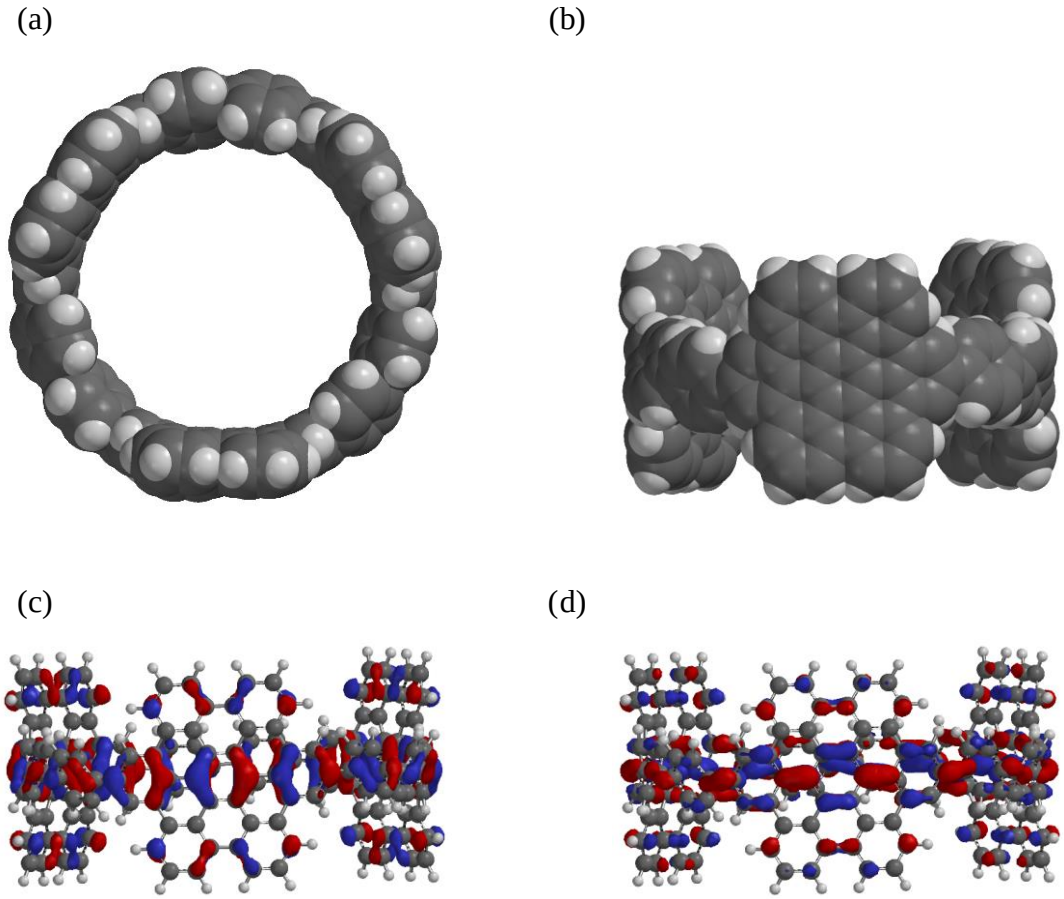


Figure S-52. Optimized structure of cyclic trimer **2** without the mesityl substituents optimized by DFT calculations at the B3LYP/6-31G* level: −6217.274260 hartrees (a.u.); (a) top view of the molecular structure; (b) side view of the molecular structure; (c) HOMO of the carbon nanohoop **2** (HOMO −5.06 eV); (d) LUMO of the carbon nanohoop **2** (LUMO −1.92 eV).

Comparison of the results on the calculations at HF/3-21G and the DFT at B3LYP/6-31G* levels for the model HBC structure 17

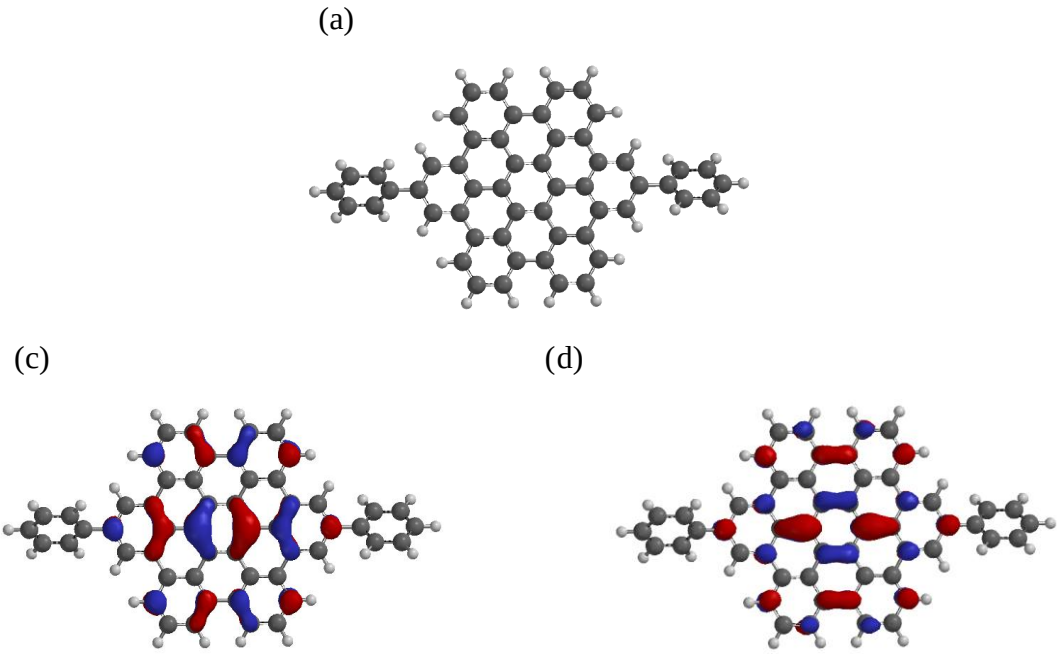


Figure S-53. Optimized structure of the model HBC structure **17** without the mesityl substituents optimized at the HF/3-21G level: −2048.736190 hartrees (a.u.); (a) top view of the model HBC structure; (b) side view of the model HBC structure; (c) HOMO of the model HBC structure (HOMO −6.92 eV); (d) LUMO of the model HBC structure (LUMO 1.39 eV).

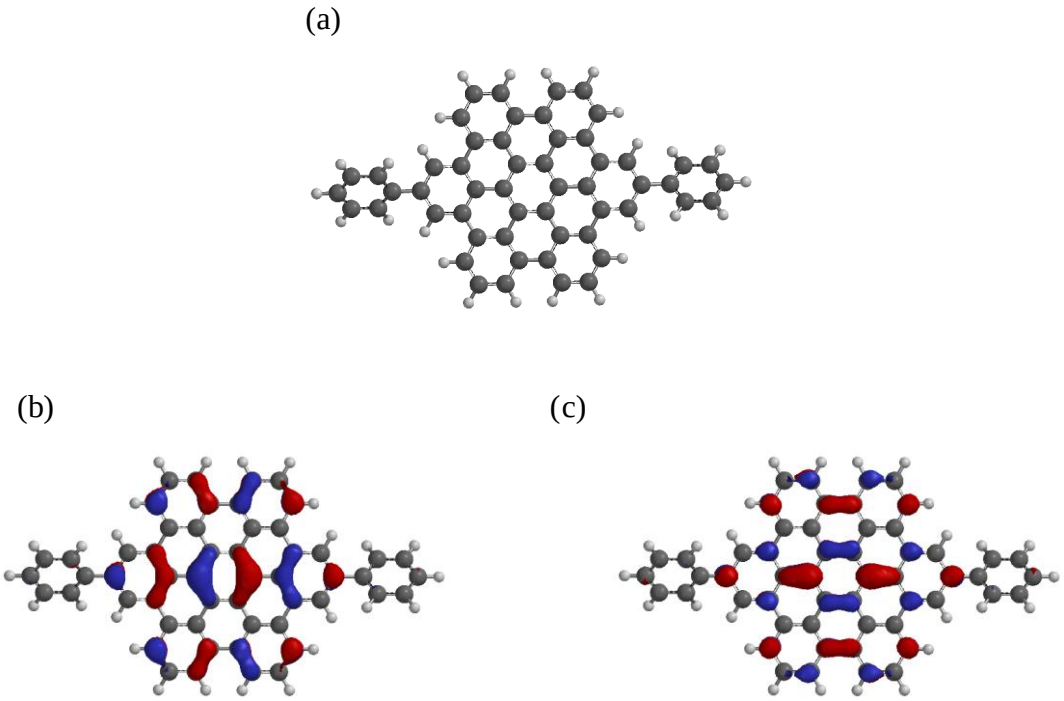
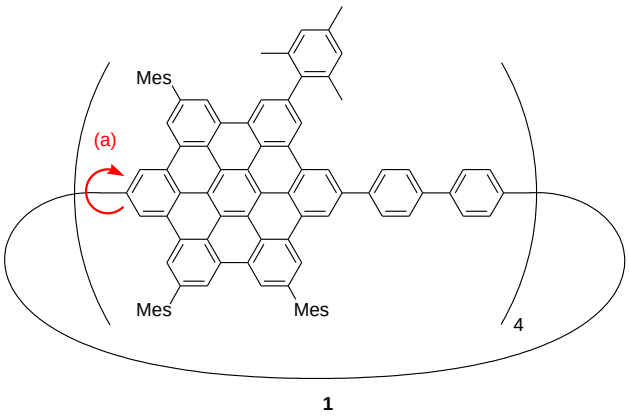


Figure S-54. Optimized structure of the model HBC structure **17** without the mesityl substituents optimized by DFT calculations at the B3LYP/6-31G* level: −2073.636359 hartrees (a.u.); (a) top view of the model HBC structure; (b) HOMO of the model HBC structure (HOMO −5.19 eV); (c) LUMO of the model HBC structure (LUMO −1.72 eV).

Dihedral angle scan for cyclic tetramer 1



1

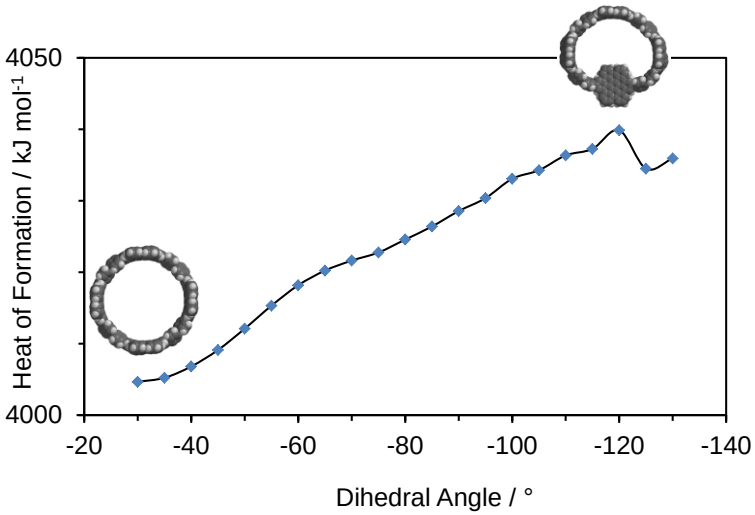


Figure S-55. Results on the dihedral angle scan for cyclic tetramer **1** by (a) starting from the highly symmetrical structure, Conformer **A**, by using semiempirical calculations (AM1) without the mesityl substituents on the calculated structure. Because the molecule takes symmetrical structure, the similar structure is repeated by each 90° scan. Therefore, the dihedral angle scan was performed from −30° (for the optimized structure) to −130° by each −5° interval.

Relative heat of formation (kcal mol^{-1}) of presumed transition structure for cyclic tetramer 1

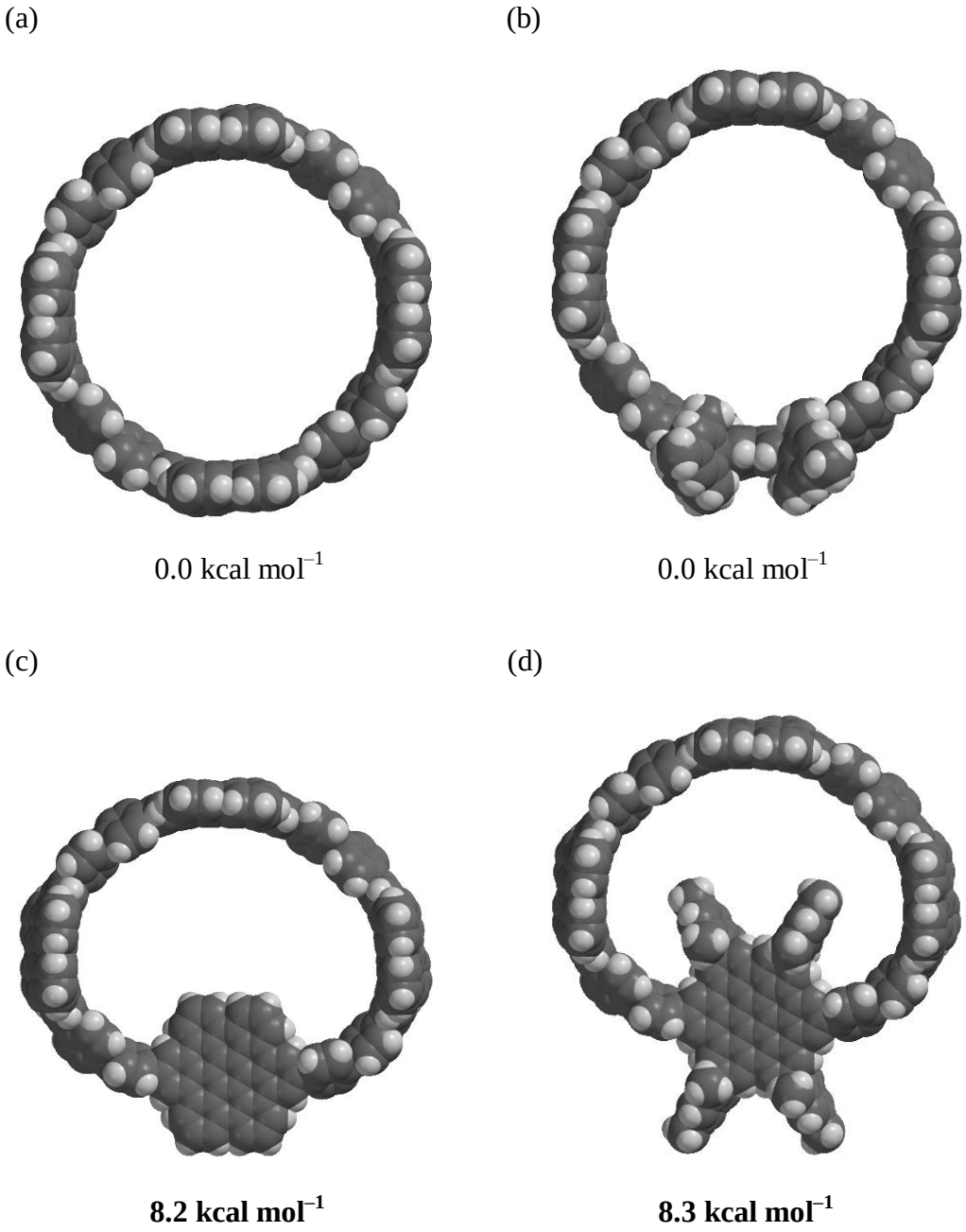


Figure S-56. Relative heat of formation (kcal mol^{-1}) of presumed transition structure optimized starting from the structure obtained by the dihedral angle scan (dihedral angle = 120°) by using semiempirical calculations (AM1) for cyclic tetramer **1**; (a) and (c) without mesityl substituents; (b) and (d) calculated structures with four mesityl substituents and the relative heat of formation to that from the optimized ground state structures.

Relative heat of formation (kcal mol^{-1}) of presumed transition structure for cyclic trimer 2

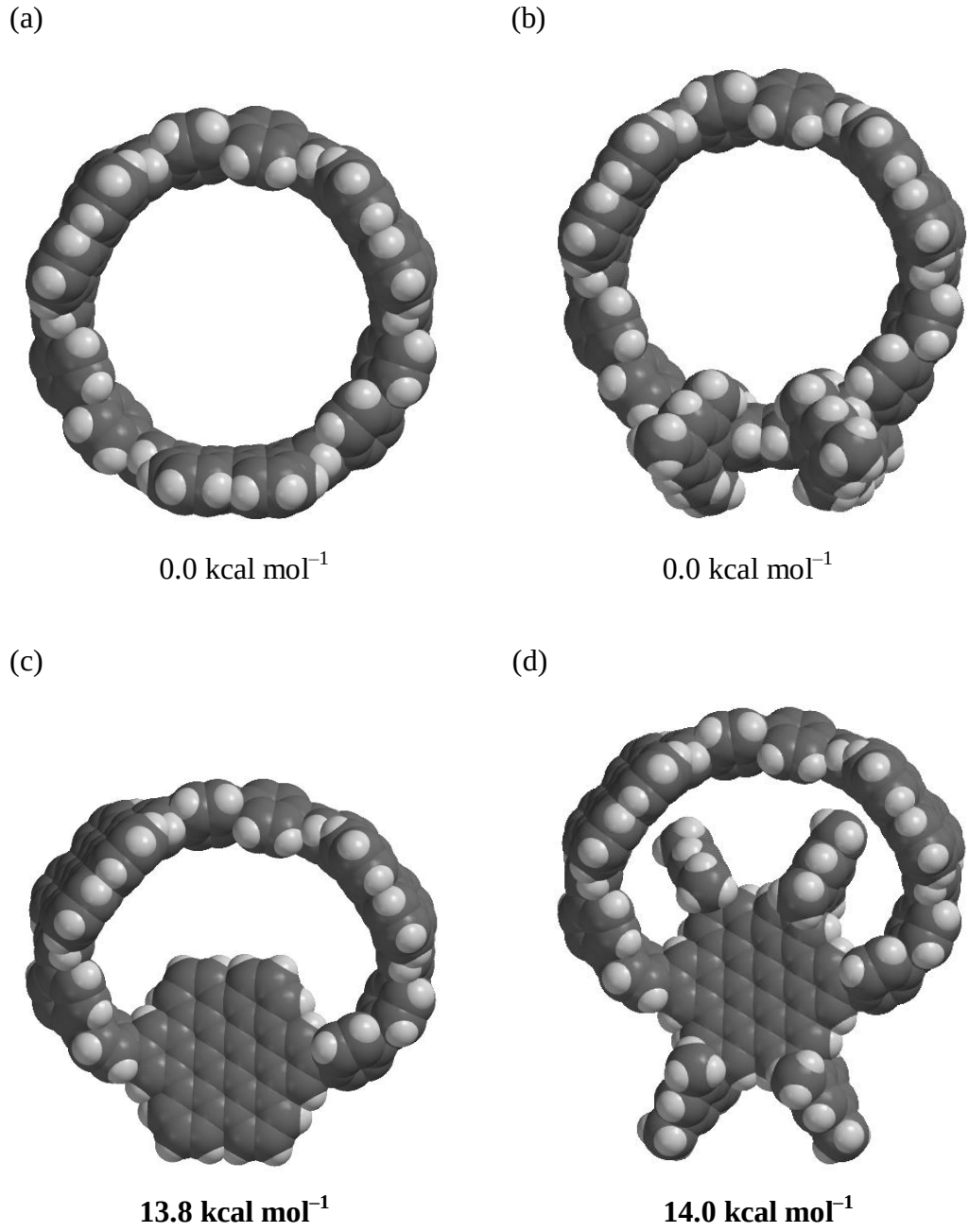


Figure S-57. Relative heat of formation (kcal mol^{-1}) of presumed transition structure optimized starting from the structure with the dihedral angle = 120° by using semiempirical calculations (AM1) for cyclic trimer **2**; (a) and (c) without mesityl substituents; (b) and (d) calculated structures with four mesityl substituents and the relative heat of formation to that from the optimized ground state structures.

(11) Copies of ^{1}H and ^{13}C NMR Spectra of 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 17, 1, 2, 20, and 21

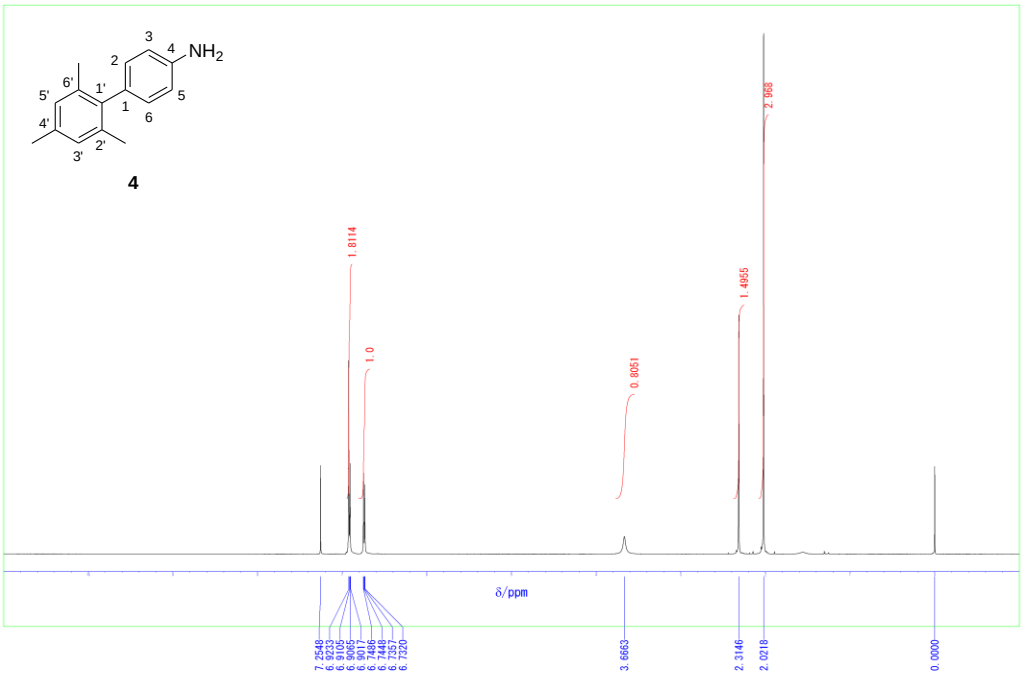


Figure S-58. ^{1}H NMR spectrum (500 MHz) of 4-mesitylaniline (**4**) in $CDCl_3$.

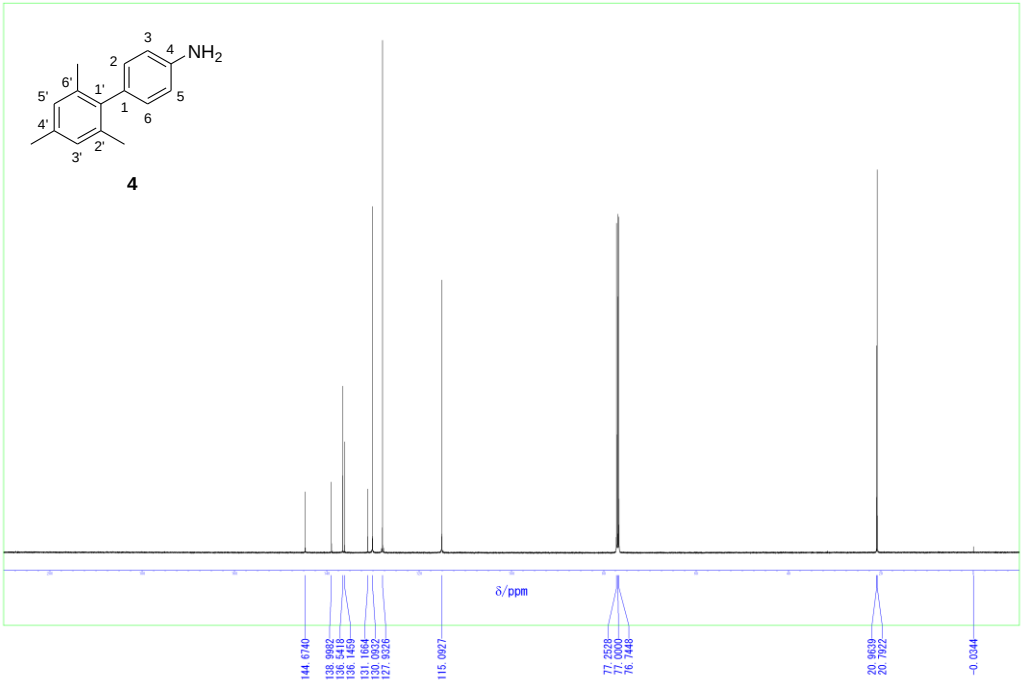


Figure S-59. ^{13}C NMR spectrum (125 MHz) of 4-mesitylaniline (**4**) in $CDCl_3$.

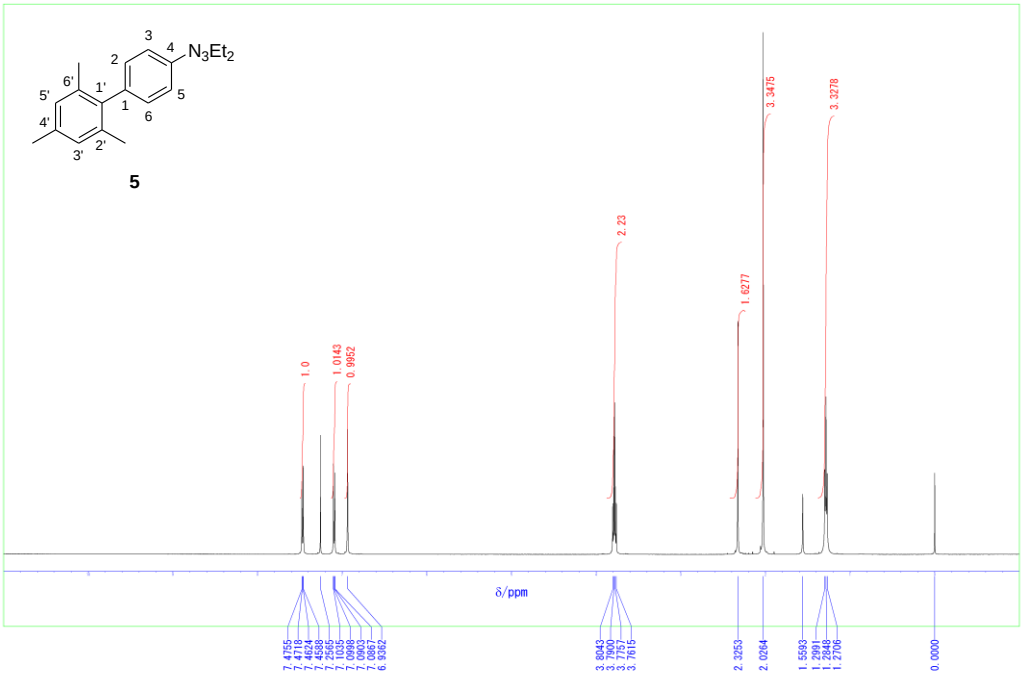


Figure S-60. ^{1}H NMR spectrum (500 MHz) of 4-mesitylphenyl-3,3'-diethyltriazene (**5**) in $CDCl_3$.

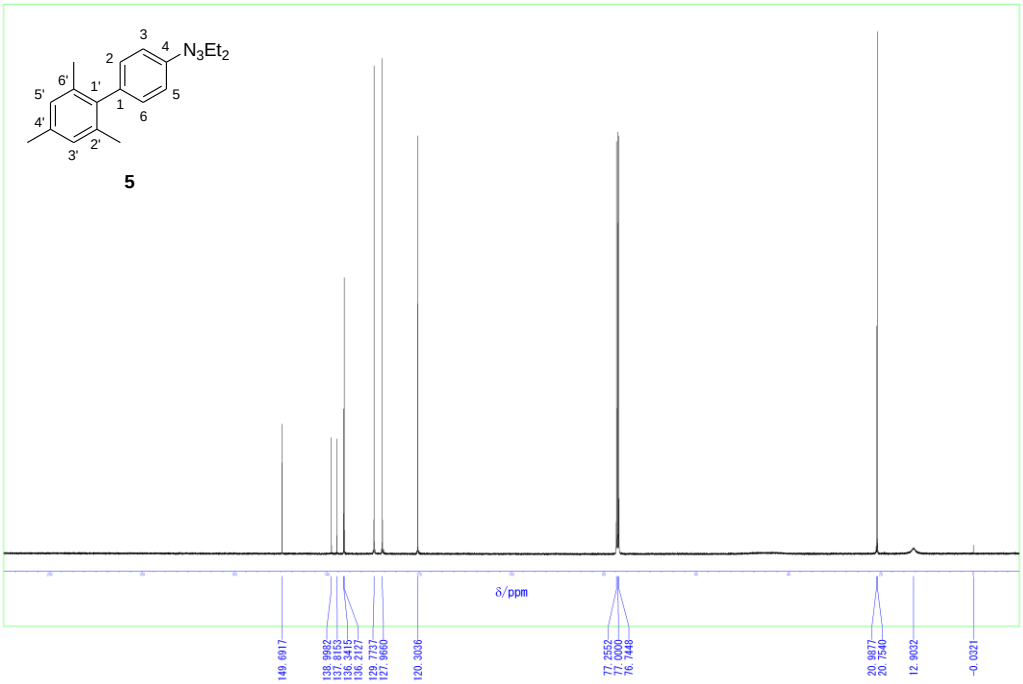


Figure S-61. ^{13}C NMR spectrum (125 MHz) of 4-mesitylphenyl-3,3'-diethyltriazene (**5**) in $CDCl_3$.

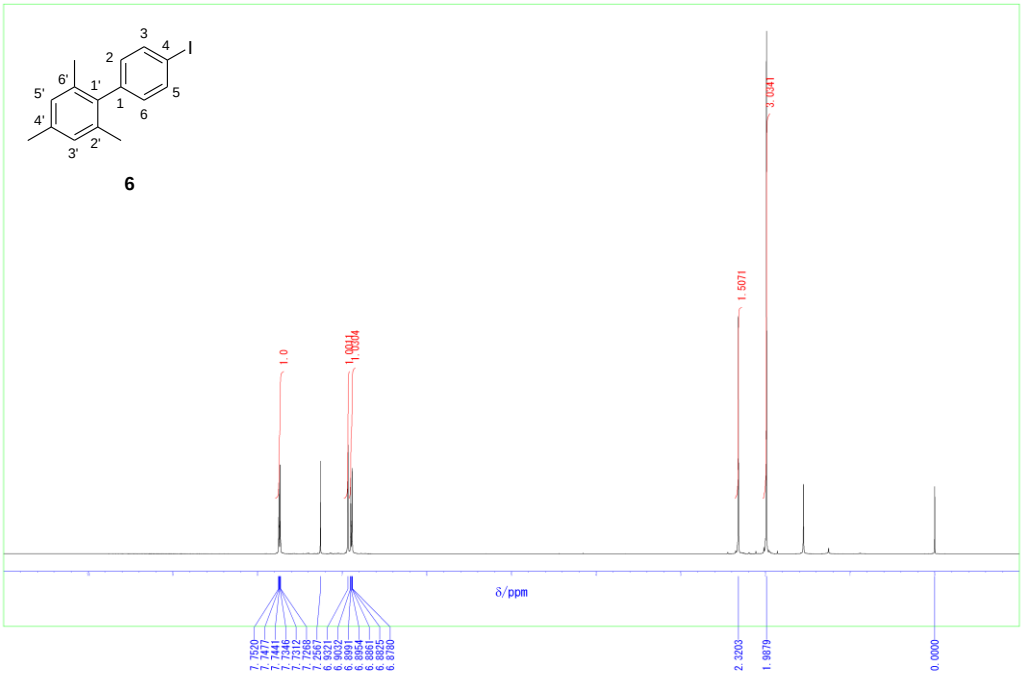


Figure S-62. ^{1}H NMR spectrum (500 MHz) of 1-iodo-4-mesitylbenzene (**6**) in $CDCl_3$.

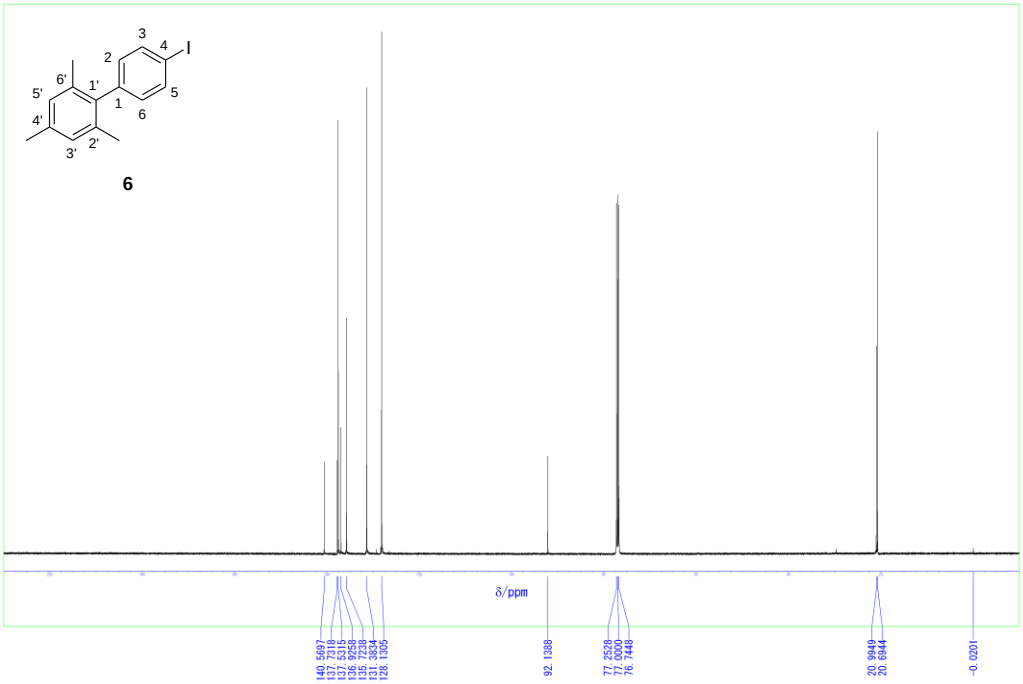


Figure S-63. ^{13}C NMR spectrum (125 MHz) of 1-iodo-4-mesitylbenzene (**6**) in $CDCl_3$.

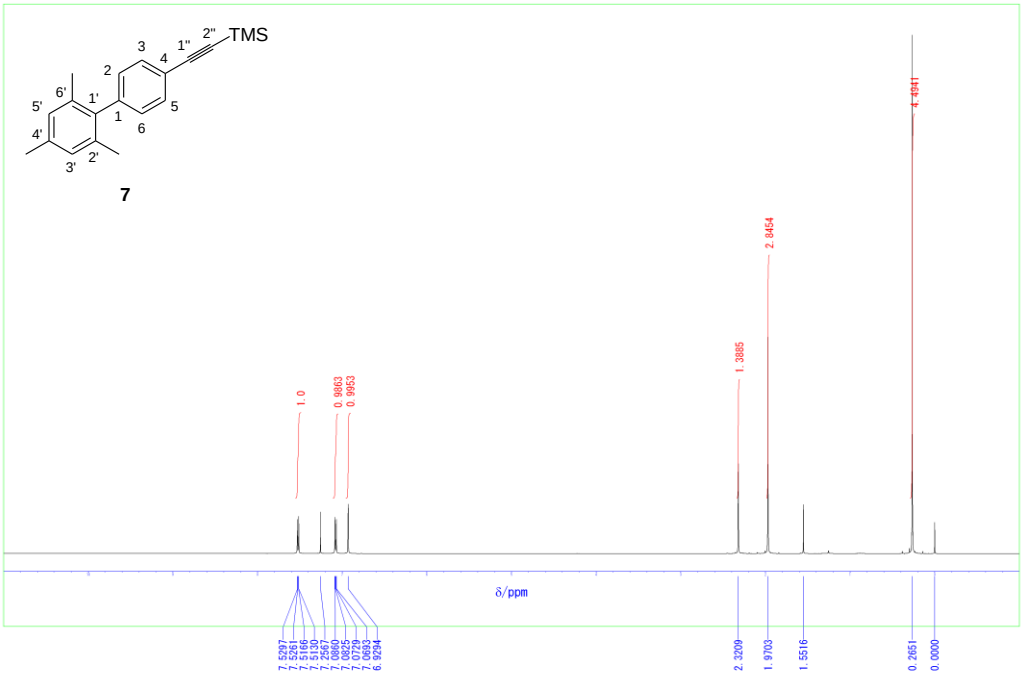


Figure S-64. ^{1}H NMR spectrum (500 MHz) of (4-mesitylphenylethynyl)trimethylsilane (**7**) in $CDCl_3$.

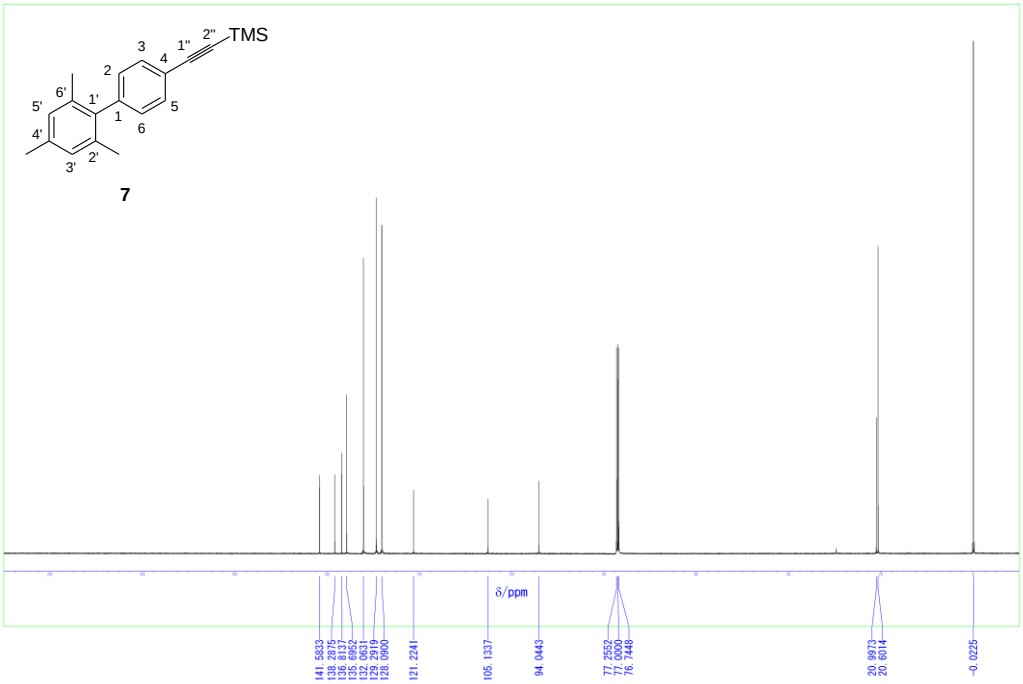


Figure S-65. ^{13}C NMR spectrum (125 MHz) of (4-mesitylphenylethynyl)trimethylsilane (**7**) in $CDCl_3$.

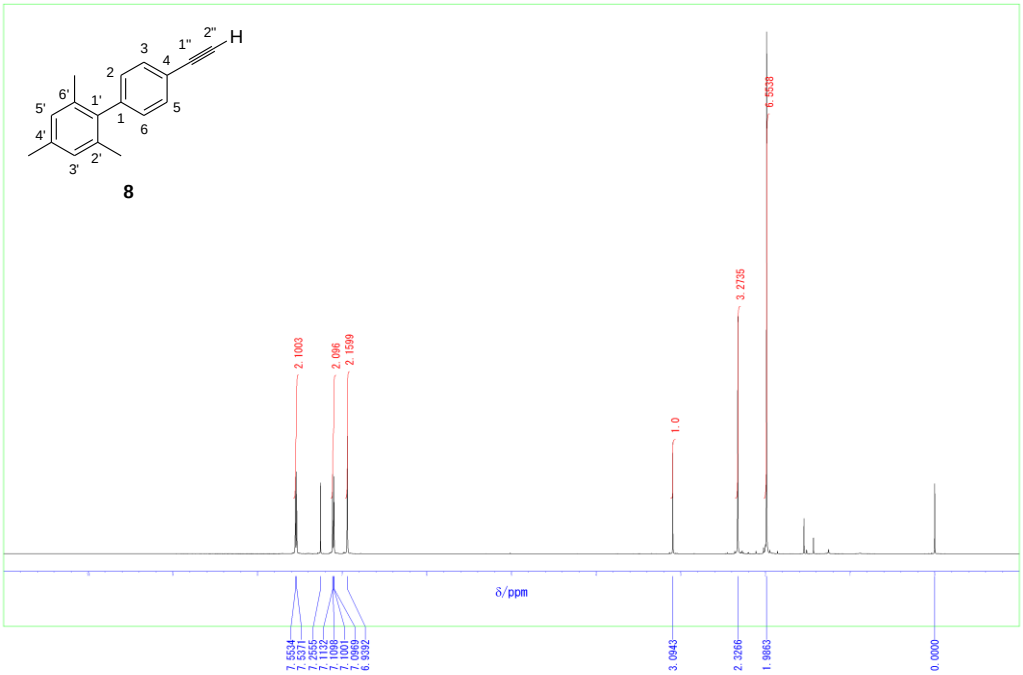


Figure S-66. ^{1}H NMR spectrum (500 MHz) of 1-ethynyl-4-mesitylbenzene (**8**) in $CDCl_3$.

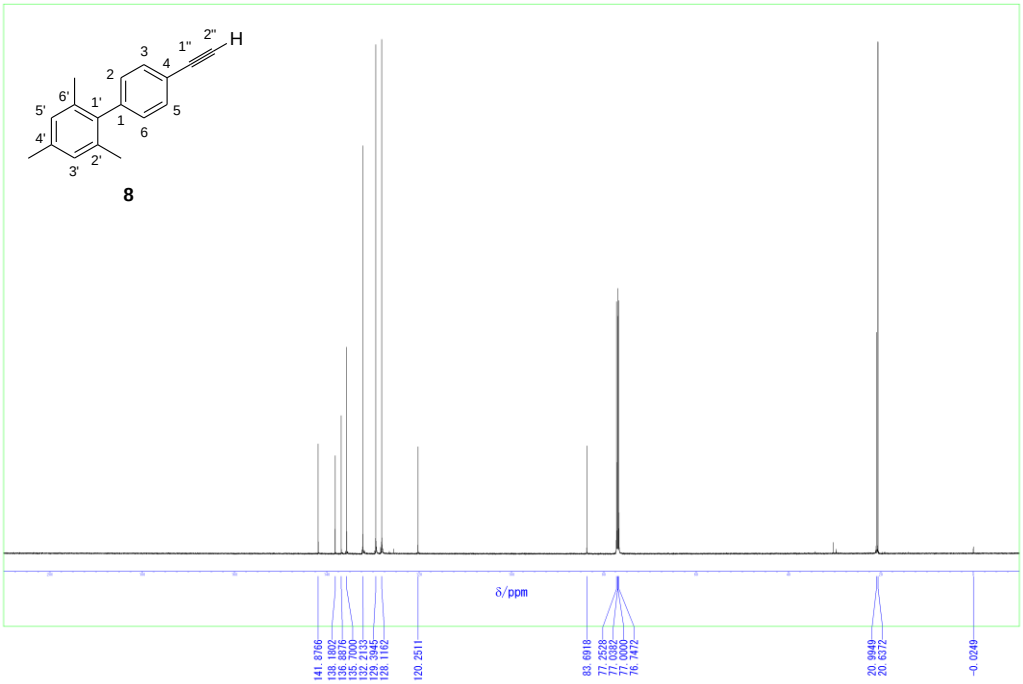


Figure S-67. ^{13}C NMR spectrum (125 MHz) of 1-ethynyl-4-mesitylbenzene (**8**) in $CDCl_3$.

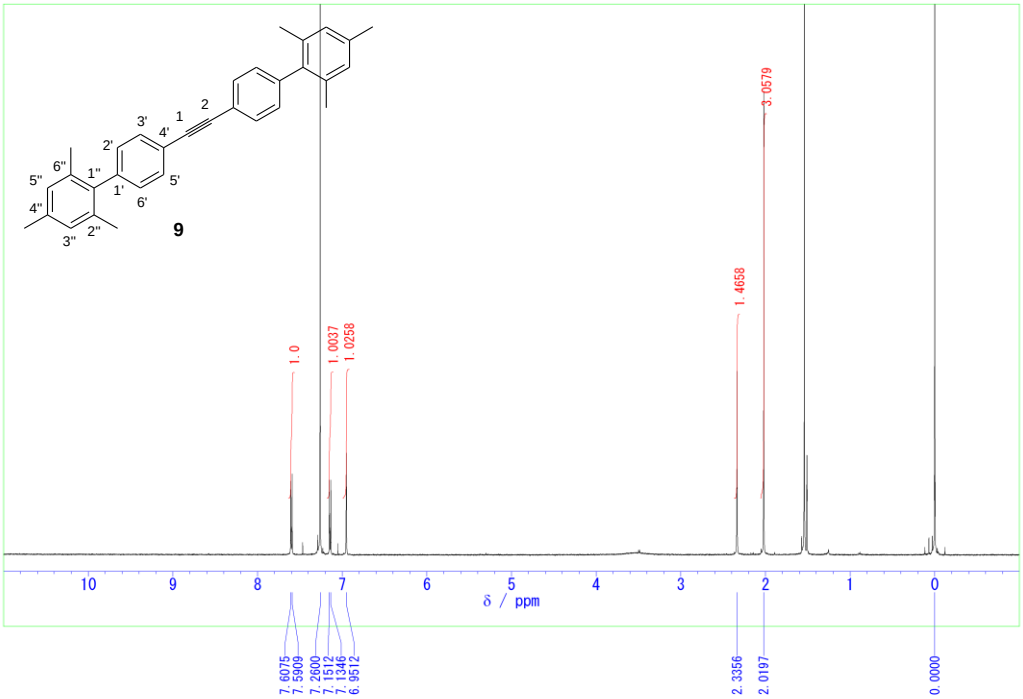


Figure S-68. ^{1}H NMR spectrum (500 MHz) of bis(4-mesitylphenyl)acetylene (**9**) in $CDCl_3$.

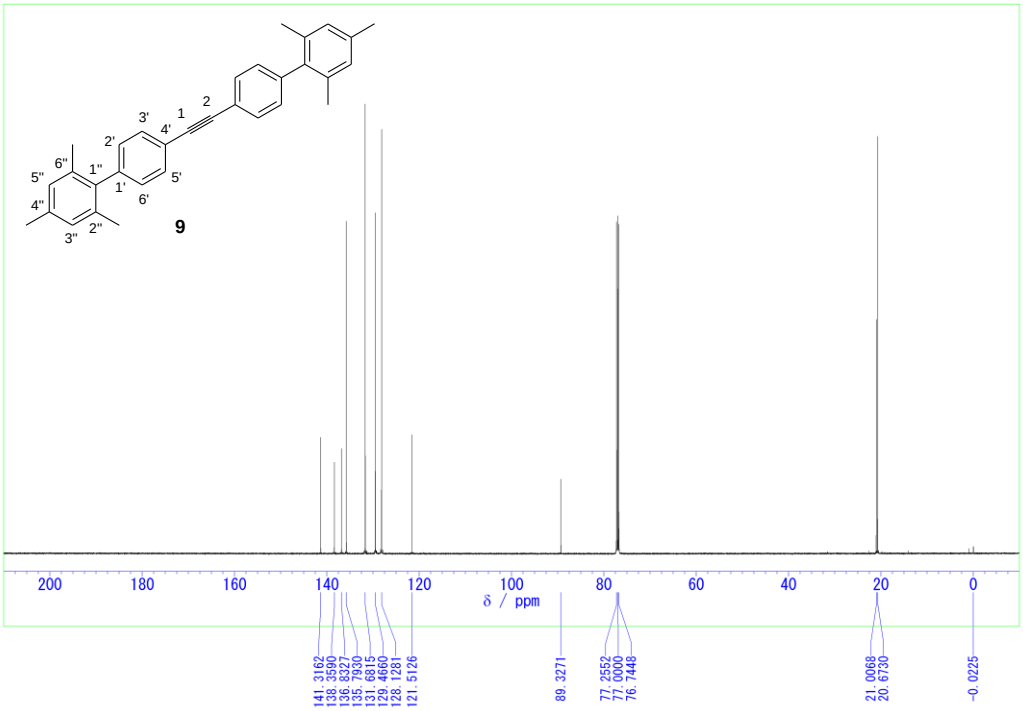


Figure S-69. ^{13}C NMR spectrum (125 MHz) of bis(4-mesitylphenyl)acetylene (**9**) in $CDCl_3$.

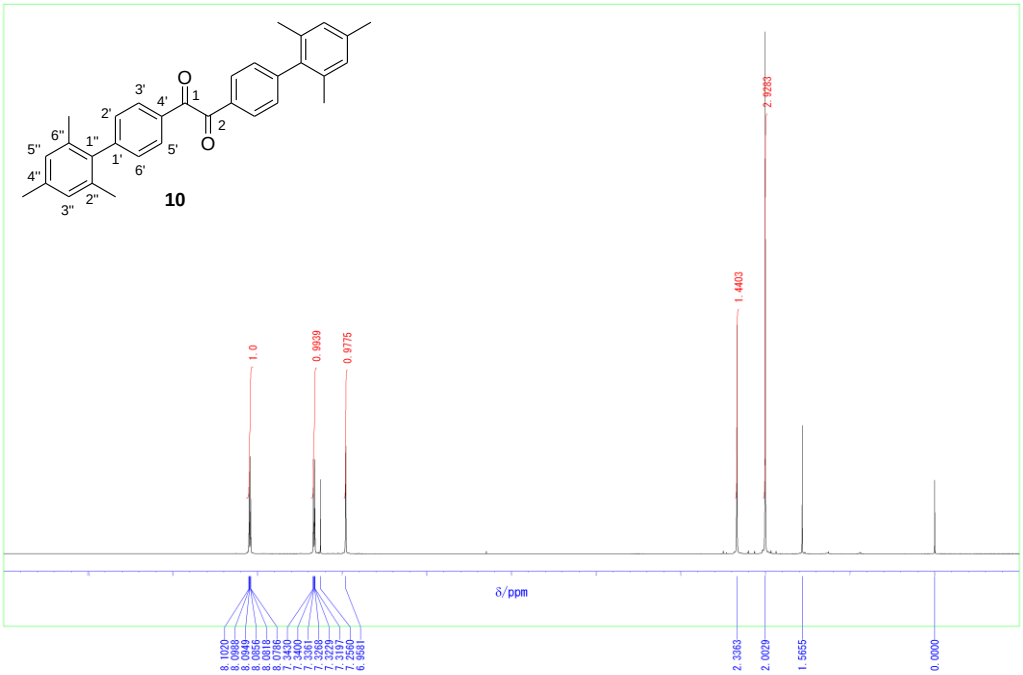


Figure S-70. ^{1}H NMR spectrum (500 MHz) of 1,2-bis(4-mesitylphenyl)ethane-1,2-dione (**10**) in $CDCl_3$.

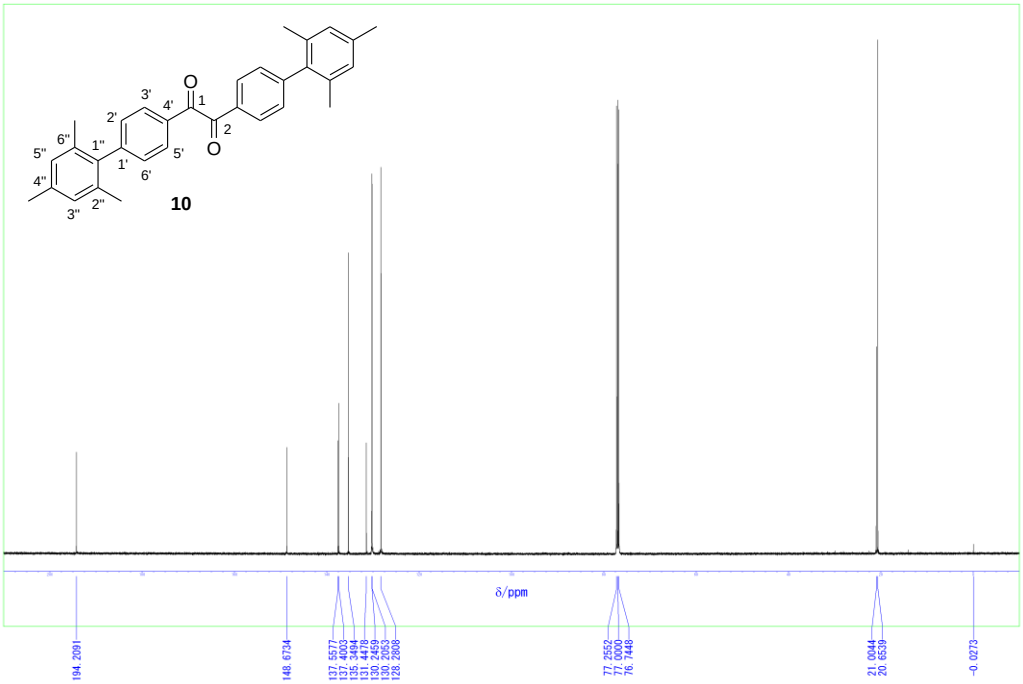


Figure S-71. ^{13}C NMR spectrum (125 MHz) of 1,2-bis(4-mesitylphenyl)ethane-1,2-dione (**10**) in $CDCl_3$.

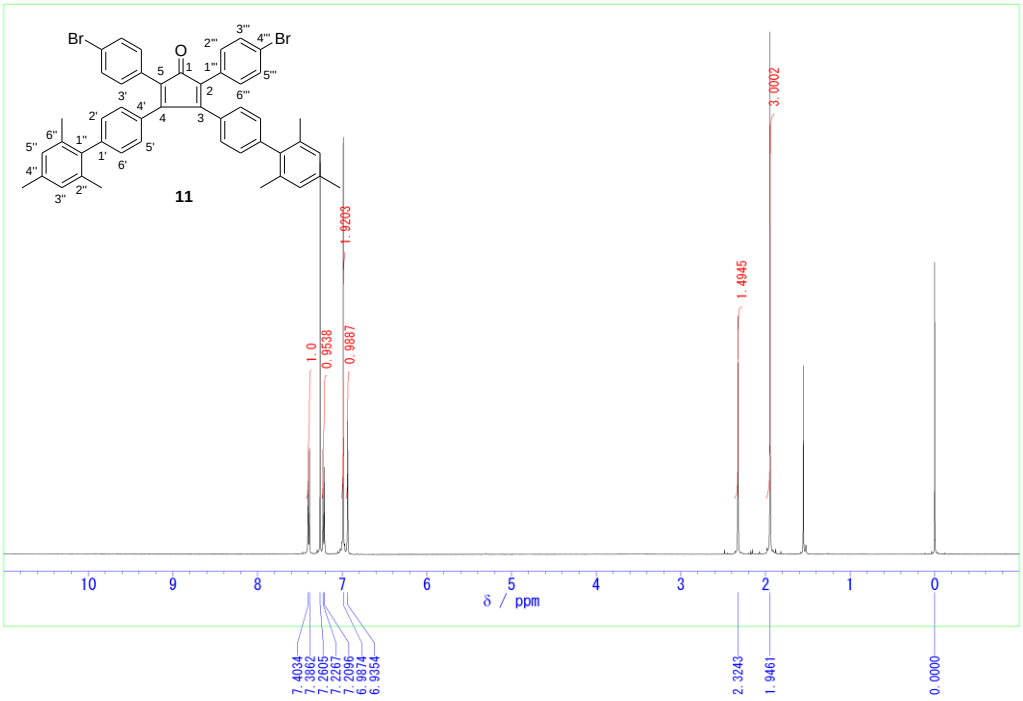


Figure S-72. ^{1}H NMR spectrum (500 MHz) of 2,3-bis(4-bromophenyl)-4,5-bis(4-mesitylphenyl)cyclopentadienone (**11**) in $CDCl_3$.

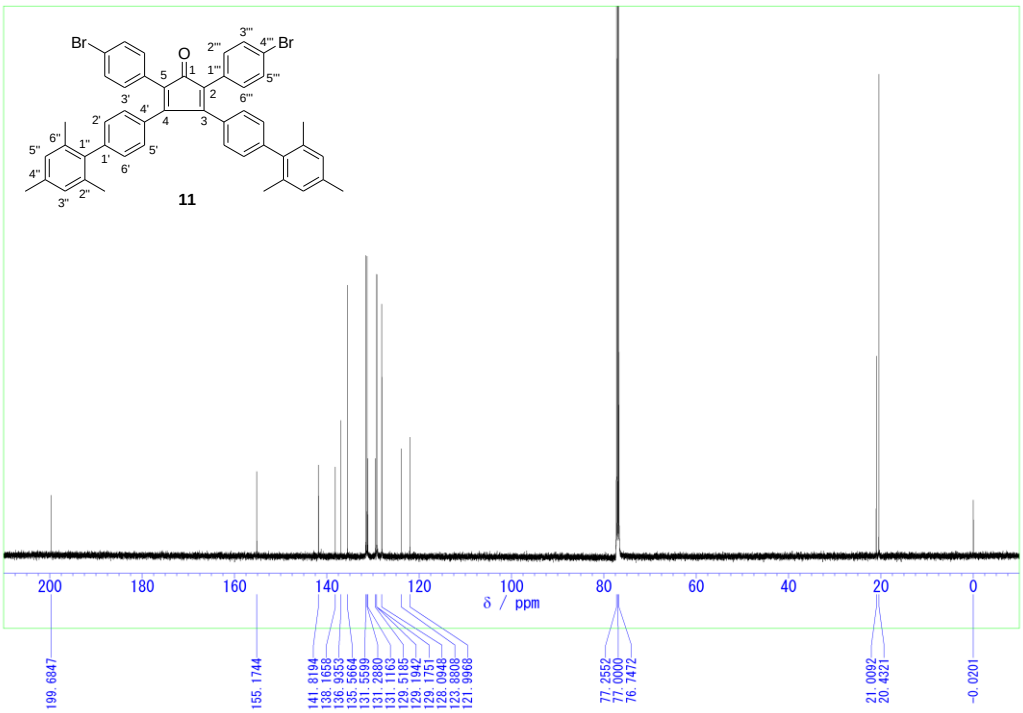


Figure S-73. ^{13}C NMR spectrum (125 MHz) of 2,3-bis(4-bromophenyl)-4,5-bis(4-mesitylphenyl)cyclopentadienone (**11**) in $CDCl_3$.

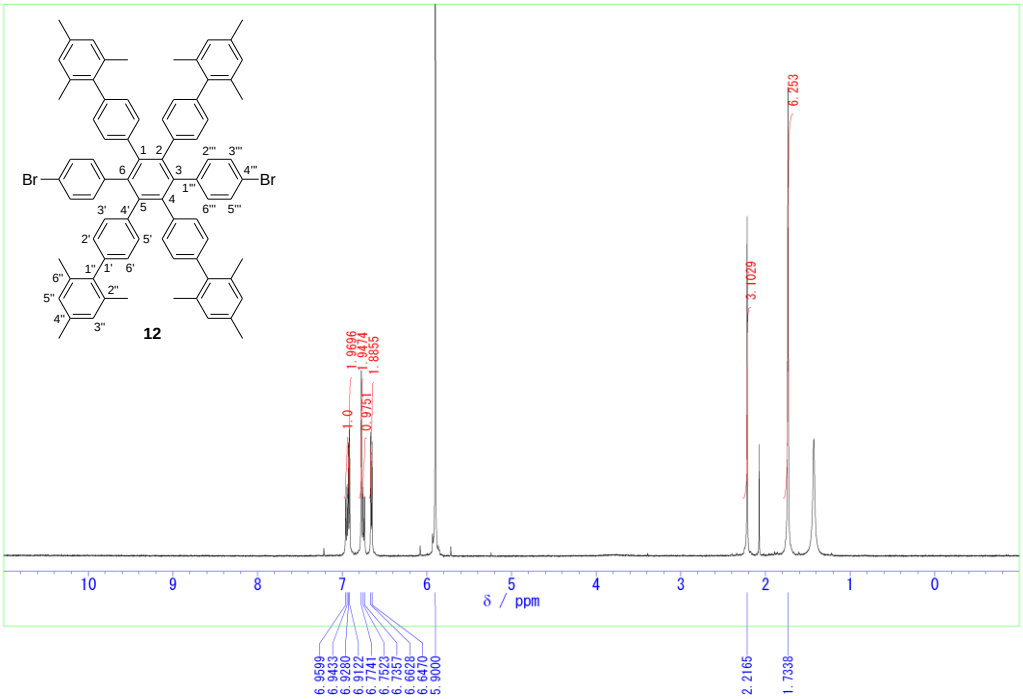


Figure S-74. ^{1}H NMR spectrum (500 MHz) of 1,4-bis(4-bromophenyl)-2,3,5,6-tetrakis(4-mesitylphenyl)benzene (**12**) in $C_2D_2Cl_4$ at 80 °C

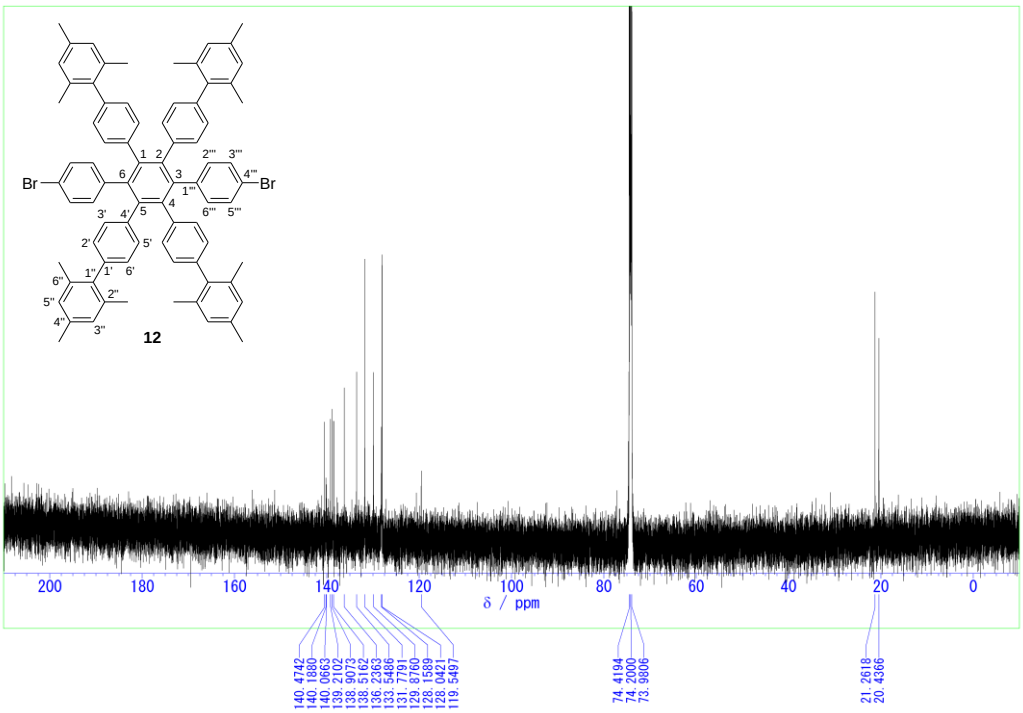


Figure S-75. ^{13}C NMR spectrum (125 MHz) of 1,4-bis(4-bromophenyl)-2,3,5,6-tetrakis(4-mesitylphenyl)benzene (**12**) in $C_2D_2Cl_4$ at 80 °C.

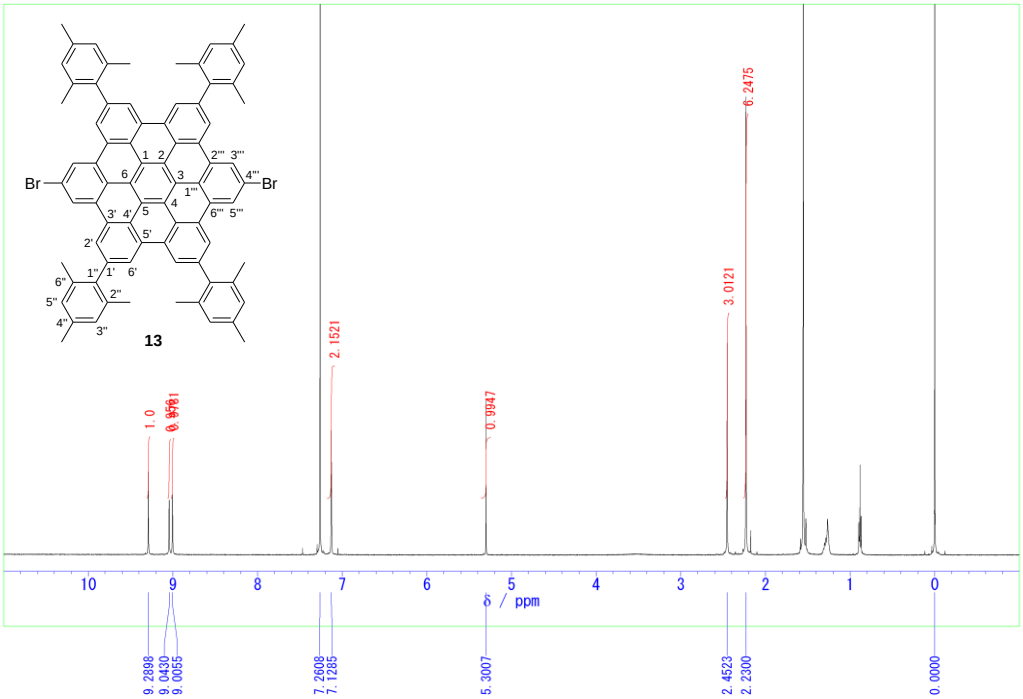


Figure S-76. ^{1}H NMR spectrum (500 MHz) of 2,11-dibromo-5,8,14,17-tetramesitylhexabenzo-[*bc*,*ef*,*hi*,*kl*,*no*,*qr*]coronene (**13**) in $CDCl_3$.

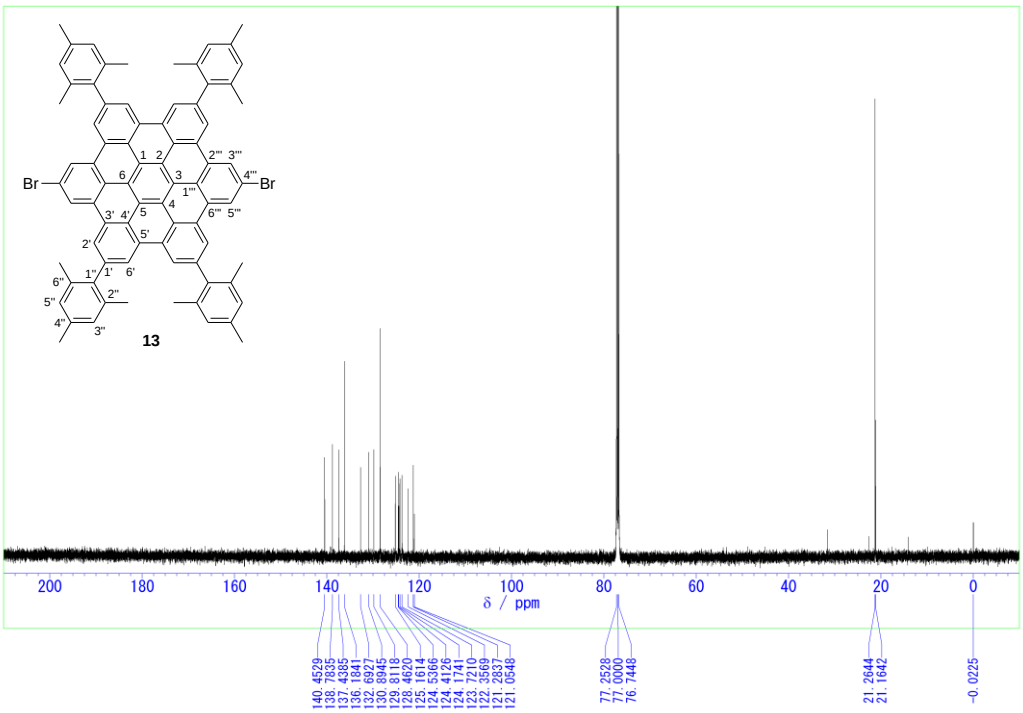


Figure S-77. ^{13}C NMR spectrum (125 MHz) of 2,11-dibromo-5,8,14,17-tetramesitylhexabenzo-[*bc*,*ef*,*hi*,*kl*,*no*,*qr*]coronene (**13**) in $CDCl_3$.

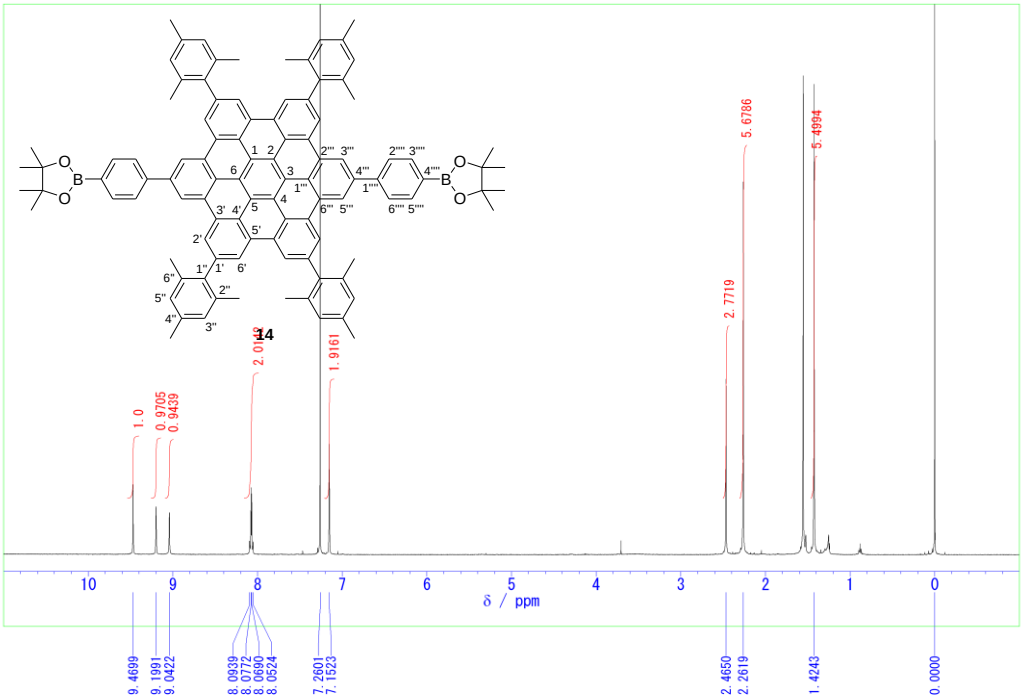


Figure S-78. ^{1}H NMR spectrum (500 MHz) of 2,11-bis[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-5,8,14,17-tetramesitylhexabenzo[*bc*,*ef*,*hi*,*kl*,*no*,*qr*]coronene (**15**) in $CDCl_3$.

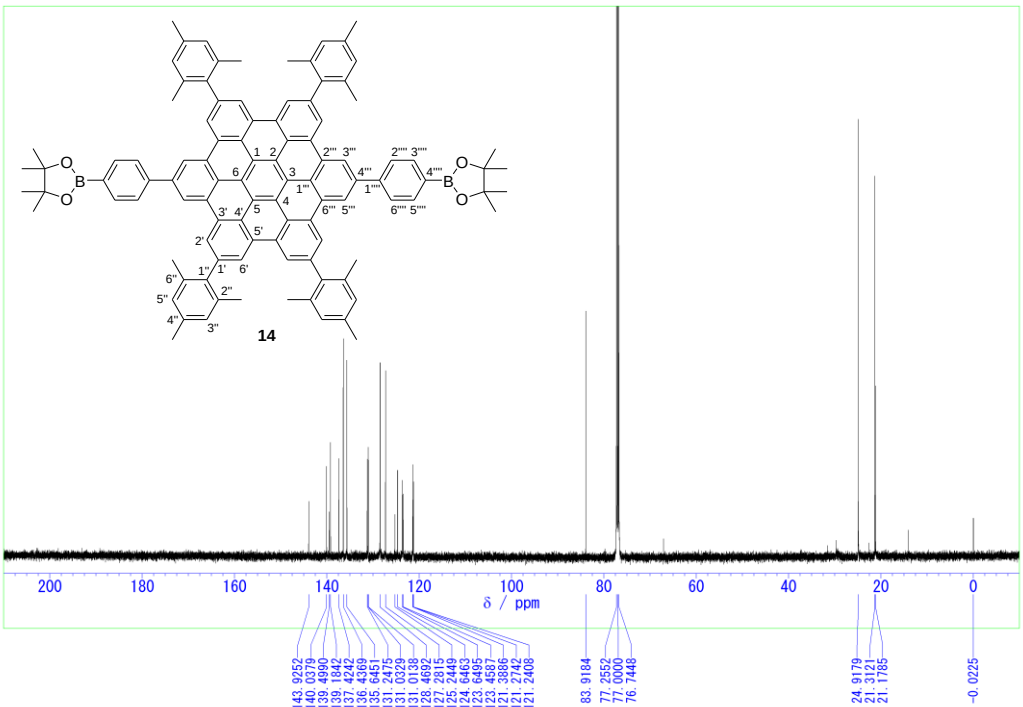


Figure S-79. ^{13}C NMR spectrum (125 MHz) of 2,11-bis[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-5,8,14,17-tetramesitylhexabenzo[*bc*,*ef*,*hi*,*kl*,*no*,*qr*]coronene (**15**) in $CDCl_3$.

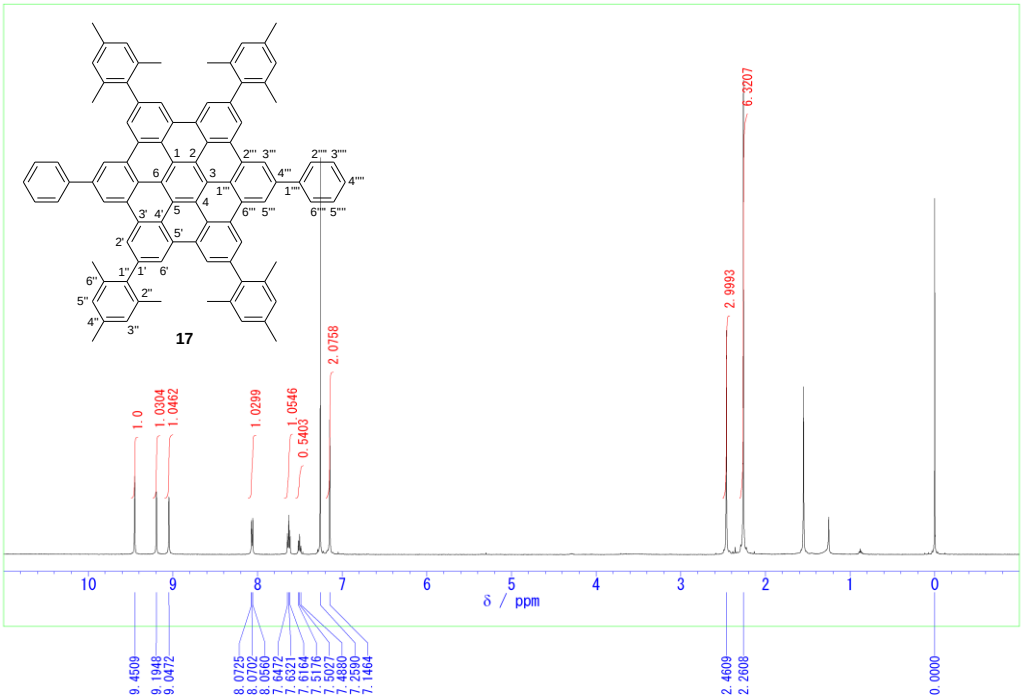


Figure S-80. ^{1}H NMR spectrum (500 MHz) of 2,5,11,14-tetramesityl-8,17-diphenylhexabenzo[*bc*,*ef*,*hi*,*kl*,*no*,*qr*]coronene (**2a**) in $CDCl_3$.

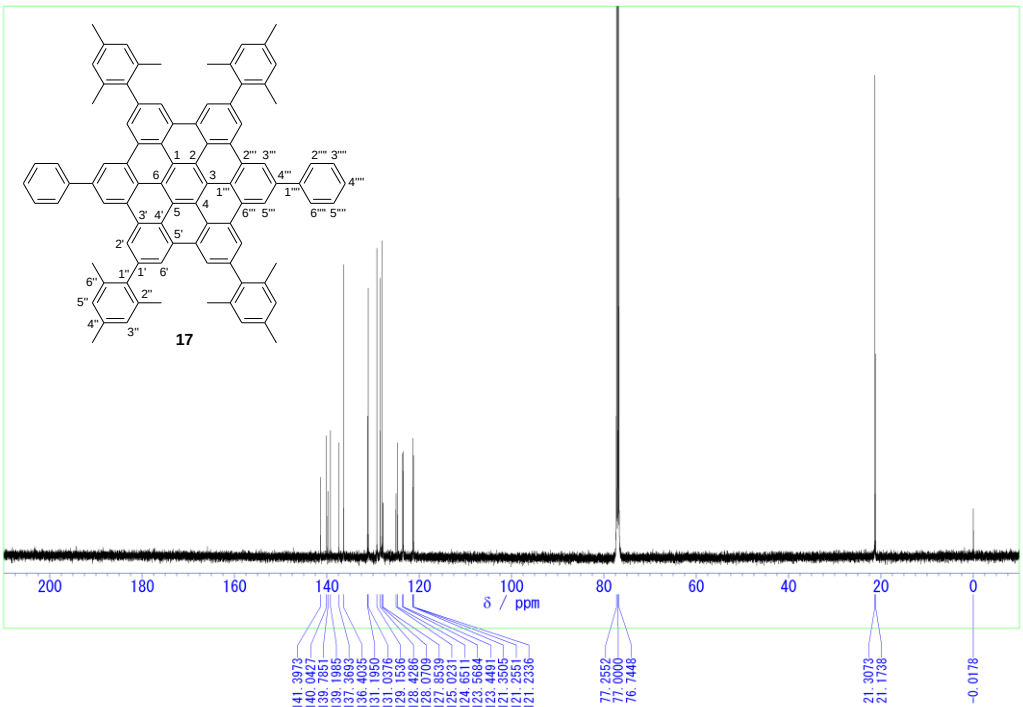


Figure S-81. ^{13}C NMR spectrum (125 MHz) of 2,5,11,14-tetramesityl-8,17-diphenylhexabenzo[*bc*,*ef*,*hi*,*kl*,*no*,*qr*]coronene (**17**) in $CDCl_3$.

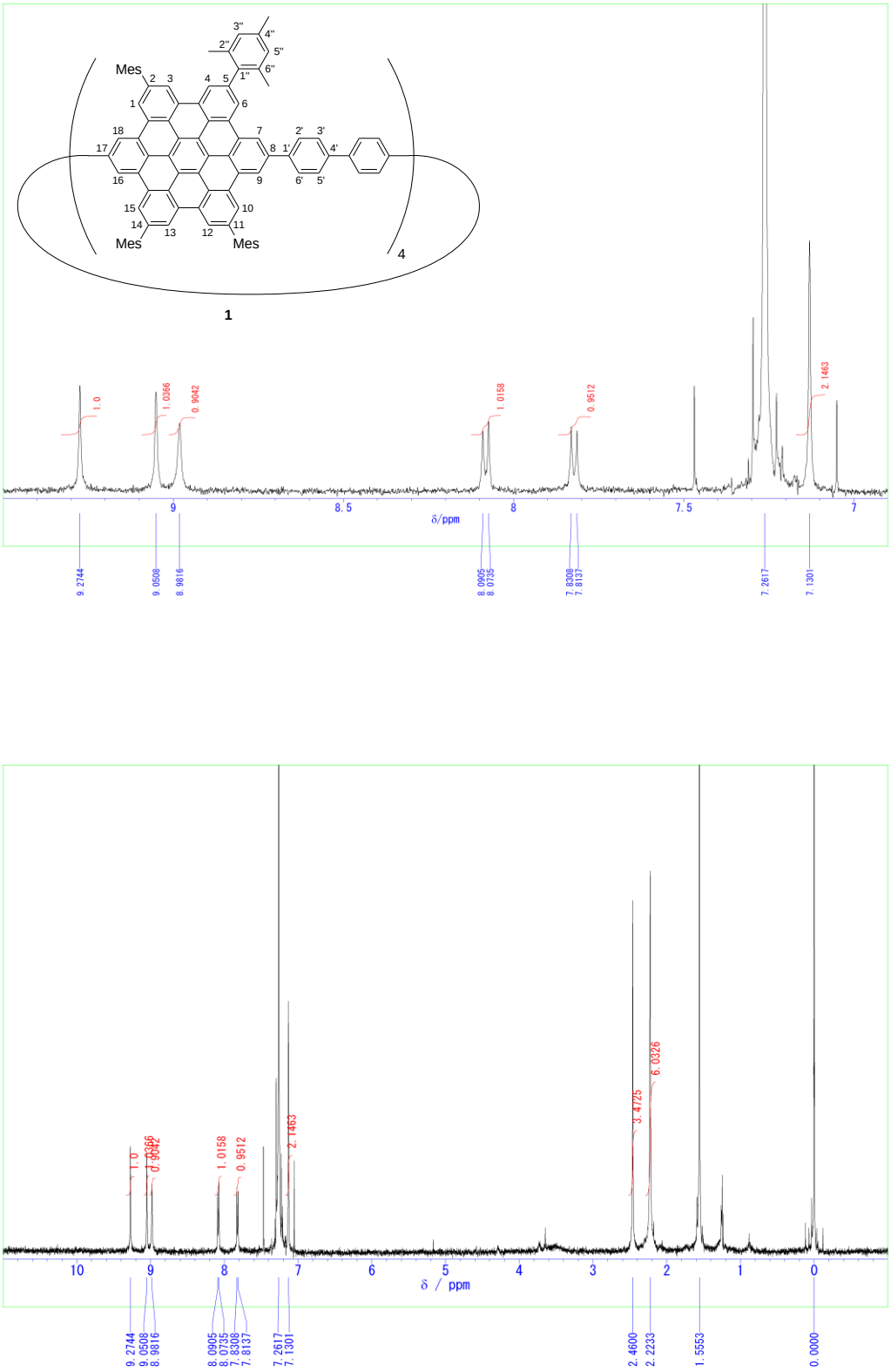


Figure S-82. ^{1}H NMR spectrum (500 MHz) of [4]cyclo(2,5,11,14-tetramesityl-8,17-diphenylhexabenzo[*bc*,*ef*,*hi*,*kl*,*no*,*qr*]coronene) (**1**) in $CDCl_3$.

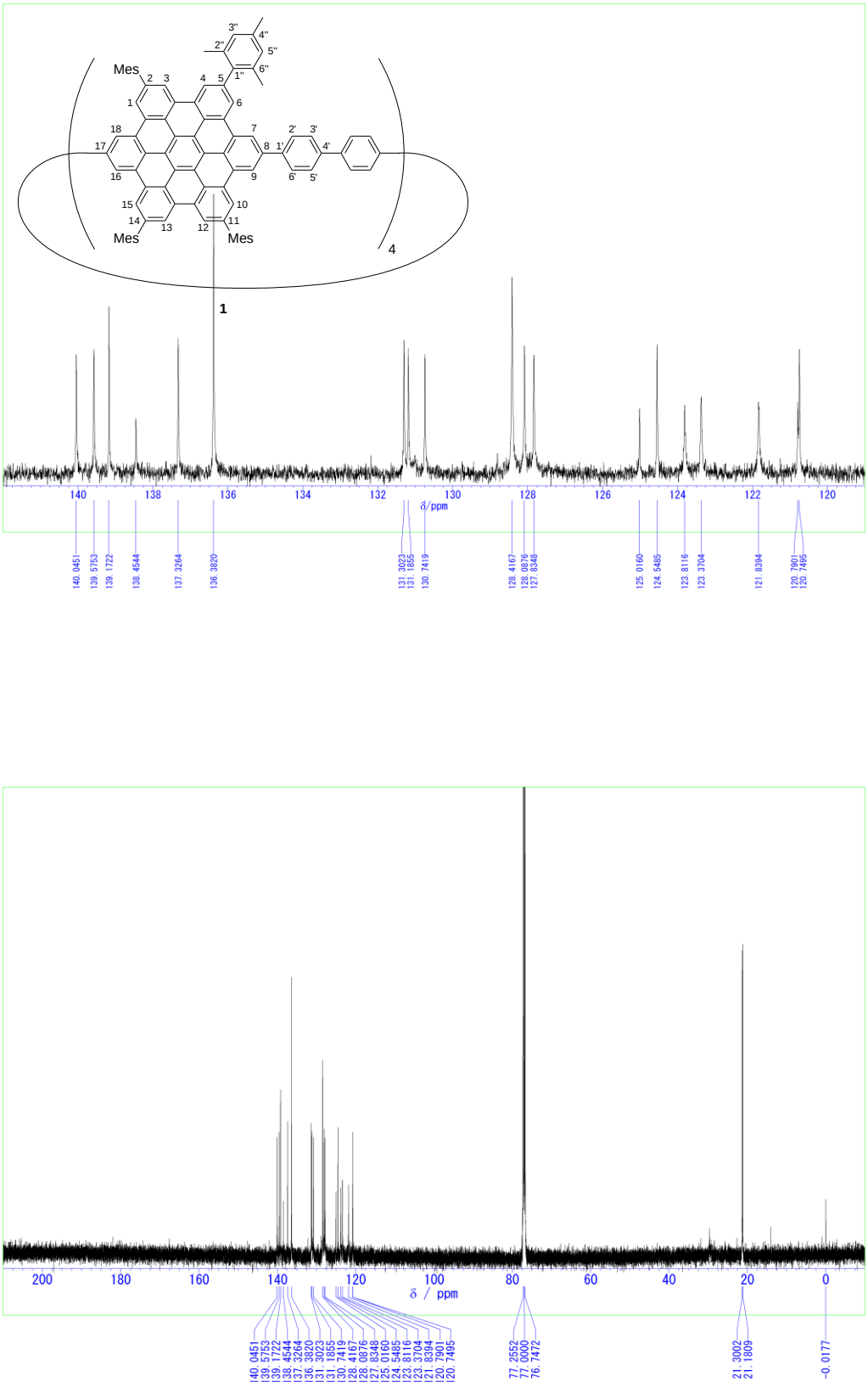


Figure S-83. ^{13}C NMR spectrum (125 MHz) of [4]cyclo(2,5,11,14-tetramesityl-8,17-diphenylhexabenzo[*bc*,*ef*,*hi*,*kl*,*no*,*qr*]coronene) (**1**) in $CDCl_3$.

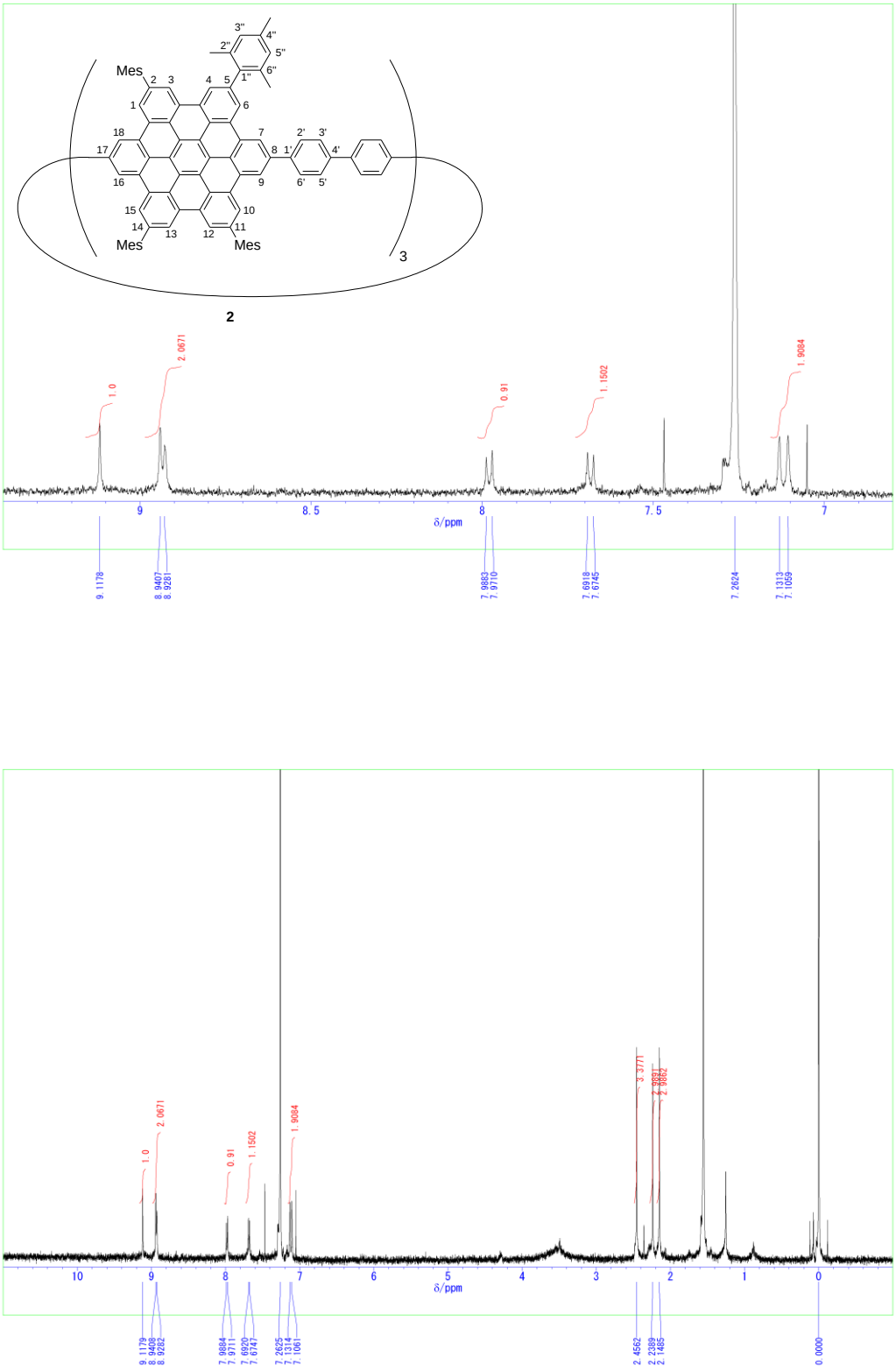


Figure S-84. ^{1}H NMR spectrum (500 MHz) of [3]cyclo(2,5,11,14-tetramesityl-8,17-diphenylhexabenzo[*bc*,*ef*,*hi*,*kl*,*no*,*qr*]coronene) (**2**) in $CDCl_3$.

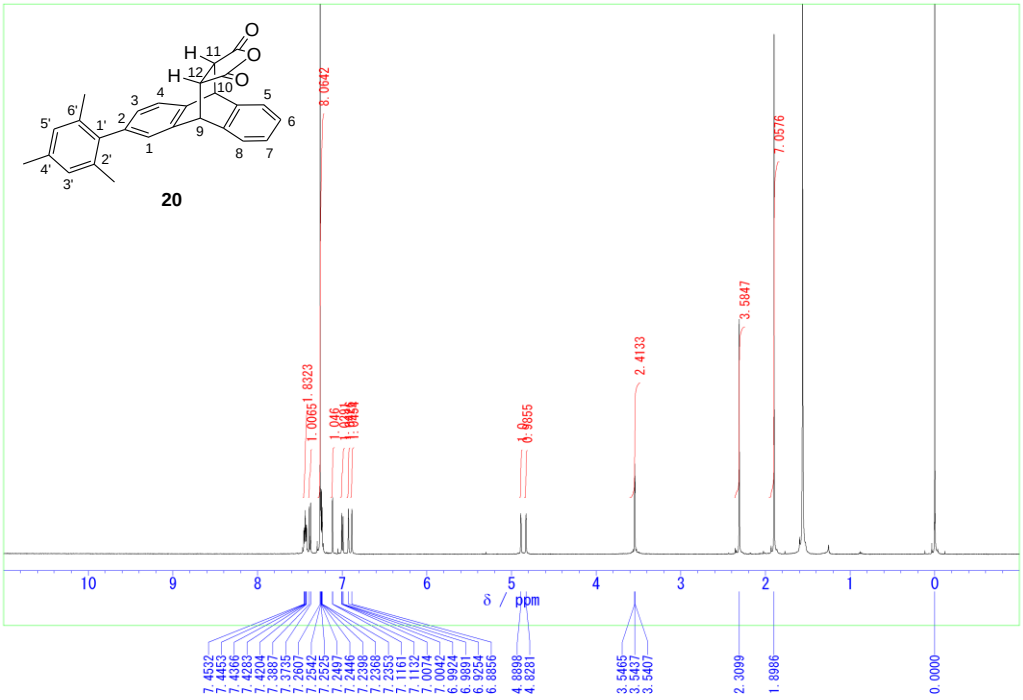


Figure S-85. ^{1}H NMR spectrum (500 MHz) of *anti*-2-mesityl-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylic anhydride (major isomer **20**) in $CDCl_3$.

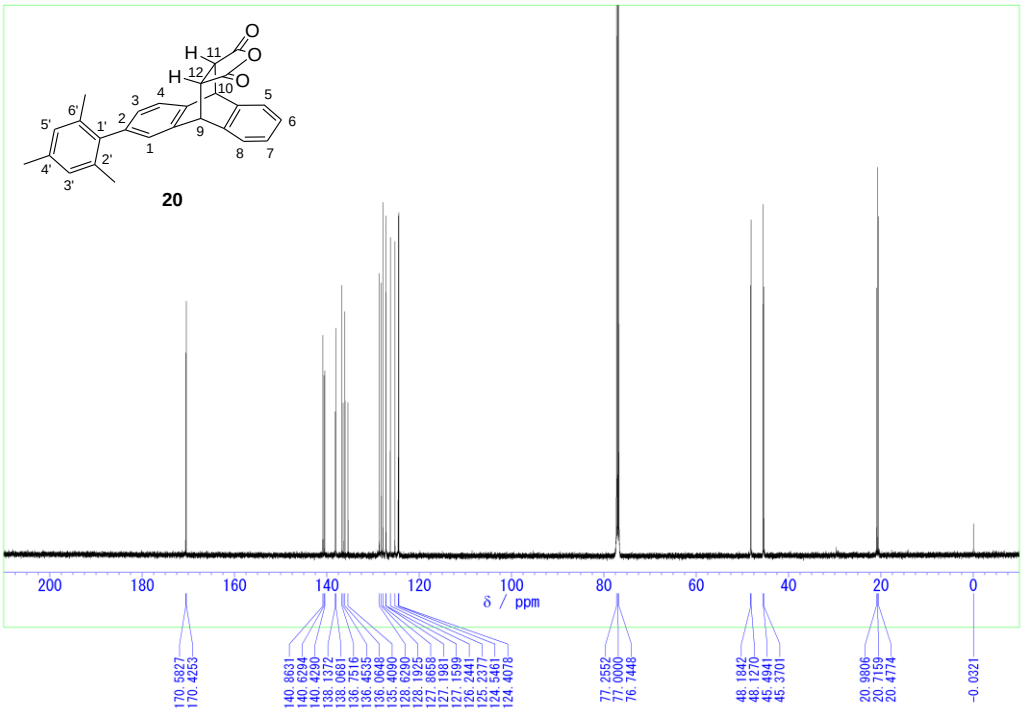


Figure S-86. ^{13}C NMR spectrum (125 MHz) of *anti*-2-mesityl-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylic anhydride (major isomer **20**) in $CDCl_3$.

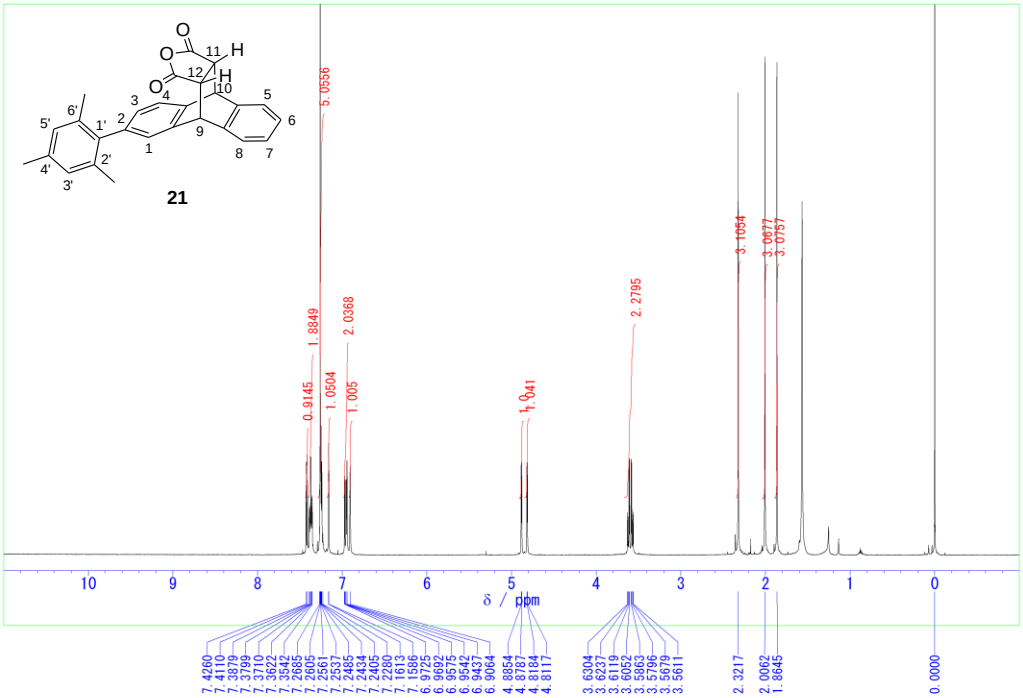


Figure S-87. ^{1}H NMR spectrum (500 MHz) of *syn*-2-mesityl-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylic anhydride (minor isomer **21**) in $CDCl_3$.

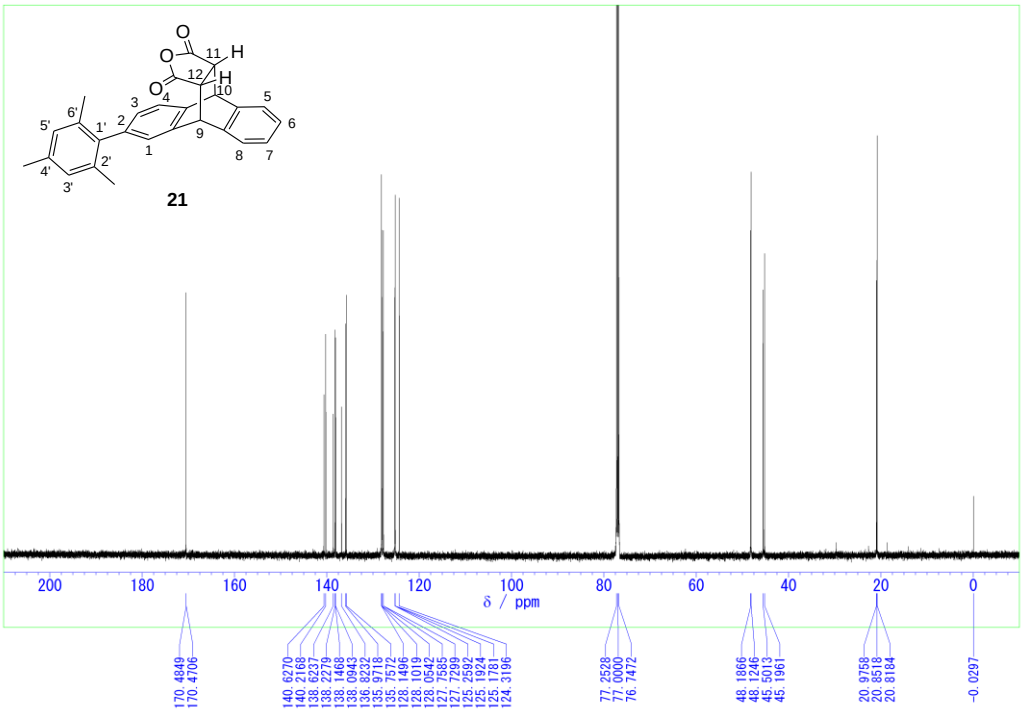


Figure S-88. ^{13}C NMR spectrum (125 MHz) of *syn*-2-mesityl-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylic anhydride (minor isomer **21**) in $CDCl_3$.

(12) Cartesian Coordinates (Angstroms) for 1, 2, and the Model HBC Derivative 17

Cartesian Coordinates (Angstroms) for the Cyclic Tetramer **1** (Conformer **A**) without the Mesityl Substituents Optimized at the HF/3-21G Level (-8190.289024 hartrees)

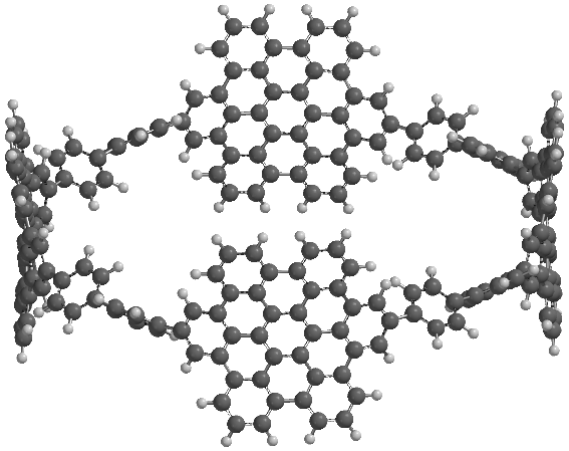


Figure S-89. Optimized structure of cyclic tetramer **1** (Conformer **A**) without the mesityl substituents optimized at the HF/3-21G level.

Coordinates (Angstroms)

ATOM X Y Z

1 C -10.5183435080 8.8243000927 1.1348377972	20 C -12.5114446740 6.9399812010 3.6709073407
2 C -9.5494676709 9.7254999189 -1.3377585078	21 C -11.3096821310 8.6803903235 4.7839700482
3 C -9.5518555967 9.8365353579 1.0894919765	22 H -13.2189068830 6.1396683973 3.7172326315
4 C -10.9754666330 8.2401539938 -0.0550316384	23 H -11.0823672260 9.1889162488 5.6950167857
5 C -10.5161553320 8.7135887448 -1.2924346762	24 H -12.6832977360 7.3756660567 5.7445390409
6 C -9.0434185345 10.2631428810 -0.1456590524	25 C -7.9190856022 11.1724137450 -0.1860836666
7 C -9.0786499032 10.4431813540 2.3163705381	26 C -5.4187175424 12.4059588330 -0.2407754981
8 C -8.2775842695 11.7439239970 4.6366780251	27 C -7.3257625932 11.5029393830 -1.4147817371
9 C -9.6883945302 10.1257143840 3.5439982474	28 C -7.3305711793 11.6189684440 1.0067999454
10 C -8.0183090917 11.3672465850 2.2786016916	29 C -6.0759713280 12.2141308840 0.9613452525
11 C -7.6447227462 12.0209137730 3.4443015985	30 C -6.0734937032 12.1006547140 -1.4219357038
12 C -9.2756577858 10.7963847320 4.6902576596	31 H -5.5580557302 12.4422418290 1.8684479416
13 H -6.8743688506 12.7619296800 3.4221538914	32 H -5.5655311350 12.2734141540 -2.3468078675
14 H -9.7295352594 10.5872790560 5.6339323709	33 C -9.0752445945 10.2187502430 -2.6142556450
15 H -7.9875403890 12.2627489010 5.5283195632	34 C -8.2774396232 11.3108731770 -5.0407666599
16 C -11.0479963250 8.3834648905 2.4087282375	35 C -8.0159385592 11.1434129300 -2.6590975134
17 C -12.2140837290 7.6423535538 4.8187808083	36 C -9.6836286833 9.7917219705 -3.8086995253
18 C -10.7058397750 9.0643504540 3.5912850376	37 C -9.2728978091 10.3596854720 -5.0099965183
19 C -11.9235723540 7.2833952174 2.4617139419	38 C -7.6440357683 11.6928302450 -3.8778799195

39 H -9.7271224054 10.0674757280 -5.9311705415
40 H -6.8760756336 12.4354246670 -3.9214623477
41 H -7.9897842467 11.7506508210 -5.9746425293
42 C -11.0421948020 8.1574319030 -2.5217807610
43 C -12.1957322230 7.1920379530 -4.8576493574
44 C -11.9159267710 7.0557662339 -2.4757126671
45 C -10.6973998530 8.7270349905 -3.7612443312
46 C -11.2945547420 8.2318753637 -4.9156401320
47 C -12.4971025450 6.5995414541 -3.6504622021
48 H -11.0638189630 8.6535699734 -5.8692125263
49 H -13.2015386430 5.7956860508 -3.6250132553
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51 C -11.8317681800 7.0755401808 -0.0026885750
52 C -12.9473723520 4.5216932739 0.1128082312
53 C -12.1933650770 6.4135189307 -1.1856719379
54 C -12.1918965440 6.5216198130 1.2361330131
55 C -12.7307430450 5.2432045806 1.2747589275
56 C -12.7288826330 5.1342143033 -1.1086175257
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59 C -3.9684911801 12.7534444190 -0.2482882871
60 C -1.2001006787 13.1204452980 -0.0779842607
61 C -3.4413838806 13.8476689280 0.4229356712
62 C -3.0947118509 11.8681847020 -0.8701353317
63 C -1.7316919379 12.0488272290 -0.7851263255
64 C -2.0681644068 14.0319949550 0.5038857694
65 H -4.1013324793 14.5487325980 0.8952755635
66 H -3.4890940175 11.0131880230 -1.3818448184
67 H -1.0684464742 11.3438869890 -1.2455196306
68 H -1.6733626630 14.8666142920 1.0488205493
69 C -13.2262597540 3.0578953525 0.1669304858
70 C -13.4342257760 0.2699393692 0.0751636069
71 C -12.3569891250 2.2562381624 0.8987121377
72 C -14.2308446820 2.4480108792 -0.5719293635
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75 H -11.5684509880 2.7134242749 1.4619771285
76 H -14.9216903990 3.0514167223 -1.1274391641
77 H -15.0976579950 0.6059520229 -1.2137441949
78 H -11.7609790590 0.2752032013 1.3920044279
79 C 9.5478845848 -9.8414368192 1.1092772769
80 C 10.5305295460 -8.7326225540 -1.2716918133
81 C 10.5120192420 -8.8270922034 1.1560950319
82 C 9.0504507081 -10.2768354520 -0.1272473146
83 C 9.5656583128 -9.7461983038 -1.3184921750
84 C 10.9783563360 -8.2500844098 -0.0336673281
85 C 11.0293664030 -8.3763955947 2.4315242470
86 C 12.1718076790 -7.6152913864 4.8464926889
87 C 11.9010783850 -7.2733155527 2.4846599308
88 C 10.6788237150 -9.0503301313 3.6155930382
89 C 11.2709326970 -8.6564057801 4.8108551799
90 C 12.4771925660 -6.9197710107 3.6965229944
91 H 11.0369959180 -9.1593021746 5.7233503138
92 H 13.1817069950 -6.1168954595 3.7435262345
93 H 12.6319393260 -7.3407966143 5.7745251143
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95 C 8.2486672739 -11.7296897630 4.6575527071
96 C 8.0073384788 -11.3672903710 2.2954063328
97 C 9.6646861673 -10.1147820970 3.5665949741
98 C 9.2442631101 -10.7796477840 4.7134718676
99 C 7.6257319547 -12.0148852510 3.4618821223
100 H 9.6902349714 -10.5640219090 5.6594531211
101 H 6.8569763892 -12.7575230220 3.4379007205
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103 C 11.8314716740 -7.0830796748 0.0181563293
104 C 12.9365642790 -4.5247755353 0.1257475905
105 C 12.2022891480 -6.4284923188 -1.1661130222
106 C 12.1780145840 -6.5192423796 1.2562971700
107 C 12.7111425980 -5.2383557439 1.2908052658
108 C 12.7331288670 -5.1468691817 -1.0932816291
109 H 12.8932423800 -4.7571672087 2.2281673549
110 H 12.8984629150 -4.5844363859 -1.9873707562
111 C 11.0663577090 -8.1839753797 -2.5001254186
112 C 12.2393009600 -7.2333104510 -4.8321091411
113 C 10.7330999960 -8.7625688358 -3.7385635781
114 C 11.9380620040 -7.0806554987 -2.4539480351
115 C 12.5290638760 -6.6318173563 -3.6265437454
116 C 11.3399531210 -8.2747260967 -4.8909281030

117 H 13.2320084250 -5.8266655762 -3.6004396506
118 H 11.1182639180 -8.7033360671 -5.8435361273
119 H 12.7100934790 -6.8850436489 -5.7295578940
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126 H 6.9153064640 -12.4744349240 -3.9066625682
127 H 8.0458560512 -11.8024137620 -5.9549896563
128 C 7.9273814679 -11.1874729300 -0.1710923177
129 C 5.4273300808 -12.4209872940 -0.2378042294
130 C 7.3298237169 -11.6271467120 1.0197945123
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132 C 6.0912615710 -12.1230048030 -1.4157257701
133 C 6.0756019278 -12.2224804560 0.9681594390
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135 H 5.5506837157 -12.4449268920 1.8726398116
136 C 13.2061721370 -3.0588720957 0.1730571483
137 C 13.4026985260 -0.2704839187 0.0695242734
138 C 14.2283505120 -2.4487016093 -0.5406022350
139 C 12.3113683340 -2.2573016594 0.8733358072
140 C 12.4081468680 -0.8838642048 0.8210955568
141 C 14.3276951530 -1.0653149387 -0.5894437119
142 H 14.9378247920 -3.0521268267 -1.0722766404
143 H 11.5100175070 -2.7155596818 1.4174898074
144 H 11.6916148320 -0.2765478228 1.3372915586
145 H 15.1050137940 -0.6061430663 -1.1678225768
146 C 3.9765546895 -12.7660705310 -0.2527467815
147 C 1.2063651520 -13.1229985760 -0.0906781912
148 C 3.1081507546 -11.8824049030 -0.8844660162
149 C 3.4432347444 -13.8545152270 0.4230549690
150 C 2.0692080070 -14.0338122290 0.4999566858
151 C 1.7441998600 -12.0582026990 -0.8035566009
152 H 3.5073164735 -11.0321021960 -1.4001431439
153 H 4.0989149554 -14.5542491770 0.9028702020
154 H 1.6695462946 -14.8633689170 1.0491594449
155 H 1.0851772966 -11.3544862490 -1.2711893062
156 C 8.8593785146 10.3998578710 1.3166222351
157 C 9.8666010706 9.5484338070 -1.1581026808
158 C 9.8930563219 9.4565809694 1.2697324379
159 C 8.3073956408 10.8923186800 0.1254357633
160 C 8.8334651956 10.4923670750 -1.1111881679
161 C 10.3730410270 9.0062185633 0.0316595241
162 C 10.4666880700 8.9473903640 2.4980904907
163 C 11.7043319250 8.0819895113 4.8298127176
164 C 11.4135814370 7.9079006548 2.4518769102
165 C 10.0942743080 9.5016498931 3.7364616160
166 C 10.7342760700 9.0578662302 4.8886970707
167 C 12.0350705580 7.5019518357 3.6243280537
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169 H 12.7926975950 6.7480390250 3.5981642088
170 H 12.1986902860 7.7678094792 5.7271354027
171 C 8.3628814079 10.8687275820 2.5937752724
172 C 7.5116810459 11.9211656870 5.0195213711
173 C 9.0096233707 10.4940324940 3.7856182663
174 C 7.2421180941 11.7177534520 2.6416023113
175 C 6.8432424094 12.2492407570 3.8597525233
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178 H 9.0518849979 10.7883777950 5.9056204809
179 H 7.2021091387 12.3470336270 5.9528499610
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182 C 11.6909726560 7.3637010419 -1.2582881018
183 C 11.7224145810 7.2755331971 1.1641242886
184 C 12.3419050980 6.0343410270 1.0914159610
185 C 12.3129256350 6.1235269104 -1.2926418165
186 H 12.5464769320 5.4851109654 1.9855855259
187 H 12.5281917760 5.6561580767 -2.2299672797
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189 C 11.6059010760 8.4551626131 -4.8489571266
190 C 10.0159191590 9.7817320835 -3.6178223277
191 C 11.3610722960 8.0959452989 -2.4867904447
192 C 11.9601215090 7.7834465628 -3.6988477431
193 C 10.6338014610 9.4300646767 -4.8132546263
194 H 12.7195051390 7.0322618106 -3.7458982897

195 H 10.3645143740 9.9147939176 -5.7258313105
196 H 12.0838374600 8.2134359054 -5.7771036022
197 C 8.3093991188 11.0558398470 -2.3379793506
198 C 7.4019673717 12.2821156740 -4.6596747496
199 C 7.1883716366 11.9050264050 -2.2971492031
200 C 8.9291730621 10.7719207480 -3.5687312519
201 C 8.4621115858 11.4047224670 -4.7157084328
202 C 6.7612485971 12.5233527730 -3.4637423918
203 H 8.9215804714 11.2205357880 -5.6618652711
204 H 5.9420176167 13.2099055950 -3.4396293552
205 H 7.0698567194 12.7736298800 -5.5521060325
206 C 7.1230576648 11.7216782810 0.1695350355
207 C 4.5423019800 12.7760471330 0.2372704857
208 C 6.4951165585 12.1172756340 -1.0212089038
209 C 6.5179841571 12.0188033790 1.4010059690
210 C 5.2265903826 12.5267052130 1.4149013935
211 C 5.2020547726 12.6226257170 -0.9690687259
212 H 4.7152673228 12.6698143030 2.3430215322
213 H 4.6620380432 12.8065526090 -1.8733298152
214 C 12.9601250800 3.9844532682 -0.1746235383
215 C 13.3507109380 1.2164242481 -0.0706138362
216 C 14.0211337500 3.4472633947 0.5408920913
217 C 12.1248118230 3.1221020463 -0.8765123318
218 C 12.3172505540 1.7587302197 -0.8241080351
219 C 14.2166897750 2.0741201710 0.5900184762
220 H 14.6855983090 4.0987798381 1.0739162681
221 H 11.2944077260 3.5231462866 -1.4221518877
222 H 11.6461055560 1.1028520652 -1.3417522688
223 H 15.0229427110 1.6704271061 1.1699939450
224 C 3.0708698029 13.0181032050 0.2528503847
225 C 0.2823353680 13.1773246680 0.0904404402
226 C 2.4616817936 14.0628642470 -0.4280015970
227 C 2.2673546756 12.0788517050 0.8896539932
228 C 0.8943492688 12.1572720400 0.8085934914
229 C 1.0784254675 14.1439955820 -0.5052241142
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232 H 0.2868220678 11.4105118510 1.2797390705
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235 C -8.8390273021 -10.4864249040 -1.0890675234
236 C -8.8458085395 -10.3808936840 1.3384098906
237 C -10.3721666630 -8.9968619620 0.0579786373
238 C -9.8744115149 -9.5447468406 -1.1328424297
239 C -8.3024937973 -10.8788797670 0.1454922052
240 C -8.3387744111 -10.8424106050 2.6141388960
241 C -7.4678276663 -11.8816447470 5.0386764848
242 C -7.2170570451 -11.6903127760 2.6576857592
243 C -8.9763601016 -10.4619713500 3.8090463792
244 C -8.5276184807 -11.0026587010 5.0093368418
245 C -6.8082711606 -12.2152168990 3.8754386916
246 H -9.0019677694 -10.7454344050 5.9308008938
247 H -5.9900206063 -12.9020849160 3.9178682866
248 H -7.1506787861 -12.3024845640 5.9717378817
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251 C -11.3944410060 -7.8864261585 2.4804786234
252 C -10.0621920860 -9.4708052999 3.7631785080
253 C -10.6927894030 -9.0208831203 4.9181406119
254 C -12.0065141470 -7.4743905550 3.6557183301
255 H -10.4331752960 -9.4270305911 5.8709261068
256 H -12.7655233990 -6.7218157798 3.6315802935
257 H -12.1515781280 -7.7275981719 5.7613495278
258 C -7.1168056947 -11.7065817410 0.1847082670
259 C -4.5352949755 -12.7598765900 0.2385190298
260 C -6.4974180545 -12.1075745250 -1.0087432082
261 C -6.5023650772 -11.9971865900 1.4131137223
262 C -5.2108394952 -12.5046146450 1.4198822016
263 C -5.2037815663 -12.6123963030 -0.9636790743
264 H -4.6924685402 -12.6429939740 2.3447742612
265 H -4.6704373409 -12.8010465610 -1.8709185111
266 C -8.3234574496 -11.0553558990 -2.3169586570
267 C -7.4309868191 -12.2908203290 -4.6396487372
268 C -8.9533577585 -10.7789602720 -3.5443190361
269 C -7.2004678227 -11.9022088600 -2.2805002582
270 C -6.7808814093 -12.5251242910 -3.4474159084
271 C -8.4935160521 -11.4161060350 -4.6918060702
272 H -5.9600614917 -13.2098626930 -3.4263260619

273 H -8.9604588108 -11.2373795190 -5.6353463870

274 H -7.1044256601 -12.7857345160 -5.5322485582

275 C -10.4331135810 -9.1395462533 -2.4061236161

276 C -11.6474273850 -8.4772709622 -4.8152611997

277 C -11.3839997970 -8.1038236120 -2.4572655754

278 C -10.0432074910 -9.7920142093 -3.5899333538

279 C -10.6720915850 -9.4490123153 -4.7821494684

280 C -11.9940717280 -7.8000864166 -3.6660642043

281 H -10.4090769930 -9.9382248896 -5.6941583077

282 H -12.7561253210 -7.0514942566 -3.7111227199

283 H -12.1338755150 -8.2423111791 -5.7407260300

284 C -11.3081750620 -7.8952057075 0.0075766492

285 C -12.5997397180 -5.4255183904 -0.1033161258

286 C -11.7157403740 -7.2625517381 1.1916563983

287 C -11.7057320440 -7.3653810192 -1.2302616611

288 C -12.3327701410 -6.1277825943 -1.2665265265

289 C -12.3394409750 -6.0236652157 1.1168957327

290 H -12.5592510430 -5.6676141413 -2.2047301973

291 H -12.5371353050 -5.4695416558 2.0095507799

292 C -3.0639870698 -13.0032290120 0.2463795103

293 C -0.2763965434 -13.1721230140 0.0772947568

294 C -2.2558401588 -12.0591643350 0.8705016649

295 C -2.4598927363 -14.0558503870 -0.4264725998

296 C -1.0770514142 -14.1420320700 -0.5067795602

297 C -0.8833759817 -12.1421148930 0.7860393624

298 H -2.7103784858 -11.2358308330 1.3837410633

299 H -3.0679364854 -14.8010516450 -0.9006989918

300 H -0.6235674705 -14.9455965810 -1.0529407119

301 H -0.2722546204 -11.3929045970 1.2484148156

302 C -12.9796855870 -3.9845537115 -0.1550698969

303 C -13.3816592310 -1.2179244844 -0.0604575315

304 C -12.1662914300 -3.1230580745 -0.8832330000

305 C -14.0260104250 -3.4473258118 0.5820083940

306 C -14.2267553270 -2.0749298921 0.6271812415

307 C -12.3645974950 -1.7601828543 -0.8356623388

308 H -11.3462971960 -3.5233887795 -1.4449063265

309 H -14.6745754680 -4.0982906183 1.1348373802

310 H -15.0208005770 -1.6710413631 1.2235725840

311 H -11.7084816230 -1.1044952444 -1.3724563441

312 H 9.7818893535 -10.1179525870 -5.9079138221

Cartesian Coordinates (Angstroms) for the Cyclic Tetramer **1** (Conformer **B**) without the Mesityl Substituents Optimized at the HF/3-21G Level (-8190.290655 hartrees)

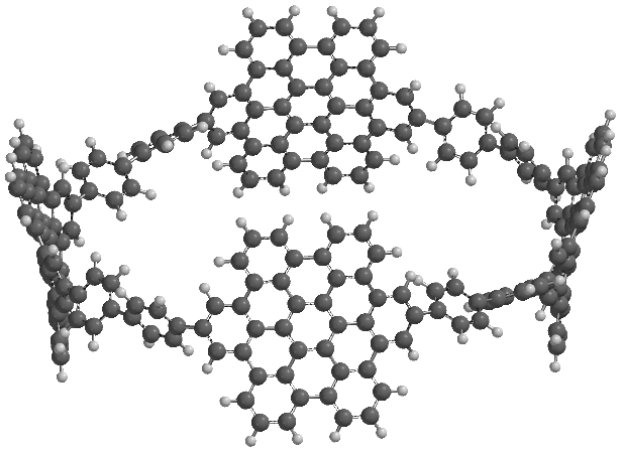

Figure S-90. Optimized structure of cyclic tetramer **1** (Conformer **B**) without the mesityl substituents optimized at the HF/3-21G level.

Coordinates (Angstroms)

ATOM X Y Z

1 C -10.8174992930 8.7315223010 0.4069437543

2 C -9.4721713971 9.2614693407 -1.9962174106

3 C -9.7906562542 9.6835386167 0.3755447750

4 C -11.1422145150 8.0153454333 -0.7537355876

5 C -10.4904732210 8.3013402371 -1.9621634932

6 C -9.0982434914 9.9262365231 -0.8191581098

7 C -9.4435525757 10.4163703190 1.5753625620

8 C -8.8564566751 11.9404038330 3.8227957894

9 C -10.2299461410 10.2871846260 2.7350805916

10 C -8.3255186035 11.2712478630 1.5773725262

11 C -8.0592339937 12.0379177560 2.7031681126

12 C -9.9195347772 11.0651716610 3.8451942110

13 H -7.2423660813 12.7275390090 2.7035482238

14 H -10.5033648320 10.9956617050 4.7365332162

15 H -8.6452668515 12.5437150390 4.6828552720

16 C -11.5489077140 8.4919191206 1.6339064556

17 C -13.1010711270 8.1561699278 3.9130295768

18 C -11.3245326990 9.3043367447 2.7604318435

19 C -12.5055004360 7.4611105652 1.6921650983

20 C -13.2849524780 7.3216931609 2.8317224809

21 C -12.1213793830 9.1236550570 3.8859683434

22 H -14.0523191210 6.5782737989 2.8715423358

23 H -11.9888508920 9.7388899056 4.7486091237

24 H -13.7185005420 8.0477103386 4.7821271923

25 C -7.9285484805 10.7771964000 -0.8142065956

26 C -5.3792089762 11.9023953480 -0.6849294537

27 C -7.1711313389 10.9379236350 -1.9853048114

28 C -7.4687865175 11.3379263890 0.3871953404

29 C -6.1872220491 11.8739321410 0.4376937699

30 C -5.9008585590 11.4873655440 -1.8988902337

31 H -5.7736409888 12.1856774100 1.3730137316

32 H -5.2772122801 11.5370670950 -2.7657934059

33 C -8.8110536213 9.5731834486 -3.2467196159

34 C -7.6626363967 10.3380332060 -5.6579886003

35 C -7.7149392284 10.4544453600 -3.2596233781

36 C -9.2767042622 9.0175251121 -4.4522164959

37 C -8.6924606377 9.4238035000 -5.6472495419

38 C -7.1669381737 10.8409701650 -4.4744770481

39 H -9.0383985800 9.0348001395 -6.5795840213

40 H -6.3684403346 11.5513600390 -4.5031325051

41 H -7.2404265110 10.6538787320 -6.5908585184

42 C -10.8707462230 7.6047271031 -3.1736163092

43 C -11.7263088010 6.3620671900 -5.5067305790

44 C -11.7951322670 6.5462379747 -3.1126131978

45 C -10.3306900430 7.9927510443 -4.4134173245

46 C -10.7792796930 7.3599639058 -5.5677289984

47 C -12.2250141680 5.9504375001 -4.2899258400

48 H -10.3947101620 7.6397425980 -6.5237623653

49 H -12.9649263800 5.1792735327 -4.2636707034

50 H -12.0722055530 5.9001892094 -6.4096755422

51 C -12.0690986850 6.9078063689 -0.6796395374

52 C -13.3647059210 4.4484196564 -0.4044264119

53 C -12.2916931620 6.1012305194 -1.8054458781

54 C -12.6489167160 6.5515605323 0.5483050468

55 C -13.2841349190 5.3230489774 0.6675170708

56 C -12.9099641140 4.8695431958 -1.6427814247

57 H -13.6656589900 5.0089117780 1.6153666000

58 H -12.9557673160 4.1871462185 -2.4638234160

59 C -3.9243704009 12.2028032320 -0.5600926773

60 C -1.1710187402 12.5180827910 -0.1569460771

61 C -3.4278878992 13.3304372550 0.0792602888

62 C -3.0229967247 11.2528592280 -1.0283976037

63 C -1.6690061705 11.4090879300 -0.8315410651

64 C -2.0636132941 13.4880165260 0.2764457439

65 H -4.1062882052 14.0815481580 0.4337430253

66 H -3.3924901362 10.3718275500 -1.5134608954

67 H -0.9884494745 10.6606801380 -1.1852148155

68 H -1.6972751732 14.3508614350 0.7970271624

69 C -13.7644980820 3.0251586604 -0.2138844369

70 C -14.1073610640 0.2509589101 -0.0097474286

71 C -13.2610678230 2.3224520878 0.8754071618

72 C -14.5027534380 2.3277141230 -1.1636863311

73 C -14.6650113640 0.9562590149 -1.0675219471

74 C -13.4360161960 0.9576815327 0.9790832418

75 H -12.6683252590 2.8341291849 1.6065418958

76 H -14.9350566300 2.8544346995 -1.9914859744

77 H -15.2095722250 0.4291669239 -1.8259682691

78 H -12.9889435350 0.4241695096 1.7939989989

79 C 9.7903845380 -9.6824318506 0.3850505786

80 C 10.4840359660 -8.2999972697 -1.9543764102

81 C 10.8168343920 -8.7298979662 0.4139962123

82 C 9.0952953835 -9.9255419525 -0.8080156484

83 C 9.4660975740 -9.2606103862 -1.9859789020

84 C 11.1384936130 -8.0136354693 -0.7474895872

85 C 11.5509843150 -8.4898735923 1.6392425043

86 C 13.1080978550 -8.1530952022 3.9148511680

87 C 12.5072740460 -7.4586644988 1.6951957913

88 C 11.3295593000 -9.3022767318 2.7663680084

89 C 12.1288128450 -9.1210489488 3.8901047214

90 C 13.2892023900 -7.3187319955 2.8329989536

91 H 11.9984931420 -9.7362146975 4.7531289647

92 H 14.0563345040 -6.5749826471 2.8710037036

93 H 13.7273971200 -8.0442009520 4.7825626957

94 C 9.4464761541 -10.4154254360 1.5856940458

95 C 8.8655294686 -11.9397842730 3.8344999268

96 C 8.3289586318 -11.2709851630 1.5903249175

97 C 10.2354778870 -10.2857442910 2.7435792450

98 C 9.9281287514 -11.0639071030 3.8544134958

99 C 8.0657557255 -12.0377958450 2.7167399033

100 H 10.5140061900 -10.9940608260 4.7443800783

101 H 7.2493135264 -12.7279140520 2.7190302563

102 H 8.6567215988 -12.5432235550 4.6950520671

103 C 12.0652137380 -6.9057983810 -0.6756894898

104 C 13.3618063730 -4.4465035737 -0.4040523183

105 C 12.2850637350 -6.0993600039 -1.8021467611

106 C 12.6478834760 -6.5493049168 0.5508397381

107 C 13.2834867180 -5.3208137965 0.6682947299

108 C 12.9039554600 -4.8677518586 -1.6412005057

109 H 13.6672903180 -5.0064762936 1.6151554924

110 H 12.9480158780 -4.1855352801 -2.4624866244

111 C 10.8610938640 -7.6032465336 -3.1667696550

112 C 11.7101235600 -6.3599717560 -5.5019969766

113 C 10.3180798900 -7.9913984782 -4.4052507855

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115 C 12.2118352000 -5.9483407806 -4.2864385387

116 C 10.7633830680 -7.3582663102 -5.5606501246

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119 H 12.0534420440 -5.8977928156 -6.4057702717

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123 C 9.2645696327 -9.0167361611 -4.4415123589
124 C 8.6777124160 -9.4233436923 -5.6351509809
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127 H 7.2241687595 -10.6542799660 -6.5753066537
128 C 7.9261116899 -10.7772051780 -0.8003036703
129 C 5.3778185969 -11.9040746640 -0.6651124490
130 C 7.4694979407 -11.3382330700 0.4021540215
131 C 7.1660762291 -10.9384360590 -1.9696363093
132 C 5.8963753808 -11.4886897810 -1.8802639978
133 C 6.1883954398 -11.8751141890 0.4556344165
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138 C 14.5006028820 -2.3271870950 -1.1660070008
139 C 13.2616273780 -2.3197573046 0.8747366543
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141 C 14.6644046280 -0.9558620347 -1.0706500819
142 H 14.9312814280 -2.8547377100 -1.9941283870
143 H 12.6693797590 -2.8305698995 1.6068823887
144 H 12.9924625540 -0.4207642516 1.7927330482
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146 C 3.9233854057 -12.2052595230 -0.5372654528
147 C 1.1708659785 -12.5224822360 -0.1300903835
148 C 3.0207911794 -11.2550341040 -1.0026418378
149 C 3.4285444291 -13.3339435800 0.1014746697
150 C 2.0646314266 -13.4925038530 0.3006310813
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153 H 4.1078914105 -14.0852241330 0.4537824743
154 H 1.6995679020 -14.3563137880 0.8205098422
155 H 0.9857066329 -10.6636885970 -1.1553538001
156 C 8.7983115931 9.9070401261 1.9825643846
157 C 10.1817805700 9.4689721901 -0.4174382351
158 C 9.8816028572 9.0207710995 1.9518864678
159 C 8.3805993111 10.5418541670 0.8036919608
160 C 9.0904438065 10.3464206270 -0.3894433673
161 C 10.5539706800 8.7793144500 0.7450479305
162 C 10.3076189210 8.3544380217 3.1651505171
163 C 11.2435856620 7.1780064645 5.5017579282
164 C 11.3039205510 7.3631474816 3.1074595758
165 C 9.7394619513 8.7055697080 4.4033851126
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169 H 12.5642498740 6.0829864366 4.2627465053
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172 C 6.9119527662 10.8607664950 5.6395469161
173 C 8.6163499871 9.6542145977 4.4386974080
174 C 6.9596820843 10.9760539590 3.2410494491
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177 H 5.5377025428 11.9782717830 4.4804412220
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189 C 12.5070550200 9.0506139496 -3.9183375897
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192 C 12.7471400400 8.2327948081 -2.8353188842
193 C 11.4614500490 9.9465534009 -3.8947636884
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195 H 11.2876089570 10.5496262650 -4.7586554038
196 H 13.1323985750 8.9847255615 -4.7860461622
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198 C 8.0050387978 12.5250311600 -3.8427357688

199 C 7.5190252912 11.8246309580 -1.5966680893
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201 C 9.1273588142 11.7270870840 -3.8616749625
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207 C 4.5320467478 12.2514126270 0.6601261143
208 C 6.6578059607 11.8331461050 -0.4078841642
209 C 6.3852892735 11.4177647270 1.9649938148
210 C 5.0796892809 11.8764074320 1.8756577725
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213 H 4.9087879570 12.5578141650 -1.3978191819
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215 C 14.0571143330 1.2409617377 0.0161248072
216 C 14.3040052550 3.3412577739 1.1688620254
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218 C 13.3393154460 1.8981081854 -0.9742861346
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221 H 12.4429605280 3.7156077089 -1.6045764477
222 H 12.9319619300 1.3339183387 -1.7893587046
223 H 15.1412548870 1.4974901466 1.8338651543
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225 C 0.2914751355 12.5694682160 0.1275105157
226 C 2.4859874317 13.5378806520 -0.1081200296
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228 C 0.8655662607 11.4987590000 0.8034983632
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239 C -8.3793860040 -10.5431528510 0.8198229797
240 C -8.1181801814 -10.1746329700 3.2480041102
241 C -6.9207140851 -10.8620205040 5.6587195040
242 C -6.9638040680 -10.9780910460 3.2601693589
243 C -8.6215503136 -9.6542203153 4.4540706856
244 C -8.0111809555 -10.0210322430 5.6488054756
245 C -6.3909364417 -11.3277088810 4.4747223260
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247 H -5.5453004890 -11.9813126660 4.5027256886
248 H -6.4781340494 -11.1494286320 6.5913459789
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250 C -11.2487981730 -7.1755402226 5.5112471323
251 C -11.3044313200 -7.3611141135 3.1168502356
252 C -9.7437236297 -8.7045642364 4.4162324891
253 C -10.2351147880 -8.1057030926 5.5712280732
254 C -11.7746055240 -6.7979138637 4.2948338129
255 H -9.8322439429 -8.3594116981 6.5269995602
256 H -12.5660527680 -6.0797159271 4.2693816664
257 H -11.6258815130 -6.7397490108 6.4146703863
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259 C -4.5322290295 -12.2564857940 0.6844491596
260 C -6.6555658230 -11.8367036740 -0.3878190968
261 C -6.3873009400 -11.4208113020 1.9854183271
262 C -5.0819485094 -11.8807364160 1.8988152203
263 C -5.3398590011 -12.2823476410 -0.4385253056
264 H -4.4567478443 -11.8884843060 2.7659881116
265 H -4.9052609862 -12.5629973120 -1.3741647588
266 C -8.6890275718 -11.0524701440 -1.5755669687
267 C -7.9968305612 -12.5287744150 -3.8249294209
268 C -9.4820442460 -10.9763906900 -2.7354683717
269 C -7.5144103634 -11.8277761830 -1.5782960463
270 C -7.1951872884 -12.5724648510 -2.7050582409
271 C -9.1180220306 -11.7293185410 -3.8465672492
272 H -6.3324839655 -13.2038095650 -2.7060405546
273 H -9.7049228499 -11.6991287630 -4.7380870159
274 H -7.7439974440 -13.1147122930 -4.6857682986
275 C -10.9227947510 -9.2786331573 -1.6322685196
276 C -12.4936824730 -9.0480208899 -3.9116563292

277 C -11.9486726930 -8.3167078170 -1.6894329072
278 C -10.6421609980 -10.0718140090 -2.7598957671
279 C -11.4491842850 -9.9451705623 -3.8855619505
280 C -12.7355000870 -8.2300296590 -2.8291673160
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285 C -13.0162824100 -5.3742947250 0.4111380279
286 C -11.8305713030 -6.9500110582 1.8101357483
287 C -12.1553253970 -7.4210384908 -0.5442982374
288 C -12.8747435540 -6.2397425006 -0.6619419024
289 C -12.5332284380 -5.7642153196 1.6489855251
290 H -13.2772967820 -5.9517602773 -1.6093906966
291 H -12.6266411930 -5.0877620739 2.4709092874
292 C -3.0599598986 -12.4544800140 0.5596129227
293 C -0.2913874697 -12.5750595200 0.1554316916
294 C -2.2271433296 -11.4452903430 1.0309266670
295 C -2.4858884652 -13.5427419200 -0.0830293186
296 C -1.1139780513 -13.6038425780 -0.2807534098
297 C -0.8655897716 -11.5057870870 0.8335754149
298 H -2.6572548474 -10.5936800400 1.5185568547
299 H -3.1101291031 -14.3384090050 -0.4398150127
300 H -0.6882791571 -14.4373128090 -0.8040291176
301 H -0.2390021994 -10.7126168840 1.1894221953
302 C -13.5151381170 -3.9824520848 0.2221459426
303 C -14.0540781760 -1.2394539404 0.0195853715
304 C -13.0627704670 -3.2451171046 -0.8666683304
305 C -14.3007605950 -3.3396435025 1.1724868414
306 C -14.5599738150 -1.9830899257 1.0771037411
307 C -13.3341687830 -1.8961799021 -0.9695670929
308 H -12.4352979330 -3.7130261584 -1.5981410429
309 H -14.6945614330 -3.8961860892 1.9999855647
310 H -15.1405376750 -1.4964247350 1.8358628946
311 H -12.9262084830 -1.3318227801 -1.7842212505
312 H 9.0211929401 -9.0341385084 -6.5683072081

Cartesian Coordinates (Angstroms) for the Cyclic Tetramer **1** (Conformer **C**) without the Mesityl Substituents Optimized at the HF/3-21G Level (-8190.295233 hartrees)

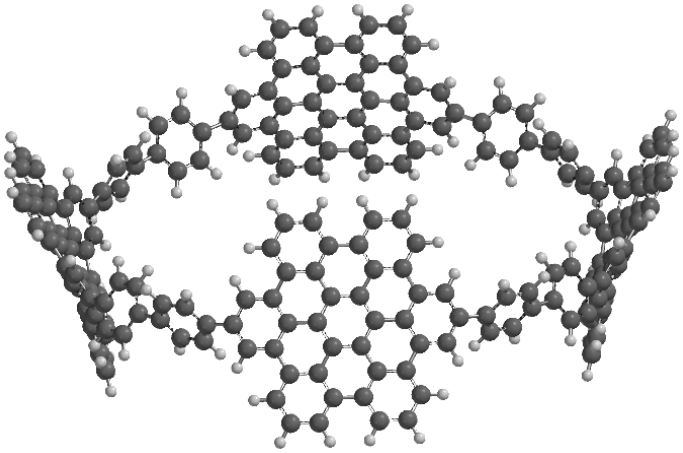

Figure S-91. Optimized structure of cyclic tetramer **1** (Conformer **C**) without the mesityl substituents optimized at the HF/3-21G level.

Coordinates (Angstroms)

ATOM X Y Z

1 C 8.5569474274 10.9445604660 -0.0541777045
2 C 6.8732694006 10.9855547730 2.1894045084
3 C 7.4111999862 11.7507567630 -0.0540261054
4 C 8.8428217301 10.1352815140 1.0549079914
5 C 8.0186822859 10.1796416120 2.1892742297
6 C 6.5530760625 11.7464314240 1.0551890939
7 C 7.1160043092 12.5942069620 -1.1942595378
8 C 6.6198617828 14.3485627000 -3.2912270797
9 C 8.0438492011 12.7112003090 -2.2455806177
10 C 5.9087315691 13.3166841870 -1.2414090625
11 C 5.6878182511 14.2020895530 -2.2870736746
12 C 7.7761565299 13.6010572200 -3.2803424083
13 H 4.7997584638 14.7965732780 -2.3111551741
14 H 8.4681275043 13.7219861050 -4.0844219038
15 H 6.4422308670 15.0434733110 -4.0873729114
16 C 9.4503037475 10.9516031160 -1.1946036464
17 C 11.2683988530 11.0768569290 -3.2922191532
18 C 9.2468680365 11.8645459510 -2.2458172213
19 C 10.5379688900 10.0591684350 -1.2420834381
20 C 11.4455766230 10.1501320140 -2.2880960961
21 C 10.1744493670 11.9129497110 -3.2809284264
22 H 12.3049664980 9.5149245187 -2.3125219968
23 H 10.0543749090 12.6050769530 -4.0849998062
24 H 11.9821634750 11.1441820480 -4.0886605640
25 C 5.2881151280 12.4452389260 0.9901091681
26 C 2.6525055098 13.3086069340 0.6573552746
27 C 4.3780005716 12.3527015610 2.0538198489
28 C 4.9100375110 13.1172833370 -0.1835805286
29 C 3.5923333272 13.5287319110 -0.3357427833
30 C 3.0672022415 12.7637859070 1.8602700521
31 H 3.2722205521 13.9749528930 -1.2528677370
32 H 2.3340080797 12.5778968650 2.6149937665
33 C 6.0237503298 11.0377628010 3.3617100729
34 C 4.4694952078 11.2906639890 5.6518166256
35 C 4.8146377178 11.7548458660 3.3202572580
36 C 6.4128434853 10.3912689450 4.5491055079
37 C 5.6224301630 10.5385785410 5.6837502570
38 C 4.0615905027 11.8866116110 4.4786417871
39 H 5.9000577257 10.0709269000 6.6025519638
40 H 3.1666783055 12.4711250550 4.4754378319
41 H 3.8846962825 11.4075729450 6.5421004567
42 C 8.3548435878 9.3975548813 3.3614569229

43 C 9.1176878999 8.0193519709 5.6511914659
44 C 9.4381186517 8.5016512780 3.3197725579
45 C 7.6150082364 9.5452688430 4.5489406695
46 C 8.0205072501 8.8506640158 5.6833687509
47 C 9.8163954459 7.8370082082 4.4779833362
48 H 7.4865302563 8.9537889670 6.6021744002
49 H 10.6687316890 7.1920072135 4.4746134709
50 H 9.4251215730 7.5080494023 6.5413077481
51 C 9.9278061968 9.1806975568 0.9895947540
52 C 11.6313424990 6.9921116147 0.6568513349
53 C 10.1483461240 8.2928639071 2.0532975919
54 C 10.6879168510 9.0518901110 -0.1842166181
55 C 11.5205622240 7.9508211065 -0.3363918050
56 C 10.9784171810 7.1982556344 1.8597579132
57 H 12.0486210730 7.8002951388 -1.2535571212
58 H 11.0515130640 6.4454504174 2.6145175440
59 C 1.1955618316 13.4945899230 0.4064648620
60 C -1.5840137663 13.4335711390 0.0547086342
61 C 0.6364261767 12.9757582310 -0.7554692054
62 C 0.3465563890 14.0440352640 1.3603963539
63 C -1.0259792727 14.0097967010 1.1889281499
64 C -0.7325228547 12.9494000790 -0.9301335762
65 H 1.2720832331 12.5272972050 -1.4923793721
66 H 0.7595686219 14.4845591770 2.2464212993
67 H -1.6677235824 14.4170997230 1.9451702307
68 H -1.1476758233 12.4868438630 -1.8031709802
69 C 12.2993735560 5.6839631068 0.4064032703
70 C 13.1824545310 3.0474940319 0.0563718365
71 C 11.9997204190 4.9812854866 -0.7547740192
72 C 13.1043891180 5.0718819198 1.3603338374
73 C 13.5366091820 3.7686336520 1.1897054921
74 C 12.4380995390 3.6840285412 -0.9285823187
75 H 11.3621500070 5.4270451283 -1.4916740698
76 H 13.3796375920 5.6104072574 2.2457200130
77 H 14.1375468700 3.3032597278 1.9459644750
78 H 12.1427488790 3.1360628483 -1.8009394825
79 C -7.4123998016 -11.7510124620 -0.0366506669
80 C -8.0227352532 -10.1765168440 2.2034751676
81 C -8.5585527531 -10.9454119750 -0.0391908824
82 C -6.5552183100 -11.7443042200 1.0732862521
83 C -6.8768397825 -10.9817257060 2.2059461143
84 C -8.8458678666 -10.1344775250 1.0682960745
85 C -9.4508193798 -10.9547170460 -1.1804534873
86 C -11.2667963690 -11.0840707410 -3.2796619669
87 C -10.5387031020 -10.0626860490 -1.2305319751
88 C -9.2460627557 -11.8693810420 -2.2299006495
89 C -10.1726088080 -11.9198129100 -3.2658588859
90 C -11.4452471390 -10.1556914680 -2.2772901566
91 H -10.0515089930 -12.6132495050 -4.0686497315
92 H -12.3047977140 -9.5207717185 -2.3036349864
93 H -11.9797423140 -11.1529597990 -4.0767015719
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96 C -5.9082120526 -13.3183557820 -1.2199421561
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115 C -9.8245472500 -7.8320232393 4.4869831852
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118 H -7.4962464312 -8.9443329891 6.6152642178
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124 C -5.6289393327 -10.5275961640 5.7004355299
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139 C -12.0004499570 -4.9840587233 -0.7533237132
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161 C -11.7458813420 6.5507834360 -1.0732133322
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164 C -11.7510272780 4.8105649683 -3.3369348442
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193 C -13.6067331660 7.7774295771 3.2586356489
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202 C -10.1534103610 11.4453064310 2.2689628158
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205 H -11.1498311990 11.9832548480 4.0678072089
206 C -9.1798219234 9.9252436358 -1.0064126537
207 C -6.9913348805 11.6285485390 -0.6718139898
208 C -9.0524350045 10.6860692710 0.1670895165
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252 C 10.3885635280 -6.4153036133 -4.5473202957
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259 C 6.9917915047 -11.6284914530 -0.6461930829
260 C 9.0530907983 -10.6854314460 0.1915436233
261 C 8.2919093498 -10.1478386670 -2.0457111677
262 C 7.1970380483 -10.9770633060 -1.8500705596
263 C 7.9516539828 -11.5172079470 0.3458795862
264 H 6.4433815575 -11.0505596060 -2.6039455451
265 H 7.8018032604 -12.0441388420 1.2638083437
266 C 10.9547438360 -9.4479150141 1.1983939084
267 C 11.0816307730 -11.2641108180 3.2975593970
268 C 11.8691385920 -9.2440035465 2.2482452054
269 C 10.0617438720 -10.5350243810 1.2480364786
270 C 10.1535161590 -11.4416983110 2.2947918191
271 C 11.9183344020 -10.1706510330 3.2841674303
272 H 9.5178434283 -12.3006992920 2.3208289574
273 H 12.6115532210 -10.0502085070 4.0872449278
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280 C 14.2084778400 -5.6860448337 2.2832747276
281 H 13.7295698230 -8.4646729182 4.0835805610
282 H 14.8033997000 -4.7982364852 2.3058057751
283 H 15.0520166250 -6.4393970316 4.0830091483
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289 C 12.7654024070 -3.0681567548 -1.8641408606
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294 C 5.0700783456 -13.1013352920 -1.3459426282
295 C 4.9819111520 -11.9935993650 0.7676658976
296 C 3.6844896655 -12.4308717770 0.9431470472
297 C 3.7666901997 -13.5324488790 -1.1736440722
298 H 5.6077074682 -13.3781882100 -2.2313740586
299 H 5.4287081339 -11.3552900420 1.5032988185
300 H 3.1374277997 -12.1339405350 1.8155376773
301 H 3.3003077841 -14.1341610060 -1.9286640150
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303 C 13.4375249140 1.5844102244 -0.0641136127
304 C 12.9811526200 -0.6352091479 0.7491344294
305 C 14.0466278960 -0.3474898212 -1.3684465544
306 C 14.0124384590 1.0252106081 -1.1984344323
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310 H 14.4186635660 1.6661841432 -1.9559073440
311 H 12.4933268510 1.1499670199 1.7955043461
312 H -5.9075681817 -10.0584636080 6.6181793200

Cartesian Coordinates (Angstroms) for the Cyclic Tetramer **1** (Conformer **A**) without the Mesityl Substituents Optimized by DFT at the B3LYP/6-31G* Level (-8289.735764 hartrees)

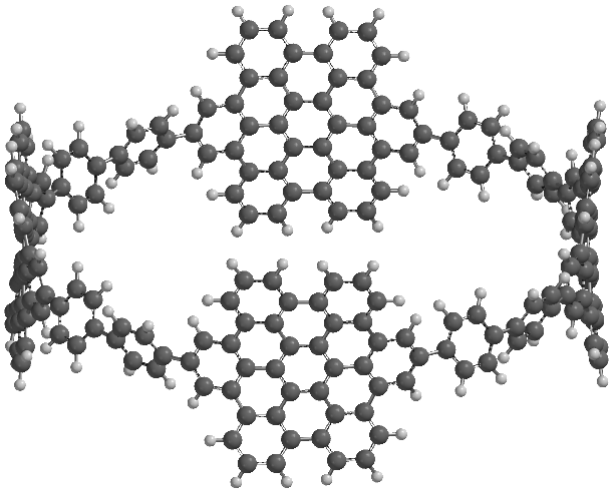

Figure S-92. Optimized structure of cyclic tetramer **1** (Conformer **A**) without the mesityl substituents optimized by DFT at the B3LYP/6-31G* level.

Coordinates (Angstroms)

ATOM	X	Y	Z	ATOM	X	Y	Z
1 C C1	-10.4884956	8.7928461	1.2599115	21 C C18	-11.2797761	8.5307474	4.9205555
2 C C4	-9.5482300	9.8298058	-1.2116443	22 H H12	-13.2850772	6.0644499	3.7540098
3 C C2	-9.5113631	9.8198877	1.2494207	23 H H13	-11.0407218	9.0102217	5.8623627
4 C C6	-10.9444470	8.2398031	0.0342040	24 H H14	-12.7172757	7.2292827	5.8433499
5 C C5	-10.4988059	8.7782441	-1.2016058	25 C C19	-7.9215609	11.2468697	-0.0015690
6 C C3	-9.0191263	10.3149642	0.0133188	26 C C20	-5.4489126	12.6269789	-0.0564741
7 C C7	-9.0107369	10.3553304	2.4928502	27 C C21	-7.3913686	11.7133233	-1.2345486
8 C C8	-8.0963092	11.4778807	4.8966593	28 C C22	-7.2923304	11.6296112	1.2129067
9 C C9	-9.5991336	9.9622909	3.7291224	29 C C23	-6.0546285	12.2810531	1.1581936
10 C C10	-7.9266848	11.2792454	2.4839735	30 C C24	-6.1715633	12.3979995	-1.2348388
11 C C11	-7.4992603	11.8394838	3.6949902	31 H H16	-5.5011942	12.4331763	2.0768083
12 C C12	-9.1232082	10.5422250	4.9150809	32 H H17	-5.7374955	12.7052121	-2.1785415
13 H H8	-6.7099087	12.5829101	3.7001975	33 C C25	-9.1212208	10.4096895	-2.4626970
14 H H9	-9.5486051	10.2615454	5.8711850	34 C C26	-8.4476772	11.7023116	-4.8590209
15 H H10	-7.7560290	11.9246396	5.8267537	35 C C27	-8.1039538	11.4067106	-2.4754725
16 C C13	-11.0219094	8.3124740	2.5123137	36 C C28	-9.7310441	10.0028635	-3.6838363
17 C C14	-12.2272079	7.5144798	4.9165635	37 C C29	-9.3851760	10.6769710	-4.8650976
18 C C15	-10.6493546	8.9403248	3.7355398	38 C C30	-7.7998035	12.0532920	-3.6803346
19 C C16	-11.9385466	7.2221983	2.5250235	39 H H20	-9.8554050	10.4125463	-5.8047721
20 C C17	-12.5422647	6.8543636	3.7346411	40 H H21	-7.0722969	12.8572030	-3.6985427

41	H	H22	-8.2137672	12.2258857	-5.7818224	80	C	C56	10.4940346	-8.7676241	-1.1863486
42	C	C31	-11.0073004	8.2509544	-2.4453405	81	C	C57	10.4841252	-8.7848349	1.2752034
43	C	C32	-12.0787155	7.2768186	-4.8492203	82	C	C58	9.0117961	-10.3031615	0.0271712
44	C	C33	-11.8513332	7.1038333	-2.4390428	83	C	C59	9.5412238	-9.8172575	-1.1974274
45	C	C34	-10.6691952	8.8774273	-3.6792508	84	C	C60	10.9409835	-8.2313643	0.0500260
46	C	C35	-11.2209247	8.3695172	-4.8652858	85	C	C61	11.0183454	-8.3063604	2.5280561
47	C	C36	-12.3878938	6.6465213	-3.6499790	86	C	C62	12.2244838	-7.5120273	4.9332311
48	H	H24	-10.9788032	8.8219906	-5.8194887	87	C	C63	11.9365062	-7.2173414	2.5418497
49	H	H25	-13.0715310	5.8048655	-3.6565218	88	C	C64	10.6450230	-8.9348509	3.7507252
50	H	H26	-12.5056908	6.9114745	-5.7790878	89	C	C65	11.2758400	-8.5271232	4.9361810
51	C	C37	-11.7955859	7.0786836	0.0466735	90	C	C66	12.5405299	-6.8513501	3.7519043
52	C	C38	-13.0074125	4.5178377	0.0881315	91	H	H41	11.0361207	-9.0071562	5.8775279
53	C	C39	-12.1464655	6.4360868	-1.1707656	92	H	H42	13.2844767	-6.0625301	3.7721163
54	C	C40	-12.2098231	6.5040735	1.2787298	93	H	H43	12.7148224	-7.2282662	5.8603178
55	C	C41	-12.8110142	5.2409310	1.2719232	94	C	C67	9.0047546	-10.3469180	2.5067836
56	C	C42	-12.7131436	5.1570429	-1.1229569	95	C	C68	8.0899709	-11.4710932	4.9098200
57	H	H28	-13.0779173	4.7781617	2.2140073	96	C	C69	7.9200799	-11.2700767	2.4973033
58	H	H29	-12.8376778	4.6044367	-2.0461418	97	C	C70	9.5937541	-9.9556800	3.7433798
59	C	C43	-4.0363803	13.0864558	-0.0921823	98	C	C71	9.1176076	-10.5362954	4.9288771
60	C	C44	-1.2297142	13.5829168	-0.0432563	99	C	C72	7.4924970	-11.8311187	3.7079170
61	C	C45	-3.4249281	13.7234491	1.0028445	100	H	H46	9.5434711	-10.2568625	5.8851282
62	C	C46	-3.2182022	12.7801589	-1.1941031	101	H	H47	6.7025379	-12.5738725	3.7125741
63	C	C47	-1.8512817	13.0331507	-1.1756734	102	H	H48	7.7494222	-11.9183645	5.8395600
64	C	C48	-2.0521479	13.9535043	1.0332213	103	C	C73	11.7946194	-7.0719791	0.0636132
65	H	H18	-4.0272778	14.0339068	1.8517827	104	C	C74	13.0132064	-4.5143372	0.1068741
66	H	H31	-3.6391722	12.2628695	-2.0504418	105	C	C75	12.1477377	-6.4296732	-1.1532831
67	H	H32	-1.2410800	12.7207857	-2.0186319	106	C	C76	12.2095387	-6.4988429	1.2961580
68	H	H33	-1.6082473	14.4226796	1.9076095	107	C	C77	12.8137067	-5.2370609	1.2903555
69	C	C49	-13.3830059	3.0804387	0.1127155	108	C	C78	12.7180460	-5.1523257	-1.1045941
70	C	C50	-13.7232721	0.2514064	0.0373402	109	H	H51	13.0809774	-4.7751109	2.2327692
71	C	C51	-13.0227219	2.2694683	1.2035971	110	H	H52	12.8447607	-4.5996236	-2.0274197
72	C	C52	-13.9935303	2.4457489	-0.9841183	111	C	C79	11.0037241	-8.2402267	-2.4295917
73	C	C53	-14.1470447	1.0627097	-1.0278670	112	C	C80	12.0789549	-7.2672065	-4.8323362
74	C	C54	-13.2000522	0.8908573	1.1723682	113	C	C81	10.6635944	-8.8641343	-3.6643038
75	H	H30	-12.5233411	2.7098035	2.0608934	114	C	C82	11.8512187	-7.0956505	-2.4221136
76	H	H35	-14.3442944	3.0389372	-1.8236686	115	C	C83	12.3896576	-6.6389042	-3.6323873
77	H	H36	-14.5969280	0.6024233	-1.9039575	116	C	C84	11.2174868	-8.3570012	-4.8496815
78	H	H37	-12.8487490	0.2899372	2.0066750	117	H	H55	13.0760576	-5.7994691	-3.6378530
79	C	C55	9.5054559	-9.8104927	1.2637648	118	H	H56	10.9744725	-8.8079308	-5.8044158

119	H	H57	12.5076226	-6.9025825	-5.7617200	158	C	C111	9.8737501	9.4874084	1.1813187
120	C	C85	9.1119510	-10.3940462	-2.4492668	159	C	C112	8.2594743	10.8857655	-0.0297080
121	C	C86	8.4304640	-11.6781077	-4.8483501	160	C	C113	8.7868204	10.4314601	-1.2672776
122	C	C87	8.0922129	-11.3885556	-2.4631276	161	C	C114	10.3578259	8.9855421	-0.0553361
123	C	C88	9.7214085	-9.9862044	-3.6703113	162	C	C115	10.4339464	9.0105502	2.4233006
124	C	C89	9.3712326	-10.6557669	-4.8529770	163	C	C116	11.6088932	8.1478193	4.8211932
125	C	C90	7.7840581	-12.0308273	-3.6694278	164	C	C117	11.3732995	7.9398840	2.4149951
126	H	H61	7.0542295	-12.8326086	-3.6888434	165	C	C118	10.0507811	9.6096975	3.6574965
127	H	H62	8.1927358	-12.1977909	-5.7724827	166	C	C119	10.6574348	9.1600608	4.8403972
128	C	C91	7.9130919	-11.2338374	0.0116234	167	C	C120	11.9596718	7.5384455	3.6224910
129	C	C92	5.4411911	-12.6151722	-0.0431047	168	H	H79	10.3866100	9.5954770	5.7948073
130	C	C93	7.2850368	-11.6187340	1.2261260	169	H	H80	12.7154028	6.7608319	3.6267123
131	C	C94	7.3812240	-11.6974443	-1.2218268	170	H	H81	12.0765515	7.8285685	5.7484603
132	C	C95	6.1616298	-12.3824438	-1.2220501	171	C	C121	8.3631269	10.9927953	2.4464688
133	C	C96	6.0478197	-12.2711164	1.1715905	172	C	C122	7.5755598	12.2101515	4.8484469
134	H	H65	5.7260886	-12.6878474	-2.1656874	173	C	C123	9.0117838	10.6430365	3.6656659
135	H	H66	5.4952842	-12.4260016	2.0903152	174	C	C124	7.2604099	11.8943152	2.4631653
136	C	C97	13.3928359	-3.0780590	0.1310730	175	C	C125	6.8976939	12.5042637	3.6712679
137	C	C98	13.7383699	-0.2498663	0.0509558	176	C	C126	8.6063617	11.2786085	4.8493419
138	C	C99	14.0084218	-2.4467955	-0.9649040	177	H	H84	6.0970292	13.2354047	3.6928199
139	C	C100	13.0311383	-2.2643766	1.2194200	178	H	H85	9.0998353	11.0555729	5.7878325
140	C	C101	13.2109808	-0.8860736	1.1858529	179	H	H86	7.2931582	12.7042330	5.7739950
141	C	C102	14.1645814	-1.0641788	-1.0109859	180	C	C127	11.3030124	7.8993116	-0.0692323
142	H	H67	14.3607151	-3.0424025	-1.8020830	181	C	C128	12.7101705	5.4414085	-0.1106735
143	H	H68	12.5283935	-2.7021673	2.0760503	182	C	C129	11.7575802	7.3574409	-1.3015418
144	H	H69	12.8580705	-0.2828094	2.0177780	183	C	C130	11.7116679	7.2917798	1.1477907
145	H	H70	14.6181266	-0.6065259	-1.8865610	184	C	C131	12.3759851	6.0606360	1.1005509
146	C	C103	4.0297623	-13.0777846	-0.0779789	185	C	C132	12.4563318	6.1455431	-1.2952576
147	C	C104	1.2253236	-13.5848648	-0.0262141	186	H	H89	12.5475425	5.5219496	2.0245139
148	C	C105	3.2078155	-12.7649784	-1.1752081	187	H	H90	12.7549433	5.7024720	-2.2375007
149	C	C106	3.4234581	-13.7252298	1.0136511	188	C	C133	10.4160994	9.0556479	-2.5336189
150	C	C107	2.0516259	-13.9609157	1.0453983	189	C	C134	11.6792621	8.3613644	-4.9401230
151	C	C108	1.8419141	-13.0229432	-1.1553218	190	C	C135	9.9848910	9.6442630	-3.7568369
152	H	H72	3.6249832	-12.2390713	-2.0282108	191	C	C136	11.4241101	8.0491706	-2.5474335
153	H	H73	4.0292116	-14.0396454	1.8586901	192	C	C137	12.0555705	7.7347563	-3.7577611
154	H	H74	1.6116716	-14.4387515	1.9170879	193	C	C138	10.6440819	9.2879730	-4.9435264
155	H	H75	1.2282549	-12.7055405	-1.9939314	194	H	H93	12.8670669	7.0157967	-3.7781716
156	C	C109	8.8342494	10.4513071	1.1939274	195	H	H94	10.3597670	9.7410453	-5.8858076
157	C	C110	9.8491883	9.4928333	-1.2800246	196	H	H95	12.1905530	8.1190899	-5.8677123

197	C	C139	8.2379720	10.9195495	-2.5099389	236	C	C165	-8.8310665	-10.4549995	1.2187889
198	C	C140	7.2233590	11.9545546	-4.9131693	237	C	C166	-10.3536337	-8.9909240	-0.0337249
199	C	C141	7.0836089	11.7536527	-2.4984370	238	C	C167	-9.8509963	-9.5071677	-1.2571800
200	C	C142	8.8510834	10.5722769	-3.7481230	239	C	C168	-8.2618680	-10.8983091	-0.0042199
201	C	C143	8.3230149	11.1057839	-4.9336873	240	C	C169	-8.3578415	-10.9915051	2.4726742
202	C	C144	6.6060223	12.2722272	-3.7093668	241	C	C170	-7.5691517	-12.2009111	4.8781446
203	H	H98	8.7653470	10.8569128	-5.8909113	242	C	C171	-7.2588414	-11.8975806	2.4906555
204	H	H99	5.7584218	12.9484921	-3.7128554	243	C	C172	-9.0010048	-10.6323967	3.6920172
205	H	H100	6.8424846	12.3678360	-5.8430167	244	C	C173	-8.5954023	-11.2643529	4.8775559
206	C	C145	7.0893151	11.7245251	-0.0119676	245	C	C174	-6.8956464	-12.5035069	3.7005741
207	C	C146	4.5189675	12.9149022	0.0473678	246	H	H117	-9.0854994	-11.0347963	5.8162700
208	C	C147	6.4291076	12.0570821	-1.2252168	247	H	H118	-6.0983382	-13.2382506	3.7233942
209	C	C148	6.5248735	12.1449966	1.2227606	248	H	H119	-7.2868262	-12.6922306	5.8051532
210	C	C149	5.2560088	12.7340563	1.2247903	249	C	C175	-10.4205564	-9.0008000	2.4453535
211	C	C150	5.1463009	12.6143211	-1.1682037	250	C	C176	-11.5798116	-8.1164488	4.8430079
212	H	H103	4.8003429	13.0051663	2.1691823	251	C	C177	-11.3555263	-7.9263549	2.4341671
213	H	H104	4.5818310	12.7266259	-2.0857723	252	C	C178	-10.0345986	-9.5937266	3.6817292
214	C	C151	13.1815430	4.0324909	-0.1335005	253	C	C179	-10.6330981	-9.1330768	4.8645114
215	C	C152	13.6947714	1.2295418	-0.0507533	254	C	C180	-11.9340897	-7.5140530	3.6417867
216	C	C153	13.8340198	3.4399824	0.9627692	255	H	H122	-10.3590163	-9.5627983	5.8206235
217	C	C154	12.8695201	3.1972500	-1.2209361	256	H	H123	-12.6861025	-6.7328706	3.6444177
218	C	C155	13.1308477	1.8322728	-1.1861346	257	H	H124	-12.0409339	-7.7882365	5.7704512
219	C	C156	14.0720877	2.0689904	1.0100474	258	C	C181	-7.0941183	-11.7402984	0.0144555
220	H	H105	14.1495253	4.0555203	1.8002985	259	C	C182	-4.5250351	-12.9341633	0.0727130
221	H	H106	12.3409802	3.6026907	-2.0777278	260	C	C183	-6.4378910	-12.0801225	-1.1988374
222	H	H107	12.8134789	1.2085429	-2.0172216	261	C	C184	-6.5273646	-12.1564451	1.2494960
223	H	H108	14.5523331	1.6402066	1.8859634	262	C	C185	-5.2597110	-12.7480838	1.2509219
224	C	C157	3.0803113	13.2839803	0.0848360	263	C	C186	-5.1554534	-12.6382143	-1.1425005
225	C	C158	0.2508952	13.6226700	0.0384192	264	H	H127	-4.8029434	-13.0158934	2.1956239
226	C	C159	2.4347278	13.8962215	-1.0044060	265	H	H128	-4.5940188	-12.7545938	-2.0613614
227	C	C160	2.2805230	12.9176297	1.1819675	266	C	C187	-8.2483681	-10.9459785	-2.4841884
228	C	C161	0.9014725	13.0935488	1.1645945	267	C	C188	-7.2448368	-11.9980988	-4.8845709
229	C	C162	1.0513748	14.0498531	-1.0335906	268	C	C189	-8.8648695	-10.6044601	-3.7222853
230	H	H110	3.0199495	14.2479868	-1.8490665	269	C	C190	-7.0959365	-11.7827123	-2.4716502
231	H	H111	2.7304852	12.4145230	2.0323634	270	C	C191	-6.6239030	-12.3098890	-3.6810134
232	H	H112	0.3085066	12.7366862	2.0024327	271	C	C192	-8.3423980	-11.1466463	-4.9064220
233	H	H113	0.5820505	14.5021159	-1.9035667	272	H	H131	-5.7780542	-12.9883659	-3.6832100
234	C	C163	-9.8670669	-9.4873813	1.2041623	273	H	H132	-8.7875118	-10.9025154	-5.8636093
235	C	C164	-8.7916876	-10.4491566	-1.2425859	274	H	H133	-6.8684265	-12.4181336	-5.8132333

275	C	C193	-10.4207466	-9.0755285	-2.5114268	294	C	C207	-2.2864424	-12.9442065	1.2083822
276	C	C194	-11.6899774	-8.3914537	-4.9175898	295	C	C208	-2.4387801	-13.9042326	-0.9858677
277	C	C195	-11.4252326	-8.0656256	-2.5277492	296	C	C209	-1.0549415	-14.0525886	-1.0173773
278	C	C196	-9.9958717	-9.6730415	-3.7325696	297	C	C210	-0.9068536	-13.1160577	1.1889445
279	C	C197	-10.6581258	-9.3217612	-4.9190343	298	H	H143	-2.7369188	-12.4511627	2.0641649
280	C	C198	-12.0598267	-7.7562583	-3.7377610	299	H	H144	-3.0229803	-14.2533441	-1.8323297
281	H	H136	-10.3788595	-9.7816934	-5.8595177	300	H	H145	-0.5848700	-14.4972075	-1.8909214
282	H	H137	-12.8688190	-7.0345380	-3.7597138	301	H	H146	-0.3149122	-12.7663580	2.0303222
283	H	H138	-12.2037564	-8.1530563	-5.8448076	302	C	C211	-13.1662142	-4.0313874	-0.1309540
284	C	C199	-11.2951406	-7.9015383	-0.0507527	303	C	C212	-13.6788555	-1.2283258	-0.0596604
285	C	C200	-12.6963501	-5.4406389	-0.1020201	304	C	C213	-12.8500648	-3.2003029	-1.2202564
286	C	C201	-11.6975024	-7.2855089	1.1641417	305	C	C214	-13.8220863	-3.4350174	0.9612265
287	C	C202	-11.7521157	-7.3655044	-1.2848317	306	C	C215	-14.0600449	-2.0638395	1.0028137
288	C	C203	-12.4473690	-6.1516037	-1.2834443	307	C	C216	-13.1109933	-1.8350521	-1.1910290
289	C	C204	-12.3594339	-6.0532720	1.1117374	308	H	H148	-12.3187598	-3.6094438	-2.0737051
290	H	H141	-12.7474946	-5.7126000	-2.2271508	309	H	H149	-14.1405492	-4.0478686	1.7995897
291	H	H142	-12.5270846	-5.5084093	2.0328284	310	H	H150	-14.5434081	-1.6317603	1.8753835
292	C	C205	-3.0859107	-13.3021232	0.1082530	311	H	H151	-12.7907086	-1.2142177	-2.0231817
293	C	C206	-0.2550092	-13.6313857	0.0574319	312	H	H154	9.8401404	-10.3897909	-5.7928776

Cartesian Coordinates (Angstroms) for the Cyclic Tetramer **1** (Conformer **A**) without the Mesityl Substituents Optimized at the AM1 Level (4004.6592 kJ/mol)

(a) (b)

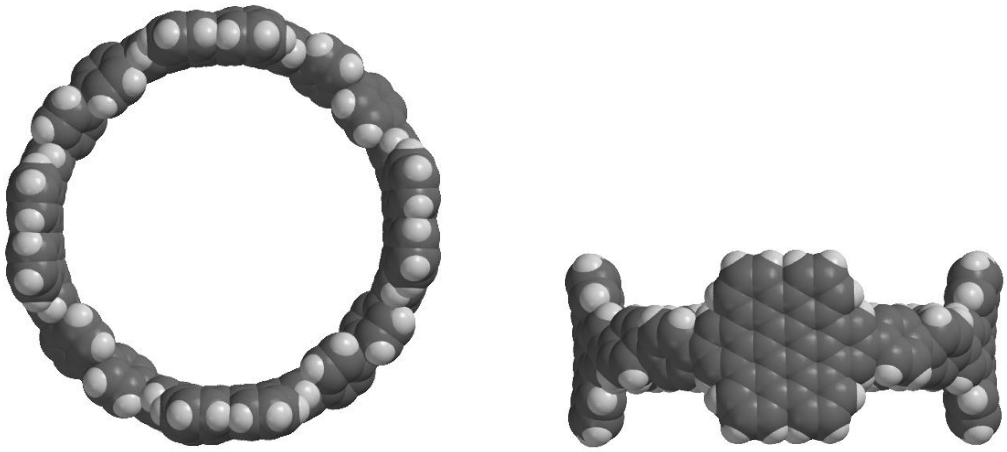

Figure S-93. Optimized structure of cyclic tetramer **1** (Conformer **A**) without the mesityl substituents optimized at the AM1 level: (a) top view of the molecular structure; (b) side view of the molecular structure.

Cartesian Coordinates (Angstroms)

Atom X Y Z

1	C	C1	-10.4107557	8.7343787	1.1633612		
2	C	C4	-9.4377166	9.7073748	-1.3053980		
3	C	C2	-9.4332005	9.7521875	1.1433250		
4	C	C6	-10.8520446	8.1598722	-0.0495497		
5	C	C5	-10.3930807	8.6687032	-1.2848507		
6	C	C3	-8.9226650	10.2125773	-0.0907165		
7	C	C7	-8.9524526	10.3155407	2.3797693		
8	C	C8	-8.0926816	11.5077334	4.7601460		
9	C	C9	-9.5611834	9.9534585	3.6083393		
10	C	C10	-7.8744386	11.2364371	2.3621182		
11	C	C11	-7.4693518	11.8366273	3.5611946		
12	C	C12	-9.1183934	10.5689822	4.7878902		
13	H	H8	-6.6622892	12.5840866	3.5660762		
14	H	H9	-9.5725555	10.3189448	5.7576935		
15	H	H10	-7.7690433	11.9904859	5.6947338		
16	C	C13	-10.9601687	8.2846932	2.4174727		
17	C	C14	-12.2016920	7.5514868	4.8141018		
18	C	C15	-10.6014501	8.9378889	3.6239193		
19	C	C16	-11.8773293	7.2034719	2.4385386		
20	C	C17	-12.5067642	6.8653520	3.6431746		
21	C	C18	-11.2490679	8.5648287	4.8105290		
22	H	H12	-13.2596653	6.0637944	3.6733500		
23	H	H13	-11.0191639	9.0703152	5.7597140		
24	H	H14	-12.7132690	7.2863745	5.7518045		
25	C	C19	-7.8221279	11.1401623	-0.1111537		
26	C	C20	-5.3617889	12.4948404	-0.1600519		
27	C	C21	-7.2790506	11.5710735	-1.3459486		
28	C	C22	-7.2184187	11.5475127	1.1032339		
29	C	C23	-5.9770290	12.1923073	1.0611241		
30	C	C24	-6.0541535	12.2476773	-1.3521093		
31	H	H16	-5.4456959	12.4227172	1.9972834		
32	H	H17	-5.6016589	12.5599096	-2.3056765		
33	C	C25	-8.9913067	10.2538235	-2.5619740		
34	C	C26	-8.2757539	11.4808185	-4.9713578		
35	C	C27	-7.9691686	11.2365266	-2.5805239		
36	C	C28	-9.5899619	9.8258567	-3.7742087		
37	C	C29	-9.2276547	10.4668014	-4.9677331		
38	C	C30	-7.6401963	11.8566608	-3.7924803		

39 H H20 -9.6933436 10.1827480 -5.9225867
40 H H21 -6.8865705 12.6575102 -3.8228447
41 H H22 -8.0189276 11.9851139 -5.9152250
42 C C31 -10.8939460 8.1241543 -2.5218101
43 C C32 -11.9695150 7.1344932 -4.9073953
44 C C33 -11.7464207 6.9913515 -2.4987464
45 C C34 -10.5390994 8.7246775 -3.7564743
46 C C35 -11.0956881 8.2159537 -4.9387807
47 C C36 -12.2896774 6.5208606 -3.7011474
48 H H24 -10.8495659 8.6613975 -5.9135736
49 H H25 -12.9852726 5.6686967 -3.7032953
50 H H26 -12.4072405 6.7588867 -5.8447159
51 C C37 -11.7095242 7.0040025 -0.0232791
52 C C38 -12.9071157 4.4645230 0.0559042
53 C C39 -12.0478241 6.3472318 -1.2313507
54 C C40 -12.1363198 6.4641948 1.2143345
55 C C41 -12.7337471 5.1989872 1.2356640
56 C C42 -12.6145293 5.0689177 -1.1730620
57 H H28 -13.0396352 4.7496948 2.1927893
58 H H29 -12.7884020 4.5020791 -2.1005773
59 C C43 -3.9718915 12.9492327 -0.1851364
60 C C44 -1.2026964 13.4489352 -0.0785026
61 C C45 -3.4189632 13.6833077 0.8742495
62 C C46 -3.1320055 12.5529458 -1.2388563
63 C C47 -1.7665598 12.8096955 -1.1920946
64 C C48 -2.0472793 13.9194659 0.9341065
65 H H18 -4.0684073 14.0633920 1.6771973
66 H H31 -3.5460236 11.9979622 -2.0947145
67 H H32 -1.1153000 12.4755728 -2.0141585
68 H H33 -1.6208280 14.4633768 1.7903088
69 C C49 -13.2712143 3.0488911 0.1051205
70 C C50 -13.5834853 0.2507780 0.0517114
71 C C51 -12.8414494 2.2602783 1.1848634
72 C C52 -13.9465155 2.4258202 -0.9545048
73 C C53 -14.0901609 1.0405596 -0.9875115
74 C C54 -13.0055262 0.8800126 1.1639755
75 H H30 -12.3326297 2.7289346 2.0412251
76 H H35 -14.3528708 3.0314031 -1.7786137
77 H H36 -14.5885804 0.5606794 -1.8431640
78 H H37 -12.6445796 0.2702090 2.0063292
79 C C55 9.4330852 -9.7488648 1.1589154
80 C C56 10.3907871 -8.6690251 -1.2717265
81 C C57 10.4107164 -8.7311318 1.1766260
82 C C58 8.9214452 -10.2110657 -0.0740690
83 C C59 9.4354077 -9.7076905 -1.2899826
84 C C60 10.8509227 -8.1584175 -0.0375019
85 C C61 10.9613855 -8.2797464 2.4296123
86 C C62 12.2055334 -7.5436152 4.8238984
87 C C63 11.8788086 -7.1987137 2.4482897
88 C C64 10.6036868 -8.9311294 3.6373312
89 C C65 11.2526434 -8.5566905 4.8227091
90 C C66 12.5095490 -6.8591104 3.6517672
91 H H41 11.0236722 -9.0608864 5.7728015
92 H H42 13.2626856 -6.0577103 3.6800838
93 H H43 12.7181902 -7.2774127 5.7606983
94 C C67 8.9533144 -10.3103054 2.3966759
95 C C68 8.0950369 -11.4983326 4.7798462
96 C C69 7.8751617 -11.2311156 2.3813550
97 C C70 9.5630956 -9.9463690 3.6242581
98 C C71 9.1209743 -10.5597542 4.8052576
99 C C72 7.4708497 -11.8292111 3.5818200
100 H H46 9.5758364 -10.3080745 5.7743255
101 H H47 6.6636639 -12.5765342 3.5885515
102 H H48 7.7719049 -11.9793765 5.7155027
103 C C73 11.7086098 -7.0026428 -0.0136200
104 C C74 12.9072927 -4.4633416 0.0608973
105 C C75 12.0458720 -6.3476656 -1.2229077
106 C C76 12.1367847 -6.4611628 1.2228464
107 C C77 12.7346676 -5.1960083 1.2418540
108 C C78 12.6131736 -5.0693979 -1.1669146
109 H H51 13.0415429 -4.7454295 2.1980659
110 H H52 12.7864060 -4.5039376 -2.0954152
111 C C79 10.8904669 -8.1262868 -2.5099248
112 C C80 11.9635237 -7.1398465 -4.8980856
113 C C81 10.5343860 -8.7285342 -3.7435660
114 C C82 11.7429852 -6.9934998 -2.4891918
115 C C83 12.2849047 -6.5246118 -3.6928698
116 C C84 11.0897404 -8.2213787 -4.9271989

117 H H55 12.9804639 -5.6723920 -3.6968659
118 H H56 10.8425753 -8.6680951 -5.9011731
119 H H57 12.4002147 -6.7653804 -5.8363370
120 C C85 8.9878722 -10.2560015 -2.5454344
121 C C86 8.2701511 -11.4863593 -4.9523233
122 C C87 7.9658391 -11.2387336 -2.5615942
123 C C88 9.5853190 -9.8297608 -3.7588593
124 C C89 9.2219552 -10.4723042 -4.9510876
125 C C90 7.6357743 -11.8606004 -3.7722972
126 H H61 6.8821795 -12.6615391 -3.8007736
127 H H62 8.0124626 -11.9920114 -5.8952061
128 C C91 7.8209122 -11.1386916 -0.0921415
129 C C92 5.3606943 -12.4937454 -0.1368883
130 C C93 7.2181794 -11.5442420 1.1234430
131 C C94 7.2768518 -11.5714854 -1.3258563
132 C C95 6.0519951 -12.2481825 -1.3299263
133 C C96 5.9768518 -12.1893244 1.0833474
134 H H65 5.5986634 -12.5618398 -2.2826184
135 H H66 5.4462700 -12.4185605 2.0202193
136 C C97 13.2723222 -3.0478191 0.1076746
137 C C98 13.5863468 -0.2500944 0.0495970
138 C C99 13.9476543 -2.4269033 -0.9532567
139 C C100 12.8434819 -2.2572485 1.1863630
140 C C101 13.0083936 -0.8771618 1.1631447
141 C C102 14.0922274 -1.0418496 -0.9885177
142 H H67 14.3532709 -3.0341126 -1.7765318
143 H H68 12.3346967 -2.7242354 2.0435897
144 H H69 12.6480270 -0.2657368 2.0045550
145 H H70 14.5907278 -0.5636682 -1.8450516
146 C C103 3.9708000 -12.9485563 -0.1604012
147 C C104 1.2019508 -13.4497905 -0.0516892
148 C C105 3.1299945 -12.5526919 -1.2134774
149 C C106 3.4189885 -13.6826934 0.8995777
150 C C107 2.0474195 -13.9197422 0.9603986
151 C C108 1.7647439 -12.8101577 -1.1656631
152 H H72 3.5431644 -11.9976408 -2.0696717
153 H H73 4.0692905 -14.0622765 1.7021270
154 H H74 1.6218586 -14.4639978 1.8168935
155 H H75 1.1126831 -12.4763854 -1.9872730
156 C C109 8.7300687 10.3497472 1.2878565
157 C C110 9.7724533 9.4437819 -1.1781276
158 C C111 9.7562894 9.3809748 1.2701545
159 C C112 8.1821141 10.8152596 0.0717499
160 C C113 8.7253471 10.3899457 -1.1609447
161 C C114 10.2516431 8.9038440 0.0362308
162 C C115 10.2925039 8.8749458 2.5085919
163 C C116 11.4307813 7.9662579 4.8972964
164 C C117 11.2225569 7.8048481 2.4884124
165 C C118 9.8944488 9.4508596 3.7418774
166 C C119 10.4832123 8.9838412 4.9258266
167 C C120 11.7954019 7.3751877 3.6923502
168 H H79 10.2045880 9.4120556 5.8996408
169 H H80 12.5491692 6.5739978 3.6967818
170 H H81 11.8920437 7.6233373 5.8358434
171 C C121 8.2448694 10.8657001 2.5429702
172 C C122 7.4427994 12.0446207 4.9492368
173 C C123 8.8706422 10.4830637 3.7565895
174 C C124 7.1563293 11.7743039 2.5586525
175 C C125 6.7835915 12.3725205 3.7690547
176 C C126 8.4632605 11.0996271 4.9484898
177 H H84 5.9757129 13.1187239 3.7970091
178 H H85 8.9468652 10.8508280 5.9042739
179 H H86 7.1505190 12.5317787 5.8918056
180 C C127 11.1887048 7.8114331 0.0128472
181 C C128 12.5630899 5.3629229 -0.0609714
182 C C129 11.6545033 7.3014409 -1.2233964
183 C C130 11.5707303 7.1818859 1.2223604
184 C C131 12.2265543 5.9467496 1.1667029
185 C C132 12.3400191 6.0816665 -1.2420584
186 H H89 12.4387260 5.3948778 2.0952735
187 H H90 12.6784235 5.6538662 -2.1980774
188 C C133 10.3540358 9.0321744 -2.4308546
189 C C134 11.6482207 8.3858649 -4.8246551
190 C C135 9.9515337 9.6564121 -3.6388276
191 C C136 11.3456487 8.0187971 -2.4490458
192 C C137 11.9993861 7.7246479 -3.6523055
193 C C138 10.6259525 9.3288475 -4.8239400
194 H H93 12.8073571 6.9785394 -3.6802004

195 H H94 10.3622253 9.8155529 -5.7741429
196 H H95 12.1788915 8.1566349 -5.7611876
197 C C139 8.2072730 10.9156098 -2.3989610
198 C C140 7.2670961 12.0385701 -4.7826824
199 C C141 7.0665885 11.7577249 -2.3841706
200 C C142 8.8414850 10.5952750 -3.6262736
201 C C143 8.3570289 11.1751384 -4.8075701
202 C C144 6.6209667 12.3249772 -3.5849084
203 H H98 8.8286578 10.9558185 -5.7764727
204 H H99 5.7628424 13.0131950 -3.5920653
205 H H100 6.9106804 12.4949345 -5.7185957
206 C C145 7.0188398 11.6629255 0.0893251
207 C C146 4.4690190 12.8406778 0.1334042
208 C C147 6.3890018 12.0242711 -1.1264838
209 C C148 6.4455923 12.0568881 1.3227973
210 C C149 5.1759926 12.6453215 1.3266010
211 C C150 5.1051451 12.5800440 -1.0867218
212 H H103 4.7016185 12.9266638 2.2791663
213 H H104 4.5596746 12.7708021 -2.0236841
214 C C151 13.0264982 3.9765898 -0.1075969
215 C C152 13.5354179 1.2076781 -0.0496679
216 C C153 13.7427622 3.4044001 0.9537341
217 C C154 12.6550149 3.1580411 -1.1867831
218 C C155 12.9160756 1.7928756 -1.1636820
219 C C156 13.9837747 2.0328374 0.9889935
220 H H105 14.1042613 4.0383701 1.7773898
221 H H106 12.1155521 3.5883751 -2.0443949
222 H H107 12.6001295 1.1578643 -2.0054845
223 H H108 14.5137380 1.5905810 1.8459397
224 C C157 3.0503738 13.1958044 0.1568338
225 C C158 0.2532411 13.4998102 0.0481084
226 C C159 2.4480177 13.8895488 -0.9027897
227 C C160 2.2398108 12.7407215 1.2095662
228 C C161 0.8598768 12.9009836 1.1618221
229 C C162 1.0632642 14.0288256 -0.9636957
230 H H110 3.0699192 14.3149320 -1.7048370
231 H H111 2.6912936 12.2158049 2.0653809
232 H H112 0.2330614 12.5218044 1.9833362
233 H H113 0.6002801 14.5418819 -1.8199279
234 C C163 -9.7566768 -9.3802538 1.2884308
235 C C164 -8.7251299 -10.3936040 -1.1405840
236 C C165 -8.7308747 -10.3494197 1.3081192
237 C C166 -10.2511690 -8.9047866 0.0535549
238 C C167 -9.7716775 -9.4469053 -1.1597204
239 C C168 -8.1825994 -10.8171321 0.0929894
240 C C169 -8.2464071 -10.8634737 2.5642487
241 C C170 -7.4456282 -12.0386145 4.9727062
242 C C171 -7.1580047 -11.7721821 2.5818455
243 C C172 -8.8727527 -10.4788231 3.7769808
244 C C173 -8.4660211 -11.0935208 4.9700261
245 C C174 -6.7858561 -12.3684415 3.7933395
246 H H117 -8.9500411 -10.8431854 5.9251806
247 H H118 -5.9780383 -13.1146578 3.8228697
248 H H119 -7.1538385 -12.5243392 5.9161717
249 C C175 -10.2934073 -8.8721572 2.5258261
250 C C176 -11.4331368 -7.9599081 4.9124152
251 C C177 -11.2230230 -7.8016940 2.5035375
252 C C178 -9.8963738 -9.4464951 3.7601643
253 C C179 -10.4859324 -8.9778022 4.9430263
254 C C180 -11.7965852 -7.3701901 3.7064285
255 H H122 -10.2082996 -9.4049089 5.9176074
256 H H123 -12.5500326 -6.5686968 3.7092663
257 H H124 -11.8950644 -7.6156658 5.8501560
258 C C181 -7.0196682 -11.6651691 0.1124365
259 C C182 -4.4700930 -12.8432962 0.1593243
260 C C183 -6.3896967 -12.0289776 -1.1024466
261 C C184 -6.4468230 -12.0570059 1.3467431
262 C C185 -5.1772564 -12.6455749 1.3519348
263 C C186 -5.1060425 -12.5849355 -1.0613411
264 H H127 -4.7031939 -12.9251172 2.3051622
265 H H128 -4.5605600 -12.7776024 -1.9978813
266 C C187 -8.2069265 -10.9217009 -2.3774631
267 C C188 -7.2670353 -12.0499608 -4.7587984
268 C C189 -8.8404748 -10.6031134 -3.6054988
269 C C190 -7.0668398 -11.7645621 -2.3607910
270 C C191 -6.6213576 -12.3345096 -3.5603544
271 C C192 -8.3562471 -11.1856776 -4.7855554
272 H H131 -5.7637368 -13.0233760 -3.5659706

273 H H132 -8.8275075 -10.9679020 -5.7549754

274 H H133 -6.9108374 -12.5084817 -5.6937448

275 C C193 -10.3523236 -9.0368827 -2.4132974

276 C C194 -11.6444347 -8.3927793 -4.8088298

277 C C195 -11.3431714 -8.0227426 -2.4335233

278 C C196 -9.9496271 -9.6632485 -3.6200847

279 C C197 -10.6229723 -9.3366691 -4.8061085

280 C C198 -11.9958704 -7.7297107 -3.6376261

281 H H136 -10.3589846 -9.8248392 -5.7554891

282 H H137 -12.8032170 -6.9829813 -3.6670980

283 H H138 -12.1742196 -8.1643226 -5.7460587

284 C C199 -11.1876172 -7.8118698 0.0280900

285 C C200 -12.5606529 -5.3627045 -0.0499640

286 C C201 -11.5700464 -7.1803504 1.2364478

287 C C202 -11.6523497 -7.3034077 -1.2090874

288 C C203 -12.3371721 -6.0832300 -1.2298471

289 C C204 -12.2251550 -5.9449231 1.1786668

290 H H141 -12.6746896 -5.6565690 -2.1866892

291 H H142 -12.4375530 -5.3916002 2.1062981

292 C C205 -3.0515126 -13.1983883 0.1835122

293 C C206 -0.2539346 -13.5014201 0.0753734

294 C C207 -2.2410266 -12.7425149 1.2362234

295 C C208 -2.4487839 -13.8926407 -0.8756314

296 C C209 -1.0638135 -14.0315498 -0.9361995

297 C C210 -0.8608584 -12.9021889 1.1887141

298 H H143 -2.6927225 -12.2172461 2.0918740

299 H H144 -3.0702893 -14.3185756 -1.6777345

300 H H145 -0.6005326 -14.5452051 -1.7920761

301 H H146 -0.2342812 -12.5217809 2.0099782

302 C C211 -13.0234581 -3.9762633 -0.0988490

303 C C212 -13.5320213 -1.2071127 -0.0451055

304 C C213 -12.6505324 -3.1592739 -1.1786046

305 C C214 -13.7406629 -3.4023855 0.9610106

306 C C215 -13.9815516 -2.0306902 0.9941498

307 C C216 -12.9113851 -1.7939960 -1.1575251

308 H H148 -12.1102440 -3.5909400 -2.0351102

309 H H149 -14.1030787 -4.0351572 1.7851526

310 H H150 -14.5123902 -1.5871631 1.8498733

311 H H151 -12.5944655 -1.1602175 -1.9998423

312 H H154 9.6866557 -10.1895100 -5.9067853

Cartesian Coordinates (Angstroms) for the Cyclic Tetramer **1** (Conformer **A**) with Four Mesityl Substituents Optimized at the AM1 Level (4112.7351 kJ/mol)

(a) (b)

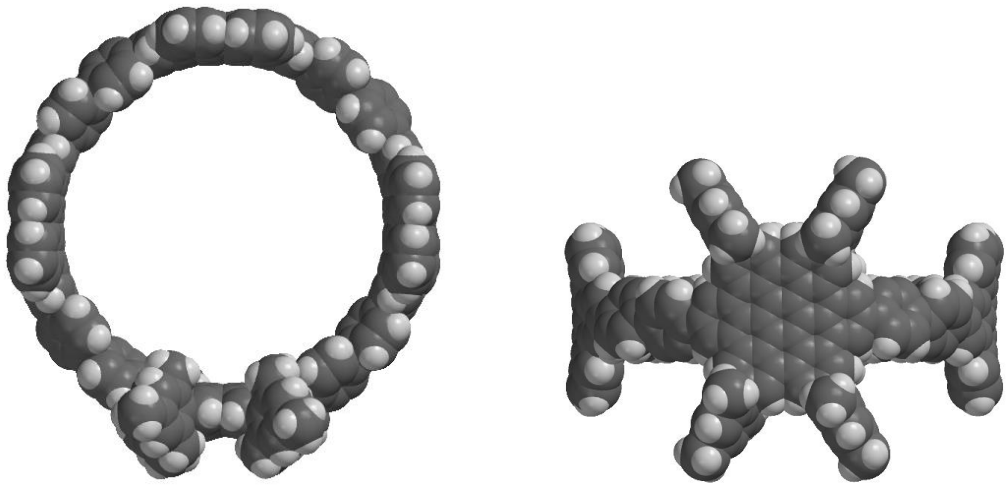

Figure S-94. Optimized structure of cyclic tetramer **1** (Conformer **A**) with four mesityl substituents optimized at the AM1 level: (a) top view of the molecular structure; (b) side view of the molecular structure.

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
1 C	C1	-8.3490254	6.8295098	1.1884171
2 C	C4	-7.3945010	7.8202861	-1.2800642
3 C	C2	-7.3729274	7.8486384	1.1682889
4 C	C6	-8.7986414	6.2628167	-0.0249521
5 C	C5	-8.3485588	6.7804665	-1.2597076
6 C	C3	-6.8716570	8.3183538	-0.0659511
7 C	C7	-6.8847613	8.4039744	2.4049256
8 C	C8	-6.0093724	9.5886918	4.7954487
9 C	C9	-7.4829243	8.0331152	3.6356114
10 C	C10	-5.8095805	9.3273794	2.3869906
11 C	C11	-5.3950109	9.9202725	3.5851790
12 C	C12	-7.0384067	8.6435466	4.8158030
13 H	H8	-4.5874866	10.6680268	3.5902165
14 H	H9	-7.4890288	8.3907874	5.7873326
15 C	C13	-8.8874280	6.3699894	2.4432546
16 C	C14	-10.1092733	5.6102044	4.8539123
17 C	C15	-8.5194419	7.0122386	3.6522577
18 C	C16	-9.8035335	5.2884853	2.4644894
19 C	C17	-10.4235044	4.9387336	3.6693579
20 C	C18	-9.1503343	6.6266982	4.8424533
21 H	H12	-11.1782262	4.1380995	3.6990658
22 H	H13	-8.9085097	7.1201952	5.7958095
23 C	C19	-5.7733591	9.2484502	-0.0879439
24 C	C20	-3.3190756	10.6134879	-0.1440769
25 C	C21	-5.2395953	9.6882372	-1.3237948
26 C	C22	-5.1631459	9.6497976	1.1253016
27 C	C23	-3.9248206	10.3001374	1.0790939
28 C	C24	-4.0177248	10.3703356	-1.3332574
29 H	H16	-3.3884462	10.5278505	2.0130886
30 H	H17	-3.5728221	10.6918197	-2.2873698
31 C	C25	-6.9572660	8.3746157	-2.5359347
32 C	C26	-6.2560010	9.6210441	-4.9513374
33 C	C27	-5.9363824	9.3578439	-2.5564789
34 C	C28	-7.5629005	7.9546445	-3.7469451
35 C	C29	-7.2128226	8.6027013	-4.9388425
36 C	C30	-5.6123421	9.9841286	-3.7653207

37 H H20 -7.6870829 8.3265412 -5.8925787
38 H H21 -4.8566261 10.7836961 -3.7972887
39 C C31 -8.8561213 6.2433221 -2.4965892
40 C C32 -9.9461415 5.2608511 -4.8907079
41 C C33 -9.7059810 5.1091665 -2.4763951
42 C C34 -8.5105938 6.8508543 -3.7300185
43 C C35 -9.0717684 6.3506076 -4.9123892
44 C C36 -10.2536324 4.6415222 -3.6765325
45 H H24 -8.8332026 6.8030555 -5.8866709
46 H H25 -10.9461193 3.7861287 -3.6804971
47 C C37 -9.6550644 5.1061964 -0.0004894
48 C C38 -10.8535935 2.5668721 0.0699767
49 C C39 -10.0006904 4.4572521 -1.2107459
50 C C40 -10.0730481 4.5580488 1.2365954
51 C C41 -10.6715590 3.2932211 1.2534560
52 C C42 -10.5678318 3.1789752 -1.1568512
53 H H28 -10.9718071 2.8378795 2.2096075
54 H H29 -10.7486338 2.6183170 -2.0868510
55 C C43 -1.9318018 11.0757618 -0.1747256
56 C C44 0.8355142 11.5891049 -0.0815506
57 C C45 -1.3757299 11.8037061 0.8874198
58 C C46 -1.0968455 10.6935280 -1.2373643
59 C C47 0.2674815 10.9568758 -1.1971044
60 C C48 -0.0050101 12.0465943 0.9403996
61 H H18 -2.0217889 12.1738522 1.6978339
62 H H31 -1.5135777 10.1450392 -2.0959862
63 H H32 0.9149415 10.6336701 -2.0265242
64 H H33 0.4238975 12.5858355 1.7983479
65 C C49 -11.2199119 1.1515184 0.1115400
66 C C50 -11.5350012 -1.6458943 0.0410883
67 C C51 -10.7925319 0.3559833 1.1871504
68 C C52 -11.8952217 0.5354178 -0.9522839
69 C C53 -12.0399331 -0.8494497 -0.9938463
70 C C54 -10.9581116 -1.0239305 1.1578914
71 H H30 -10.2851080 0.8187140 2.0475250
72 H H35 -12.3008828 1.1460153 -1.7731125
73 H H36 -12.5379022 -1.3235546 -1.8529532
74 H H37 -10.5995069 -1.6389816 1.9973793
75 C C55 11.4352941 -11.6327446 1.2613465
76 C C56 12.4187878 -10.5778398 -1.1700121
77 C C57 12.4085321 -10.6107439 1.2789255
78 C C58 10.9409230 -12.1117537 0.0277928
79 C C59 11.4679416 -11.6207104 -1.1875815
80 C C60 12.8614821 -10.0506633 0.0635359
81 C C61 12.9417188 -10.1421066 2.5331406
82 C C62 14.1526228 -9.3719759 4.9338288
83 C C63 13.8545809 -9.0571760 2.5502239
84 C C64 12.5715073 -10.7804706 3.7440182
85 C C65 13.2039493 -10.3890433 4.9328810
86 C C66 14.4686795 -8.7004445 3.7573889
87 H H41 12.9650334 -10.8827577 5.8860168
88 H H42 15.2181481 -7.8956203 3.7855466
89 H H43 14.6522340 -9.0922699 5.8737178
90 C C67 10.9423759 -12.1814086 2.4996598
91 C C68 10.0593300 -13.3446767 4.8859231
92 C C69 9.8682278 -13.1068076 2.4819630
93 C C70 11.5353100 -11.8002940 3.7301876
94 C C71 11.0810293 -12.4014864 4.9128364
95 C C72 9.4514426 -13.6923633 3.6843040
96 H H46 11.5227869 -12.1363966 5.8843747
97 H H47 8.6473047 -14.4429558 3.6898833
98 H H48 9.7265789 -13.8159513 5.8231590
99 C C73 13.7142317 -8.8911635 0.0841257
100 C C74 14.9034579 -6.3469904 0.1430194
101 C C75 14.0638235 -8.2491747 -1.1286396
102 C C76 14.1251666 -8.3334566 1.3192022
103 C C77 14.7187280 -7.0662650 1.3303638
104 C C78 14.6259089 -6.9683646 -1.0809360
105 H H51 15.0125806 -6.6034714 2.2847963
106 H H52 14.8082202 -6.4132480 -2.0138753
107 C C79 12.9314668 -10.0476686 -2.4083604
108 C C80 14.0289677 -9.0845464 -4.7948232
109 C C81 12.5930360 -10.6660401 -3.6388570
110 C C82 13.7788881 -8.9109945 -2.3907425
111 C C83 14.3332747 -8.4538447 -3.5931992
112 C C84 13.1602823 -10.1702981 -4.8216178
113 H H55 15.0252961 -7.5987849 -3.5989391
114 H H56 12.9266950 -10.6295162 -5.7931450

115 H H57 14.4752108 -8.7191497 -5.7321530
116 C C85 11.0383301 -12.1859446 -2.4417396
117 C C86 10.3565152 -13.4492135 -4.8421459
118 C C87 10.0205888 -13.1731613 -2.4587941
119 C C88 11.6491659 -11.7718651 -3.6525994
120 C C89 11.3038284 -12.4308775 -4.8413158
121 C C90 9.7086124 -13.8114913 -3.6657771
122 H H61 8.9588306 -14.6160305 -3.6938024
123 H H62 10.1132624 -13.9678292 -5.7818810
124 C C91 9.8443162 -13.0439812 0.0071593
125 C C92 7.3892630 -14.4076559 -0.0521017
126 C C93 9.2280404 -13.4373758 1.2198372
127 C C94 9.3172050 -13.4934557 -1.2279172
128 C C95 8.0945893 -14.1740883 -1.2392454
129 C C96 7.9894635 -14.0872398 1.1719623
130 H H65 7.6540628 -14.5002091 -2.1937344
131 H H66 7.4481878 -14.3073889 2.1048706
132 C C97 15.2648423 -4.9302273 0.1776662
133 C C98 15.5773287 -2.1329418 0.0935268
134 C C99 15.9497645 -4.3197276 -0.8830922
135 C C100 14.8240988 -4.1286254 1.2433306
136 C C101 14.9883371 -2.7487218 1.2074392
137 C C102 16.0934577 -2.9349387 -0.9314863
138 H H67 16.3640926 -4.9349972 -1.6959467
139 H H68 14.3068869 -4.5869004 2.1002496
140 H H69 14.6193143 -2.1288578 2.0388470
141 H H70 16.5996787 -2.4652774 -1.7881846
142 C C103 6.0007709 -14.8657827 -0.0873361
143 C C104 3.2314246 -15.3692995 -0.0051345
144 C C105 5.1718789 -14.4830337 -1.1545542
145 C C106 5.4375775 -15.5890495 0.9741392
146 C C107 4.0658284 -15.8272430 1.0216071
147 C C108 3.8064826 -14.7415540 -1.1196384
148 H H72 5.5943621 -13.9371025 -2.0120488
149 H H73 6.0789344 -15.9587850 1.7883322
150 H H74 3.6311018 -16.3627920 1.8789082
151 H H75 3.1636302 -14.4175874 -1.9523619
152 C C109 10.7725291 8.5026798 1.2469909
153 C C110 11.7894456 7.5616569 -1.2164727
154 C C111 11.7949351 7.5298406 1.2324647
155 C C112 10.2154980 8.9549335 0.0299691
156 C C113 10.7462334 8.5121475 -1.2020016
157 C C114 12.2773209 7.0351376 0.0003741
158 C C115 12.3403634 7.0374893 2.4724152
159 C C116 13.4971286 6.1552657 4.8620759
160 C C117 13.2657754 5.9633102 2.4575598
161 C C118 11.9558709 7.6308723 3.7016786
162 C C119 12.5539195 7.1770293 4.8860911
163 C C120 13.8480440 5.5469148 3.6616281
164 H H79 12.2862679 7.6192223 5.8567266
165 H H80 14.5985601 4.7427257 3.6694803
166 H H81 13.9657828 5.8227586 5.8007103
167 C C121 10.3002862 9.0361329 2.4997234
168 C C122 9.5238019 10.2483300 4.8976008
169 C C123 10.9358465 8.6669334 3.7123784
170 C C124 9.2146785 9.9482600 2.5135411
171 C C125 8.8547326 10.5630438 3.7193879
172 C C126 10.5413080 9.3001120 4.8998137
173 H H84 8.0492876 11.3119489 3.7450432
174 H H85 11.0328634 9.0621204 5.8542888
175 H H86 9.2418176 10.7487172 5.8363915
176 C C127 13.2095169 5.9384687 -0.0174140
177 C C128 14.5721706 3.4828682 -0.0722187
178 C C129 13.6619936 5.4107702 -1.2511478
179 C C130 13.5995979 5.3226067 1.1965410
180 C C131 14.2491427 4.0837853 1.1508143
181 C C132 14.3420098 4.1877939 -1.2602627
182 H H89 14.4668067 3.5428349 2.0844954
183 H H90 14.6702039 3.7466310 -2.2137464
184 C C133 12.3580826 7.1317803 -2.4689865
185 C C134 13.6277366 6.4492134 -4.8657426
186 C C135 11.9473746 7.7424519 -3.6810815
187 C C136 13.3451840 6.1138774 -2.4830881
188 C C137 13.9867101 5.8014836 -3.6882620
189 C C138 12.6095988 7.3967474 -4.8679035
190 H H93 14.7911728 5.0515372 -3.7139234
191 H H94 12.3393547 7.8724332 -5.8218388
192 H H95 14.1488111 6.2056157 -5.8040259

193 C C139 10.2192884 9.0243555 -2.4419003
194 C C140 9.2630987 10.1221399 -4.8309249
195 C C141 9.0819951 9.8710016 -2.4275559
196 C C142 10.8415012 8.6863292 -3.6705618
197 C C143 10.3492870 9.2538914 -4.8546446
198 C C144 8.6283179 10.4255911 -3.6312184
199 H H98 10.8117202 9.0209317 -5.8247927
200 H H99 7.7728602 11.1171133 -3.6392785
201 H H100 8.9006047 10.5687523 -5.7692045
202 C C145 9.0551977 9.8066238 0.0471831
203 C C146 6.5084233 10.9904314 0.0988776
204 C C147 8.4160055 10.1548957 -1.1674155
205 C C148 8.4936170 10.2172309 1.2805937
206 C C149 7.2252468 10.8083271 1.2881518
207 C C150 7.1338520 10.7141432 -1.1233466
208 H H103 6.7596529 11.1020676 2.2412557
209 H H104 6.5809936 10.8949146 -2.0579279
210 C C151 15.0290699 2.0939332 -0.1056294
211 C C152 15.5286411 -0.6760381 -0.0200293
212 C C153 15.7496243 1.5307255 0.9576829
213 C C154 14.6474096 1.2646595 -1.1729389
214 C C155 14.9039354 -0.1010687 -1.1362959
215 C C156 15.9858925 0.1587115 1.0067799
216 H H105 16.1186552 2.1723230 1.7720062
217 H H106 14.1038327 1.6872043 -2.0319016
218 H H107 14.5806438 -0.7441937 -1.9690750
219 H H108 16.5193243 -0.2759665 1.8654281
220 C C157 5.0902938 11.3467851 0.1294624
221 C C158 2.2917674 11.6457251 0.0364531
222 C C159 4.4795855 12.0261858 -0.9347480
223 C C160 4.2877422 10.9056240 1.1942479
224 C C161 2.9071861 11.0632570 1.1539768
225 C C162 3.0942717 12.1630682 -0.9875597
226 H H110 5.0951558 12.4415204 -1.7468545
227 H H111 4.7459076 10.3932445 2.0540992
228 H H112 2.2866837 10.6941736 1.9848820
229 H H113 2.6246078 12.6647378 -1.8469513
230 C C163 -7.7343639 -11.2926683 1.2463797
231 C C164 -6.6768436 -12.2876755 -1.1791534
232 C C165 -6.7104557 -12.2637856 1.2696747
233 C C166 -8.2141261 -10.8062707 0.0099440
234 C C167 -7.7216983 -11.3391341 -1.2023217
235 C C168 -6.1491428 -12.7224155 0.0569883
236 C C169 -6.2411366 -12.7890673 2.5269682
237 C C170 -5.4697429 -13.9854468 4.9345219
238 C C171 -5.1546751 -13.6999910 2.5494200
239 C C172 -6.8803666 -12.4131253 3.7356190
240 C C173 -6.4882563 -13.0383512 4.9280666
241 C C174 -4.7973510 -14.3068989 3.7600358
242 H H117 -6.9825850 -12.7948988 5.8797330
243 H H118 -3.9913593 -15.0549318 3.7925451
244 H H119 -5.1895846 -14.4794911 5.8772127
245 C C175 -8.2840916 -10.7936768 2.4817909
246 C C176 -9.4485899 -9.8984972 4.8629451
247 C C177 -9.2115366 -9.7214203 2.4578204
248 C C178 -7.9018466 -11.3786599 3.7157681
249 C C179 -8.5035679 -10.9183246 4.8958005
250 C C180 -9.7976760 -9.2985453 3.6577535
251 H H122 -8.2374098 -11.3536947 5.8699217
252 H H123 -10.5497897 -8.4958020 3.6586655
253 H H124 -9.9202027 -9.5608696 5.7982632
254 C C181 -4.9879420 -13.5727040 0.0826617
255 C C182 -2.4412340 -14.7561596 0.1490646
256 C C183 -4.3446624 -13.9274599 -1.1279183
257 C C184 -4.4299770 -13.9759261 1.3201564
258 C C185 -3.1616312 -14.5669126 1.3350370
259 C C186 -3.0625957 -14.4863635 -1.0766318
260 H H127 -2.6989184 -14.8550458 2.2912500
261 H H128 -2.5066476 -14.6722099 -2.0083712
262 C C187 -6.1451981 -12.8061305 -2.4144634
263 C C188 -5.1790441 -13.9149129 -4.7944701
264 C C189 -6.7639913 -12.4759705 -3.6469943
265 C C190 -5.0066795 -13.6509630 -2.3917945
266 C C191 -4.5479928 -14.2110896 -3.5909997
267 C C192 -6.2666968 -13.0487842 -4.8264175
268 H H131 -3.6914467 -14.9012893 -3.5926158
269 H H132 -6.7262035 -12.8217175 -5.7993514
270 H H133 -4.8124315 -14.3656190 -5.7291796

271 C C193 -8.2875514 -10.9178244 -2.4590115
272 C C194 -9.5517953 -10.2524079 -4.8634854
273 C C195 -9.2769764 -9.9023397 -2.4820207
274 C C196 -7.8718719 -11.5346086 -3.6663060
275 C C197 -8.5313824 -11.1974627 -4.8570912
276 C C198 -9.9157353 -9.5986255 -3.6908875
277 H H136 -8.2572044 -11.6780697 -5.8074242
278 H H137 -10.7219317 -8.8507966 -3.7233274
279 H H138 -10.0707760 -10.0156533 -5.8046793
280 C C199 -9.1486372 -9.7117448 -0.0171104
281 C C200 -10.5175949 -7.2599672 -0.0906097
282 C C201 -9.5434627 -9.0893456 1.1919669
283 C C202 -9.5990352 -9.1926344 -1.2552344
284 C C203 -10.2823333 -7.9715748 -1.2736573
285 C C204 -10.1960236 -7.8524974 1.1369010
286 H H141 -10.6092510 -7.5371599 -2.2306719
287 H H142 -10.4174608 -7.3062701 2.0666217
288 C C205 -1.0236555 -15.1140819 0.1865166
289 C C206 1.7744305 -15.4205919 0.1066571
290 C C207 -0.2241881 -14.6674798 1.2513623
291 C C208 -0.4103858 -15.8015600 -0.8709910
292 C C209 0.9747976 -15.9422242 -0.9173692
293 C C210 1.1561045 -14.8288180 1.2176663
294 H H143 -0.6844876 -14.1480090 2.1058252
295 H H144 -1.0237575 -16.2204048 -1.6829633
296 H H145 1.4465652 -16.4504131 -1.7717367
297 H H146 1.7742002 -14.4554051 2.0484241
298 C C211 -10.9783497 -5.8725711 -0.1334685
299 C C212 -11.4842733 -3.1032295 -0.0646224
300 C C213 -10.5969370 -5.0486456 -1.2049819
301 C C214 -11.7023731 -5.3049323 0.9251441
302 C C215 -11.9418283 -3.9332194 0.9659582
303 C C216 -10.8566053 -3.6833243 -1.1766139
304 H H148 -10.0510480 -5.4748721 -2.0606303
305 H H149 -12.0716204 -5.9426899 1.7423750
306 H H150 -12.4779171 -3.4947750 1.8210607
307 H H151 -10.5335238 -3.0442369 -2.0125899
308 H H154 11.7796341 -12.1579365 -5.7944221
309 C C217 -10.5355821 4.7637067 -6.1410097
310 C C218 -11.6648093 3.8133529 -8.5322550
311 C C219 -11.6354227 5.4265832 -6.7143430
312 C C220 -10.0024587 3.6241112 -6.7689791
313 C C221 -10.5714774 3.1595674 -7.9584057
314 C C222 -12.1894862 4.9460449 -7.9042678
315 H H5 -10.1512516 2.2684439 -8.4491651
316 H H3 -13.0492807 5.4671692 -8.3522664
317 C C223 -10.7794329 5.2436168 6.1086236
318 C C224 -12.0658558 4.5469974 8.5076986
319 C C225 -12.0843131 5.6999970 6.3681438
320 C C226 -10.1205907 4.4379997 7.0540954
321 C C227 -10.7694076 4.0974083 8.2447183
322 C C228 -12.7151721 5.3482561 7.5646870
323 H H11 -10.2512751 3.4679476 8.9841988
324 H H14 -13.7355067 5.7080517 7.7670540
325 C C229 -5.5702769 10.2266714 6.0435759
326 C C230 -4.7268072 11.4452291 8.4305354
327 C C231 -6.3142647 11.2836991 6.5967938
328 C C232 -4.4025574 9.7816539 6.6887653
329 C C233 -3.9912900 10.3945741 7.8755472
330 C C234 -5.8855358 11.8835894 7.7845367
331 H H23 -3.0770629 10.0453256 8.3791154
332 H H26 -6.4684083 12.7118921 8.2153806
333 C C235 -5.9216537 10.3020510 -6.2091919
334 C C236 -5.2816817 11.6071228 -8.6134349
335 C C237 -6.7566205 11.3199272 -6.7029894
336 C C238 -4.7655085 9.9392962 -6.9226859
337 C C239 -4.4558557 10.5947809 -8.1176763
338 C C240 -6.4288551 11.9636172 -7.8997249
339 H H38 -3.5504668 10.3098845 -8.6749043
340 H H39 -7.0824393 12.7617047 -8.2836314
341 C C241 -12.7502492 4.1676843 9.7654815
342 H H15 -12.0124574 3.9956710 10.5873906
343 H H44 -13.3307077 3.2227133 9.6125832
344 H H45 -13.4620515 4.9661530 10.0901315
345 C C242 -8.7495690 3.9340554 6.7997994
346 H H7 -8.1012024 4.7483606 6.3890205
347 H H49 -8.7804821 3.1036406 6.0501366
348 H H50 -8.2806481 3.5446555 7.7364016

349 C C243 -12.7937041 6.5594959 5.3902858

350 H H1 -12.3313187 7.5784513 5.3694489

351 H H53 -13.8741881 6.6680664 5.6533647

352 H H54 -12.7194201 6.1242289 4.3618966

353 C C244 -4.2907575 12.0774927 9.6971788

354 H H27 -3.1796197 12.0278905 9.8080077

355 H H58 -4.7532172 11.5453487 10.5667333

356 H H59 -4.6030263 13.1500093 9.7377407

357 C C245 -7.5419944 11.7785385 5.9290230

358 H H10 -7.2696023 12.3811770 5.0258509

359 H H60 -8.1441456 12.4238353 6.6144202

360 H H63 -8.1795177 10.9214770 5.5948690

361 C C246 -3.6086164 8.6629739 6.1263561

362 H H19 -2.6407875 8.5370279 6.6700859

363 H H64 -3.3888019 8.8473580 5.0444903

364 H H71 -4.1843601 7.7064848 6.2038426

365 C C247 -8.8342997 2.9155988 -6.1930215

366 H H6 -7.8993735 3.4996172 -6.3871567

367 H H76 -8.7143318 1.8999390 -6.6432538

368 H H77 -8.9491540 2.8028407 -5.0855908

369 C C248 -12.2226833 6.6232032 -6.0652202

370 H H2 -11.4165355 7.3222410 -5.7279957

371 H H78 -12.8156879 6.3179987 -5.1663413

372 H H82 -12.9001148 7.1720869 -6.7641455

373 C C249 -12.2700696 3.3044081 -9.7847770

374 H H4 -11.5125377 2.7677323 -10.4072632

375 H H83 -12.6977816 4.1406610 -10.3908019

376 H H87 -13.0963793 2.5884285 -9.5444804

377 C C250 -3.8771174 8.8613134 -6.4258379

378 H H34 -2.9135080 8.8361546 -6.9905926

379 H H88 -4.3793598 7.8676667 -6.5404157

380 H H91 -3.6506264 9.0113712 -5.3402716

381 C C251 -7.9753625 11.7247246 -5.9622303

382 H H22 -7.6922444 12.2912473 -5.0393084

383 H H92 -8.5599600 10.8228853 -5.6496047

384 H H96 -8.6331586 12.3761552 -6.5877842

385 C C252 -4.9517607 12.2847606 -9.8886563

386 H H40 -3.8461958 12.3172147 -10.0503231

387 H H97 -5.3418116 13.3322216 -9.8986301

388 H H101 -5.4143685 11.7309090 -10.7444682

Cartesian Coordinates (Angstroms) of Transition Structure for the Rotation of the HBC Core for the Cyclic Tetramer **1** without the Mesityl Substituents Optimized at the AM1 Level (4038.8452 kJ/mol)

(a) (b)

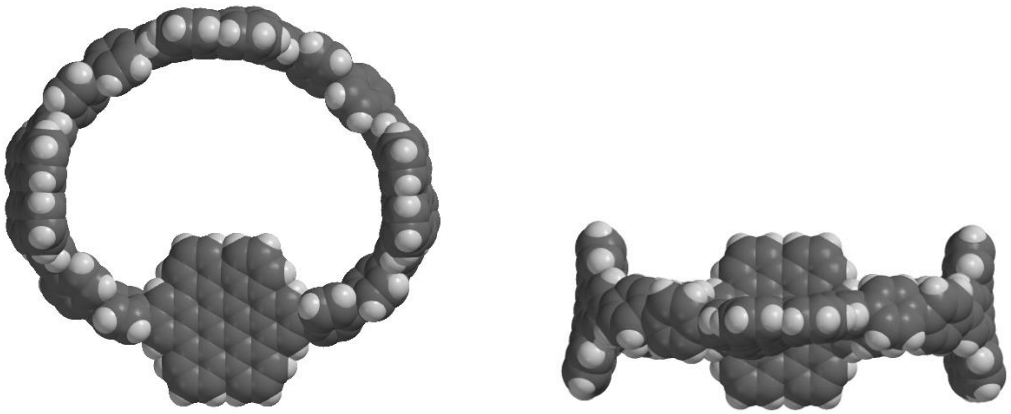

Figure S-95. Optimized structure of the transition for the rotation of the HBC core for cyclic tetramer **1** without the mesityl substituents optimized at the AM1 level: (a) top view of the molecular structure; (b) side view of the molecular structure.

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
1 C C1	-9.4297133	0.1786980	-7.6262344
2 C C4	-6.7067691	-0.1858051	-6.9578823
3 C C2	-8.4606544	0.0585145	-8.6505298
4 C C6	-9.0284755	0.1756754	-6.2706859
5 C C5	-7.6647581	0.0011471	-5.9362256
6 C C3	-7.1006045	-0.1289671	-8.3157690
7 C C7	-8.8548431	0.1332267	-10.0363947
8 C C8	-9.6272240	0.3230000	-12.7253268
9 C C9	-10.2260384	0.2684123	-10.3733374
10 C C10	-7.8751657	0.0835798	-11.0624277
11 C C11	-8.2843785	0.1719067	-12.4007497
12 C C12	-10.5892227	0.3746900	-11.7236420
13 H H8	-7.5525588	0.1195973	-13.2198799
14 H H9	-11.6403496	0.5061805	-12.0189787
15 H H10	-9.9305528	0.4012883	-13.7805667
16 C C13	-10.8281638	0.2921317	-7.9615788
17 C C14	-13.5511115	0.3942029	-8.6208869
18 C C15	-11.2293555	0.3014274	-9.3223129
19 C C16	-11.8047357	0.3719231	-6.9346946
20 C C17	-13.1611959	0.4175754	-7.2872638
21 C C18	-12.5967971	0.3398523	-9.6297028
22 H H12	-13.9446941	0.4707127	-6.5176485
23 H H13	-12.9437491	0.3207819	-10.6730372
24 H H14	-14.6205734	0.4213444	-8.8795771
25 C C19	-6.1087984	-0.2341324	-9.3575389
26 C C20	-4.1294924	-0.2168359	-11.3583002
27 C C21	-4.7527992	-0.4680116	-9.0173743
28 C C22	-6.4713642	-0.0679532	-10.7172793
29 C C23	-5.4682760	-0.0430960	-11.7010847
30 C C24	-3.7825907	-0.4426674	-10.0203663
31 H H16	-5.7165458	0.1255121	-12.7590862
32 H H17	-2.7169182	-0.5774118	-9.7779923
33 C C25	-5.3336548	-0.4636529	-6.6127581
34 C C26	-2.7310265	-1.2741513	-5.9500776
35 C C27	-4.3782362	-0.6906833	-7.6327937
36 C C28	-4.9393422	-0.5494982	-5.2546741
37 C C29	-3.6407130	-0.9765187	-4.9422133
38 C C30	-3.0900813	-1.1200860	-7.2848429

39	H	H20	-3.3257875	-1.0987436	-3.8952910	78	H	H37	-13.0973420	2.5887914	0.8367576
40	H	H21	-2.3466837	-1.3563806	-8.0602706	79	C	C55	8.5416832	0.4681396	8.7089351
41	H	H22	-1.7216289	-1.6283995	-5.6911160	80	C	C56	9.3890638	-1.9792088	7.5739415
42	C	C31	-7.2447190	0.0317708	-4.5558255	81	C	C57	9.5467559	0.4608795	7.7173753
43	C	C32	-6.3977833	0.2657705	-1.8904098	82	C	C58	7.9517120	-0.7476804	9.1217199
44	C	C33	-8.1845279	0.3159030	-3.5347207	83	C	C59	8.4075358	-1.9746837	8.5890943
45	C	C34	-5.8879384	-0.1974394	-4.2152564	84	C	C60	9.9352119	-0.7585823	7.1179850
46	C	C35	-5.4800117	-0.0623979	-2.8806634	85	C	C61	10.1829665	1.6932618	7.3244168
47	C	C36	-7.7387843	0.4448861	-2.2112248	86	C	C62	11.5864753	4.0348781	6.7085648
48	H	H24	-4.4257197	-0.1988346	-2.5980214	87	C	C63	11.1430748	1.6913030	6.2810873
49	H	H25	-8.4365121	0.6941090	-1.3987441	88	C	C64	9.8691571	2.9007280	7.9981762
50	H	H26	-6.0632420	0.3808612	-0.8479828	89	C	C65	10.5959530	4.0582905	7.6843275
51	C	C37	-10.0093850	0.3464280	-5.2272469	90	C	C66	11.8525883	2.8665066	6.0025493
52	C	C38	-11.9188604	0.6415551	-3.1793026	91	H	H41	10.4010597	5.0050369	8.2087102
53	C	C39	-9.5910282	0.4410821	-3.8754678	92	H	H42	12.6389682	2.8757153	5.2333339
54	C	C40	-11.3897963	0.4174408	-5.5422340	93	H	H43	12.1599154	4.9484404	6.4899758
55	C	C41	-12.3304697	0.5393306	-4.5057169	94	C	C67	8.1168625	1.7141014	9.2969219
56	C	C42	-10.5512978	0.6188853	-2.8777657	95	C	C68	7.3491783	4.1127967	10.5196461
57	H	H28	-13.4094580	0.5656977	-4.7169002	96	C	C69	7.0229156	1.7321888	10.1988197
58	H	H29	-10.2601897	0.7171936	-1.8206775	97	C	C70	8.7963812	2.9174870	8.9787935
59	C	C43	-3.0173415	-0.1083718	-12.3059990	98	C	C71	8.3963944	4.1067535	9.6049342
60	C	C44	-0.5514662	0.2423740	-13.5927565	99	C	C72	6.6645165	2.9388801	10.8140900
61	C	C45	-2.7228816	1.1030930	-12.9426698	100	H	H46	8.9015988	5.0578751	9.3826682
62	C	C46	-2.1402187	-1.1928294	-12.4572130	101	H	H47	5.8451583	2.9715504	11.5472187
63	C	C47	-0.9139864	-1.0163832	-13.0875754	102	H	H48	7.0585507	5.0534998	11.0114397
64	C	C48	-1.4942223	1.2787046	-13.5776657	103	C	C73	10.8390113	-0.7499844	5.9969675
65	H	H18	-3.4415186	1.9349383	-12.8951640	104	C	C74	12.1935211	-0.6718637	3.5340081
66	H	H31	-2.4037557	-2.1707708	-12.0269622	105	C	C75	11.1376307	-1.9557710	5.3169328
67	H	H32	-0.2034324	-1.8540151	-13.1570992	106	C	C76	11.3660712	0.4744200	5.5188054
68	H	H33	-1.2447470	2.2497861	-14.0308579	107	C	C77	12.0382059	0.4953188	4.2918960
69	C	C49	-12.8331050	0.7588336	-2.0413406	108	C	C78	11.7864618	-1.8958513	4.0776238
70	C	C50	-14.0983267	0.7001191	0.4576212	109	H	H51	12.4260929	1.4442608	3.8912122
71	C	C51	-12.6397334	1.8067562	-1.1268501	110	H	H52	11.9408735	-2.8142830	3.4909151
72	C	C52	-13.7915907	-0.2221930	-1.7624941	111	C	C79	9.8316177	-3.2264280	7.0020202
73	C	C53	-14.4112859	-0.2587868	-0.5126649	112	C	C80	10.7766662	-5.6438623	5.9534735
74	C	C54	-13.2768421	1.7847564	0.1068488	113	C	C81	9.3803640	-4.4557176	7.5463149
75	H	H30	-11.9501052	2.6272051	-1.3775253	114	C	C82	10.7237082	-3.2210826	5.8996287
76	H	H35	-14.0123056	-0.9997197	-2.5089545	115	C	C83	11.1995572	-4.4404188	5.3999203
77	H	H36	-15.1167761	-1.0684261	-0.2735734	116	C	C84	9.8692829	-5.6543308	7.0070918

117	H	H55	11.9228459	-4.4611451	4.5714548	156	C	C109	9.3576476	1.6855526	-11.2273404
118	H	H56	9.5428910	-6.6258965	7.4055557	157	C	C110	10.3955949	-0.8652095	-10.5916810
119	H	H57	11.1599759	-6.5946405	5.5530388	158	C	C111	10.3613321	1.5587725	-10.2442465
120	C	C85	7.8783749	-3.2190984	9.0883953	159	C	C112	8.8372677	0.5308245	-11.8526432
121	C	C86	6.9998514	-5.6222173	10.2217727	160	C	C113	9.3858258	-0.7392469	-11.5690316
122	C	C87	6.8460170	-3.2089473	10.0606262	161	C	C114	10.8466596	0.2785078	-9.8965565
123	C	C88	8.4085179	-4.4509482	8.6274340	162	C	C115	10.8816915	2.7324295	-9.5899086
124	C	C89	7.9640759	-5.6417004	9.2199576	163	C	C116	12.0278569	4.9991445	-8.4212691
125	C	C90	6.4355081	-4.4196557	10.6334215	164	C	C117	11.7864828	2.5903369	-8.5077963
126	H	H61	5.6729914	-4.4333511	11.4261739	165	C	C118	10.4960141	4.0228603	-10.0340290
127	H	H62	6.6776141	-6.5654451	10.6883732	166	C	C119	11.0942652	5.1446284	-9.4421270
128	C	C91	6.8414294	-0.7329011	10.0386523	167	C	C120	12.3657777	3.7356337	-7.9473501
129	C	C92	4.4042241	-0.6856863	11.4435388	168	H	H79	10.8349924	6.1604691	-9.7741518
130	C	C93	6.3045105	0.5008138	10.4806142	169	H	H80	13.1031585	3.6461178	-7.1359050
131	C	C94	6.2315389	-1.9470785	10.4380874	170	H	H81	12.4979086	5.8914371	-7.9806534
132	C	C95	5.0208914	-1.9051741	11.1395301	171	C	C121	8.8594983	2.9890449	-11.5867784
133	C	C96	5.0734960	0.5076655	11.1464365	172	C	C122	8.0132771	5.5103241	-12.4486025
134	H	H65	4.5206503	-2.8402746	11.4339094	173	C	C123	9.4714210	4.1535323	-11.0576006
135	H	H66	4.5942557	1.4638445	11.4066406	174	C	C124	7.7647047	3.1015791	-12.4805906
136	C	C97	12.6868693	-0.6023402	2.1588485	175	C	C125	7.3678370	4.3709194	-12.9187240
137	C	C98	13.3095496	-0.5594192	-0.5884580	176	C	C126	9.0415116	5.4068259	-11.5174248
138	C	C99	13.3651965	-1.6750987	1.5627234	177	H	H84	6.5516387	4.4771417	-13.6488205
139	C	C100	12.3938973	0.5263540	1.3758874	178	H	H85	9.5111146	6.3311035	-11.1505472
140	C	C101	12.7105298	0.5521387	0.0230485	179	H	H86	7.7028658	6.5022745	-12.8105886
141	C	C102	13.6667401	-1.6577706	0.2023105	180	C	C127	11.7319313	0.1290385	-8.7719607
142	H	H67	13.6552537	-2.5462103	2.1694392	181	C	C128	12.9362689	-0.2183862	-6.2614415
143	H	H68	11.8757963	1.3882360	1.8238188	182	C	C129	12.1514335	-1.1611968	-8.3659226
144	H	H69	12.4591500	1.4355530	-0.5837956	183	C	C130	12.0932612	1.2621043	-8.0036670
145	H	H70	14.1741914	-2.5187935	-0.2580441	184	C	C131	12.6711692	1.0700087	-6.7443259
146	C	C103	3.0448182	-0.6473206	11.9822006	185	C	C132	12.7441974	-1.3177671	-7.1076237
147	C	C104	0.3348518	-0.4235919	12.7185449	186	H	H89	12.8675312	1.9362018	-6.0938112
148	C	C105	2.1227517	-1.6462020	11.6311757	187	H	H90	13.0303096	-2.3201182	-6.7541542
149	C	C106	2.6057599	0.4211592	12.7783299	188	C	C133	10.9598892	-2.1582408	-10.2986823
150	C	C107	1.2637135	0.5396678	13.1308665	189	C	C134	12.2085406	-4.6180742	-9.8475482
151	C	C108	0.7876254	-1.5435320	12.0069797	190	C	C135	10.6008580	-3.2824061	-11.0853570
152	H	H72	2.4460622	-2.5052443	11.0235096	191	C	C136	11.8845560	-2.2975659	-9.2325067
153	H	H73	3.3227846	1.1829212	13.1199400	192	C	C137	12.5160856	-3.5317934	-9.0346313
154	H	H74	0.9265147	1.4016278	13.7260101	193	C	C138	11.2520670	-4.5020687	-10.8508933
155	H	H75	0.0719168	-2.3264646	11.7132090	194	H	H93	13.2717788	-3.6500034	-8.2438630

195	H	H94	11.0191279	-5.3891867	-11.4576524	234	C	C163	-10.8938290	1.5600607	9.9396803
196	H	H95	12.7214174	-5.5792837	-9.6914350	235	C	C164	-9.9306179	-0.9360109	10.8502655
197	C	C139	8.9079131	-1.9047317	-12.2686156	236	C	C165	-9.7839091	1.5080978	10.8090676
198	C	C140	8.0816945	-4.1191345	-13.7613219	237	C	C166	-11.5071470	0.3624599	9.5108857
199	C	C141	7.7994650	-1.7935331	-13.1461144	238	C	C167	-11.0609678	-0.8819978	10.0078523
200	C	C142	9.5516653	-3.1548589	-12.0845617	239	C	C168	-9.2713493	0.2573100	11.2191299
201	C	C143	9.1291714	-4.2478847	-12.8549868	240	C	C169	-9.1735198	2.7274355	11.2744007
202	C	C144	7.4116337	-2.9078778	-13.9003370	241	C	C170	-8.1143267	5.0692753	12.3725814
203	H	H98	9.6184804	-5.2277881	-12.7559804	242	C	C171	-7.9999517	2.6686445	12.0682553
204	H	H99	6.5816848	-2.8312136	-14.6183643	243	C	C172	-9.7586804	3.9794318	10.9556311
205	H	H100	7.7762578	-4.9849635	-14.3682597	244	C	C173	-9.2212190	5.1388943	11.5329342
206	C	C145	7.6828446	0.6377965	-12.7048890	245	C	C174	-7.4969763	3.8491613	12.6292470
207	C	C146	5.1001451	0.7677736	-13.7823457	246	H	H117	-9.6682130	6.1240403	11.3350602
208	C	C147	7.0870109	-0.5300140	-13.2394560	247	H	H118	-6.6176029	3.8215422	13.2897506
209	C	C148	7.0722470	1.8987398	-12.9117861	248	H	H119	-7.7192877	5.9882491	12.8316824
210	C	C149	5.7805211	1.9457247	-13.4458228	249	C	C175	-11.3910280	2.8316268	9.4788798
211	C	C150	5.7920398	-0.4500823	-13.7657136	250	C	C176	-12.4573861	5.2870391	8.6725472
212	H	H103	5.2675609	2.9126230	-13.5628713	251	C	C177	-12.4001012	2.8728723	8.4836180
213	H	H104	5.2777961	-1.3628984	-14.1033269	252	C	C178	-10.8720301	4.0344768	10.0215203
214	C	C151	13.2625841	-0.4037774	-4.8478667	253	C	C179	-11.4297861	5.2535430	9.6095984
215	C	C152	13.4477498	-0.5720771	-2.0438378	254	C	C180	-12.9352192	4.1103049	8.1046753
216	C	C153	13.9423110	0.5822316	-4.1173036	255	H	H122	-11.0620653	6.2060822	10.0181745
217	C	C154	12.7812470	-1.5331926	-4.1662474	256	H	H123	-13.7466637	4.1612125	7.3635462
218	C	C155	12.8774345	-1.6191832	-2.7815191	257	H	H124	-12.8915563	6.2532377	8.3736389
219	C	C156	14.0240548	0.5051894	-2.7294234	258	C	C181	-8.0265532	0.1963243	11.9385123
220	H	H105	14.3979262	1.4368393	-4.6398335	259	C	C182	-5.3587038	0.0739429	12.8031295
221	H	H106	12.2797188	-2.3396358	-4.7229299	260	C	C183	-7.4365965	-1.0595156	12.2218040
222	H	H107	12.4677133	-2.4946739	-2.2550251	261	C	C184	-7.3389235	1.3893385	12.2687724
223	H	H108	14.5245127	1.3053936	-2.1636546	262	C	C185	-6.0117607	1.3096339	12.7050462
224	C	C157	3.6545553	0.7852543	-14.0039733	263	C	C186	-6.0945645	-1.1031996	12.6163662
225	C	C158	0.8575239	0.4999175	-13.8881591	264	H	H127	-5.4526216	2.2291069	12.9363271
226	C	C159	3.0024341	-0.1753414	-14.7893196	265	H	H128	-5.5893674	-2.0741003	12.7346086
227	C	C160	2.8741607	1.6852983	-13.2571583	266	C	C187	-9.4429935	-2.2075004	11.3213062
228	C	C161	1.4937233	1.5471530	-13.2028381	267	C	C188	-8.5503284	-4.6498780	12.3480211
229	C	C162	1.6150121	-0.3099917	-14.7412077	268	C	C189	-10.1874850	-3.3886342	11.0719067
230	H	H110	3.5890089	-0.8415345	-15.4396966	269	C	C190	-8.2200095	-2.2698537	12.0360619
231	H	H111	3.3597670	2.4772084	-12.6663185	270	C	C191	-7.7972011	-3.4992167	12.5574031
232	H	H112	0.8954979	2.2335939	-12.5838787	271	C	C192	-9.7250517	-4.6005038	11.6047324
233	H	H113	1.1177120	-1.0849027	-15.3433031	272	H	H131	-6.8718379	-3.5646245	13.1486676

273	H	H132	-10.2817286	-5.5347426	11.4411716	293	C	C206	-1.1006157	-0.2384849	12.9284718
274	H	H133	-8.2114529	-5.6084514	12.7694752	294	C	C207	-3.1039987	1.0310873	12.4301487
275	C	C193	-11.7562535	-2.0926564	9.6518756	295	C	C208	-3.2788327	-1.0922412	13.5634864
276	C	C194	-13.2643983	-4.3885519	9.1369594	296	C	C209	-1.8922132	-1.2247888	13.5287308
277	C	C195	-12.8262680	-2.0432301	8.7226307	297	C	C210	-1.7188883	0.9139480	12.4219262
278	C	C196	-11.3822584	-3.3249759	10.2451224	298	H	H143	-3.5709466	1.9182183	11.9752847
279	C	C197	-12.1662044	-4.4591271	9.9880680	299	H	H144	-3.8839186	-1.8729109	14.0486931
280	C	C198	-13.5859018	-3.1970157	8.4942693	300	H	H145	-1.4152249	-2.1152695	13.9650899
281	H	H136	-11.9286957	-5.4242582	10.4587943	301	H	H146	-1.1019277	1.7127442	11.9826201
282	H	H137	-14.4514252	-3.1671765	7.8156914	302	C	C211	-14.3523175	0.3749733	4.6782880
283	H	H138	-13.8790514	-5.2850515	8.9641924	303	C	C212	-14.4331571	0.5267671	1.8706178
284	C	C199	-12.5218147	0.4012847	8.4914630	304	C	C213	-13.9705232	-0.7259673	3.8922295
285	C	C200	-13.9613450	0.4056098	6.0872928	305	C	C214	-14.9256489	1.4853643	4.0413082
286	C	C201	-12.8581793	1.6329320	7.8793356	306	C	C215	-14.9546880	1.5664475	2.6500547
287	C	C202	-13.0948037	-0.8025494	8.0144623	307	C	C216	-14.0194923	-0.6551145	2.5058507
288	C	C203	-13.8205313	-0.7816098	6.8182167	308	H	H148	-13.5742933	-1.6346489	4.3710352
289	C	C204	-13.5521436	1.6155056	6.6644804	309	H	H149	-15.3230363	2.3179716	4.6410157
290	H	H141	-14.2395005	-1.7147361	6.4117292	310	H	H150	-15.3546078	2.4673609	2.1610675
291	H	H142	-13.7246624	2.5556298	6.1182258	311	H	H151	-13.6787723	-1.5074604	1.8980393
292	C	C205	-3.9066063	0.0115447	12.9680984	312	H	H154	8.3741681	-6.6132760	8.9082857

Cartesian Coordinates (Angstroms) of Transition Structure for the Rotation of the HBC Core for the Cyclic Tetramer **1** with Four Mesityl Substituents Optimized at the AM1 Level (4147.5696 kJ/mol)

(a) (b)

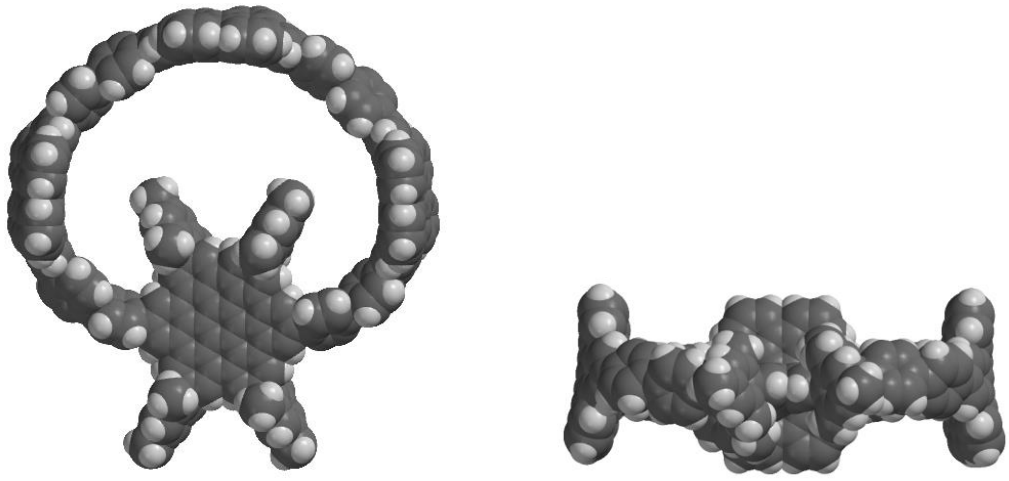

Figure S-96. Optimized structure of the transition for the rotation of the HBC core for cyclic tetramer **1** with four mesityl substituents optimized at the AM1 level: (a) top view of the molecular structure; (b) side view of the molecular structure.

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
1 C C1	-7.8269880	0.2069409	-6.3097112
2 C C4	-5.0959458	-0.1725260	-5.6889321
3 C C2	-6.8758647	0.0871086	-7.3505115
4 C C6	-7.4035565	0.1975634	-4.9613229
5 C C5	-6.0360371	0.0121916	-4.6505619
6 C C3	-5.5112419	-0.1049467	-7.0396275
7 C C7	-7.2934675	0.1650023	-8.7286234
8 C C8	-8.1142706	0.3539997	-11.4134556
9 C C9	-8.6695927	0.2985873	-9.0430615
10 C C10	-6.3323536	0.1178207	-9.7715466
11 C C11	-6.7613238	0.2076875	-11.1021124
12 C C12	-9.0579113	0.4004306	-10.3851798
13 H H8	-6.0426982	0.1597943	-11.9338749
14 H H9	-10.1151074	0.5244666	-10.6636094
15 C C13	-9.2299132	0.3236682	-6.6213440
16 C C14	-11.9736324	0.4120295	-7.2346581
17 C C15	-9.6554208	0.3325337	-7.9741853
18 C C16	-10.1889207	0.4037519	-5.5787441
19 C C17	-11.5513252	0.4332048	-5.9043447
20 C C18	-11.0263046	0.3701751	-8.2596005
21 H H12	-12.3220822	0.4701689	-5.1202816
22 H H13	-11.3922890	0.3590299	-9.2971729
23 C C19	-4.5371008	-0.2042397	-8.0982726
24 C C20	-2.5906871	-0.1710517	-10.1301230
25 C C21	-3.1755610	-0.4369800	-7.7808533
26 C C22	-4.9222072	-0.0327386	-9.4510531
27 C C23	-3.9352185	-0.0018193	-10.4511277
28 C C24	-2.2214866	-0.3998505	-8.7985407
29 H H16	-4.2009853	0.1677326	-11.5047482
30 H H17	-1.1513761	-0.5303782	-8.5737698
31 C C25	-3.7196456	-0.4596743	-5.3680187
32 C C26	-1.1008933	-1.2912472	-4.7552583
33 C C27	-2.7797772	-0.6743582	-6.4043422
34 C C28	-3.3049923	-0.5686220	-4.0183242
35 C C29	-2.0053711	-1.0054350	-3.7304304
36 C C30	-1.4876211	-1.1094122	-6.0852530

37	H	H20	-1.6744414	-1.1467400	-2.6904280	76	C	C56	10.9686231	-1.9809138	9.1974385
38	H	H21	-0.7551134	-1.3332706	-6.8754138	77	C	C57	11.1314008	0.4577275	9.3579303
39	C	C31	-5.5942041	0.0253476	-3.2774218	78	C	C58	9.5679733	-0.7618735	10.7876818
40	C	C32	-4.7071240	0.1933841	-0.6102548	79	C	C59	10.0104512	-1.9845226	10.2344729
41	C	C33	-6.5136912	0.3122917	-2.2392336	80	C	C60	11.5041734	-0.7566457	8.7387649
42	C	C34	-4.2370376	-0.2284708	-2.9587033	81	C	C61	11.7583924	1.6932406	8.9602478
43	C	C35	-3.8093231	-0.1311137	-1.6284632	82	C	C62	13.1463461	4.0395294	8.3285524
44	C	C36	-6.0517290	0.4085073	-0.9200956	83	C	C63	12.6900207	1.7002697	7.8914501
45	H	H24	-2.7546608	-0.2944616	-1.3600039	84	C	C64	11.4637873	2.8943775	9.6537961
46	H	H25	-6.7337841	0.6559615	-0.0932116	85	C	C65	12.1827007	4.0543927	9.3310774
47	C	C37	-8.3651271	0.3771975	-3.9016301	86	C	C66	13.3924579	2.8777357	7.6046620
48	C	C38	-10.2338119	0.7264890	-1.8250781	87	H	H41	12.0024796	4.9963919	9.8690531
49	C	C39	-7.9224416	0.4709706	-2.5576336	88	H	H42	14.1575768	2.8936612	6.8144103
50	C	C40	-9.7495667	0.4635679	-4.1937563	89	H	H43	13.7142239	4.9548660	8.1029519
51	C	C41	-10.6701053	0.6161782	-3.1429844	90	C	C67	9.7415984	1.6976178	10.9829246
52	C	C42	-8.8621751	0.6801854	-1.5461579	91	C	C68	9.0120551	4.0830029	12.2531388
53	H	H28	-11.7517482	0.6637343	-3.3363330	92	C	C69	8.6679082	1.7084922	11.9089095
54	H	H29	-8.5520369	0.7873189	-0.4952110	93	C	C70	10.4171356	2.9025854	10.6624526
55	C	C43	-1.4908033	-0.0528061	-11.0911143	94	C	C71	10.0372572	4.0849355	11.3137096
56	C	C44	0.9689828	0.3174135	-12.3831568	95	C	C72	8.3286902	2.9083135	12.5478015
57	C	C45	-1.2064106	1.1623153	-11.7251185	96	H	H46	10.5413913	5.0368130	11.0922467
58	C	C46	-0.6109751	-1.1334197	-11.2551434	97	H	H47	7.5261560	2.9340077	13.2996050
59	C	C47	0.6132962	-0.9466242	-11.8861377	98	H	H48	8.7376341	5.0182112	12.7643061
60	C	C48	0.0192547	1.3474464	-12.3634901	99	C	C73	12.3788841	-0.7386471	7.5951470
61	H	H18	-1.9295711	1.9897803	-11.6717788	100	C	C74	13.6647541	-0.6399308	5.0968837
62	H	H31	-0.8687436	-2.1152762	-10.8304454	101	C	C75	12.6602155	-1.9389883	6.8983179
63	H	H32	1.3284958	-1.7798567	-11.9611004	102	C	C76	12.8919005	0.4900520	7.1127632
64	H	H33	0.2616471	2.3217023	-12.8135474	103	C	C77	13.5292993	0.5212921	5.8676603
65	C	C49	-11.1258362	0.8710539	-0.6725335	104	C	C78	13.2749484	-1.8687855	5.6423405
66	C	C50	-12.3455971	0.8491688	1.8494722	105	H	H51	13.9046369	1.4738833	5.4636747
67	C	C51	-10.8970431	1.9203167	0.2320073	106	H	H52	13.4146432	-2.7827345	5.0450422
68	C	C52	-12.0971365	-0.0905492	-0.3708212	107	C	C79	11.3976514	-3.2235323	8.6057750
69	C	C53	-12.6930808	-0.1097179	0.8906950	108	C	C80	12.3214987	-5.6319803	7.5193838
70	C	C54	-11.5118777	1.9168989	1.4774245	109	C	C81	10.9600961	-4.4570657	9.1517337
71	H	H30	-10.1967908	2.7262215	-0.0354953	110	C	C82	12.2630708	-3.2090914	7.4824296
72	H	H35	-12.3463522	-0.8671660	-1.1091759	111	C	C83	12.7289642	-4.4242053	6.9635639
73	H	H36	-13.4080039	-0.9054226	1.1477148	112	C	C84	11.4387891	-5.6511547	8.5936744
74	H	H37	-11.3041088	2.7213318	2.1993317	113	H	H55	13.4323425	-4.4379455	6.1179856
75	C	C55	10.1502343	0.4569101	10.3730099	114	H	H56	11.1236047	-6.6258581	8.9935155

115	H	H57	12.6973197	-6.5793942	7.1041773	154	C	C111	11.7737935	1.6527494	-8.7641902
116	C	C85	9.4908074	-3.2326579	10.7342924	155	C	C112	10.2934994	0.6265938	-10.4143900
117	C	C86	8.6346378	-5.6437764	11.8669372	156	C	C113	10.8322792	-0.6441678	-10.1154903
118	C	C87	8.4772306	-3.2296935	11.7261218	157	C	C114	12.2483690	0.3719437	-8.4036033
119	C	C88	10.0114644	-4.4608554	10.2533545	158	C	C115	12.2779322	2.8260036	-8.0964391
120	C	C89	9.5789443	-5.6558836	10.8461518	159	C	C116	13.3928335	5.0924929	-6.8967499
121	C	C90	8.0778513	-4.4444442	12.2980292	160	C	C117	13.1553136	2.6834438	-6.9920239
122	H	H61	7.3305436	-4.4634389	13.1050514	161	C	C118	11.9044081	4.1168012	-8.5498782
123	H	H62	8.3219740	-6.5904156	12.3331481	162	C	C119	12.4861494	5.2383725	-7.9414393
124	C	C91	8.4759113	-0.7538652	11.7261120	163	C	C120	13.7194322	3.8286633	-6.4160050
125	C	C92	6.0563860	-0.7143355	13.1595087	164	H	H79	12.2350444	6.2544049	-8.2790643
126	C	C93	7.9496947	0.4766572	12.1890698	165	H	H80	14.4362868	3.7393227	-5.5863771
127	C	C94	7.8698051	-1.9705458	12.1235168	166	H	H81	13.8505447	5.9845859	-6.4429651
128	C	C95	6.6675814	-1.9326048	12.8394157	167	C	C121	10.3110034	3.0846900	-10.1477044
129	C	C96	6.7270112	0.4802550	12.8699860	168	C	C122	9.4923165	5.6071300	-11.0331340
130	H	H65	6.1689559	-2.8695033	13.1308640	169	C	C123	10.9086898	4.2485434	-9.6013325
131	H	H66	6.2546622	1.4353243	13.1464267	170	C	C124	9.2424867	3.1986810	-11.0725580
132	C	C97	14.1211718	-0.5594539	3.7095962	171	C	C125	8.8596229	4.4684175	-11.5217841
133	C	C98	14.6789000	-0.4925106	0.9486511	172	C	C126	10.4933340	5.5023567	-10.0729610
134	C	C99	14.7856722	-1.6266165	3.0883730	173	H	H84	8.0649658	4.5754906	-12.2751459
135	C	C100	13.8063132	0.5743433	2.9427244	174	H	H85	10.9532393	6.4261255	-9.6928295
136	C	C101	14.0907923	0.6119275	1.5829268	175	H	H86	9.1934318	6.5994175	-11.4037146
137	C	C102	15.0551100	-1.5973276	1.7215194	176	C	C127	13.1061916	0.2220092	-7.2578435
138	H	H67	15.0911662	-2.5023551	3.6806779	177	C	C128	14.2693542	-0.1242973	-4.7265734
139	H	H68	13.2970540	1.4312563	3.4099228	178	C	C129	13.5165443	-1.0682688	-6.8426151
140	H	H69	13.8232009	1.4996895	0.9895424	179	C	C130	13.4518110	1.3550428	-6.4822151
141	H	H70	15.5529626	-2.4535684	1.2421302	180	C	C131	14.0083398	1.1633875	-5.2131175
142	C	C103	4.6975763	-0.6768996	13.6996770	181	C	C132	14.0877341	-1.2241625	-5.5742421
143	C	C104	1.9838909	-0.4413187	14.4170919	182	H	H89	14.1926933	2.0294752	-4.5589833
144	C	C105	3.7722252	-1.6681402	13.3354369	183	H	H90	14.3672597	-2.2263196	-5.2150076
145	C	C106	4.2601975	0.3862890	14.5036906	184	C	C133	12.3692634	-2.0650789	-8.8024752
146	C	C107	2.9162179	0.5107623	14.8470477	185	C	C134	13.5997397	-4.5277980	-8.3165014
147	C	C108	2.4349903	-1.5594889	13.7014843	186	C	C135	12.0287043	-3.1892366	-9.5973849
148	H	H72	4.0947003	-2.5245897	12.7236576	187	C	C136	13.2666946	-2.2052873	-7.7133756
149	H	H73	4.9797982	1.1400357	14.8574142	188	C	C137	13.8896960	-3.4409982	-7.4980038
150	H	H74	2.5802633	1.3695835	15.4474027	189	C	C138	12.6699197	-4.4104497	-9.3443913
151	H	H75	1.7163380	-2.3351759	13.3958813	190	H	H93	14.6252735	-3.5604765	-6.6886955
152	C	C109	10.7974397	1.7806314	-9.7744008	191	H	H94	12.4502947	-5.2978260	-9.9556878
153	C	C110	11.8146216	-0.7713182	-9.1105423	192	H	H95	14.1054854	-5.4902635	-8.1456675

193	C	C139	10.3727119	-1.8088630	-10.8286697	232	C	C165	-8.0682203	1.5821000	12.2959264
194	C	C140	9.5857895	-4.0225520	-12.3440406	233	C	C166	-9.7701364	0.4583975	10.9509098
195	C	C141	9.2909633	-1.6959600	-11.7387086	234	C	C167	-9.3442743	-0.7928230	11.4489095
196	C	C142	11.0081817	-3.0602201	-10.6256165	235	C	C168	-7.5743964	0.3246684	12.7088975
197	C	C143	10.6059113	-4.1528811	-11.4072657	236	C	C169	-7.4604490	2.7936151	12.7847717
198	C	C144	8.9230910	-2.8098670	-12.5035195	237	C	C170	-6.4120723	5.1199319	13.9261947
199	H	H98	11.0898031	-5.1338194	-11.2934559	238	C	C171	-6.3075074	2.7207301	13.6071974
200	H	H99	8.1148983	-2.7318790	-13.2458331	239	C	C172	-8.0283015	4.0521778	12.4607614
201	H	H100	9.2962055	-4.8881401	-12.9590071	240	C	C173	-7.4970677	5.2035855	13.0597083
202	C	C145	9.1646402	0.7351874	-11.3001286	241	C	C174	-5.8102204	3.8934537	14.1892658
203	C	C146	6.6152491	0.8686934	-12.4539482	242	H	H117	-7.9320248	6.1933609	12.8581270
204	C	C147	8.5838317	-0.4313447	-11.8536077	243	H	H118	-4.9479861	3.8546870	14.8714679
205	C	C148	8.5616372	1.9968196	-11.5241697	244	H	H119	-6.0220651	6.0326667	14.4017958
206	C	C149	7.2862458	2.0456210	-12.0958048	245	C	C175	-9.6343033	2.9269046	10.9383069
207	C	C150	7.3058275	-0.3494649	-12.4196747	246	C	C176	-10.6609505	5.3965006	10.1229045
208	H	H103	6.7775267	3.0129810	-12.2263983	247	C	C177	-10.6209534	2.9828167	9.9214529
209	H	H104	6.8011741	-1.2610151	-12.7747423	248	C	C178	-9.1181495	4.1220856	11.5003495
210	C	C151	14.5888419	-0.3092065	-3.3113182	249	C	C179	-9.6554057	5.3484722	11.0829310
211	C	C152	14.7928299	-0.4912651	-0.5089030	250	C	C180	-11.1364491	4.2272119	9.5379495
212	C	C153	15.2684540	0.6760279	-2.5796129	251	H	H122	-9.2886261	6.2953711	11.5052598
213	C	C154	14.1105315	-1.4409562	-2.6316495	252	H	H123	-11.9307688	4.2899321	8.7793420
214	C	C155	14.2158920	-1.5336795	-1.2479415	253	H	H124	-11.0794443	6.3682117	9.8195403
215	C	C156	15.3596005	0.5921120	-1.1927391	254	C	C181	-6.3479346	0.2496262	13.4579695
216	H	H105	15.7186081	1.5344918	-3.1005695	255	C	C182	-3.7036853	0.1024834	14.3892078
217	H	H106	13.6058598	-2.2449993	-3.1889482	256	C	C183	-5.7735627	-1.0122818	13.7462500
218	H	H107	13.8103104	-2.4121211	-0.7231770	257	C	C184	-5.6607584	1.4353136	13.8147300
219	H	H108	15.8619219	1.3906575	-0.6262425	258	C	C185	-4.3458048	1.3432934	14.2841450
220	C	C157	5.1764777	0.8867697	-12.7158778	259	C	C186	-4.4423410	-1.0681188	14.1746140
221	C	C158	2.3795490	0.5880634	-12.6588077	260	H	H127	-3.7866349	2.2571197	14.5368433
222	C	C159	4.5450420	-0.0719441	-13.5201859	261	H	H128	-3.9466201	-2.0432278	14.2981757
223	C	C160	4.3766803	1.7822504	-11.9841543	262	C	C187	-7.7652691	-2.1395311	12.7884897
224	C	C161	2.9963215	1.6370347	-11.9582426	263	C	C188	-6.9118540	-4.5964536	13.8147097
225	C	C162	3.1572843	-0.2116462	-13.5031940	264	C	C189	-8.5113960	-3.3137225	12.5124734
226	H	H110	5.1481210	-0.7329420	-14.1606505	265	C	C190	-6.5598813	-2.2158736	13.5313028
227	H	H111	4.8463234	2.5747262	-11.3813408	266	C	C191	-6.1569877	-3.4523335	14.0517725
228	H	H112	2.3822715	2.3179530	-11.3488157	267	C	C192	-8.0687437	-4.5331257	13.0449627
229	H	H113	2.6758098	-0.9847200	-14.1202777	268	H	H131	-5.2462954	-3.5287229	14.6641392
230	C	C163	-9.1573566	1.6483918	11.4014935	269	H	H132	-8.6271133	-5.4624537	12.8603846
231	C	C164	-8.2333498	-0.8611684	12.3160164	270	H	H133	-6.5886672	-5.5607986	14.2353486

271	C	C193	-10.0409206	-1.9957192	11.0697321	310	C	C218	-9.3632129	0.6537194	-15.4953049
272	C	C194	-11.5537367	-4.2774420	10.5061838	311	C	C219	-9.0853616	-0.6621748	-13.4706477
273	C	C195	-11.0922884	-1.9314965	10.1202527	312	C	C220	-8.4134059	1.6758016	-13.5047585
274	C	C196	-9.6875809	-3.2352932	11.6606830	313	C	C221	-8.8247281	1.7629921	-14.8378725
275	C	C197	-10.4732995	-4.3621975	11.3784657	314	C	C222	-9.4906384	-0.5538809	-14.8041785
276	C	C198	-11.8548435	-3.0784237	9.8676533	315	H	H5	-8.7240739	2.7179387	-15.3758311
277	H	H136	-10.2515941	-5.3327469	11.8457617	316	H	H3	-9.9156710	-1.4312726	-15.3151371
278	H	H137	-12.7069512	-3.0375999	9.1728382	317	C	C223	-13.4070042	0.4356827	-7.5552277
279	H	H138	-12.1704258	-5.1684818	10.3134800	318	C	C224	-16.1480172	0.4754425	-8.1673679
280	C	C199	-10.7639617	0.5122025	9.9116696	319	C	C225	-14.1523111	-0.7566340	-7.5310702
281	C	C200	-12.1701740	0.5455778	7.4869349	320	C	C226	-14.0373009	1.6481594	-7.8868129
282	C	C201	-11.0785362	1.7505505	9.3012617	321	C	C227	-15.4020516	1.6573179	-8.1887908
283	C	C202	-11.3394220	-0.6833948	9.4172894	322	C	C228	-15.5157343	-0.7264978	-7.8373040
284	C	C203	-12.0491362	-0.6475486	8.2117044	323	H	H10	-15.8953412	2.6071621	-8.4462316
285	C	C204	-11.7542277	1.7472847	8.0759452	324	H	H11	-16.0977215	-1.6607230	-7.8180592
286	H	H141	-12.4718542	-1.5738302	7.7935798	325	C	C229	-4.2441640	0.2993354	0.7796299
287	H	H142	-11.9084147	2.6920535	7.5321903	326	C	C230	-3.3654895	0.4982646	3.4396985
288	C	C205	-2.2565621	0.0289449	14.5890945	327	C	C231	-4.1442866	-0.8548031	1.5770700
289	C	C206	0.5472016	-0.2438782	14.6060527	328	C	C232	-3.9032716	1.5527533	1.3169910
290	C	C207	-1.4347076	1.0466666	14.0773370	329	C	C233	-3.4667359	1.6412081	2.6421338
291	C	C208	-1.6504229	-1.0837024	15.1902759	330	C	C234	-3.7069249	-0.7452031	2.8996376
292	C	C209	-0.2644632	-1.2272129	15.1838279	331	H	H23	-3.2008524	2.6234567	3.0618977
293	C	C210	-0.0508473	0.9181519	14.0970137	332	H	H26	-3.6316922	-1.6481242	3.5247424
294	H	H143	-1.8848219	1.9412941	13.6202545	333	C	C235	0.2490185	-1.7752942	-4.4381125
295	H	H144	-2.2719159	-1.8628164	15.6568689	334	C	C236	2.8317453	-2.7041492	-3.8359034
296	H	H145	0.1961043	-2.1245424	15.6237109	335	C	C237	0.4516688	-3.1239668	-4.0951953
297	H	H146	0.5816881	1.7151904	13.6771218	336	C	C238	1.3433807	-0.8930972	-4.4786703
298	C	C211	-12.5572336	0.5275409	6.0765715	337	C	C239	2.6241937	-1.3652455	-4.1778372
299	C	C212	-12.6566275	0.6854132	3.2691137	338	C	C240	1.7405287	-3.5760262	-3.7977451
300	C	C213	-12.1896130	-0.5744675	5.2855014	339	H	H38	3.4799172	-0.6736903	-4.2116332
301	C	C214	-13.1187534	1.6470602	5.4451366	340	H	H39	1.8972463	-4.6323680	-3.5312576
302	C	C215	-13.1565446	1.7311961	4.0541656	341	C	C241	-17.5902121	0.4972476	-8.5051147
303	C	C216	-12.2493916	-0.5011509	3.8996566	342	H	H14	-17.7222511	0.4270522	-9.6145723
304	H	H148	-11.7979468	-1.4876172	5.7595185	343	H	H44	-18.0670029	1.4463615	-8.1561797
305	H	H149	-13.5015527	2.4835958	6.0488417	344	H	H45	-18.1269544	-0.3625397	-8.0339064
306	H	H150	-13.5481333	2.6381623	3.5696797	345	C	C242	-13.5009315	-2.0435075	-7.1875654
307	H	H151	-11.9225150	-1.3561384	3.2879924	346	H	H1	-12.7165091	-2.2923647	-7.9462448
308	H	H154	9.9828570	-6.6250529	10.5193178	347	H	H49	-14.2408154	-2.8801836	-7.1559520
309	C	C217	-8.5429977	0.4573000	-12.8147069	348	H	H50	-13.0030046	-1.9691190	-6.1878327

349	C	C243	-13.2703570	2.9169207	-7.9103813	369	C	C248	-3.9993100	2.7782169	0.4881634
350	H	H7	-12.3144009	2.7839443	-8.4772114	370	H	H19	-3.2514857	2.7387538	-0.3434339
351	H	H53	-13.0136989	3.2287313	-6.8662817	371	H	H78	-3.8059272	3.6966902	1.0941578
352	H	H54	-13.8574995	3.7383014	-8.3894443	372	H	H82	-5.0185523	2.8588861	0.0329449
353	C	C244	-7.8585209	2.8751118	-12.8322957	373	C	C249	-4.5042838	-2.1829594	1.0253100
354	H	H6	-6.9604972	2.6040060	-12.2218905	374	H	H15	-3.9098800	-2.3901575	0.0999358
355	H	H58	-8.6245952	3.3168147	-12.1458023	375	H	H83	-5.5891984	-2.2044820	0.7510979
356	H	H59	-7.5610698	3.6548299	-13.5757472	376	H	H87	-4.3094609	-2.9983831	1.7638458
357	C	C245	-9.7809388	0.7550032	-16.9128792	377	C	C250	1.1538677	0.5358662	-4.8257474
358	H	H4	-8.9075853	0.5495024	-17.5824113	378	H	H34	2.1297277	1.0306696	-5.0531003
359	H	H60	-10.1647137	1.7792298	-17.1439341	379	H	H88	0.6749257	1.0767432	-3.9707743
360	H	H63	-10.5842407	0.0144661	-17.1488425	380	H	H91	0.4865243	0.6376484	-5.7183733
361	C	C246	4.1913907	-3.1896931	-3.5045254	381	C	C251	-0.6840509	-4.0763552	-4.0577876
362	H	H40	4.9690646	-2.6171628	-4.0676615	382	H	H22	-0.4027163	-5.0221615	-3.5333548
363	H	H64	4.3013878	-4.2740780	-3.7524356	383	H	H92	-1.0031004	-4.3323221	-5.0997554
364	H	H71	4.3853419	-3.0594058	-2.4096624	384	H	H96	-1.5595679	-3.6225076	-3.5285139
365	C	C247	-2.8902192	0.5974562	4.8392320	385	C	C252	-9.2221170	-1.9607589	-12.7682740
366	H	H27	-1.7922322	0.3840235	4.8843388	386	H	H2	-8.2183811	-2.4441982	-12.6595308
367	H	H76	-3.4167513	-0.1421162	5.4917529	387	H	H97	-9.8896285	-2.6579485	-13.3314424
368	H	H77	-3.0651122	1.6210594	5.2525765	388	H	H101	-9.6473687	-1.8100462	-11.7440651

Cartesian Coordinates (Angstroms) for the Cyclic Trimer **2** without Mesityl Substituents Optimized at the HF/3-21G Level (-6142.681541 hartrees)

(a) (b)

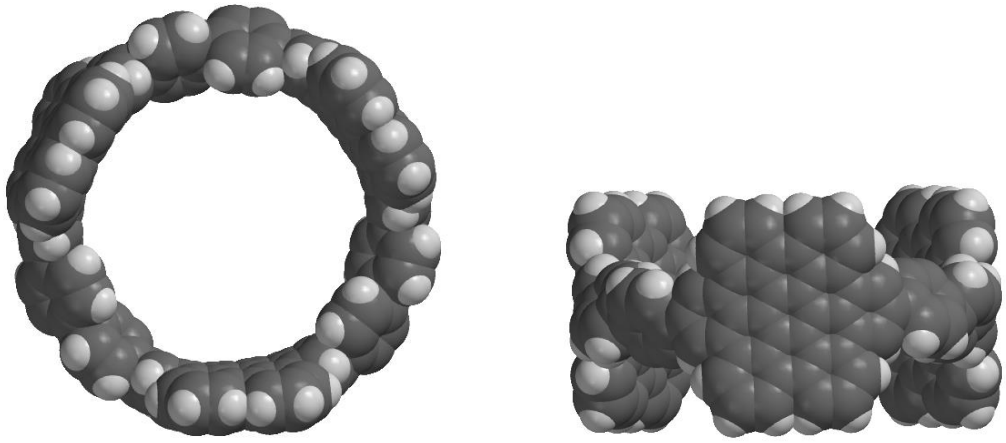

Figure S-97. Optimized structure of cyclic trimer **2** without the mesityl substituents optimized at the HF/3-21G level: (a) top view of the molecular structure; (b) side view of the molecular structure.

Coordinates (Angstroms)

ATOM X Y Z

1 C 1.8339906995 9.9206734308 -1.2316013843
2 C 0.5044835697 10.0755744311 1.2313812549
3 C 0.4430841581 10.0682774029 -1.1964154710
4 C 2.5527236988 9.7941144835 -0.0352303184
5 C 1.8920687650 9.8994733058 1.1961960434
6 C -0.2241021104 10.1176215554 0.0350114333
7 C -0.3070262801 10.1589861137 -2.4306728354
8 C -1.7607285467 10.4696955167 -4.7754691296
9 C 0.3662521737 10.2780992779 -3.6601956511
10 C -1.7133817830 10.1336733531 -2.3977798778
11 C -2.4230210872 10.3089483196 -3.5770498009
12 C -0.3841589009 10.4389945452 -4.8201667721
13 H -3.4918358194 10.3422018122 -3.5608708067
14 H 0.0978999515 10.5383114718 -5.7680237920
15 H -2.3191727652 10.6123984604 -5.6788721961
16 C 2.5302438925 9.9011626111 -2.5006211495
17 C 3.9199508509 10.0942578247 -4.8957891071
18 C 1.8339730127 10.1710858384 -3.6926840001
19 C 3.9121475918 9.6388918471 -2.5381231462
20 C 4.5940339661 9.7604990881 -3.7400138808
21 C 2.5545360232 10.2767556501 -4.8778686741
22 H 5.6535796592 9.6179436618 -3.7738248522
23 H 2.0582070156 10.5077323581 -5.7949859957
24 H 4.4591138764 10.2024509229 -5.8155495073
25 C -1.6681931521 10.0774250629 0.0740461960
26 C -4.3476978137 9.3004561363 0.1702192134
27 C -2.3394939576 10.0243974232 1.3051519613
28 C -2.3973626016 9.9309286508 -1.1145353831
29 C -3.7185576313 9.5090470614 -1.0470151425
30 C -3.6720779715 9.6400094672 1.3334852211
31 H -4.2296719076 9.2356349115 -1.9450433907
32 H -4.1693965991 9.5198139191 2.2721595723
33 C -0.1775947088 10.2166737310 2.5004038116
34 C -1.4856573525 10.7241350850 4.8955743565
35 C -1.5827800648 10.2791446291 2.5379131859
36 C 0.5620948440 10.3193204181 3.6924605048
37 C -0.1148606674 10.5878338017 4.8776464724
38 C -2.2184269422 10.5542820902 3.7398081056

39 H 0.4212788626 10.6985323603 5.7947603555
40 H -3.2823622389 10.6591523458 3.7736342538
41 H -1.9854963054 10.9533960416 5.8153360694
42 C 2.6429483385 9.8153178675 2.4304496094
43 C 4.1291781151 9.7835706930 4.7752264191
44 C 4.0058057011 9.4673455341 2.3975528360
45 C 2.0151053081 10.0860529862 3.6599697822
46 C 2.7824229871 10.0701595133 4.8199321820
47 C 4.7367539127 9.4748198289 3.5768082244
48 H 2.3361206861 10.2776726439 5.7677872617
49 H 5.7845850714 9.2614623202 3.5606126181
50 H 4.7054859661 9.7941046765 5.6786193481
51 C 3.9488750763 9.4229680868 -0.0742614842
52 C 6.3777412523 8.0503913107 -0.1704377455
53 C 4.6248070277 9.1127054584 1.1143144955
54 C 4.5899866987 9.2169679366 -1.3053600074
55 C 5.7983944290 8.5363322230 -1.3336983658
56 C 5.8134894660 8.3981729631 1.0467980317
57 H 6.2546950123 8.3049499304 -2.2723844432
58 H 6.2479472926 8.0144842933 1.9448362194
59 C -5.6208002706 8.5236757937 0.2217498319
60 C -7.7131095829 6.6607837913 0.0902651708
61 C -6.6072157784 8.6274471233 -0.7532228453
62 C -5.7498774726 7.5232652535 1.1803172806
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65 H -6.5568720591 9.4144838974 -1.4796335644
66 H -4.9919042176 7.4037228949 1.9272263877
67 H -6.8265934262 5.8097801613 1.8282919741
68 H -8.3579740356 7.7673840399 -1.6141819686
69 C 7.4377228772 7.0012844283 -0.2219619090
70 C 9.0441570952 4.7061913313 -0.0901860320
71 C 7.3329749471 5.9981333576 -1.1806346223
72 C 8.4213039220 6.8748339389 0.7532010082
73 C 9.2073985705 5.7357397962 0.8255522055
74 C 8.1291673056 4.8743691815 -1.1206989254
75 H 6.5680292275 6.0565469304 -1.9277122675
76 H 8.5536027255 7.6522411656 1.4796798475
77 H 9.9263807047 5.6342804037 1.6144928169
78 H 7.9857820277 4.0825989517 -1.8285226747
79 C -4.5768480627 -9.1234613714 0.2235886986
80 C -1.9152930513 -9.9974933876 0.0914100648
81 C -3.6463567939 -8.7318875148 1.1813022262
82 C -4.1717765953 -10.0292989911 -0.7509244221
83 C -2.8540250845 -10.4523958721 -0.8234643245
84 C -2.3403529383 -9.1690486823 1.1211747574
85 H -3.9232238130 -8.0157964276 1.9277881152
86 H -4.8780452939 -10.3815162021 -1.4767067978
87 H -2.5493004127 -11.1120985731 -1.6118683196
88 H -1.6235650321 -8.8021626620 1.8283462291
89 C -9.5228357960 -3.3753908443 -1.2301736931
90 C -8.9902744117 -4.6026507385 1.2331120065
91 C -8.9544023075 -4.6533348488 -1.1946417862
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93 C -9.5324237156 -3.3133400627 1.1975542726
94 C -8.6624701834 -5.2549510517 0.0369179721
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98 C -9.0990905271 -4.8262408183 -3.6582078712
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129 H -8.5009334209 -7.1953058641 5.8179970696
130 C -9.8347968736 -2.6205884171 2.4315979308
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133 C -9.7547175791 -3.2991348542 3.6613714442
134 C -10.1248306712 -2.6263711435 4.8210955518
135 C -10.5873202903 -0.6368321905 3.5772114341
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138 H -10.8480594669 -0.8229121761 5.6791098564
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140 C -10.1726093160 1.4949932657 -0.1710564413
141 C -10.2177502476 -0.5535930148 1.1146750476
142 C -10.2915584884 -0.6369579423 -1.3049171991
143 C -10.3051563606 0.7498805418 -1.3339283311
144 C -10.1921195463 0.8330471659 1.0465222329
145 H -10.3327433993 1.2602676728 -2.2728894629
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155 H -7.5338779086 4.8651211297 -1.8313631472
156 H -9.8434257774 5.7756715264 1.6131744247
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158 C 7.6390292759 -6.5889143309 1.1946803355
159 C 7.6855283769 -6.5476931731 -1.2330771202
160 C 8.8881732148 -4.8665734557 0.0341519360
161 C 8.4870369613 -5.4766736923 1.2302570700
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165 C 6.3988639373 -8.2031844444 -2.5401893592
166 C 7.9014163867 -6.6717214722 -3.6942917494
167 C 7.6310148453 -7.3473560202 -4.8797938416
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173 C 9.9618416624 -3.7105340290 -4.7757490612
174 C 9.6474188303 -3.5842826048 -2.3980181135
175 C 8.7300160922 -5.4555810277 -3.6613064416
176 C 9.2453076462 -4.8863002442 -4.8210172201
177 C 10.1546628239 -3.0574102920 -3.5770150673
178 H 9.0895778458 -5.3527390303 -5.7691029849
179 H 10.7190469542 -2.1491491954 -3.5603198875
180 H 10.3652094529 -3.2983954690 -5.6789614588
181 C 6.1946454233 -8.1283190410 -0.0762047798
182 C 3.7883526045 -9.5399645944 -0.1723291920
183 C 5.5876304429 -8.5581203029 1.1123384338
184 C 5.6941894171 -8.5785439023 -1.3074139364
185 C 4.4989098154 -9.2819670183 -1.3357382782
186 C 4.3729566637 -9.2275253672 1.0448881152
187 H 4.0692891850 -9.5597382156 -2.2744399079
188 H 3.8234606068 -9.4114192014 1.9430491042
189 C 7.1902525306 -7.1971659052 2.4287034574
190 C 6.4187063392 -8.4688871537 4.7728565229
191 C 7.7399771244 -6.7906718614 3.6582419827
192 C 6.2056512266 -8.2016180822 2.3955326833
193 C 5.8461604083 -8.8386689890 3.5744659283
194 C 7.3420882353 -7.4475016313 4.8178873204

195 H 5.1359950919 -9.6381198857 3.5579868812

196 H 7.7459704008 -7.1662162401 5.7657456829

197 H 6.1393167900 -8.9735000974 5.6759961394

198 C 8.9514495063 -4.9579940525 2.4994126516

199 C 10.0472702093 -4.0819680677 4.8945989081

200 C 9.7094942912 -3.7732020943 2.5373832368

201 C 8.6702046338 -5.6503821018 3.6911034909

202 C 9.2424371081 -5.1999606704 4.8763032557

203 C 10.2667376804 -3.3618095907 3.7392492646

204 H 9.0700622424 -5.7200694737 5.7931331351

205 H 10.8905323240 -2.4935748204 3.7733160012

206 H 10.4966406794 -3.7649784608 5.8143459081

207 C 9.5767729752 -3.5966680379 0.0737520370

208 C 10.2439354834 -0.8878704357 0.1714041219

209 C 9.8145326193 -2.8913777816 -1.1144482848

210 C 9.8672301247 -2.9897211803 1.3051175878

211 C 10.2008078603 -1.6435333017 1.3342166008

212 C 10.1098970564 -1.5363295436 -1.0462053271

213 H 10.3456021496 -1.1534007019 2.2732072536

214 H 10.1282725992 -0.9565079183 -1.9439356140

215 C 2.3489127612 -9.9301234659 -0.2235414111

216 C -0.4422743380 -10.1690122149 -0.0913829683

217 C 1.5333376789 -9.3348699503 -1.1810703141

218 C 1.7464822725 -10.7188267516 0.7507930850

219 C 0.3667643767 -10.8277320925 0.8233229775

220 C 0.1618160998 -9.4601482164 -1.1209513732

221 H 1.9673987702 -8.7014268855 -1.9274144448

222 H 2.3529084019 -11.2241493333 1.4764121875

223 H -0.0814407533 -11.3999469681 1.6115676903

224 H -0.4514696620 -8.9381573165 -1.8279804921

225 C 10.2061085332 0.6030096166 0.2237149086

226 C 9.6332111120 3.3452676400 0.0925505762

227 C 9.4041540474 1.2135021872 1.1831443537

228 C 10.7867666098 1.4065356781 -0.7517633752

229 C 10.4947423342 2.7593885733 -0.8238110238

230 C 9.1302352168 2.5632432488 1.1235112833

231 H 8.9234927435 0.6159606435 1.9305299565

232 H 11.4433192518 0.9707026644 -1.4788224142

233 H 10.9124097751 3.3529271677 -1.6130660589

234 H 8.4555353010 3.0008073588 1.8318872227

Cartesian Coordinates (Angstroms) for the Cyclic Trimer **2** without Mesityl Substituents Optimized by DFT at the B3LPY/6-31G* Level (-6217.274260 hartrees)

(a) (b)

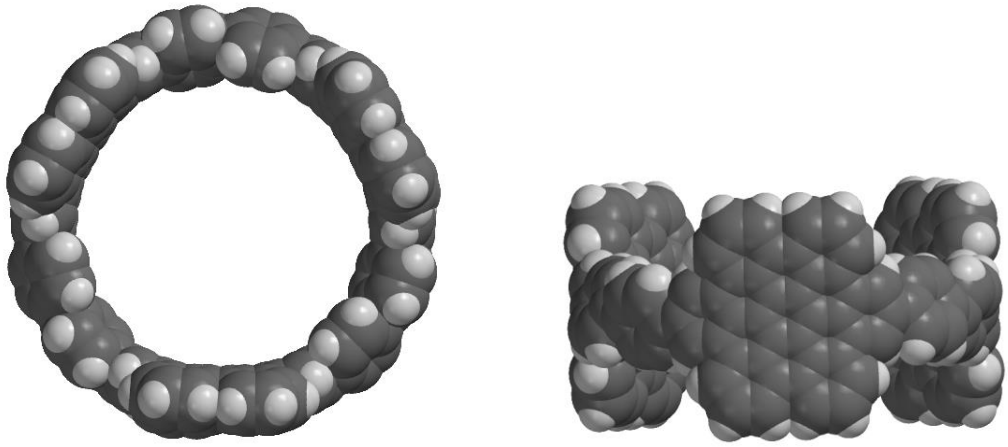

Figure S-98. Optimized structure of cyclic trimer **2** without the mesityl substituents optimized by DFT at the B3LPY/6-31G* level: (a) top view of the molecular structure; (b) side view of the molecular structure.

Coordinates (Angstroms)

ATOM	X	Y	Z
1 C C1	1.8620829	9.9073576	-1.2412797
2 C C4	0.4929377	10.0621042	1.2419444
3 C C2	0.4529954	10.0502398	-1.2189849
4 C C6	2.5769890	9.7770873	-0.0223612
5 C C5	1.8986539	9.8883546	1.2191666
6 C C3	-0.2335992	10.0907918	0.0227594
7 C C7	-0.2844618	10.1358646	-2.4560816
8 C C8	-1.7300638	10.4188677	-4.8425429
9 C C9	0.4086455	10.2373539	-3.6966582
10 C C10	-1.7082933	10.1169858	-2.4352274
11 C C11	-2.4089184	10.2784072	-3.6373916
12 C C12	-0.3411354	10.3829595	-4.8739864
13 H H8	-3.4927980	10.3187389	-3.6311615
14 H H9	0.1563627	10.4642568	-5.8331675
15 H H10	-2.2875017	10.5503316	-5.7659126
16 C C13	2.5692003	9.8896302	-2.4991233
17 C C14	3.9892959	10.0662858	-4.9101505
18 C C15	1.8711159	10.1380061	-3.7152502
19 C C16	3.9707304	9.6364261	-2.5228790
20 C C17	4.6626145	9.7506916	-3.7351463
21 C C18	2.6100162	10.2366515	-4.9046981
22 H H12	5.7389286	9.6174100	-3.7606192
23 H H13	2.1119093	10.4540534	-5.8422679
24 H H14	4.5422865	10.1695237	-5.8397861
25 C C19	-1.6716724	10.0556620	0.0484986
26 C C20	-4.4079023	9.3399348	0.1187372
27 C C21	-2.3666851	10.0218550	1.2871482
28 C C22	-2.4034776	9.9278253	-1.1615096
29 C C23	-3.7479429	9.5424248	-1.1009242
30 C C24	-3.7215110	9.6730459	1.2949862
31 H H16	-4.2575509	9.2789338	-2.0199017
32 H H17	-4.2350715	9.5753580	2.2441132
33 C C25	-0.1998545	10.2004269	2.5001908
34 C C26	-1.5444934	10.6802337	4.9132393
35 C C27	-1.6227616	10.2632599	2.5248329
36 C C28	0.5374148	10.2899243	3.7159615
37 C C29	-0.1613803	10.5440674	4.9062159
38 C C30	-2.2716516	10.5244962	3.7382892

39	H	H20	0.3720409	10.6443514	5.8440431	78	H	H37	8.4924707	4.4057894	-2.0399347
40	H	H21	-3.3508208	10.6318774	3.7647473	79	C	C103	-4.6120586	-9.2360444	0.1873240
41	H	H22	-2.0604791	10.8983802	5.8442670	80	C	C104	-1.9263462	-10.1849721	0.0909497
42	C	C31	2.6385805	9.8142289	2.4554004	81	C	C105	-3.7438656	-9.0913650	1.2838485
43	C	C32	4.1185191	9.7974039	4.8374731	82	C	C106	-4.1365701	-9.9749542	-0.9116586
44	C	C33	4.0241630	9.4844790	2.4338595	83	C	C107	-2.8210970	-10.4276086	-0.9645459
45	C	C34	1.9870199	10.0711061	3.6954411	84	C	C108	-2.4370400	-9.5635722	1.2418394
46	C	C35	2.7548128	10.0632193	4.8705572	85	H	H72	-4.0585825	-8.5131795	2.1468425
47	C	C36	4.7470734	9.5003486	3.6333876	86	H	H73	-4.7936099	-10.1720338	-1.7539286
48	H	H24	2.2906394	10.2626525	5.8292162	87	H	H74	-2.4740638	-10.9558602	-1.8486819
49	H	H25	5.8139278	9.3047692	3.6250339	88	H	H75	-1.7693785	-9.3527632	2.0727371
50	H	H26	4.6941194	9.8147888	5.7588516	89	C	C109	-9.5403587	-3.3565954	-1.2420299
51	C	C37	3.9721995	9.4248461	-0.0479848	90	C	C110	-8.9938101	-4.6111462	1.2455613
52	C	C38	6.4724136	8.1026521	-0.1186244	91	C	C111	-8.9558249	-4.6460196	-1.2144792
53	C	C39	4.6575621	9.1374171	1.1615830	92	C	C112	-9.7866131	-2.6679764	-0.0259520
54	C	C40	4.6416090	9.2336146	-1.2858868	93	C	C113	-9.5479453	-3.3082771	1.2176593
55	C	C41	5.8813527	8.5852847	-1.2948795	94	C	C114	-8.6480918	-5.2562351	0.0294506
56	C	C42	5.8769890	8.4529741	1.1011083	95	C	C115	-8.6546155	-5.3293168	-2.4488710
57	H	H28	6.3585515	8.3742755	-2.2443520	96	C	C116	-8.1560358	-6.7226768	-4.8302962
58	H	H29	6.3107177	8.0791123	2.0207697	97	C	C117	-7.9137089	-6.5449445	-2.4228828
59	C	C43	-5.7064513	8.6166409	0.1580162	98	C	C118	-9.0930055	-4.7872056	-3.6913609
60	C	C44	-7.8718029	6.7658176	0.0562072	99	C	C119	-8.8343221	-5.5101041	-4.8662070
61	C	C45	-6.5825350	8.5758171	-0.9422282	100	C	C120	-7.6917768	-7.2326039	-3.6230400
62	C	C46	-6.0167711	7.7904571	1.2527993	101	H	H79	-9.1544892	-5.1249022	-5.8272155
63	C	C47	-7.0793494	6.8956337	1.2080642	102	H	H80	-7.1728330	-8.1851281	-3.6137075
64	C	C48	-7.6329171	7.6634789	-0.9978174	103	H	H81	-7.9819319	-7.2707619	-5.7522385
65	H	H18	-6.4229109	9.2446449	-1.7832286	104	C	C121	-9.8797004	-2.7403253	-2.5018281
66	H	H31	-5.3604179	7.7711711	2.1168438	105	C	C122	-10.7567311	-1.6143009	-4.9138168
67	H	H32	-7.2316015	6.2111311	2.0381051	106	C	C123	-9.7486234	-3.4759719	-3.7143029
68	H	H33	-8.2622382	7.6292022	-1.8833272	107	C	C124	-10.3599042	-1.3995016	-2.5308078
69	C	C49	7.5671447	7.0976323	-0.1578768	108	C	C125	-10.8108002	-0.8642853	-3.7439377
70	C	C50	9.2394078	4.7909789	-0.0549550	109	C	C126	-10.2138555	-2.8939250	-4.9039928
71	C	C51	7.6803593	6.2244096	-1.2547475	110	H	H84	-11.2333920	0.1344276	-3.7723317
72	C	C52	8.4068101	6.8509258	0.9441391	111	H	H85	-10.1614868	-3.4412729	-5.8380357
73	C	C53	9.2139072	5.7176525	1.0008076	112	H	H86	-11.1299407	-1.1940595	-5.8437088
74	C	C54	8.5035040	5.1055295	-1.2087888	113	C	C127	-7.8906418	-6.4786732	0.0612651
75	H	H30	7.0419096	6.3607532	-2.1219755	114	C	C128	-5.8892387	-8.4760415	0.1440283
76	H	H35	8.4068177	7.5363444	1.7869035	115	C	C129	-7.5153180	-7.0586696	1.3027973
77	H	H36	9.8134335	5.5333352	1.8886808	116	C	C130	-7.4035770	-7.0456592	-1.1458753

117	C	C131	-6.3905843	-8.0089928	-1.0785570	156	H	H113	-9.6889985	5.7202927	1.8645305
118	C	C132	-6.5281323	-8.0502661	1.3173616	157	C	C163	8.4856263	-5.3997615	-1.2261234
119	H	H89	-5.9002392	-8.3150529	-1.9946553	158	C	C164	7.6346651	-6.5868236	1.2087949
120	H	H90	-6.1882913	-8.4419850	2.2689921	159	C	C165	7.6555080	-6.5472433	-1.2518958
121	C	C133	-8.7723881	-5.2783243	2.5054399	160	C	C166	8.8724537	-4.8352683	0.0175078
122	C	C134	-8.5386382	-6.6854542	4.9185976	161	C	C167	8.4884455	-5.4567462	1.2345960
123	C	C135	-9.2309776	-4.6856733	3.7171211	162	C	C168	7.1910158	-7.1090380	-0.0340596
124	C	C136	-8.1094092	-6.5385095	2.5359648	163	C	C169	7.2792504	-7.1421810	-2.5116829
125	C	C137	-8.0209784	-7.2323393	3.7494746	164	C	C170	6.7088814	-8.4441671	-4.9286161
126	C	C138	-9.1168925	-5.4214747	4.9067985	165	C	C171	6.3593443	-8.2295104	-2.5379319
127	H	H93	-7.5692447	-8.2181283	3.7780837	166	C	C172	7.8386451	-6.6549113	-3.7275099
128	H	H94	-9.4868439	-5.0131782	5.8400168	167	C	C173	7.5462002	-7.3350517	-4.9200705
129	H	H95	-8.4814217	-7.2434849	5.8491009	168	C	C174	6.1063697	-8.8783269	-3.7530418
130	C	C139	-9.8550333	-2.6266972	2.4514828	169	H	H117	7.9773845	-7.0057257	-5.8581078
131	C	C140	-10.5723072	-1.3252523	4.8296440	170	H	H118	5.4546958	-9.7450329	-3.7808023
132	C	C141	-10.2519634	-1.2591486	2.4260001	171	H	H119	6.5158410	-8.9676629	-5.8610026
133	C	C142	-9.7595429	-3.3180102	3.6930679	172	C	C175	8.9276581	-4.7991325	-2.4613926
134	C	C143	-10.1320957	-2.6431380	4.8662285	173	C	C176	9.9025938	-3.6861101	-4.8431567
135	C	C144	-10.6226565	-0.6347881	3.6238741	174	C	C177	9.6325616	-3.5620992	-2.4354308
136	H	H98	-10.0741322	-3.1420643	5.8265181	175	C	C178	8.6624518	-5.4426689	-3.7043843
137	H	H99	-10.9779313	0.3900002	3.6126770	176	C	C179	9.1678951	-4.8651521	-4.8794883
138	H	H100	-10.8707007	-0.8306752	5.7499032	177	C	C180	10.1255948	-3.0340969	-3.6355556
139	C	C145	-10.1732389	-1.2823004	-0.0566560	178	H	H122	8.9883716	-5.3326231	-5.8404885
140	C	C146	-10.2702522	1.5433138	-0.1362911	179	H	H123	10.7095000	-2.1201163	-3.6258467
141	C	C147	-10.2639244	-0.5417793	1.1509217	180	H	H124	10.2985880	-3.2686555	-5.7648517
142	C	C148	-10.3408167	-0.6113236	-1.2972695	181	C	C181	6.1886085	-8.1411843	-0.0612740
143	C	C149	-10.3955749	0.7866339	-1.3105416	182	C	C182	3.7962549	-9.6498847	-0.1276758
144	C	C150	-10.2774685	0.8561396	1.0857753	183	C	C183	5.6063718	-8.6017151	1.1487569
145	H	H103	-10.4504468	1.3029911	-2.2617067	184	C	C184	5.6822674	-8.6179343	-1.2996270
146	H	H104	-10.1690089	1.4208708	2.0039172	185	C	C185	4.5025530	-9.3699493	-1.3063381
147	C	C157	-9.9399693	2.9922992	-0.1783877	186	C	C186	4.4056578	-9.3189123	1.0907100
148	C	C158	-8.7614326	5.5860788	-0.0793413	187	H	H127	4.0752727	-9.6705853	-2.2554885
149	C	C159	-10.1406021	3.8454733	0.9224382	188	H	H128	3.8725813	-9.5176188	2.0127666
150	C	C160	-9.2375736	3.5211384	-1.2760638	189	C	C187	7.2077441	-7.1995512	2.4433300
151	C	C161	-8.6720433	4.7902131	-1.2325819	190	C	C188	6.4693114	-8.4911588	4.8205499
152	C	C162	-9.5536592	5.1069292	0.9772961	191	C	C189	7.7628564	-6.7720524	3.6833494
153	H	H110	-10.7368870	3.5084686	1.7654165	192	C	C190	6.2308240	-8.2357540	2.4200844
154	H	H111	-9.0409400	2.8963990	-2.1416539	193	C	C191	5.8919480	-8.8796515	3.6168938
155	H	H112	-8.0591976	5.1260400	-2.0644210	194	C	C192	7.3789584	-7.4410970	4.8560656

195	H	H131	5.1923513	-9.7084145	3.6073423	215	C	C205	2.3759323	-10.0886743	-0.1612396
196	H	H132	7.7874125	-7.1443074	5.8148894	216	C	C206	-0.4599208	-10.3635753	-0.0471472
197	H	H133	6.2031194	-9.0057232	5.7397561	217	C	C207	1.5603943	-9.7405400	-1.2529140
198	C	C193	8.9628968	-4.9354355	2.4937940	218	C	C208	1.7425596	-10.6912332	0.9414219
199	C	C194	10.0639085	-4.0283717	4.9079928	219	C	C209	0.3566746	-10.8132497	1.0037491
200	C	C195	9.7320877	-3.7371294	2.5227249	220	C	C210	0.1791064	-9.8848407	-1.2021066
201	C	C196	8.6770143	-5.6262524	3.7064644	221	H	H143	1.9968211	-9.2546023	-2.1197394
202	C	C197	9.2527446	-5.1567311	4.8972259	222	H	H144	2.3367336	-11.0417347	1.7803883
203	C	C198	10.2887222	-3.3140634	3.7363816	223	H	H145	-0.1016201	-11.2394655	1.8925917
204	H	H136	9.0760173	-5.6747566	5.8324882	224	H	H146	-0.4222350	-9.5197315	-2.0301181
205	H	H137	10.9226913	-2.4342874	3.7647120	225	C	C211	10.3508482	0.6345834	0.1763950
206	H	H138	10.5153244	-3.6971033	5.8391511	226	C	C212	9.8247228	3.4343509	0.0792899
207	C	C199	9.5684297	-3.5766112	0.0482715	227	C	C213	9.7997381	1.3154973	1.2766945
208	C	C200	10.3244475	-0.8512991	0.1312593	228	C	C214	10.7457878	1.4154168	-0.9255649
209	C	C201	9.8231320	-2.8730587	-1.1586279	229	C	C215	10.4777846	2.7806293	-0.9790061
210	C	C202	9.8932740	-2.9652743	1.2890259	230	C	C216	9.5525748	2.6826895	1.2336100
211	C	C203	10.2718109	-1.6183291	1.3035431	231	H	H148	9.4635902	0.7564431	2.1442421
212	C	C204	10.1643656	-1.5172815	-1.0915390	232	H	H149	11.2392051	0.9439879	-1.7708835
213	H	H141	10.4486444	-1.1314081	2.2550892	233	H	H150	10.7548719	3.3441102	-1.8661970
214	H	H142	10.1883865	-0.9388012	-2.0072012	234	H	H151	9.0400443	3.1549333	2.0672372

Cartesian Coordinates (Angstroms) for the Cyclic Trimer **2** without Mesityl Substituents Optimized at the AM1 Level (3071.1922 kJ/mol)

(a) (b)

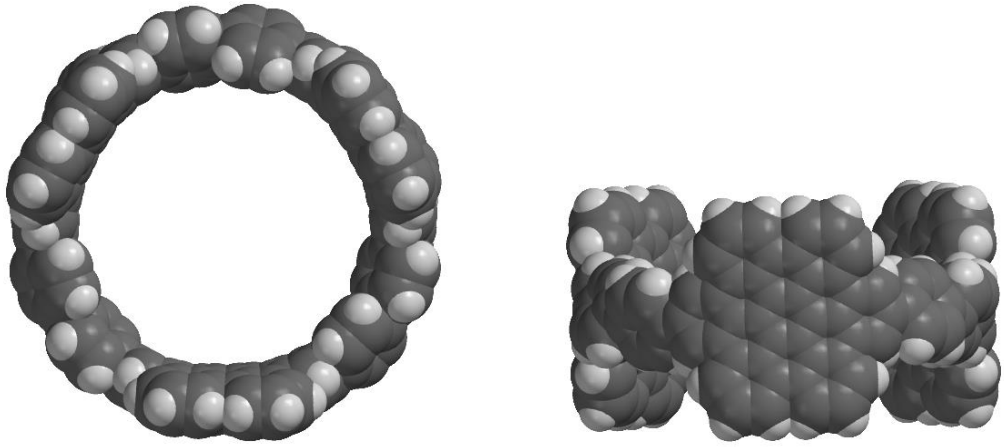

Figure S-99. Optimized structure of cyclic trimer **2** without the mesityl substituents optimized at the AM1 level: (a) top view of the molecular structure; (b) side view of the molecular structure.

Cartesian Coordinates (Angstroms)

Atom X Y Z

1 C C1 1.8329526 9.8233802 -1.2392923	21 C C18 2.5554104 10.1772514 -4.8959130
2 C C4 0.4842878 9.9804608 1.2389462	22 H H12 5.7057043 9.5216691 -3.7759218
3 C C2 0.4304871 9.9716751 -1.2091244	23 H H13 2.0485326 10.4112185 -5.8434008
4 C C6 2.5500204 9.6848194 -0.0304891	24 H H14 4.4909522 10.1085965 -5.8512943
5 C C5 1.8833205 9.8026834 1.2087828	25 C C19 -1.6834437 9.9792934 0.0636862
6 C C3 -0.2454506 10.0101895 0.0301474	26 C C20 -4.3929882 9.2603547 0.1485840
7 C C7 -0.3112506 10.0675655 -2.4405938	27 C C21 -2.3635343 9.9508941 1.3052523
8 C C8 -1.7614951 10.3932790 -4.8076754	28 C C22 -2.4136591 9.8552619 -1.1429481
9 C C9 0.3769369 10.1764524 -3.6757372	29 C C23 -3.7563905 9.4663752 -1.0829636
10 C C10 -1.7287570 10.0546953 -2.4094468	30 C C24 -3.7175200 9.5988116 1.3290486
11 C C11 -2.4388768 10.2370206 -3.6025881	31 H H16 -4.3060589 9.2573451 -2.0135323
12 C C12 -0.3716309 10.3506519 -4.8487229	32 H H17 -4.2513637 9.5365083 2.2895383
13 H H8 -3.5384553 10.2707013 -3.5952784	33 C C25 -0.1989615 10.1242993 2.4991400
14 H H9 0.1275047 10.4534804 -5.8232477	34 C C26 -1.5213535 10.6333825 4.9075908
15 H H10 -2.3299957 10.5455262 -5.7376749	35 C C27 -1.6151803 10.1915557 2.5282172
16 C C13 2.5309715 9.8063411 -2.4994894	36 C C28 0.5459655 10.2158321 3.7023206
17 C C14 3.9349199 9.9979750 -4.9079628	37 C C29 -0.1375370 10.4910591 4.8955407
18 C C15 1.8269731 10.0664140 -3.7026835	38 C C30 -2.2597413 10.4703324 3.7395910
19 C C16 3.9247776 9.5465356 -2.5285623	39 H H20 0.4095313 10.6024141 5.8430194
20 C C17 4.6161285 9.6697620 -3.7399497	40 H H21 -3.3542039 10.5764449 3.7755723

41 H H22 -2.0371141 10.8687874 5.8509167
42 C C31 2.6272728 9.7257660 2.4402503
43 C C32 4.1136199 9.7100168 4.8072903
44 C C33 4.0039202 9.3876580 2.4091131
45 C C34 1.9825189 9.9899374 3.6753769
46 C C35 2.7511186 9.9877301 4.8483397
47 C C36 4.7369700 9.4021806 3.6022284
48 H H24 2.2889698 10.2025868 5.8228468
49 H H25 5.8148892 9.1824106 3.5949036
50 H H26 4.7019205 9.7277759 5.7372674
51 C C37 3.9424616 9.3244428 -0.0640162
52 C C38 6.4141878 8.0019854 -0.1488531
53 C C39 4.6246473 9.0360534 1.1426359
54 C C40 4.5978345 9.1404701 -1.3055759
55 C C41 5.8346543 8.4866719 -1.3293420
56 C C42 5.8420177 8.3489521 1.0826920
57 H H28 6.3399139 8.3033795 -2.2898218
58 H H29 6.3288988 8.0192551 2.0132981
59 C C43 -5.6676227 8.5444426 0.1954543
60 C C44 -7.7913091 6.6985319 0.0766847
61 C C45 -6.5629256 8.5540959 -0.8847268
62 C C46 -5.9387697 7.6941911 1.2807942
63 C C47 -6.9933036 6.7908062 1.2273003
64 C C48 -7.6055713 7.6322977 -0.9503406
65 H H18 -6.4276348 9.2752181 -1.7047547
66 H H31 -5.2827567 7.6995986 2.1647171
67 H H32 -7.1728352 6.1048560 2.0693828
68 H H33 -8.2700729 7.6175650 -1.8272174
69 C C49 7.4898466 7.0118990 -0.1956646
70 C C50 9.1305658 4.7260050 -0.0764440
71 C C51 7.5583999 6.1224233 -1.2813258
72 C C52 8.3627484 6.8146233 0.8849845
73 C C53 9.1646856 5.6772300 0.9508117
74 C C54 8.3761660 5.0002045 -1.2275996
75 H H30 6.9218809 6.2791732 -2.1656776
76 H H35 8.3969489 7.5473140 1.7052280
77 H H36 9.8073602 5.5094416 1.8280575
78 H H37 8.3932126 4.2915666 -2.0699153
79 C C103 -4.5739288 -9.1729760 0.1972694
80 C C104 -1.9103097 -10.0800322 0.0779767
81 C C105 -3.7025477 -8.9802155 1.2828525
82 C C106 -4.1319850 -9.9511154 -0.8834650
83 C C107 -2.8108451 -10.3885445 -0.9493749
84 C C108 -2.3913311 -9.4372909 1.2291136
85 H H72 -4.0370667 -8.4163503 2.1672583
86 H H73 -4.8232940 -10.1965288 -1.7036608
87 H H74 -2.4638738 -10.9548927 -1.8266913
88 H H75 -1.7080920 -9.2479156 2.0714389
89 C C109 -9.4439420 -3.3289136 -1.2378734
90 C C110 -8.9030983 -4.5735612 1.2407286
91 C C111 -8.8699681 -4.6170666 -1.2073221
92 C C112 -9.6823056 -2.6381833 -0.0293227
93 C C113 -9.4499524 -3.2736627 1.2101504
94 C C114 -8.5639027 -5.2206355 0.0321003
95 C C115 -8.5822150 -5.3077512 -2.4385729
96 C C116 -8.1399019 -6.7278538 -4.8048661
97 C C117 -7.8605940 -6.5278781 -2.4071459
98 C C118 -9.0223727 -4.7675559 -3.6736902
99 C C119 -8.7994444 -5.5037015 -4.8462671
100 C C120 -7.6637710 -7.2347274 -3.5998990
101 H H79 -9.1396611 -5.1240930 -5.8207226
102 H H80 -7.1417720 -8.2030889 -3.5923016
103 H H81 -7.9879224 -7.2969593 -5.7345423
104 C C121 -9.7792438 -2.7167778 -2.4982028
105 C C122 -10.6494224 -1.5985001 -4.9066140
106 C C123 -9.6530622 -3.4572219 -3.7010148
107 C C124 -10.2513973 -1.3798906 -2.5277148
108 C C125 -10.7048930 -0.8436265 -3.7390631
109 C C126 -10.1145317 -2.8826901 -4.8942195
110 H H84 -11.1215624 0.1739654 -3.7752683
111 H H85 -10.0643354 -3.4392620 -5.8413839
112 H H86 -11.0242195 -1.1730119 -5.8498979
113 C C127 -7.8161382 -6.4492648 0.0658907
114 C C128 -5.8337402 -8.4311784 0.1506957
115 C C129 -7.4494864 -7.0224829 1.3075905
116 C C130 -7.3433035 -7.0193777 -1.1407408
117 C C131 -6.3326575 -7.9851647 -1.0808374
118 C C132 -6.4651011 -8.0165715 1.3313316

119 H H89 -5.8766742 -8.3561238 -2.0115625
120 H H90 -6.1427199 -8.4464482 2.2918979
121 C C133 -8.6844799 -5.2361758 2.5011665
122 C C134 -8.4609789 -6.6342876 4.9101438
123 C C135 -9.1366041 -4.6368147 3.7042078
124 C C136 -8.0325347 -6.4951984 2.5305693
125 C C137 -7.9500490 -7.1920117 3.7422516
126 C C138 -9.0316445 -5.3656091 4.8977180
127 H H93 -7.4929795 -8.1920960 3.7785444
128 H H94 -9.4018822 -4.9475925 5.8451280
129 H H95 -8.4057344 -7.1980997 5.8537303
130 C C139 -9.7552972 -2.5905517 2.4413937
131 C C140 -10.4857016 -1.2950039 4.8078399
132 C C141 -10.1514835 -1.2294897 2.4097011
133 C C142 -9.6609281 -3.2804173 3.6767863
134 C C143 -10.0439903 -2.6134992 4.8494532
135 C C144 -10.5310196 -0.6016544 3.6025379
136 H H98 -9.9987378 -3.1207917 5.8241460
137 H H99 -10.8801685 0.4415644 3.5947026
138 H H100 -10.7957569 -0.7943018 5.7375900
139 C C145 -10.0666658 -1.2522045 -0.0633896
140 C C146 -10.1540094 1.5496022 -0.1496065
141 C C147 -10.1572904 -0.5166117 1.1429388
142 C C148 -10.2351640 -0.5932016 -1.3052134
143 C C149 -10.2857650 0.8049390 -1.3296593
144 C C150 -10.1694092 0.8812531 1.0822986
145 H H103 -10.3795371 1.3336725 -2.2904203
146 H H104 -10.1266130 1.4680407 2.0126962
147 C C157 -9.8305972 2.9752911 -0.1971859
148 C C158 -8.6617435 5.5348369 -0.0788954
149 C C159 -10.0922915 3.8308151 0.8836906
150 C C160 -9.0939581 3.4769640 -1.2836893
151 C C161 -8.5262101 4.7441980 -1.2304141
152 C C162 -9.5034710 5.0918052 0.9490910
153 H H110 -10.7444936 3.4964852 1.7044765
154 H H111 -8.9147011 2.8468554 -2.1684016
155 H H112 -7.9205466 5.1111921 -2.0733672
156 H H113 -9.6763326 5.7328456 1.8265668
157 C C163 8.4387546 -5.3594037 -1.2100790
158 C C164 7.5644177 -6.5328418 1.2073527
159 C C165 7.6065337 -6.4979155 -1.2407039
160 C C166 8.8116861 -4.7948958 0.0294233
161 C C167 8.4203159 -5.4120201 1.2379456
162 C C168 7.1272163 -7.0493506 -0.0320889
163 C C169 7.2407582 -7.0920263 -2.5011819
164 C C170 6.7002387 -8.4004088 -4.9103109
165 C C171 6.3158967 -8.1666388 -2.5306281
166 C C172 7.8188301 -6.6130194 -3.7042382
167 C C173 7.5482886 -7.2976781 -4.8978280
168 C C174 6.0746386 -8.8254015 -3.7423798
169 H H117 8.0048205 -6.9762157 -5.8452637
170 H H118 5.3991538 -9.6930413 -3.7787240
171 H H119 6.5161814 -8.9360654 -5.8539652
172 C C175 8.8934991 -4.7651257 -2.4412972
173 C C176 9.9030188 -3.6729425 -4.8077368
174 C C177 9.5934074 -3.5324097 -2.4095343
175 C C178 8.6421657 -5.4143429 -3.6767532
176 C C179 9.1686842 -4.8537421 -4.8494168
177 C C180 10.1075099 -3.0090349 -3.6023566
178 H H122 9.0072968 -5.3366820 -5.8241682
179 H H123 10.6882274 -2.0747030 -3.5944771
180 H H124 10.3201649 -3.2572353 -5.7374943
181 C C181 6.1161704 -8.0723329 -0.0658990
182 C C182 3.7305004 -9.5442467 -0.1506806
183 C C183 5.5246893 -8.5181938 1.1407317
184 C C184 5.6271473 -8.5454445 -1.3076177
185 C C185 4.4401950 -9.2859639 -1.3313569
186 C C186 4.3187465 -9.2252140 1.0808438
187 H H127 4.0272165 -9.6297654 -2.2919106
188 H H128 3.7895395 -9.4812565 2.0115287
189 C C187 7.1250460 -7.1385355 2.4385841
190 C C188 6.3667624 -8.4181214 4.8048935
191 C C189 7.6779843 -6.7145448 3.6737181
192 C C190 6.1413430 -8.1592163 2.4071439
193 C C191 5.7866257 -8.8015020 3.5999008
194 C C192 7.2910574 -7.3792678 4.8463013
195 H H131 5.0552427 -9.6232573 3.5923221
196 H H132 7.7096120 -7.0883782 5.8207766

197 H H133 6.0874271 -8.9367036 5.7345805

198 C C193 8.8880114 -4.8939761 2.4982927

199 C C194 9.9930849 -4.0071106 4.9067319

200 C C195 9.6562612 -3.7023494 2.5278657

201 C C196 8.5942412 -5.5852978 3.7010775

202 C C197 9.1759765 -5.1329769 4.8942932

203 C C198 10.2214315 -3.2854345 3.7392106

204 H H136 8.9985902 -5.6629443 5.8414347

205 H H137 10.8619556 -2.3916581 3.7754442

206 H H138 10.4560662 -3.6797694 5.8500182

207 C C199 9.5058792 -3.5352185 0.0635624

208 C C200 10.2386709 -0.8294877 0.1500143

209 C C201 9.7639881 -2.8403424 -1.1427095

210 C C202 9.8222194 -2.9331149 1.3054243

211 C C203 10.1946806 -1.5845316 1.3299930

212 C C204 10.0990143 -1.4831413 -1.0819498

213 H H141 10.4081194 -1.0918449 2.2907834

214 H H142 10.1929951 -0.9022167 -2.0122699

215 C C205 2.3338673 -9.9762659 -0.1972166

216 C C206 -0.4668010 -10.2476099 -0.0777777

217 C C207 1.5299055 -9.5869332 -1.2816982

218 C C208 1.7252185 -10.6333835 0.8825610

219 C C209 0.3389359 -10.7558950 0.9485185

220 C C210 0.1488131 -9.7307625 -1.2278821

221 H H143 1.9848686 -9.1137602 -2.1652011

222 H H144 2.3418779 -11.0320158 1.7019943

223 H H145 -0.1286594 -11.2286833 1.8250890

224 H H146 -0.4727772 -9.3884240 -2.0693226

225 C C211 10.2537158 0.6322984 0.1977216

226 C C212 9.7084677 3.3927030 0.0794077

227 C C213 9.6523929 1.2905741 1.2837378

228 C C214 10.7068518 1.4041998 -0.8825919

229 C C215 10.4256334 2.7671766 -0.9479978

230 C C216 9.3930789 2.6547273 1.2304476

231 H H148 9.3318079 0.7188746 2.1680246

232 H H149 11.2646042 0.9281812 -1.7029678

233 H H150 10.7426604 3.3509834 -1.8250874

234 H H151 8.8881892 3.1517292 2.0729656

Cartesian Coordinates (Angstroms) for the Cyclic Trimer **2** with Four Mesityl Substituents Optimized at the AM1 Level (3178.9098 kJ/mol)

(a) (b)

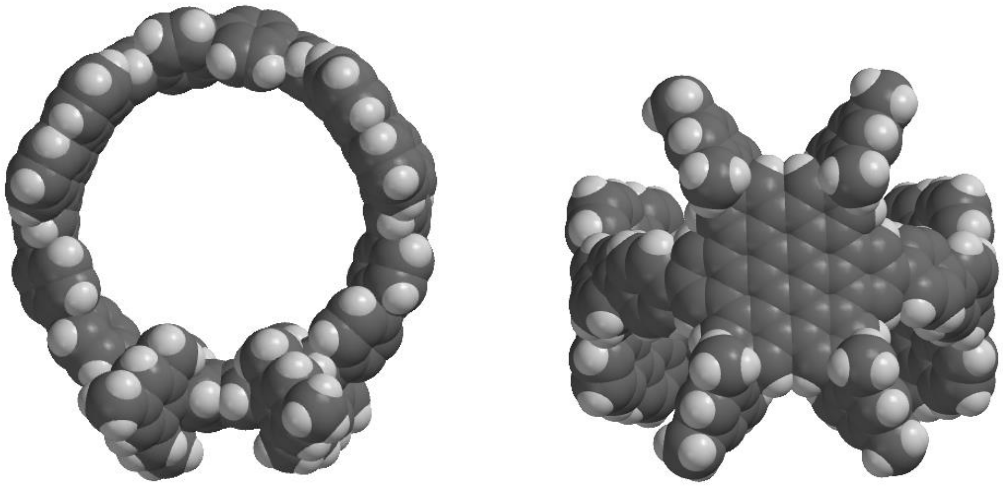

Figure S-100. Optimized structure of cyclic trimer **2** with four mesityl substituents optimized at the AM1 level: (a) top view of the molecular structure; (b) side view of the molecular structure.

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
1 C	C1	-0.2281202	11.3885609	-1.2452330
2 C	C4	-1.5809002	11.5484595	1.2305828
3 C	C2	-1.6307098	11.5361008	-1.2175544
4 C	C6	0.4870102	11.2519118	-0.0350898
5 C	C5	-0.1817524	11.3712719	1.2029340
6 C	C3	-2.3086949	11.5759482	0.0205774
7 C	C7	-2.3704809	11.6295548	-2.4503945
8 C	C8	-3.8170868	11.9500513	-4.8203564
9 C	C9	-1.6803111	11.7372431	-3.6845448
10 C	C10	-3.7880225	11.6153143	-2.4215308
11 C	C11	-4.4963262	11.7949596	-3.6161595
12 C	C12	-2.4271093	11.9088786	-4.8590362
13 H	H8	-5.5959488	11.8274114	-3.6107340
14 H	H9	-1.9264134	12.0107528	-5.8328594
15 H	H10	-4.3841992	12.1001750	-5.7515433
16 C	C13	0.4719921	11.3701508	-2.5042185
17 C	C14	1.8800329	11.5600690	-4.9103190
18 C	C15	-0.2301180	11.6284406	-3.7089035
19 C	C16	1.8659308	11.1107328	-2.5305904
20 C	C17	2.5593678	11.2331647	-3.7408278
21 C	C18	0.5003849	11.7385523	-4.9009298
22 H	H12	3.6490715	11.0854589	-3.7746552
23 H	H13	-0.0049594	11.9713151	-5.8495270
24 H	H14	2.4377030	11.6702411	-5.8527354
25 C	C19	-3.7467070	11.5438373	0.0518519
26 C	C20	-6.4555962	10.8222153	0.1335436
27 C	C21	-4.4287223	11.5166542	1.2924056
28 C	C22	-4.4748163	11.4172046	-1.1558019
29 C	C23	-5.8172678	11.0270081	-1.0973305
30 C	C24	-5.7823823	11.1631858	1.3145805
31 H	H16	-6.3652382	10.8159619	-2.0284506
32 H	H17	-6.3176842	11.1017724	2.2743098
33 C	C25	-2.2662009	11.6937699	2.4894694
34 C	C26	-3.5926925	12.2057642	4.8949471
35 C	C27	-3.6825162	11.7599082	2.5161863
36 C	C28	-1.5231585	11.7877940	3.6936458
37 C	C29	-2.2087361	12.0645912	4.8853039
38 C	C30	-4.3291683	12.0400733	3.7261057

39 H H20 -1.6631912 12.1781031 5.8334031
40 H H21 -5.4237791 12.1452099 3.7602233
41 H H22 -4.1101085 12.4423532 5.8370642
42 C C31 0.5602718 11.2963241 2.4356785
43 C C32 2.0430983 11.2851900 4.8048479
44 C C33 1.9369439 10.9580302 2.4071900
45 C C34 -0.0864287 11.5625828 3.6693283
46 C C35 0.6804979 11.5628274 4.8433955
47 C C36 2.6682392 10.9748499 3.6013381
48 H H24 0.2168932 11.7795995 5.8167816
49 H H25 3.7461495 10.7549383 3.5959254
50 H H26 2.6300759 11.3050089 5.7356184
51 C C37 1.8794542 10.8913494 -0.0658506
52 C C38 4.3492609 9.5650837 -0.1451519
53 C C39 2.5594381 10.6038559 1.1422604
54 C C40 2.5367749 10.7055642 -1.3060872
55 C C41 3.7728114 10.0501683 -1.3270622
56 C C42 3.7758674 9.9147426 1.0851050
57 H H28 4.2796334 9.8657336 -2.2865001
58 H H29 4.2607364 9.5855655 2.0169541
59 C C43 -7.7295968 10.1050934 0.1794944
60 C C44 -9.8518875 8.2575779 0.0605124
61 C C45 -8.6233941 10.1126072 -0.9019098
62 C C46 -8.0014833 9.2559682 1.2655799
63 C C47 -9.0553673 8.3518194 1.2120008
64 C C48 -9.6653070 9.1899944 -0.9676482
65 H H18 -8.4874802 10.8326914 -1.7227321
66 H H31 -7.3465132 9.2629149 2.1502543
67 H H32 -9.2355338 7.6668531 2.0547439
68 H H33 -10.3286152 9.1735786 -1.8453966
69 C C49 5.4218411 8.5715838 -0.1896619
70 C C50 7.0537378 6.2793334 -0.0677083
71 C C51 5.4900302 7.6824669 -1.2756806
72 C C52 6.2911639 8.3703765 0.8930020
73 C C53 7.0886772 7.2299319 0.9601733
74 C C54 6.3034342 6.5571866 -1.2206276
75 H H30 4.8565310 7.8420335 -2.1616074
76 H H35 6.3260984 9.1024020 1.7137586
77 H H36 7.7285481 7.0592658 1.8389035
78 H H37 6.3202207 5.8491439 -2.0634208
79 C C103 -6.6727849 -7.6340214 0.2026874
80 C C104 -4.0115791 -8.5482678 0.0860207
81 C C105 -5.8016766 -7.4425985 1.2885364
82 C C106 -6.2325582 -8.4151115 -0.8764231
83 C C107 -4.9125917 -8.8562555 -0.9410050
84 C C108 -4.4916804 -7.9032091 1.2361200
85 H H72 -6.1352268 -6.8768822 2.1719169
86 H H73 -6.9241712 -8.6598498 -1.6964828
87 H H74 -4.5667551 -9.4250781 -1.8171104
88 H H75 -3.8084597 -7.7148376 2.0785082
89 C C109 -11.5191006 -1.7727344 -1.2442638
90 C C110 -10.9853727 -3.0167457 1.2362533
91 C C111 -10.9495537 -3.0628319 -1.2117438
92 C C112 -11.7565295 -1.0799581 -0.0366916
93 C C113 -11.5276442 -1.7149472 1.2037229
94 C C114 -10.6471032 -3.6662747 0.0286718
95 C C115 -10.6626077 -3.7557125 -2.4419810
96 C C116 -10.2214042 -5.1792207 -4.8065367
97 C C117 -9.9453264 -4.9783514 -2.4084845
98 C C118 -11.0991385 -3.2151306 -3.6782017
99 C C119 -10.8768042 -3.9529201 -4.8498867
100 C C120 -9.7490040 -5.6867831 -3.6004110
101 H H79 -11.2142256 -3.5729314 -5.8251601
102 H H80 -9.2303167 -6.6569146 -3.5912472
103 H H81 -10.0697442 -5.7494971 -5.7355426
104 C C121 -11.8510222 -1.1608269 -2.5055943
105 C C122 -12.7150793 -0.0424270 -4.9161368
106 C C123 -11.7256864 -1.9028570 -3.7075316
107 C C124 -12.3191699 0.1774188 -2.5370209
108 C C125 -12.7696915 0.7137665 -3.7494121
109 C C126 -12.1840115 -1.3281679 -4.9018314
110 H H84 -13.1833965 1.7324995 -3.7871526
111 H H85 -12.1343740 -1.8858332 -5.8483728
112 H H86 -13.0875695 0.3831943 -5.8602637
113 C C127 -9.9040238 -4.8977054 0.0645778
114 C C128 -7.9297275 -6.8876073 0.1538484
115 C C129 -9.5412330 -5.4712357 1.3072650
116 C C130 -9.4318160 -5.4708033 -1.1408952

117 C C131 -8.4251980 -6.4406853 -1.0787485
118 C C132 -8.5609580 -6.4693373 1.3332434
119 H H89 -7.9693859 -6.8144057 -2.0084664
120 H H90 -8.2414811 -6.8996305 2.2945907
121 C C133 -10.7705954 -3.6788853 2.4976096
122 C C134 -10.5549327 -5.0753729 4.9083290
123 C C135 -11.2216571 -3.0765736 3.6995776
124 C C136 -10.1235582 -4.9403916 2.5290296
125 C C137 -10.0450170 -5.6362685 3.7415307
126 C C138 -11.1206924 -3.8045223 4.8939760
127 H H93 -9.5918778 -6.6380915 3.7793142
128 H H94 -11.4903042 -3.3841035 5.8405614
129 H H95 -10.5028048 -5.6384110 5.8525484
130 C C139 -11.8319131 -1.0294791 2.4339425
131 C C140 -12.5596814 0.2711896 4.7984167
132 C C141 -12.2236257 0.3328333 2.4004195
133 C C142 -11.7409556 -1.7182854 3.6701917
134 C C143 -12.1224851 -1.0487364 4.8418315
135 C C144 -12.6019214 0.9632633 3.5922759
136 H H98 -12.0795871 -1.5550513 5.8171306
137 H H99 -12.9476780 2.0075922 3.5830422
138 H H100 -12.8686249 0.7740218 5.7273821
139 C C145 -12.1366354 0.3071686 -0.0726228
140 C C146 -12.2172779 3.1091044 -0.1619325
141 C C147 -12.2263915 1.0443125 1.1328392
142 C C148 -12.3021165 0.9653099 -1.3153220
143 C C149 -12.3493139 2.3635012 -1.3413386
144 C C150 -12.2351202 2.4421287 1.0706769
145 H H103 -12.4407458 2.8914940 -2.3027232
146 H H104 -12.1917258 3.0299127 2.0004206
147 C C157 -11.8917857 4.5342783 -0.2107115
148 C C158 -10.7218507 7.0934125 -0.0944599
149 C C159 -12.1549507 5.3916315 0.8682182
150 C C160 -11.1524406 5.0335746 -1.2963474
151 C C161 -10.5841707 6.3006147 -1.2441306
152 C C162 -11.5656123 6.6524308 0.9326522
153 H H110 -12.8089107 5.0589708 1.6882265
154 H H111 -10.9716762 4.4017505 -2.1794103
155 H H112 -9.9766037 6.6658429 -2.0863427
156 H H113 -11.7398463 7.2950385 1.8086584
157 C C163 6.3256459 -3.8061329 -1.2028554
158 C C164 5.4533107 -4.9819658 1.2136457
159 C C165 5.4937900 -4.9448805 -1.2340223
160 C C166 6.7000312 -3.2429099 0.0367331
161 C C167 6.3084667 -3.8606260 1.2447299
162 C C168 5.0163733 -5.4985273 -0.0257888
163 C C169 5.1261927 -5.5362333 -2.4947880
164 C C170 4.5767561 -6.8427666 -4.9153095
165 C C171 4.2042990 -6.6127470 -2.5255377
166 C C172 5.6981097 -5.0535701 -3.6988372
167 C C173 5.4240157 -5.7311894 -4.8942702
168 C C174 3.9599170 -7.2703221 -3.7359961
169 H H117 5.8749365 -5.4048109 -5.8435660
170 H H118 3.2881282 -8.1415491 -3.7722771
171 C C175 6.7782621 -3.2105542 -2.4337487
172 C C176 7.7889188 -2.1109980 -4.8087140
173 C C177 7.4814396 -1.9803020 -2.4020932
174 C C178 6.5226739 -3.8545576 -3.6705420
175 C C179 7.0441281 -3.2932659 -4.8437644
176 C C180 7.9970333 -1.4552035 -3.5921250
177 H H122 6.8771432 -3.7718430 -5.8205209
178 H H123 8.5836941 -0.5239436 -3.5828887
179 C C181 4.0076583 -6.5237429 -0.0598127
180 C C182 1.6269929 -8.0039644 -0.1439394
181 C C183 3.4182010 -6.9719162 1.1469896
182 C C184 3.5189617 -6.9969597 -1.3016636
183 C C185 2.3350333 -7.7423558 -1.3249317
184 C C186 2.2145544 -7.6828413 1.0874227
185 H H127 1.9231480 -8.0879510 -2.2854266
186 H H128 1.6867054 -7.9407869 2.0184799
187 C C187 5.0143063 -5.5875128 2.4445929
188 C C188 4.2514955 -6.8712407 4.8197664
189 C C189 5.5629805 -5.1620790 3.6806301
190 C C190 4.0338188 -6.6105720 2.4138079
191 C C191 3.6787694 -7.2550192 3.6039664
192 C C192 5.1751617 -5.8226669 4.8538454
193 H H131 2.9515689 -8.0812199 3.5954433
194 H H132 5.5894867 -5.5284391 5.8299423

195 C C193 6.7748941 -3.3429219 2.5051882
196 C C194 7.8829629 -2.4529600 4.9233563
197 C C195 7.5446874 -2.1529194 2.5362932
198 C C196 6.4795063 -4.0318080 3.7084721
199 C C197 7.0574936 -3.5808161 4.9026122
200 C C198 8.1111006 -1.7354730 3.7454993
201 H H136 6.8775200 -4.1093424 5.8509184
202 H H137 8.7550455 -0.8434477 3.7816523
203 C C199 7.3960153 -1.9842974 0.0715969
204 C C200 8.1369017 0.7190911 0.1590677
205 C C201 7.6553657 -1.2895162 -1.1344827
206 C C202 7.7134135 -1.3834112 1.3138373
207 C C203 8.0899809 -0.0360272 1.3389224
208 C C204 7.9944190 0.0665595 -1.0732205
209 H H141 8.3051513 0.4557652 2.2999108
210 H H142 8.0899608 0.6476509 -2.0034116
211 C C205 0.2319522 -8.4414318 -0.1897527
212 C C206 -2.5682704 -8.7175208 -0.0695754
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217 H H143 -0.1182664 -7.5955765 -2.1653275
218 H H144 0.2410566 -9.4854458 1.7165462
219 H H145 -2.2286180 -9.6856536 1.8400942
220 H H146 -2.5749924 -7.8739438 -2.0681613
221 C C211 8.1589073 2.1808648 0.2067506
222 C C212 7.6263480 4.9437698 0.0884583
223 C C213 7.5638377 2.8425397 1.2942077
224 C C214 8.6131772 2.9501644 -0.8751145
225 C C215 8.3382218 4.3143851 -0.9404400
226 C C216 7.3106909 4.2079012 1.2408586
227 H H148 7.2438680 2.2730416 2.1801966
228 H H149 9.1666681 2.4713565 -1.6968887
229 H H150 8.6560267 4.8961643 -1.8186622
230 H H151 6.8106794 4.7076312 2.0846991
231 C C55 4.3265101 -7.5539411 -6.1760541
232 C C56 3.8509005 -8.9166974 -8.5870826
233 C C57 3.4260594 -7.0270176 -7.1185881
234 C C58 4.9887216 -8.7654694 -6.4444497
235 C C59 4.7455398 -9.4350209 -7.6469130
236 C C60 3.1965690 -7.7127256 -8.3151431
237 H H5 5.2661678 -10.3818044 -7.8565536
238 H H3 2.4919197 -7.2975912 -9.0516816
239 C C61 8.3447770 -1.5540731 -6.0492274
240 C C62 9.4079269 -0.4891063 -8.4220660
241 C C63 7.5207865 -0.8287212 -6.9284374
242 C C64 9.7027180 -1.7432043 -6.3608947
243 C C65 10.2218299 -1.2091511 -7.5440591
244 C C66 8.0595283 -0.3026823 -8.1058472
245 H H11 11.2851338 -1.3584031 -7.7858045
246 H H15 7.4139976 0.2661575 -8.7922458
247 C C67 3.8775783 -7.5629492 6.0605375
248 C C68 3.1667159 -8.8862109 8.4353540
249 C C69 2.9592012 -6.9750017 6.9480781
250 C C70 4.4389241 -8.8160542 6.3653210
251 C C71 4.0789087 -9.4656757 7.5492277
252 C C72 2.6124998 -7.6414137 8.1272499
253 H H34 4.5205589 -10.4452035 7.7877164
254 H H38 1.8946390 -7.1780129 8.8210359
255 C C73 8.5014656 -2.0163639 6.1822027
256 C C74 9.6869141 -1.1818887 8.5895294
257 C C75 7.7452633 -1.3077353 7.1327228
258 C C76 9.8533994 -2.3051840 6.4403001
259 C C77 10.4336554 -1.8850019 7.6407066
260 C C78 8.3444518 -0.8968561 8.3269442
261 H H42 11.4922389 -2.1110374 7.8401981
262 H H43 7.7511640 -0.3414466 9.0691598
263 C C79 10.3073981 -0.7561180 9.8653989
264 H H44 11.4017504 -0.5691118 9.7359657
265 H H45 10.1781958 -1.5569074 10.6367878
266 H H46 9.8315074 0.1792980 10.2498331
267 C C80 10.6685701 -3.0612496 5.4594782
268 H H41 11.7582294 -2.9883125 5.6960905
269 H H47 10.5018640 -2.6687731 4.4246644
270 H H48 10.3764009 -4.1417924 5.4719795
271 C C81 6.3217815 -0.9798689 6.8786708
272 H H40 6.2469065 -0.1647349 6.1151974

273 H H49 5.8119763 -0.6360318 7.8117978

274 H H50 5.7775575 -1.8748927 6.4846505

275 C C82 5.4185712 -9.4508065 5.4513407

276 H H27 6.4045112 -8.9256774 5.5230454

277 H H51 5.0663917 -9.3839451 4.3911160

278 H H52 5.5736291 -10.5273952 5.7074511

279 C C83 2.7851720 -9.5928563 9.6801123

280 H H39 3.6599293 -10.1398123 10.1107816

281 H H53 1.9792694 -10.3387381 9.4629876

282 H H54 2.4021977 -8.8774474 10.4485343

283 C C84 2.3437599 -5.6609010 6.6438204

284 H H23 3.1182392 -4.9390589 6.2809062

285 H H55 1.8482872 -5.2266342 7.5464384

286 H H56 1.5734045 -5.7761355 5.8399250

287 C C85 3.5914199 -9.6446924 -9.8507913

288 H H4 4.5169142 -10.1569482 -10.2126400

289 H H57 3.2362537 -8.9491962 -10.6504016

290 H H58 2.8028366 -10.4222397 -9.6870360

291 C C86 5.9516490 -9.3350592 -5.4715296

292 H H6 6.9010693 -8.7424682 -5.4813531

293 H H59 6.1969772 -10.3970382 -5.7180331

294 H H60 5.5302740 -9.2981594 -4.4353377

295 C C87 2.7062886 -5.7578192 -6.8550979

296 H H2 3.4057859 -4.9875975 -6.4431529

297 H H61 1.8949421 -5.9271798 -6.1029746

298 H H62 2.2423807 -5.3538222 -7.7879803

299 C C88 10.5890554 -2.5121594 -5.4546470

300 H H7 11.6650835 -2.3594829 -5.7141681

301 H H63 10.3594006 -3.6049118 -5.5313676

302 H H64 10.4308701 -2.1984064 -4.3920675

303 C C89 6.0890736 -0.6054191 -6.6142770

304 H H1 5.9910770 0.1342782 -5.7798536

305 H H65 5.6061940 -1.5612195 -6.2885801

306 H H66 5.5354734 -0.2112551 -7.5012410

307 C C90 9.9623775 0.0599138 -9.6812164

308 H H19 11.0619755 0.2393904 -9.5919035

309 H H67 9.4664890 1.0257641 -9.9477365

310 H H68 9.7923912 -0.6631386 -10.5188403

Cartesian Coordinates (Angstroms) of Transition Structure for the Rotation of the HBC Core for the Cyclic Trimer **2** without the Mesityl Substituents Optimized at the AM1 Level (3128.9857 kJ/mol)

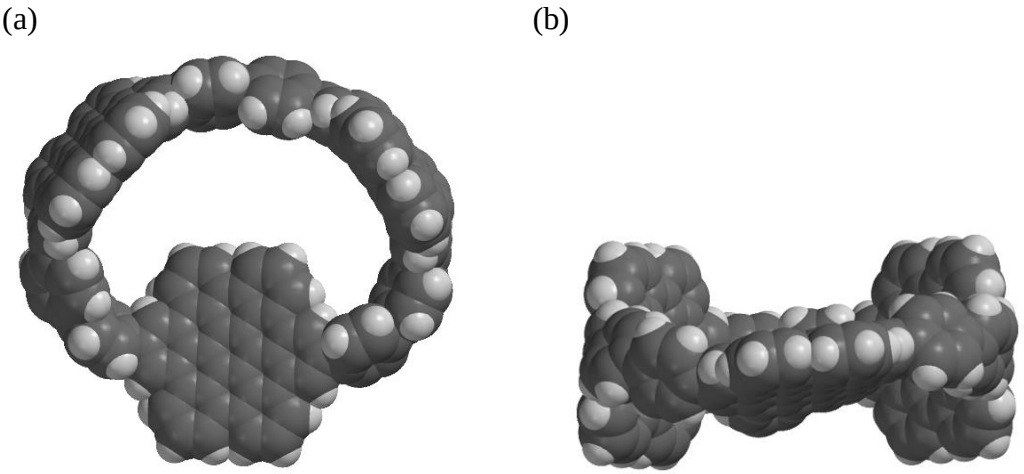

Figure S-101. Optimized structure of the transition for the rotation of the HBC core for cyclic trimer **2** without the mesityl substituents optimized at the AM1 level: (a) top view of the molecular structure; (b) side view of the molecular structure.

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
1 C C1	1.8028214	8.7537187	-1.3369925
2 C C4	0.1096778	6.4898476	-1.4354354
3 C C2	0.4117904	8.9009565	-1.1256730
4 C C6	2.3392498	7.4806067	-1.6280976
5 C C5	1.4869081	6.3550259	-1.7158114
6 C C3	-0.4276522	7.7645367	-1.1389676
7 C C7	-0.1539840	10.2095374	-0.9108755
8 C C8	-1.2638758	12.7680091	-0.6582560
9 C C9	0.6890314	11.3508098	-0.9225230
10 C C10	-1.5526373	10.3590649	-0.7181003
11 C C11	-2.0876700	11.6501631	-0.6055673
12 C C12	0.1105224	12.6225130	-0.8076098
13 H H8	-3.1691938	11.8041798	-0.4802037
14 H H9	0.7295103	13.5306389	-0.8410873
15 H H10	-1.7017371	13.7745722	-0.5784080
16 C C13	2.6780938	9.8966948	-1.2532156
17 C C14	4.3683807	12.1247586	-1.0999942
18 C C15	2.1285038	11.1884044	-1.0509191
19 C C16	4.0836923	9.7308486	-1.3678839
20 C C17	4.9101976	10.8608356	-1.3017143
21 C C18	2.9940973	12.2883529	-0.9686723
22 H H12	5.9998875	10.7667307	-1.4173442
23 H H13	2.6051212	13.3021166	-0.7952540
24 H H14	5.0310636	13.0016094	-1.0439725
25 C C19	-1.8308123	7.9024559	-0.8382716
26 C C20	-4.5596545	8.1504540	-0.1967327
27 C C21	-2.6400222	6.7428049	-0.7313466
28 C C22	-2.4028197	9.1825411	-0.6320134
29 C C23	-3.7742575	9.2897982	-0.3347870
30 C C24	-3.9770611	6.8852213	-0.3620441
31 H H16	-4.2471252	10.2719354	-0.1907036
32 H H17	-4.6211148	6.0044296	-0.2147313
33 C C25	-0.7377103	5.3222244	-1.4354190
34 C C26	-2.3550368	3.0341774	-1.3066349
35 C C27	-2.0913917	5.4324905	-1.0345714
36 C C28	-0.2178105	4.0591764	-1.8143877
37 C C29	-1.0369372	2.9248551	-1.7318928
38 C C30	-2.8812076	4.2760640	-0.9690337
39 H H20	-0.6458103	1.9292723	-1.9880516
40 H H21	-3.9325372	4.3228634	-0.6505917

41	H	H22	-2.9861160	2.1351846	-1.2382394	80	C	C104	-1.7539272	-8.5702256	0.6814023
42	C	C31	2.0164107	5.0746144	-2.1157251	81	C	C105	-3.5908916	-7.4682715	1.8171140
43	C	C32	3.0044248	2.6747959	-3.1752909	82	C	C106	-3.9736315	-8.5669221	-0.2955446
44	C	C33	3.3948894	4.9398230	-2.4066899	83	C	C107	-2.6341428	-8.9506005	-0.3384256
45	C	C34	1.1603309	3.9553076	-2.2546030	84	C	C108	-2.2614048	-7.8698780	1.7866925
46	C	C35	1.6671396	2.7707222	-2.8079408	85	H	H72	-3.9485235	-6.8679715	2.6677815
47	C	C36	3.8679420	3.7441892	-2.9627159	86	H	H73	-4.6494168	-8.8781289	-1.1063265
48	H	H24	1.0116376	1.9032172	-2.9729800	87	H	H74	-2.2609076	-9.5418973	-1.1880790
49	H	H25	4.9241994	3.6393745	-3.2510871	88	H	H75	-1.5881280	-7.6029053	2.6158523
50	H	H26	3.3833709	1.7463135	-3.6284031	89	C	C109	-10.0866287	-2.6171990	-0.6908654
51	C	C37	3.7622958	7.3179929	-1.7881753	90	C	C110	-9.2865631	-3.6813590	1.8011606
52	C	C38	6.5435334	6.8920279	-1.7343798	91	C	C111	-9.3397771	-3.8129973	-0.6431491
53	C	C39	4.2889513	6.0423386	-2.1058954	92	C	C112	-10.3673012	-1.9174601	0.5029648
54	C	C40	4.6440549	8.4041982	-1.5664137	93	C	C113	-10.0016209	-2.4666962	1.7513062
55	C	C41	6.0296368	8.1693196	-1.5177261	94	C	C114	-8.9080142	-4.3225397	0.6009183
56	C	C42	5.6678247	5.8449543	-2.0604624	95	C	C115	-9.0033893	-4.5021726	-1.8627447
57	H	H28	6.7299779	8.9839722	-1.2823386	96	C	C116	-8.4458377	-5.9254396	-4.2018306
58	H	H29	6.0910748	4.8435183	-2.2393801	97	C	C117	-8.1157051	-5.6075037	-1.8228698
59	C	C43	-5.9956132	8.1186444	0.1048156	98	C	C118	-9.5614366	-4.0735686	-3.0943202
60	C	C44	-8.5838727	7.0642668	0.2566826	99	C	C119	-9.2759573	-4.8101447	-4.2528997
61	C	C45	-6.9444900	8.4480709	-0.8715415	100	C	C120	-7.8611622	-6.3187223	-3.0022498
62	C	C46	-6.4180774	7.4511314	1.2665203	101	H	H79	-9.7008679	-4.5162217	-5.2237671
63	C	C47	-7.7080506	6.9433919	1.3502806	102	H	H80	-7.2065660	-7.2028203	-2.9879966
64	C	C48	-8.2315697	7.9138878	-0.8001626	103	H	H81	-8.2455391	-6.4982576	-5.1200615
65	H	H18	-6.6517420	9.0620497	-1.7361319	104	C	C121	-10.5538813	-2.1052826	-1.9536656
66	H	H31	-5.7030681	7.2789938	2.0852766	105	C	C122	-11.6779386	-1.2170239	-4.3513905
67	H	H32	-8.0217929	6.3727749	2.2375848	106	C	C123	-10.3755221	-2.8685003	-3.1353320
68	H	H33	-8.9508916	8.1071258	-1.6098293	107	C	C124	-11.2058489	-0.8466210	-2.0056928
69	C	C49	7.9339425	6.4883004	-1.5120861	108	C	C125	-11.7838722	-0.4279072	-3.2100184
70	C	C50	10.0508096	4.8444809	-0.7161424	109	C	C126	-10.9675724	-2.4130952	-4.3223315
71	C	C51	8.5251276	5.6035950	-2.4323282	110	H	H84	-12.3373514	0.5217485	-3.2592853
72	C	C52	8.5727256	6.7114793	-0.2856008	111	H	H85	-10.8834951	-2.9964218	-5.2508468
73	C	C53	9.6479636	5.9096124	0.0999830	112	H	H86	-12.1525384	-0.8877003	-5.2882381
74	C	C54	9.5728328	4.7833604	-2.0360791	113	C	C127	-8.0008588	-5.4384794	0.6431198
75	H	H30	8.1103985	5.5178941	-3.4479421	114	C	C128	-5.7852686	-7.1584550	0.7163476
76	H	H35	8.1874732	7.4821413	0.3986484	115	C	C129	-7.5240347	-5.9162375	1.8878975
77	H	H36	10.1188923	6.0566946	1.0829166	116	C	C130	-7.4955923	-5.9830705	-0.5624494
78	H	H37	9.9849785	4.0364239	-2.7312527	117	C	C131	-6.3693242	-6.8130244	-0.5094672
79	C	C103	-4.4581852	-7.7732265	0.7541641	118	C	C132	-6.4242225	-6.7803068	1.9055630

119	H	H89	-5.8982071	-7.1556957	-1.4434672	158	C	C164	8.0200395	-5.6351838	1.9698443
120	H	H90	-6.0228066	-7.1363709	2.8666892	159	C	C165	8.2285697	-5.8571743	-0.4599276
121	C	C133	-8.9374506	-4.2613268	3.0727514	160	C	C166	9.5693503	-4.2040454	0.7382758
122	C	C134	-8.4521915	-5.5305250	5.5138463	161	C	C167	9.0083456	-4.6289052	1.9628184
123	C	C135	-9.4190680	-3.6796327	4.2731666	162	C	C168	7.5984524	-6.2145481	0.7524264
124	C	C136	-8.1278945	-5.4247472	3.1158953	163	C	C169	7.8579161	-6.5134346	-1.6878640
125	C	C137	-7.9148723	-6.0609334	4.3449813	164	C	C170	7.2531806	-7.9311226	-4.0189677
126	C	C138	-9.1802769	-4.3454287	5.4841006	165	C	C171	6.7784716	-7.4335541	-1.6960550
127	H	H93	-7.3326941	-6.9931028	4.3956097	166	C	C172	8.5809529	-6.2467092	-2.8787071
128	H	H94	-9.5679260	-3.9432035	6.4314098	167	C	C173	8.2694934	-6.9813919	-4.0318616
129	H	H95	-8.2925665	-6.0484792	6.4717867	168	C	C174	6.5034901	-8.1498914	-2.8675678
130	C	C139	-10.3401093	-1.7781088	2.9706839	169	H	H117	8.8242834	-6.8200232	-4.9675910
131	C	C140	-11.1260930	-0.4855717	5.3202513	170	H	H118	5.7012701	-8.9025657	-2.8845553
132	C	C141	-10.9001268	-0.4769493	2.9094375	171	H	H119	7.0360287	-8.5097226	-4.9296723
133	C	C142	-10.1104327	-2.4008929	4.2235334	172	C	C175	9.8488891	-4.4654069	-1.7029825
134	C	C143	-10.5247971	-1.7383558	5.3881163	173	C	C176	11.2238083	-3.8264835	-4.0505568
135	C	C144	-11.3042983	0.1489623	4.0947413	174	C	C177	10.7314953	-3.3554281	-1.7269825
136	H	H98	-10.3774176	-2.1967673	6.3768773	175	C	C178	9.5938765	-5.2026163	-2.8871078
137	H	H99	-11.7768260	1.1420749	4.0640552	176	C	C179	10.3079777	-4.8737430	-4.0486149
138	H	H100	-11.4571665	0.0109248	6.2449765	177	C	C180	11.4272121	-3.0619082	-2.9059770
139	C	C145	-10.9262215	-0.5935101	0.4384924	178	H	H122	10.1561633	-5.4384871	-4.9799669
140	C	C146	-11.2909189	2.1780555	0.2492197	179	H	H123	12.1486770	-2.2317339	-2.9319451
141	C	C147	-11.0406746	0.1783777	1.6197702	180	H	H124	11.7863418	-3.5960014	-4.9680502
142	C	C148	-11.2316076	-0.0116242	-0.8155481	181	C	C181	6.4631597	-7.0985475	0.7352487
143	C	C149	-11.4308604	1.3716272	-0.8898808	182	C	C182	3.9280841	-8.2987990	0.6268285
144	C	C150	-11.1865899	1.5649162	1.5063206	183	C	C183	5.7625534	-7.3691838	1.9354452
145	H	H103	-11.6360422	1.8440031	-1.8625506	184	C	C184	5.9786750	-7.6079535	-0.4942028
146	H	H104	-11.1513130	2.1926262	2.4100658	185	C	C185	4.7104638	-8.1997777	-0.5310134
147	C	C157	-10.9932460	3.6048203	0.1243326	186	C	C186	4.4914408	-7.9486455	1.8615050
148	C	C158	-9.6551219	6.0758045	0.1395072	187	H	H127	4.2986223	-8.5584849	-1.4865755
149	C	C159	-11.1698072	4.5027874	1.1882572	188	H	H128	3.8957798	-8.0747383	2.7786759
150	C	C160	-10.3219956	4.0583377	-1.0250063	189	C	C187	7.4346852	-6.0610513	3.2156547
151	C	C161	-9.6709360	5.2843303	-1.0222721	190	C	C188	6.4058425	-7.0326033	5.6262135
152	C	C162	-10.4930742	5.7222638	1.2038781	191	C	C189	7.9532132	-5.5798513	4.4449612
153	H	H110	-11.8046693	4.2252369	2.0427607	192	C	C190	6.3462951	-6.9694259	3.2053383
154	H	H111	-10.2485471	3.4150927	-1.9150944	193	C	C191	5.8565087	-7.4607917	4.4218831
155	H	H112	-9.1024701	5.6077772	-1.9078759	194	C	C192	7.4315390	-6.0930070	5.6412126
156	H	H113	-10.5794810	6.3869373	2.0762109	195	H	H131	5.0417721	-8.1998462	4.4358879
157	C	C163	9.2148395	-4.8483335	-0.4671877	196	H	H132	7.8240432	-5.7605509	6.6132562

197	H	H133	6.0211230	-7.4351768	6.5755396	216	C	C206	-0.3085185	-8.7656924	0.5831111
198	C	C193	9.4349895	-4.0270101	3.2005063	217	C	C207	1.7602607	-8.2699092	-0.5788108
199	C	C194	10.4260194	-2.9759629	5.5931637	218	C	C208	1.8272581	-9.1863694	1.6511885
200	C	C195	10.3207792	-2.9203441	3.1750125	219	C	C209	0.4363549	-9.2411671	1.6707051
201	C	C196	8.9762622	-4.5462885	4.4374438	220	C	C210	0.3710856	-8.3419063	-0.5677748
202	C	C197	9.5013752	-4.0149378	5.6245321	221	H	H143	2.2704343	-7.8748335	-1.4706122
203	C	C198	10.8242686	-2.4194701	4.3814918	222	H	H144	2.3937905	-9.5610549	2.5170249
204	H	H136	9.1909726	-4.4111162	6.6023694	223	H	H145	-0.0845417	-9.6367037	2.5557163
205	H	H137	11.5485369	-1.5911955	4.3792881	224	H	H146	-0.2027381	-8.0201631	-1.4502687
206	H	H138	10.8396004	-2.5853784	6.5353789	225	C	C211	11.4290658	1.0285536	0.4134983
207	C	C199	10.4180040	-3.0427074	0.7055727	226	C	C212	10.8025630	3.7049826	-0.1934389
208	C	C200	11.4126192	-0.4270502	0.5587103	227	C	C213	10.6407459	1.7920298	1.2927137
209	C	C201	10.8827469	-2.5396157	-0.5333368	228	C	C214	12.0575258	1.6813955	-0.6561780
210	C	C202	10.6732211	-2.3227066	1.8978776	229	C	C215	11.7478176	3.0076440	-0.9577412
211	C	C203	11.1550251	-1.0134531	1.8062437	230	C	C216	10.3115787	3.1027098	0.9784642
212	C	C204	11.3702049	-1.2285988	-0.5913404	231	H	H148	10.2039615	1.3298397	2.1912122
213	H	H141	11.2921805	-0.4147025	2.7198791	232	H	H149	12.7692973	1.1327977	-1.2910400
214	H	H142	11.6466142	-0.7876491	-1.5614617	233	H	H150	12.2101161	3.4927375	-1.8302928
215	C	C205	2.5067068	-8.6372275	0.5527270	234	H	H151	9.6224881	3.6656696	1.6275423

Cartesian Coordinates (Angstroms) of Transition Structure for the Rotation of the HBC Core for the Cyclic Trimer **2** with Four Mesityl Substituents Optimized at the AM1 Level (3237.5449 kJ/mol)

(a) (b)

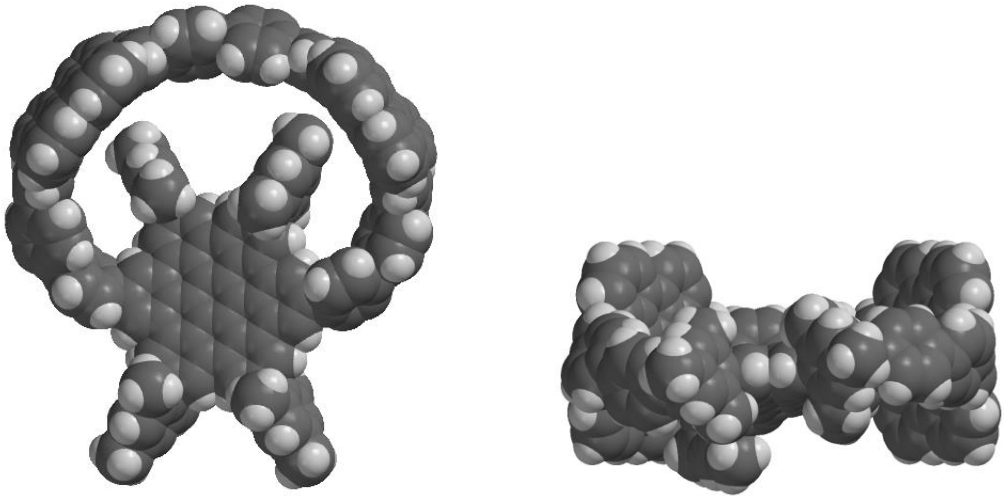

Figure S-102. Optimized structure of the transition for the rotation of the HBC core for cyclic trimer **2** with four mesityl substituents optimized at the AM1 level: (a) top view of the molecular structure; (b) side view of the molecular structure.

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
1 C C1	1.6206953	6.8782297	-0.9444663
2 C C4	-0.0524198	4.5986760	-0.9694626
3 C C2	0.2323216	7.0170759	-0.7108988
4 C C6	2.1621292	5.6065049	-1.2308628
5 C C5	1.3189865	4.4719881	-1.2796501
6 C C3	-0.5972175	5.8737577	-0.6901149
7 C C7	-0.3401841	8.3235415	-0.5050620
8 C C8	-1.4660450	10.8849241	-0.2413524
9 C C9	0.4945932	9.4703171	-0.5318834
10 C C10	-1.7378772	8.4661324	-0.3024396
11 C C11	-2.2804469	9.7524297	-0.1846782
12 C C12	-0.0869002	10.7383736	-0.4067744
13 H H8	-3.3618456	9.9012554	-0.0473489
14 H H9	0.5264826	11.6510992	-0.4424540
15 C C13	2.4883960	8.0279423	-0.8872090
16 C C14	4.1710446	10.2769403	-0.7803375
17 C C15	1.9338923	9.3172801	-0.6856370
18 C C16	3.8927849	7.8721533	-1.0250626
19 C C17	4.7137337	9.0058123	-0.9787222
20 C C18	2.7900757	10.4248251	-0.6308412
21 H H12	5.8030217	8.9181578	-1.1080572
22 H H13	2.3970248	11.4391297	-0.4656397
23 C C19	-1.9991471	6.0052285	-0.3814259
24 C C20	-4.7408842	6.2451550	0.2011012
25 C C21	-2.7971665	4.8406406	-0.2451955
26 C C22	-2.5826515	7.2852323	-0.2092421
27 C C23	-3.9604630	7.3875120	0.0585581
28 C C24	-4.1453294	4.9809337	0.0805812
29 H H16	-4.4444952	8.3683973	0.1706790
30 H H17	-4.7886852	4.0985551	0.2226237
31 C C25	-0.8830215	3.4211603	-0.9133399
32 C C26	-2.4494338	1.1032002	-0.6070370
33 C C27	-2.2269398	3.5252485	-0.4812225
34 C C28	-0.3545646	2.1523199	-1.2572809
35 C C29	-1.1434856	1.0073990	-1.0913421
36 C C30	-2.9855661	2.3594516	-0.3141417

37	H	H20	-0.7428375	0.0084239	-1.3212460	76	C	C104	-2.0624136	-10.4552589	1.1584505
38	H	H21	-4.0206742	2.4007973	0.0564257	77	C	C105	-3.9123776	-9.3582740	2.2777265
39	C	C31	1.8505869	3.1897312	-1.6685466	78	C	C106	-4.2805271	-10.4863450	0.1781140
40	C	C32	2.8343250	0.7730353	-2.7189916	79	C	C107	-2.9374377	-10.8576231	0.1424132
41	C	C33	3.2184112	3.0654177	-2.0073970	80	C	C108	-2.5788784	-9.7473785	2.2546282
42	C	C34	1.0078508	2.0551936	-1.7480753	81	H	H72	-4.2776442	-8.7517936	3.1206995
43	C	C35	1.5077745	0.8643503	-2.2909058	82	H	H73	-4.9518198	-10.8143403	-0.6297740
44	C	C36	3.6870082	1.8690227	-2.5626775	83	H	H74	-2.5569508	-11.4559465	-0.6990766
45	H	H24	0.8600054	-0.0180811	-2.4045411	84	H	H75	-1.9098502	-9.4639300	3.0817511
46	H	H25	4.7314177	1.7750875	-2.8965657	85	C	C109	-10.3700995	-4.5364051	-0.3310430
47	C	C37	3.5821038	5.4541077	-1.4234955	86	C	C110	-9.6035194	-5.5787790	2.1805504
48	C	C38	6.3657359	5.0470851	-1.4231994	87	C	C111	-9.6363950	-5.7391279	-0.2622872
49	C	C39	4.1103598	4.1803223	-1.7462535	88	C	C112	-10.6556216	-3.8202883	0.8519490
50	C	C40	4.4601416	6.5481900	-1.2267543	89	C	C113	-10.3082780	-4.3591700	2.1099697
51	C	C41	5.8481477	6.3223114	-1.2030528	90	C	C114	-9.2198213	-6.2373175	0.9915108
52	C	C42	5.4910523	3.9935880	-1.7324624	91	C	C115	-9.2959617	-6.4460181	-1.4705297
53	H	H28	6.5477927	7.1424956	-0.9850306	92	C	C116	-8.7365424	-7.9068183	-3.7856219
54	H	H29	5.9168224	2.9944343	-1.9191069	93	C	C117	-8.4185017	-7.5584426	-1.4095215
55	C	C43	-6.1850197	6.2087219	0.4588122	94	C	C118	-9.8392632	-6.0274108	-2.7120212
56	C	C44	-8.7758382	5.1535087	0.5595462	95	C	C119	-9.5541876	-6.7835707	-3.8580706
57	C	C45	-7.1068136	6.5178970	-0.5492381	96	C	C120	-8.1631433	-8.2887287	-2.5768665
58	C	C46	-6.6386037	5.5623247	1.6205870	97	H	H79	-9.9697798	-6.4990424	-4.8357496
59	C	C47	-7.9288840	5.0517295	1.6772802	98	H	H80	-7.5170085	-9.1785730	-2.5454983
60	C	C48	-8.3950490	5.9839157	-0.5027245	99	H	H81	-8.5366474	-8.4949065	-4.6942364
61	H	H18	-6.7911712	7.1164255	-1.4165211	100	C	C121	-10.8166221	-4.0329273	-1.6046443
62	H	H31	-5.9464970	5.4071757	2.4619060	101	C	C122	-11.8989388	-3.1547093	-4.0249852
63	H	H32	-8.2650946	4.4948830	2.5650408	102	C	C123	-10.6362271	-4.8119936	-2.7755969
64	H	H33	-9.0923685	6.1621262	-1.3346349	103	C	C124	-11.4487602	-2.7653426	-1.6780450
65	C	C49	7.7589611	4.6455357	-1.2149221	104	C	C125	-12.0060267	-2.3512898	-2.8936687
66	C	C50	9.8618556	2.9865389	-0.4175022	105	C	C126	-11.2074864	-4.3610368	-3.9744407
67	C	C51	8.3364585	3.7485217	-2.1322471	106	H	H84	-12.5437114	-1.3936346	-2.9598335
68	C	C52	8.4111723	4.8768517	0.0030102	107	H	H85	-11.1211251	-4.9557008	-4.8955240
69	C	C53	9.4791922	4.0657611	0.3897226	108	H	H86	-12.3571934	-2.8285049	-4.9710198
70	C	C54	9.3771870	2.9202155	-1.7348882	109	C	C127	-8.3189582	-7.3572875	1.0546568
71	H	H30	7.9145467	3.6583883	-3.1445160	110	C	C128	-6.1043019	-9.0757987	1.1644144
72	H	H35	8.0403963	5.6597091	0.6812433	111	C	C129	-7.8508245	-7.8191865	2.3086263
73	H	H36	9.9589922	4.2173393	1.3675837	112	C	C130	-7.8078610	-7.9194790	-0.1402882
74	H	H37	9.7764983	2.1622941	-2.4256479	113	C	C131	-6.6826162	-8.7492063	-0.0694291
75	C	C103	-4.7743144	-9.6832452	1.2164045	114	C	C132	-6.7508415	-8.6826457	2.3446310

115	H	H89	-6.2072322	-9.1055698	-0.9961357	154	C	C164	7.7223722	-7.4673408	2.3819509
116	H	H90	-6.3550708	-9.0253774	3.3128962	155	C	C165	7.9207338	-7.7189301	-0.0456967
117	C	C133	-9.2677678	-6.1450069	3.4618358	156	C	C166	9.2733587	-6.0576014	1.1277696
118	C	C134	-8.8067212	-7.3856064	5.9218924	157	C	C167	8.7152072	-6.4657157	2.3593297
119	C	C135	-9.7570855	-5.5466985	4.6509656	158	C	C168	7.2937423	-8.0593917	1.1731019
120	C	C136	-8.4626123	-7.3105263	3.5256977	159	C	C169	7.5435559	-8.3890698	-1.2641228
121	C	C137	-8.2614506	-7.9321002	4.7641535	160	C	C170	6.9272425	-9.8345609	-3.5751292
122	C	C138	-9.5305532	-6.1985571	5.8717456	161	C	C171	6.4616416	-9.3062869	-1.2571156
123	H	H93	-7.6826385	-8.8653547	4.8306202	162	C	C172	8.2634527	-8.1395977	-2.4605974
124	H	H94	-9.9245192	-5.7834561	6.8108825	163	C	C173	7.9462538	-8.8880477	-3.6032752
125	H	H95	-8.6569468	-7.8923810	6.8873484	164	C	C174	6.1807532	-10.0365356	-2.4186628
126	C	C139	-10.6537414	-3.6545093	3.3181262	165	H	H117	8.4990348	-8.7408568	-4.5425034
127	C	C140	-11.4594521	-2.3329886	5.6444711	166	H	H118	5.3766124	-10.7873372	-2.4235528
128	C	C141	-11.2028510	-2.3498306	3.2367086	167	H	H119	6.7057694	-10.4243761	-4.4775803
129	C	C142	-10.4421470	-4.2655159	4.5799772	168	C	C175	9.5423912	-6.3488657	-1.3111458
130	C	C143	-10.8671442	-3.5888249	5.7325195	169	C	C176	10.9107360	-5.7437502	-3.6714885
131	C	C144	-11.6173223	-1.7092781	4.4106637	170	C	C177	10.4301713	-5.2434726	-1.3515037
132	H	H98	-10.7357575	-4.0383870	6.7275576	171	C	C178	9.2798929	-7.0991774	-2.4853997
133	H	H99	-12.0818069	-0.7130056	4.3641141	172	C	C179	9.9906529	-6.7871518	-3.6534780
134	H	H100	-11.7993840	-1.8253617	6.5599485	173	C	C180	11.1221859	-4.9668458	-2.5367771
135	C	C145	-11.1977837	-2.4905953	0.7669876	174	H	H122	9.8331557	-7.3625055	-4.5773409
136	C	C146	-11.5207934	0.2831650	0.5452768	175	H	H123	11.8471156	-4.1401645	-2.5755974
137	C	C147	-11.3199856	-1.7057912	1.9389425	176	H	H124	11.4703928	-5.5263563	-4.5938935
138	C	C148	-11.4766098	-1.9173414	-0.4971824	177	C	C181	6.1558554	-8.9402695	1.1708988
139	C	C149	-11.6525398	-0.5320602	-0.5884495	178	C	C182	3.6197609	-10.1413449	1.0873237
140	C	C150	-11.4487817	-0.3188354	1.8100161	179	C	C183	5.4591079	-9.1947014	2.3768965
141	H	H103	-11.8325879	-0.0660379	-1.5691353	180	C	C184	5.6660496	-9.4643383	-0.0502326
142	H	H104	-11.4223960	0.3172246	2.7082026	181	C	C185	4.3975825	-10.0562884	-0.0746822
143	C	C157	-11.2069113	1.7057188	0.4120929	182	C	C186	4.1874219	-9.7743344	2.3150496
144	C	C158	-9.8453112	4.1645299	0.4308180	183	H	H127	3.9820674	-10.4270947	-1.0240122
145	C	C159	-11.3967355	2.6163513	1.4627763	184	H	H128	3.5948378	-9.8881261	3.2358061
146	C	C160	-10.5025508	2.1388806	-0.7252099	185	C	C187	7.1401141	-7.8761923	3.6349022
147	C	C161	-9.8389255	3.3582561	-0.7205527	186	C	C188	6.1155829	-8.8136177	6.0609104
148	C	C162	-10.7114624	3.8309727	1.4790199	187	C	C189	7.6652751	-7.3826039	4.8564305
149	H	H110	-12.0519980	2.3535221	2.3064892	188	C	C190	6.0482569	-8.7804614	3.6396045
150	H	H111	-10.4128241	1.4838385	-1.6051229	189	C	C191	5.5606571	-9.2546268	4.8638413
151	H	H112	-9.2441003	3.6643716	-1.5949536	190	C	C192	7.1453637	-7.8784312	6.0607258
152	H	H113	-10.8129156	4.5070006	2.3408445	191	H	H131	4.7431463	-9.9902711	4.8899826
153	C	C163	8.9111365	-6.7142905	-0.0686546	192	H	H132	7.5425111	-7.5355792	7.0272358

193	H	H133	5.7321990	-9.2025167	7.0164499	232	C	C56	-3.1858858	14.7880354	0.1013999
194	C	C193	9.1503298	-5.8522084	3.5883214	233	C	C57	-2.6849230	12.8188640	-1.2324162
195	C	C194	10.1577346	-4.7804155	5.9649286	234	C	C58	-1.9956654	12.9179198	1.0986480
196	C	C195	10.0428560	-4.7514330	3.5467597	235	C	C59	-2.5610126	14.1921734	1.2001761
197	C	C196	8.6937688	-6.3547429	4.8329063	236	C	C60	-3.2439848	14.0943355	-1.1099597
198	C	C197	9.2269133	-5.8132322	6.0117723	237	H	H5	-2.5141741	14.7324929	2.1579145
199	C	C198	10.5544672	-4.2402365	4.7454406	238	H	H3	-3.7360224	14.5568622	-1.9791088
200	H	H136	8.9182821	-6.1965036	6.9952665	239	C	C61	5.0484122	11.4540471	-0.7284748
201	H	H137	11.2840491	-3.4167503	4.7310706	240	C	C62	6.7270525	13.7051934	-0.6272592
202	H	H138	10.5776050	-4.3817626	6.9009331	241	C	C63	5.1809847	12.2863296	-1.8539601
203	C	C199	10.1286787	-4.9016906	1.0784905	242	C	C64	5.7580548	11.7528436	0.4484166
204	C	C200	11.1460828	-2.2960450	0.8994896	243	C	C65	6.5900748	12.8751071	0.4886301
205	C	C201	10.5917743	-4.4154002	-0.1676874	244	C	C66	6.0186380	13.4040434	-1.7931377
206	C	C202	10.3943055	-4.1705935	2.2616774	245	H	H10	7.1432804	13.1086564	1.4110051
207	C	C203	10.8873100	-2.8667431	2.1539590	246	H	H11	6.1201311	14.0544822	-2.6752485
208	C	C204	11.0900876	-3.1091738	-0.2417853	247	C	C67	-3.2535387	-0.1092074	-0.4065882
209	H	H141	11.0335963	-2.2594796	3.0605168	248	C	C68	-4.7852666	-2.4326057	-0.0197962
210	H	H142	11.3654040	-2.6807252	-1.2178084	249	C	C69	-3.8689181	-0.7387633	-1.5027531
211	C	C205	2.1994023	-10.4861430	1.0231960	250	C	C70	-3.4086203	-0.6450484	0.8844973
212	C	C206	-0.6149616	-10.6362634	1.0620810	251	C	C71	-4.1727816	-1.8008717	1.0660967
213	C	C207	1.4473132	-10.1379340	-0.1106205	252	C	C72	-4.6292793	-1.8940867	-1.2995731
214	C	C208	1.5265617	-11.0248504	2.1308403	253	H	H22	-4.2952437	-2.2188594	2.0769274
215	C	C209	0.1361370	-11.0903318	2.1544373	254	H	H23	-5.1125906	-2.3843672	-2.1584182
216	C	C210	0.0588075	-10.2207011	-0.0953012	255	C	C73	3.3346058	-0.4705953	-3.3191083
217	H	H143	1.9521306	-9.7497280	-1.0084828	256	C	C74	4.2967959	-2.8424592	-4.4755516
218	H	H144	2.0978498	-11.3834082	3.0003815	257	C	C75	3.4034503	-0.5957988	-4.7182175
219	H	H145	-0.3794748	-11.4780397	3.0459753	258	C	C76	3.7455053	-1.5371358	-2.5004494
220	H	H146	-0.5194573	-9.9141080	-0.9803299	259	C	C77	4.2236103	-2.7131851	-3.0860758
221	C	C211	11.1817379	-0.8423129	0.7398499	260	C	C78	3.8827597	-1.7801996	-5.2840757
222	C	C212	10.5961831	1.8391957	0.1125097	261	H	H38	4.5465678	-3.5471945	-2.4439598
223	C	C213	10.4091943	-0.0586437	1.6151731	262	H	H39	3.9336432	-1.8777152	-6.3792005
224	C	C214	11.8157610	-0.2088100	-0.3381370	263	C	C79	-3.7672761	16.1454603	0.2181143
225	C	C215	11.5265421	1.1197410	-0.6496222	264	H	H4	-2.9786321	16.9152761	0.0213612
226	C	C216	10.1000893	1.2545819	1.2911240	265	H	H41	-4.1752103	16.3179361	1.2445750
227	H	H148	9.9684363	-0.5060499	2.5191423	266	H	H42	-4.5929749	16.2940193	-0.5204784
228	H	H149	12.5155617	-0.7742376	-0.9714534	267	C	C80	-5.5797819	-3.6655938	0.1850633
229	H	H150	11.9927947	1.5896776	-1.5283568	268	H	H27	-4.9054561	-4.5590521	0.1743464
230	H	H151	9.4227885	1.8340753	1.9379233	269	H	H43	-6.3414921	-3.7923688	-0.6229417
231	C	C55	-2.0563557	12.2249868	-0.1236200	270	H	H44	-6.1094057	-3.6397100	1.1692247

271	C	C81	4.8209709	-4.0876981	-5.0829211	291	C	C86	3.6878338	-1.4261366	-1.0230689
272	H	H40	5.9343836	-4.0236001	-5.1801375	292	H	H34	4.5202316	-0.7737406	-0.6560364
273	H	H45	4.3893347	-4.2506748	-6.1009261	293	H	H55	3.7859288	-2.4278145	-0.5371430
274	H	H46	4.5772670	-4.9750493	-4.4481172	294	H	H56	2.7189910	-0.9671576	-0.7018984
275	C	C82	7.6241982	14.8828211	-0.5766690	295	C	C87	2.9686075	0.5185657	-5.5940368
276	H	H14	8.6682292	14.5774021	-0.8414464	296	H	H26	3.5733344	1.4357069	-5.3782762
277	H	H47	7.6401276	15.3286598	0.4484180	297	H	H57	1.8927720	0.7618264	-5.4037466
278	H	H48	7.2959636	15.6694897	-1.2997508	298	H	H58	3.0876472	0.2593795	-6.6744447
279	C	C83	5.6239765	10.8974613	1.6519826	299	C	C88	4.4520011	11.9868347	-3.1097854
280	H	H7	6.4207134	11.1245542	2.4018565	300	H	H1	4.9378522	11.1277722	-3.6381518
281	H	H49	5.6941192	9.8157128	1.3735415	301	H	H59	4.4506581	12.8678001	-3.7973847
282	H	H50	4.6277095	11.0675629	2.1332024	302	H	H60	3.3914511	11.7043875	-2.8904817
283	C	C84	-2.7607933	-0.0046648	2.0543523	303	C	C89	-2.7519518	12.1128881	-2.5344683
284	H	H19	-1.6584642	-0.1980809	2.0348825	304	H	H2	-1.7470790	12.1235306	-3.0273731
285	H	H51	-3.1714881	-0.4038810	3.0138408	305	H	H61	-3.4864905	12.5990495	-3.2219835
286	H	H52	-2.9190822	1.1030369	2.0327296	306	H	H62	-3.0543912	11.0455511	-2.3868757
287	C	C85	-3.7320107	-0.1849997	-2.8713120	307	C	C90	-1.3498224	12.3075215	2.2854622
288	H	H15	-2.6690212	0.0993291	-3.0752818	308	H	H6	-0.3724445	11.8407764	2.0035758
289	H	H53	-4.3635031	0.7330483	-2.9773839	309	H	H63	-2.0072849	11.5067464	2.7091266
290	H	H54	-4.0560589	-0.9261011	-3.6423821	310	H	H64	-1.1639097	13.0686787	3.0821909

Cartesian Coordinates (Angstroms) for the Model HBC Derivative **17** without the Mesityl Substituents Optimized at the HF/3-21G Level (-2048.736190 hartrees)

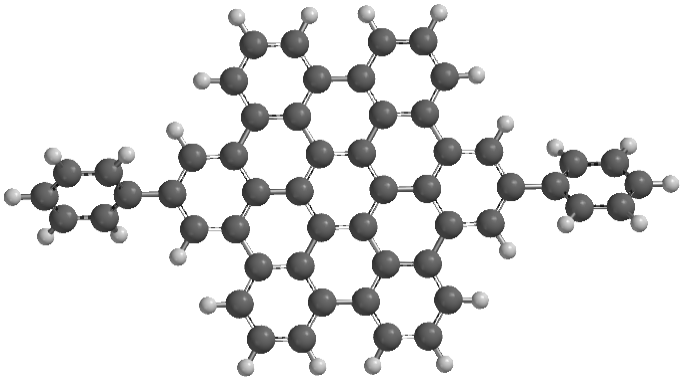

Figure S-103. Optimized structure of the model HBC derivative **17** without the mesityl substituents optimized at the HF/3-21G level.

Coordinates (Angstroms)

ATOM	X	Y	Z
1 C C55	-0.7028554	1.2177282	-0.0055104
2 C C56	0.7028558	-1.2177115	-0.0054852
3 C C57	0.7028406	1.2177151	0.0057445
4 C C58	-1.4054666	0.0000213	0.0001674
5 C C59	-0.7028405	-1.2176928	0.0057973
6 C C60	1.4054622	-0.0000012	0.0001353
7 C C61	1.4292790	2.4748004	0.0415749
8 C C62	2.8168992	4.8843601	0.2195317
9 C C63	2.8358066	2.4818006	0.0931552
10 C C64	0.7317457	3.6970606	0.0464111
11 C C65	1.4440045	4.8862520	0.1451960
12 C C66	3.5065376	3.6953124	0.1868176
13 H H41	0.9349460	5.8234134	0.1776201
14 H H42	4.5713800	3.7251349	0.2453064
15 H H43	3.3500013	5.8101257	0.3036621
16 C C67	-1.4293020	2.4748257	-0.0415178
17 C C68	-2.8169718	4.8844721	-0.2201608
18 C C69	-2.8358310	2.4818541	-0.0931058
19 C C70	-0.7317849	3.6970846	-0.0466283
20 C C71	-1.4440766	4.8863150	-0.1457563
21 C C72	-3.5065768	3.6954108	-0.1871276
22 H H46	-0.9349945	5.8234722	-0.1784492
23 H H47	-4.5714294	3.7252186	-0.2457368
24 H H48	-3.3500771	5.8102486	-0.3046242
25 C C73	2.8565190	-0.0000112	0.0001149
26 C C74	5.6584498	-0.0000331	0.0001032
27 C C75	3.5690527	-1.2120594	-0.0433381
28 C C76	3.5690490	1.2120221	0.0435203
29 C C77	4.9571896	1.1877763	0.0383343
30 C C78	4.9571899	-1.1878350	-0.0381246
31 H H51	5.5175673	2.0946628	0.0781834
32 H H52	5.5175637	-2.0947234	-0.0779568
33 C C79	1.4293043	-2.4748171	-0.0414437
34 C C80	2.8169766	-4.8844861	-0.2199120
35 C C81	0.7317995	-3.6970823	-0.0464283
36 C C82	2.8358261	-2.4818488	-0.0930934
37 C C83	3.5065704	-3.6954180	-0.1870315
38 C C84	1.4440922	-4.8863246	-0.1454597
39 H H55	4.5714206	-3.7252258	-0.2456666
40 H H56	0.9350067	-5.8234834	-0.1780182
41 H H57	3.3500798	-5.8102630	-0.3042826
42 C C85	-1.4292710	-2.4747741	0.0416959
43 C C86	-2.8168299	-4.8842581	0.2197983
44 C C87	-2.8357988	-2.4817612	0.0932656

45	C	C88	-0.7317209	-3.6970346	0.0466267	63	C	C102	9.2364194	-0.7393174	0.9411287
46	C	C89	-1.4439375	-4.8861920	0.1454777	64	H	H67	7.3161893	-1.2974884	1.6834634
47	C	C90	-3.5065091	-3.6952293	0.1870062	65	H	H68	7.3160845	1.2974647	-1.6833009
48	H	H61	-4.5713400	-3.7250576	0.2454881	66	H	H69	9.7689415	1.3081456	-1.6770176
49	H	H62	-3.3499189	-5.8100083	0.3039821	67	H	H70	9.7690454	-1.3082350	1.6770871
50	C	C91	-2.8565300	0.0000295	0.0001726	68	C	C103	-7.1482224	0.0000387	0.0000954
51	C	C92	-5.6584642	0.0000442	0.0001501	69	C	C104	-9.9316661	-0.0000934	-0.0000183
52	C	C93	-3.5690636	1.2120737	-0.0432612	70	C	C105	-7.8529726	-0.7388628	-0.9423779
53	C	C94	-3.5690600	-1.2120024	0.0435622	71	C	C106	-7.8530614	0.7389051	0.9425030
54	C	C95	-4.9572103	-1.1877639	0.0383123	72	C	C107	-9.2364696	0.7385037	0.9416746
55	C	C96	-4.9572098	1.1878480	-0.0379877	73	C	C108	-9.2363769	-0.7385978	-0.9416647
56	H	H65	-5.5175890	-2.0946592	0.0780645	74	H	H72	-7.3160545	-1.2962278	-1.6842591
57	H	H66	-5.5175907	2.0947394	-0.0777132	75	H	H73	-7.3162260	1.2963182	1.6844243
58	C	C97	7.1481953	-0.0000352	0.0000806	76	H	H74	-9.7691163	1.3068420	1.6780638
59	C	C98	9.9316327	-0.0000422	0.0000341	77	H	H75	-9.7689421	-1.3070040	-1.6780909
60	C	C99	7.8530242	-0.7396210	0.9419383	78	H	H154	-0.9348902	-5.8233498	0.1779524
61	C	C100	7.8529695	0.7395595	-0.9417997	79	H	H54	11.0034094	-0.0000505	0.0000199
62	C	C101	9.2363649	0.7392393	-0.9410405	80	H	H60	-11.0034430	-0.0001566	-0.0000540

Cartesian Coordinates (Angstroms) for the Model HBC Derivative **17** without the Mesityl Substituents Optimized by DFT at the B3LYP/6-31G* Level (-2073.636359 hartrees)

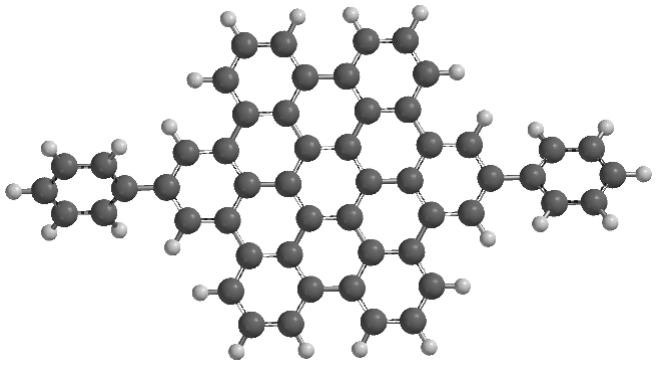

Figure S-104. Optimized structure of the model HBC derivative **17** without the mesityl substituents optimized by DFT at the B3LYP/6-31G* level.

Coordinates (Angstroms)

ATOM	X	Y	Z
1 C C55	0.7112613	-1.2332116	0.0064729
2 C C56	-0.7112575	1.2332311	0.0064799
3 C C57	-0.7112537	-1.2332138	-0.0064783
4 C C58	1.4221434	0.0000122	0.0000080
5 C C59	0.7112580	1.2332339	-0.0064630
6 C C60	-1.4221396	0.0000073	-0.0000006
7 C C61	-1.4358450	-2.4859525	-0.0325113
8 C C62	-2.8410002	-4.9216633	-0.1492002
9 C C63	-2.8600689	-2.4930913	-0.0715061
10 C C64	-0.7300912	-3.7236831	-0.0321843
11 C C65	-1.4552494	-4.9227811	-0.0947718
12 C C66	-3.5350291	-3.7208307	-0.1336451
13 H H41	-0.9421795	-5.8758387	-0.1114728
14 H H42	-4.6163547	-3.7525609	-0.1764908
15 H H43	-3.3833349	-5.8614347	-0.2034011
16 C C67	1.4358563	-2.4859488	0.0324925
17 C C68	2.8410192	-4.9216554	0.1491483
18 C C69	2.8600798	-2.4930837	0.0714909
19 C C70	0.7301066	-3.7236813	0.0321481
20 C C71	1.4552687	-4.9227770	0.0947188
21 C C72	3.5350441	-3.7208210	0.1336127
22 H H46	0.9422014	-5.8758358	0.1114044
23 H H47	4.6163700	-3.7525470	0.1764567
24 H H48	3.3833565	-5.8614245	0.2033350
25 C C73	-2.8672427	0.0000043	-0.0000032
26 C C74	-5.7067715	-0.0000035	-0.0000043
27 C C75	-3.5897734	1.2260702	0.0421594
28 C C76	-3.5897681	-1.2260652	-0.0421682
29 C C77	-4.9893816	-1.1961410	-0.0418271
30 C C78	-4.9893875	1.1961378	0.0418180
31 H H51	-5.5545759	-2.1191713	-0.0410285
32 H H52	-5.5545855	2.1191652	0.0410186
33 C C79	-1.4358532	2.4859667	0.0325084
34 C C80	-2.8410199	4.9216677	0.1491934
35 C C81	-0.7301028	3.7236987	0.0321823
36 C C82	-2.8600785	2.4930990	0.0714989
37 C C83	-3.5350447	3.7208328	0.1336350
38 C C84	-1.4552673	4.9227922	0.0947684
39 H H55	-4.6163709	3.7525574	0.1764761
40 H H56	-0.9421996	5.8758503	0.1114721
41 H H57	-3.3833589	5.8614361	0.2033933
42 C C85	1.4358502	2.4859728	-0.0324823
43 C C86	2.8410100	4.9216810	-0.1491509
44 C C87	2.8600753	2.4931108	-0.0714726
45 C C88	0.7300966	3.7237022	-0.0321474
46 C C89	1.4552578	4.9227996	-0.0947257

47	C	C90	3.5350379	3.7208480	-0.1336002	64	H	H67	-7.3762615	1.5586044	1.4801959
48	H	H61	4.6163639	3.7525746	-0.1764409	65	H	H68	-7.3762625	-1.5586213	-1.4802007
49	H	H62	3.3833458	5.8614515	-0.2033444	66	H	H69	-9.8447648	-1.5715745	-1.4679813
50	C	C91	2.8672461	0.0000141	0.0000135	67	H	H70	-9.8447633	1.5715454	1.4679838
51	C	C92	5.7067690	0.0000141	0.0000237	68	C	C103	7.1917935	0.0000092	0.0000159
52	C	C93	3.5897741	-1.2260548	0.0421710	69	C	C104	10.0118273	-0.0000596	-0.0000271
53	C	C94	3.5897733	1.2260836	-0.0421404	70	C	C105	7.9137083	0.8847042	-0.8186044
54	C	C95	4.9893865	1.1961559	-0.0417983	71	C	C106	7.9137239	-0.8847140	0.8186179
55	C	C96	4.9893853	-1.1961273	0.0418406	72	C	C107	9.3079200	-0.8846323	0.8190944
56	H	H65	5.5545858	2.1191828	-0.0410019	73	C	C108	9.3079043	0.8845548	-0.8191223
57	H	H66	5.5545854	-2.1191542	0.0410450	74	H	H72	7.3762383	1.5583489	-1.4803361
58	C	C97	-7.1918000	-0.0000060	-0.0000033	75	H	H73	7.3762621	-1.5583415	1.4803632
59	C	C98	-10.0118368	-0.0000147	0.0000013	76	H	H74	9.8447658	-1.5713452	1.4681133
60	C	C99	-7.9137252	0.8848520	0.8185225	77	H	H75	9.8447416	1.5712341	-1.4681630
61	C	C100	-7.9137265	-0.8848683	-0.8185267	78	H	H154	0.9421861	5.8758563	-0.1114227
62	C	C101	-9.3079226	-0.8847586	-0.8190212	79	H	H54	-11.0984198	-0.0000182	0.0000038
63	C	C102	-9.3079214	0.8847340	0.8190211	80	H	H60	11.0984102	-0.0000896	-0.0000488

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