Electronic Supporting Information for

Synthesis, Electronic Properties, and Self-Assembly of an Alkylated Dibenzo(biscorannulene)

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This file includes:

1. Synthesis of 1 and 2.

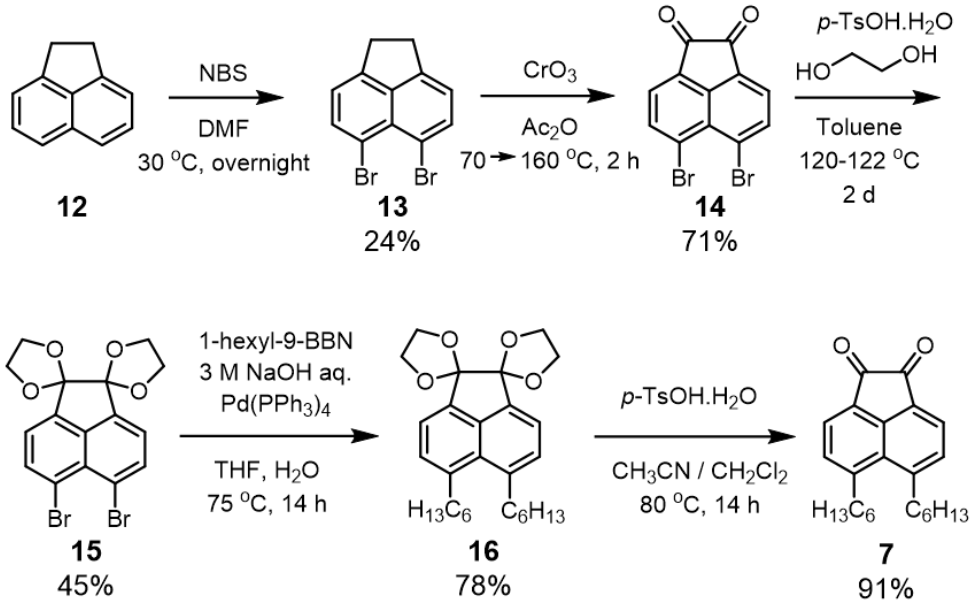
1-1. General Methods.

All solvents were distilled or passed through activated alumina and copper catalysts in a Glass Contour solvent purification system before use. Commercially available $Pd(PCy_3)_2Cl_2$ was recrystallized from CH_2Cl_2/hexane before use. Diazabicyclo[4.3.0]non-5-ene was distilled before use. Other commercially available reagents were used as received. $Pd(PPh_3)_4$ was prepared following the reported procedure.[1]

^1H (500 or 400 MHz) and ^{13}C (125 or 100 MHz) NMR spectra were measured on a JEOL ECA-500, ECA-400, or JNM-ECZ400S spectrometer. For NMR measurements, chloroform-*d* was used as the solvent, and the spectra were referenced to tetramethylsilane signals in the ^1H and ^{13}C NMR spectra (0.00 ppm). When 1,1,2,2-tetrachloroethane-d_2 was used as the solvent, the ^{13}C NMR spectrum was referenced to a residual solvent signal (73.80 ppm). When dichloromethane-d_2 was used as the solvent, the ^1H NMR spectra were referenced to a residual solvent signal (5.32 ppm). Recycling HPLC separation was undertaken with a JAI LC-5060 recycling chromatograph using 600 mm × 20 mm JAIGEL-1HR and 2HR GPC columns with $CHCl_3$ as the eluent. Analytical HPLC (ODS column; Nacalai tesque, COSMOSIL 5C_{18}-AR-II, 4.6 mm × 150 mm) was performed using a SHIMADZU LC-20AD system with a SPD-M20A photodiode array detector. Preparative HPLC (ODS column; Nacalai tesque, COSMOSIL 5C_{18}-AR-II, 20 mm × 250 mm) was performed using a SHIMADZU LC-20AR system with a SPD-20A detector. Other spectra were recorded using the following instruments: IR spectra, JACSCO FT/IR-410; mass spectra, JMS-T100GCV (TOF); melting point (mp), Stuart Scientific SMP3. Oil baths were used as the heat sources for the following reactions.

The syntheses of **1** and **2** are summarized in Schemes 1 and 2. The synthesis of compound **7** is outlined in Scheme S1.

Scheme S1. Synthesis of Compound **7**.



1-2. Synthesis of Compound 7.

Synthesis of 5,6-Dibromo-1,2-dihydroacenaphthylene (13). 1,2-Dihydoroacenaphthylene (**12**, 5.00 g, 32.4 mmol) was dissolved in DFM (30 mL) in a Schleck tube. *N*-Bromosuccinimide (NBS, 14.5 g, 81.3 mmol) was added to this solution, and the remaining NBS at the sidewall of the Schleck tube was washed with DMF (2 mL). After the mixture had been stirred at 31 °C overnight, the precipitates were collected by filtration and washed with ice-cold hexane and water. Recrystallization from hexane afforded **13** (2.46 g, 24% yield) as a yellow solid. ^{1}H NMR spectrum of **13** agreed with that in a previous report.[2]

Synthesis of 5,6-Dibromoacenaphthylene-1,2-dione (14). In a three-necked flask, compound **13** (4.46 g, 14.3 mmol) was dissolved in Ac_2O (525 mL). To this solution that was heated to 70 °C, CrO_3 (11.3 g, 113 mmol) was gradually added. The mixture had been stirred at 70 °C for 2 h and then at 160 °C for 35 min. The mixture was poured into ice, and to which conc. H_2SO_4 (20 mL) was added. The precipitates were collected by filtration and washed with water. Recrystallization from Ac_2O afforded **14** (3.43 g, 71% yield) as a brown solid. ^{1}H NMR spectrum of **14** agreed with that in a previous report.[3]

Synthesis of 5,6-Dibromo-1,2-di(1,3-dioxolan-2-yl)acenaphthylene (15). In a two-necked flask

with a Dean-Stark apparatus, compound **14** (1.93 g, 5.69 mmol) was dissolved in toluene (88 mL). Ethylene glycol (4.80 mL, 86.8 mmol) and 4-methylbenzenesulfonic acid·H_2O (266 mg, 1.40 mmol) were added to the solution. After the mixture had been stirred at 120–122 °C for 21 h, a further amount of ethylene glycol (4.80 mL, 86.8 mmol) and 4-methylbenzenesulfonic acid·H_2O (266 mg, 1.40 mmol) was added. The mixture had been stirred for additional 50 min. At that time, water generation was not observed. The products were extracted with $CHCl_3$, and the solvents were removed under vacuum. The residue was subjected to the silica gel column chromatography (hexane/CH_2Cl_2 = 1/4) to give **15** (1.10 g, 45% yield) as a light brown solid. ^{1}H NMR spectrum of **15** agrees with that in a previous report.[4]

Synthesis of 5,6-Dihexyl-1,2-bis(1,3-dioxolan-2-yl)acenaphthylene (16). Under argon atmosphere, 1-hexene (1.80 mL, 14.3 mmol) and THF (4.6 mL) were added to a two-necked flask. A solution of 9-borabicyclo[3.3.1]nonane (BBN, 0.5 M, 21.0 mL, 11 mmol) in THF was slowly added to the mixture at 0 °C. After the mixture had been stirred at 0 °C for 20 min and then at room temperature for 6 h, compound **15** (1.15 g, 2.69 mmol), $Pd(PPh_3)_4$ (121 mg, 105 μmol), THF (9.40 mL), and NaOH aq. (2.9 M, 2.50 mL) were added. The mixture had been refluxed for 17 h. The products were extracted with CH_2Cl_2. The organic phase was washed with brine and dried over $MgSO_4$. After the solvents were evaporated, the residue was subjected to the silica gel column chromatography (hexane/CH_2Cl_2 = 1/3) and recycling HPLC (chloroform) to give **16** (921 mg, 78% yield) as a white solid. m.p. 62.4–64.0 °C; ^{1}H NMR (500 MHz, $CDCl_3$, 25.1 °C) δ 7.45 (d, *J* = 7.0 Hz, 2H), 7.39 (d, *J* = 7.0 Hz, 2H), 4.22–4.11 (m, 4H), 3.77–3.66 (m, 4H), 3.09 (t, *J* = 8.0 Hz, 2H), 1.70–1.61 (m, 4H), 1.50–1.40 (m, 4H), 1.38–1.27 (m, 8H), 0.97–0.81 (m, 6H); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, 24.4 °C) δ 140.5, 137.5, 136.0, 130.2, 129.1, 118.7, 98.6, 61.8, 36.2, 33.3, 31.8, 29.5, 22.7, 14.1; IR (KBr) 3011, 2953, 2921, 2873, 2855, 1465, 1278, 1199, 1085, 1010, 978, 828 cm^{-1}; HRMS (FD) *m/z* calcd for $C_{28}H_{38}O_4$ (M^+): 438.2770, found: 438.2770.

Synthesis of 5,6-Dihexylacenaphthylene-1,2-dione (7). Compound **16** (1.02 g, 2.32 mmol) was dissolved in CH_2Cl_2 (6.5 mL). CH_3CN (35.2 mL) and water (11.2 mL) were added to this solution

followed by the addition of 4-methylbenzenesulfonic acid·H_2O (4.42 g, 23.2 mmol). After the mixture had been refluxed for 20 h, water and CH_2Cl_2 were added. The products were extracted with CH_2Cl_2, the organic phase was dried over $MgSO_4$, and the solvents were removed under vacuum. Compound **7** (0.741 g, 91% yield) was obtained as a yellow solid. m.p. 78.4–79.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 23.6 °C) δ 8.01 (d, J = 8.5 Hz, 2H), 7.62 (d, J = 8.5 Hz, 2H), 3.25 (t, J = 10.0 Hz, 4H), 1.77–1.66 (m, 4H), 1.56–1.42 (m, 4H), 1.41–1.27 (m, 8H), 0.95–0.86 (m, 6H); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, 25.4 °C) δ 188.8, 148.4, 148.3, 130.6, 129.0, 128.2, 121.8, 37.0, 33.0, 31.7, 29.4, 22.6, 14.0; IR (KBr) 2952, 2849, 1768, 1725, 1575, 1466, 1383, 1162, 1039, 832, 729 cm^{-1}; HRMS (FD) *m/z* calcd for $C_{24}H_{30}O_2$ (M^+): 350.2246, found: 350.2255.

1-3. Synthesis of Compound 1.

Synthesis of 1-[4-{2-Oxo-3-(2-bromophenyl)propyl}-2,5-dibromophenyl]-3-(2-bromophenyl)propan-2-one (4). An aqueous solution of NaOH (16.6 M, 21.5 mL) was added to a solution of 2-bromobenzylbromide (2.77 g, 11.1 mmol) and tetrabutylammonium iodide (185 mg, 0.501 mmol) in CH_2Cl_2 (125 mL). After the mixture had been stirred at room temperature for 30 min, 1,4-bis(bromomethyl)-2,5-dibromobenzene (**3**, 2.12 g, 5.02 mmol)[5] was added. The mixture had been stirred at room temperature for additional 5 h. The mixture was neutralized by the addition of an aqueous solution of HCl (6 M). The precipitates of the intermediate product of this reaction were removed by filtration. The products were extracted from the filtrate with CH_2Cl_2. The organic phase was washed with water and dried over Na_2SO_4. The solvents were removed under vacuum. The residue was subjected to the silica gel column chromatography (hexane/CH_2Cl_2 = 1/4) to give the reaction intermediate product. The total weight of the reaction intermediate product is 4.13 g, which was used for the next step without further purification.

To the reaction intermediate product, HCl aq. (1 M, 30 mL) and THF (150 mL) were added. After the mixture had been stirred at 45 °C for 3 d, the precipitates containing compound **4** were removed by filtration. From the filtrate, the products were extracted with CH_2Cl_2. The organic phase

was washed with water and dried over $MgSO_4$. After the solvents were evaporated, the residue was combined with the precipitates from the filtration. Recrystallization of the combined solid materials from toluene afforded compound **4** (1.57 g, 48% yield) as a white solid. m.p. 159.3–161.1 °C; ^{1}H NMR (500 MHz, $CDCl_3$, 23.8 °C) δ 7.58 (d, J = 8.0 Hz, 2H), 7.40 (s, 2H), 7.31–7.21 (m, 4H), 7.18–7.13 (m, 2H), 3.96 (s, 4H), 3.89 (s, 4H); ^{13}C{^{1}H} NMR (125 MHz, 1,1,2,2-tetrachloroethane-d_2, 60.0 °C) δ 202.0, 135.3, 135.2, 135.1, 134.0, 132.8, 131.7, 129.0, 127.6, 124.9, 123.7, 49.84, 49.76, 49.7, 48.8, 48.7, 48.6; IR (KBr) 3051, 2935, 2912, 1716, 1411, 1402, 1332, 1187, 1060, 881, 751 cm^{-1}; HRMS (FD) *m/z* calcd for $C_{24}H_{18}{}^{79}Br_4O_2$ (M^+): 653.8040, found: 653.8056.

Synthesis of 5. In a two-necked flask, compounds **7** (108 mg, 0.308 mmol) and **4** (104 mg, 0.157 mmol) were dissolved in a mixture of methanol (4.0 mL) and CH_2Cl_2 (5.0 mL). A solution of KOH in methanol (0.89 M, 1.0 mL) was added to the solution. The reaction vessel was wrapped in aluminum foil. After the mixture had been stirred at 64 °C for 18.5 h, the solvents were evaporated. To the residue, water and CH_2Cl_2 were added, and the products were extracted with CH_2Cl_2. The organic phase was dried over $MgSO_4$, and the solvents were removed. The separation by the silica gel column chromatography (hexane/CH_2Cl_2 = 1/1) afforded compound **5** (0.113 g, 56% yield) as a black solid. Compound **5** was obtained as a mixture of stereoisomers. m.p. 132.1–134.1 °C; ^{1}H NMR (500 MHz, $CDCl_3$, 18.3 °C) δ 7.87–7.82 (m, 2H), 7.78–7.73 (m, 2H), 7.61–7.48 (m, 4H), 7.48–7.40 (m, 6H), 7.40–7.34 (m, 2H), 7.33–7.28 (m, 2H), 3.21–3.03 (m, 8H), 1.73–1.59 (m, 8H), 1.51–1.41 (m, 8H), 1.38–1.28 (m, 16H), 0.94–0.86 (m, 12H); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, 25.0 °C) δ 199.34, 199.27, 199.12, 199.05, 156.9, 156.7, 155.8, 155.7, 143.3, 143.2, 143.0, 142.8, 136.1, 136.0, 135.7, 134.3, 133.3, 133.2, 132.91, 132.86, 132.1, 131.7, 131.1, 130.9, 130.0, 129.96, 129.8, 129.7, 127.2, 124.1, 124.0, 123.9, 123.7, 123.1, 122.9, 122.7, 122.5, 122.4, 120.6, 120.5, 118.6, 118.5, 36.6, 33.1, 31.7, 29.3, 22.6, 14.1; IR (KBr) 3402, 2953, 2924, 2855, 1710, 1639, 1573, 1466, 1384, 1129, 1064, 961, 834, 745 cm^{-1}; HRMS (FD) *m/z* calcd for $C_{72}H_{70}{}^{79}Br_4O_2$ (M^+): 1282.2109, found: 1282.2171.

Synthesis of 6. Compound **5** (467 mg, 0.363 mmol), bicyclo[2,2,1]hepta-2,5-diene (13.0 mL, 128

mmol), and *m*-xylene (37.2 mL) were added to a flask which was wrapped in aluminum foil. After the mixture had been stirred at 140 °C for 4 d, bicyclo[2,2,1]hepta-2,5-diene (2.2 mL, 22 mmol) was added. The mixture had been stirred at 140 °C for additional 10 d. The solvent and bicyclo[2,2,1]hepta-2,5-diene were removed under vacuum. The residue was subjected to the silica gel column chromatography (hexane/CH_2Cl_2 = 4/1) and HPLC (ODS column, CH_3CN/CH_2Cl_2 = 3/2) to give **6** (358 mg, 77% yield) as a yellow solid. m.p. 117.1–118.3 °C; ^{1}H NMR (500 MHz, $CDCl_3$, 22.6 °C) δ 8.05–8.02 (m, 1H), 7.99–7.95 (m, 1H), 7.84 (d, *J* = 8.0 Hz, 2H), 7.62–7.58 (m, 1H), 7.56–7.49 (m, 3H), 7.45–7.36 (m, 4H), 7.35–7.32 (m, 1H), 7.32–7.27 (m, 4H), 7.21–7.16 (m, 2H), 7.04–7.01 (m, 1H), 6.78–6.73 (m, 2H), 3.26–3.03 (m, 8H), 1.82–1.60 (m, 8H), 1.56–1.41 (m, 8H), 1.40–1.27 (m, 16H), 0.96–0.84 (m, 12H); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, 21.4 °C) δ 143.0, 142.92, 142.88, 142.85, 142.82, 141.8, 141.6, 141.51, 141.49, 141,45, 136.7, 136.5, 136.3, 135.2, 135.1, 134.9, 134.82, 134.80, 134.7, 134.50, 134.46, 134.3, 133.04, 133.00, 131.2, 131.0, 130.4, 130.3, 130.0, 129.5, 128.31, 128.28, 128.24, 128.18, 128.12, 127.8, 127.7, 123.8, 123.7, 123.3, 123.1, 123.03, 122.98, 122.9, 122.8, 122.7, 122.6, 122.5, 122.4, 36.5, 36.3, 33.6, 33.5, 31.84, 31.75, 29.7, 29.6, 22.7, 22.6, 14.1; IR (KBr) 3053, 2954, 2924, 2856, 1458, 1426, 1343, 1244, 1026, 893, 832, 758 cm^{-1}; HRMS (FD) *m/z* calcd for $C_{74}H_{74}{}^{79}Br_4$ (M^+): 1278.2524, found: 1278.2569.

Synthesis of 1. Under argon atmosphere, compound **6** (102 mg, 79.7 μmol) and $PdCl_2(PCy_3)_2$ (25.4 mg, 34.4 μmol) were added to a Schlenk tube. Deoxygenated 1,5-diazabicyclo[4.3.0]non-5-ene (45.0 μL, 350 μmol) and *N,N*-dimethylacetamide (DMA, 1.0 mL) were added. The mixture was further deoxygenated by freeze-pump-thaw cycles. After the reaction mixture had been stirred at 150 °C for 3 d, the products were extracted with CH_2Cl_2. The organic phase was washed with brine and dried over Na_2SO_4. The mixture was filtrated through a pad of silica gel (hexane/CH_2Cl_2 = 7/3). After the solvents were evaporated, a mixture of CH_3CN and CH_2Cl_2 (CH_3CN/CH_2Cl_2 = 1/1) was added, generating the precipitate, which was removed by filtration. The filtrate was separated by HPLC (ODS column, CH_3CN/CH_2Cl_2 = 1/1). The solid materials obtained by the filtration were purified by recrystallization (CH_2Cl_2 and EtOH) to afford compound **1** as a yellow solid. The supernatant solution

from the recrystallization and the samples obtained from the HPLC separation were combined, and the combined material was further purified by recrystallization (CH_2Cl_2 and EtOH) to give compound **1** as a yellow solid. The total amount of the compound **1** from the first and send recrystallizations was 15.2 mg (15% yield). m.p.160.5–162.3 °C; ^{1}H NMR (500 MHz, $CDCl_3$, 25.0 °C, the concentration of **1** at 8.4 mM determined by the internal standard of 1,1,2,2-tetrachloroethane) δ 9.28 (s, 2H), 8.50–8.43 (m, 2H), 8.43–8.38 (m, 2H), 8.14 (d, J = 8.0 Hz, 2H), 8.00 (t, J = 4.0 Hz, 4H), 7.79 (s, 2H), 7.64–7.54 (m, 4H), 3.28 (t, J = 8.0 Hz, 4H), 3.19 (t, J = 8.0 Hz, 4H), 2.00–1.92 (m, 4H), 1.91–1.80 (m, 4H), 1.73–1.64 (m, 4H), 1.63–1.56 (m, 4H), 1.54–1.36 (m, 16H), 1.02 (t, J = 7.0 Hz, 6H), 0.98 (t, J = 7.0 Hz, 6H); ^{13}C NMR (125 MHz, 1,1,2,2-tetrachloroethane-d_2, 24.9 °C) δ 143.5, 143.2, 134.6, 133.9, 133.7, 133.6, 133.3, 132.8, 132.3, 131.3, 131.0, 127.9, 127.7, 127.6, 127.5, 127.4, 127.0, 126.9, 125.01, 124.98, 124.0, 123.70, 123.67, 120.9, 36.9, 36.6, 33.9, 33.5, 31.9, 31.8, 29.9, 29.7, 22.8, 22.7, 14.24, 14.20; IR (KBr) 3015, 2952, 2925, 2853, 1617, 1538, 1467, 1433, 1376, 1215, 1114, 1040, 893, 885, 857, 819, 760, 641 cm^{-1}; HRMS (FD): *m/z* calcd for $C_{74}H_{70}$ (M^+): 958.5478, found: 958.5473.

1-4. Synthesis of Compound 2.

Synthesis of 1,3-Bis(2-bromophenyl)propan-2-one (9). An aqueous solution of NaOH (15.8 M, 31.4 mL) was added to a solution of 2-bromo-1-(bromomethyl)benzene (**3**, 1.95 g, 7.81 mmol), 4-isocyanomethanesulfonyltoluene (790 mg, 4.04 mmol), and tetra-*n*-butylammonium iodide (293 mg, 0.793 mmol) in CH_2Cl_2 (91 mL). After the mixture had been stirred at room temperature for 4 h, the mixture was neutralized by the gradual addition of an aqueous solution of HCl (6 M). The products were extracted with CH_2Cl_2. The organic phase was washed with water and dried over $MgSO_4$. After the solvents were evaporated, reaction intermediate **8** (2.24 g) was separated using the silica gel column chromatography (hexane/CH_2Cl_2 = 1/1).

Reaction intermediate **8** was suspended in a mixture of an aqueous solution of HCl (1 M, 12 mL) and THF (60 mL). The mixture had been stirred at 35 °C for 3 d. The products were extracted

with hexane. The organic phase was washed with water and dried over $MgSO_4$. The solvents were removed under vacuum. The residue was subjected to the silica gel column chromatography (hexane/CH_2Cl_2 = 1/1) and recrystallization from hexane to furnish **9** (768 mg, 53% yield) as a white solid. ^{1}H NMR spectrum of **9** agreed with that in a previous report.[6]

Synthesis of Compound 10. Compounds **7** (95.6 mg, 0.273 mmol) and **9** (101 mg, 0.275 mmol) were dissolved in a mixture of CH_3OH (1.5 mL) and CH_2Cl_2 (0.25 mL). After the addition of KOH (13.8 mg, 0.246 mmol), the rection vessel was wrapped in aluminum foil. The reaction mixture had been refluxed for 2.5 h. The mixture was washed with brine, and the products were extracted with CH_2Cl_2. The organic phase was dried over $MgSO_4$. After the solvents were evaporated, compound **10** (173 mg, 93% yield) was obtained as a black solid by the silica gel column chromatography (hexane/CH_2Cl_2 = 1/1) separation. Compound **10** was obtained as a mixture of stereoisomers. m.p. 78.2–80.1 °C; ^{1}H NMR (500 MHz, $CDCl_3$, 25.0 °C) δ 7.73 (dd, J = 8.0, 1.5 Hz, 2H), 7.50–7.45 (m, 2H), 7.44–7.38 (m, 4H), 7.38–7.33 (m, 2H), 7.30–7.24 (m, 2H), 3.18–3.04 (m, 4H), 1.70–1.60 (m, 4H), 1.48–1.39 (m, 4H), 1.37–1.27 (m, 8H), 0.94–0.84 (m, 6H); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, 25.0 °C) δ 199.6, 199.3, 155.7, 155.5, 147.3, 142.7, 133.24, 133.16, 133.05, 132.98, 132.1, 131.6, 130.89, 130.85, 130.23, 130.18, 129.8, 129.7, 129.6, 127.1, 124.1, 124.0, 123.0, 122.7, 120.4, 120.2, 36.5, 33.1, 31.7, 29.3, 22.6, 14.1; IR (KBr) 3403, 3060, 2954, 2925, 2855, 1711, 1640, 1573, 1467, 1431, 1026, 836, 747 cm^{-1}; HRMS (FD) *m/z* calcd for $C_{39}H_{38}{}^{79}Br_2O$ (M^+): 680.1289, found: 680.1275.

Synthesis of Compound 11. Compound **10** (159 mg, 0.233 mmol), *m*-xylene (1.4 mL), and bicyclo[2,2,1]hepta-2,5-diene (2.45 mL, 23.3 mmol) were added to a reaction vessel. The reaction vessel was wrapped in aluminum foil. After the reaction mixture had been refluxed for 4 d, the volatiles were removed under vacuum. The residue was subjected to the silica gel column chromatography (hexane/CH_2Cl_2, from 1/1 to 3/1) to give **11** (145 mg, 92% yield) as a yellow solid. m.p. 67.1–68.7 °C; ^{1}H NMR (500 MHz, $CDCl_3$, 25.0 °C) δ 7.82–7.79 (m, 2H), 7.56 (dd, J = 7.5, 1.5 Hz, 1H), 7.51–7.46 (m, 3H), 7.40–7.36 (m, 2H), 7.19 (d, J = 2.0 Hz, 2H), 7.13 (d, J = 7.5 Hz, 2H), 6.70 (d, J = 7.5 Hz, 2H), 3.13–2.99 (m, 4H), 1.68–1.57 (m, 4H), 1.47–1.37 (m, 4H), 1.35-1.23 (m,

8H), 0.87 (t, J = 7.5 Hz, 6H); $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$, 21.3 °C) δ 141.6, 141.3, 136.4, 135.9, 134.9, 134.3, 132.9, 131.3, 131.0, 130.1, 129.3, 128.0, 127.6, 123.7, 122.4, 36.2, 33.5, 31.7, 29.6, 22.6, 14.1; IR (KBr) 3052, 2925, 1585, 1560, 1462, 1426, 1388, 1240, 1026, 835, 754 cm^{-1}; HRMS (FD) *m/z* calcd for $C_{40}H_{40}{}^{79}Br_2$ (M^+): 678.1497, found: 678.1492.

Synthesis of 2. Under argon atmosphere, compound **11** (66.2 mg, 97.3 μmol) and $PdCl_2(PCy_3)_2$ (15.2 mg, 20.6 μmol) were added to a Schlenk tube. Deoxygenated 1,5-diazabicyclo[4.3.0]non-5-ene (45.0 μL, 350 μmol) and *N*,*N*-dimethylacetamide (DMA, 1.0 mL) were added. The mixture was further deoxygenated by freeze-pump-thaw cycles. After the reaction mixture had been stirred at 150 °C for 2 d, the products were extracted with CH_2Cl_2. The organic phase was washed with HCl aq. (0.1 M) and brine and dried over $MgSO_4$. Compound **2** (22.0 mg, 44% yield) was obtained as a yellow solid by the silica gel column chromatography (hexane/CH_2Cl_2 = 5/1), HPLC (ODS column, CH_3CN/CH_2Cl_2 = 9/1), and recycling HPLC (chloroform) separations. m.p. 56.8–57.6 °C; ^{1}H NMR (500 MHz, $CDCl_3$, 23.1 °C) δ 8.71–8.63 (m, 4H), 8.33 (s, 2H), 8.08 (s, 2H), 7.77–7.71 (m, 4H), 3.37–3.31 (m, 4H), 1.92–1.83 (m, 4H), 1.63–1.50 (m, 4H), 1.46–1.34 (m, 8H), 0.94 (t, 6H); ^{13}C NMR (125 MHz, $CDCl_3$, 21.4 °C) δ 143.3, 135.2, 134.2, 134.0, 133.3, 132.8, 128.14, 128.10, 128.0, 127.2, 127.0, 125.12, 125.09, 124.5, 124.0, 36.8, 33.9, 31.8, 29.7, 22.7, 14.1; IR (KBr) 3045, 2923, 2853, 1613, 1537, 1467, 1450, 1434, 1419, 1373, 1213, 1113, 1040, 858, 814, 773, 760, 754, 731, 667, 641 cm^{-1}; HRMS (FD) *m/z* calcd for $C_{40}H_{38}$ (M^+): 518.2974, found: 518.2968.

1-5. UV-vis Absorption and Emission Measurements.

UV-vis absorption spectra and emission spectra of **1** and **2** were recorded on a JASCO V-550 and a JASCO FP-6500 spectrometer, respectively. All measurements were performed at room temperature. The solutions were prepared in spectrograde CH_2Cl_2. The concentrations of **1** and **2** were set to 1.0×10^{-5} M for the absorption measurements and 4.0×10^{-7} M for the emission measurements (Fig. 2a). An excitation wavelength was 320 nm for **1** and **2**. A solution of 9,10-diphenylanthracene in cyclohexane (Φ = 90%) was used as an external standard for the quantum yield determination.[7,8]

2. TD-DFT Calculations of 1 and 2.

The excited-state (TD-DFT) calculations were performed at B3LYP/6-311G(d,p) level of theory using the optimized structures of model compounds in which the hexyl groups are replaced with hydrogen atoms (vide infra). The energy levels and distributions of the selected molecular orbitals are shown in Figure S1. The electronic transitions of **1** and **2** are summarized in Tables S1 and S2.

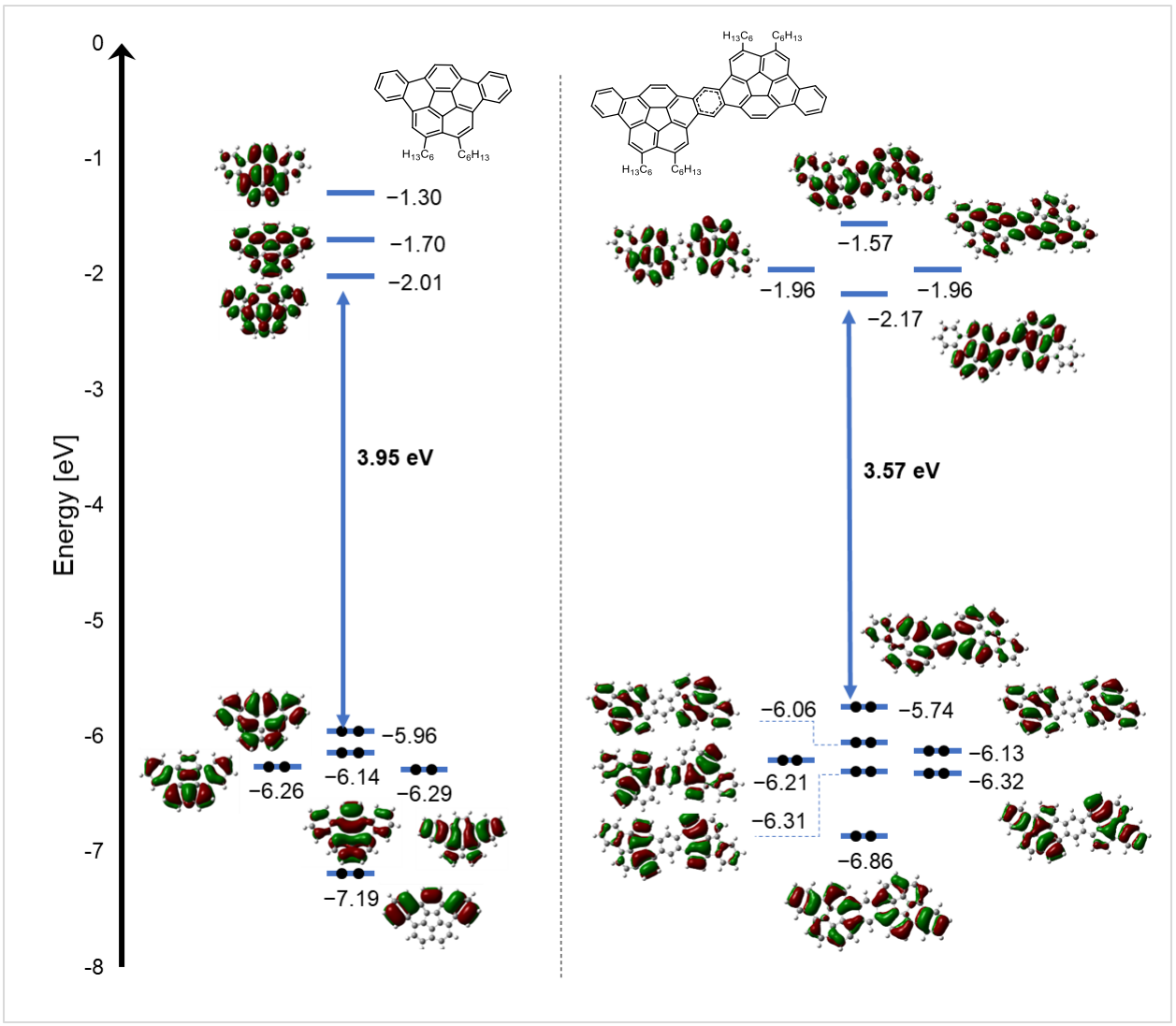


Figure S1. Energy levels and distributions of the selected molecular orbitals of the model compounds of **2** (left) and ***anti*-1** (right). Black dots indicate electron occupancy

Table S1. Major Electronic Transitions of *anti*-Geometry of Model of **1**.

excited state	wavelength (nm)	oscillation strength(*f*)	major contributions
1	399.33	0.0682	160 -> 163 (–22%), 161 (HOMO) -> 162 (LUMO, 64%), 161 -> 163 (11%)
2	383.78	0.0465	160 -> 162 (38%), 161 -> 162 (–17%), 161 -> 163 (54%)
3	375.30	0.0000	159 -> 163 (–17%), 161 -> 164 (66%)
4	365.25	0.0001	156 -> 162 (–36%), 157 -> 164 (–27%), 158 -> 162 (48%), 159 -> 164 (20%)
5	364.79	0.0000	156 -> 164 (–21%), 157 -> 162 (–42%), 158 -> 164 (23%), 159 -> 162 (45%)
6	356.51	0.0000	155 -> 163 (12%), 156 -> 164 (19%), 157 -> 162 (34%), 158 -> 164 (–12%), 159 -> 162 (36%), 160 -> 164 (37%), 161 -> 166 (–15%)
7	354.30	0.7858	158 -> 163 (–29%), 158 -> 165 (10%), 160 -> 162 (49%), 161 -> 163 (–33%), 161 -> 165 (–11%)
8	350.49	0.2619	155 -> 164 (–13%), 156 -> 162 (34%), 157 -> 164 (15%), 158 -> 162 (33%), 158 -> 163 (20%), 159 -> 166 (–11%), 160 -> 162 (21%), 161 -> 163(–17%), 161 -> 165 (28%)
9	344.20	0.000	155 -> 162 (17%), 156 -> 164 (–23%), 157 -> 162 (–12%), 157 -> 163 (24%), 158 -> 164 (–14%), 159 -> 162 (–26%), 159 -> 163 (–20%), 160 -> 164 (42%), 161 -> 164 (–11%)
10	342.42	0.3122	156 -> 163 (–19%), 156 -> 165 (–12%), 157 -> 164 (13%), 158 -> 162 (18%), 158 -> 163 (–14%), 160 -> 163 (49%), 161 -> 162 (16%), 161 -> 163 (14%), 161 -> 165 (–26%)

Table S2. Major Electronic Transitions of Model of **2**.

Excited state	wavelength (nm)	oscillation strength(*f*)	major contributions
1	363.20	0.0265	88 -> 92 (15%), 90 -> 93 (26%), 91 (HOMO) -> 92 (LUMO, 62%)
2	361.65	0.0019	89 -> 92 (52%), 90 -> 92 (48%)
3	352.24	0.0000	89 -> 92 (34%), 90 -> 92 (–39%), 91 -> 93 (45%), 91 -> 94 (–13%)
4	339.38	0.0111	88 -> 92 (56%), 89 -> 93 (22%), 90 -> 93 (27%), 91 -> 92 (–22%)
5	324.35	0.1278	88 -> 93 (47%), 88 -> 94 (20%), 89 -> 92 (24%), 90 -> 92 (–27%), 91 -> 93 (–32%)
6	315.78	0.1494	88 -> 93 (47%), 88 -> 94 (–27%), 89 -> 92 (–13%), 90 -> 92 (10%), 91 -> 93 (34%), 91 -> 94 (23%)
7	310.13	0.0634	88 -> 92 (–18%), 89 -> 93 (–31%), 89 -> 94 (–28%), 90 -> 93 (45%), 90 -> 94 (–22%), 91 -> 92 (–13%)
8	302.93	0.0078	88 -> 92 (–33%), 89 -> 93 (54%), 90 -> 93 (28%)
9	296.62	0.0193	88 -> 93 (–18%), 88 -> 94 (14%), 89 -> 92 (11%), 91 -> 94 (63%)
10	288.25	0.0552	87 -> 93 (11%), 89 -> 93 (–15%), 90 -> 93 (11%), 90 -> 94 (64%), 91 -> 92 (12%)

3. Electrochemical Measurements of 1 and 2.

The electrochemical measurements were performed on a HOKUTO DENKO HZ-7000 voltammetric analyzer under an argon atmosphere. The solvent was degassed by argon before use. As the supporting electrolyte, $Bu_4N \cdot PF_6$ was used after the recrystallization from hot EtOH. Platinum wire electrode, glassy carbon electrode, and Ag/Ag^+ electrode were used as the counter electrode, working electrode, and reference electrode, respectively. The potential was corrected against the ferrocene/ferrocenium (Fc/Fc^+) redox couple. Ferrocene was purified by sublimation before use. A scan rate of 100 mV/s was set during cyclic voltammetry (CV) measurements. The cyclic voltammograms are show in Figures S2 and S3.

The half-wave potential of the Fc/Fc^+ redox couple $E_{1/2}$ (Fc/Fc^+) is estimated by the following equation.[9,10]

$$E_{1/2}\ (Fc/Fc^+) = (E_{ap} + E_{cp})/2$$

E_{ap} and E_{cp} are the anodic and cathodic peak potentials. In our electrochemical setup, E_{ap} and E_{cp} values are 0.458 and −0.007 V for **1** as well as 0.554 and −0.049 V for **2**. The $E_{1/2}$ (Fc/Fc^+) values become 0.226 and 0.253 V relative to the Ag/Ag^+ reference electrode. The voltammograms were then calibrated based on these $E_{1/2}$ (Fc/Fc^+) values.

Using the reported energy level of the ferrocene/ferrocenium (Fc/Fc^+) couple (–4.8 eV) in vacuum,[9,10] the LUMO energy levels of the **1** and **2** were estimated according to the following equation.

$$E_{LUMO} = -(4.8 + E_{red,onset})\ \text{eV}$$

$E_{red,onset}$ is the onset potential of the first reduction wave relative to the Fc/Fc^+ reference electrode. The calculated E_{LUMO} values are –3.4 eV and –3.3 eV for **1** and **2**, respectively.

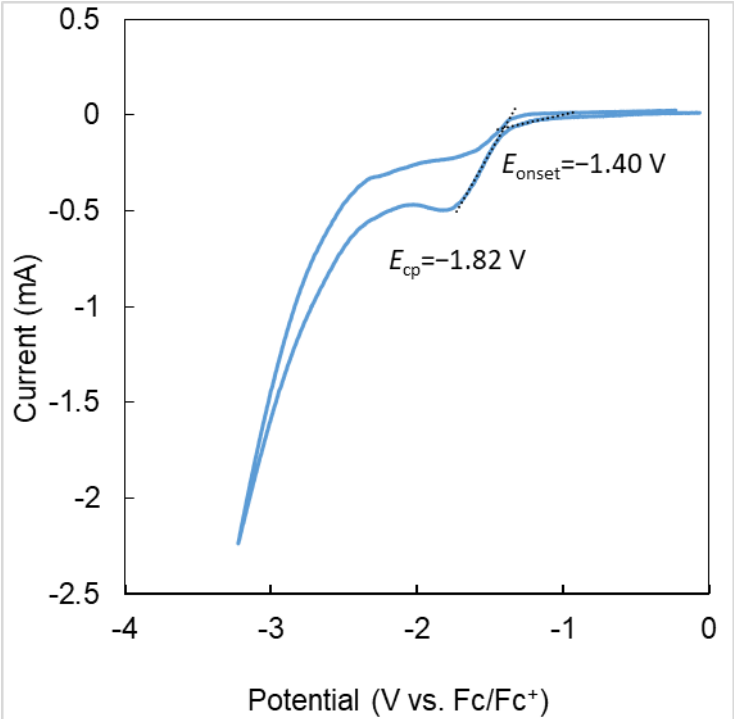


Figure S2. Cyclic voltammetric curve of **1** in a solution of nBu$_4$NPF$_6$/CH$_2$Cl$_2$ (2 mM). Working electrode: glassy carbon; counter electrode: Pt; reference electrode: Ag/Ag$^+$; T = room temperature; Scan rate: 100 mV·s^{-1} (vs. Fc$^{+/0}$).

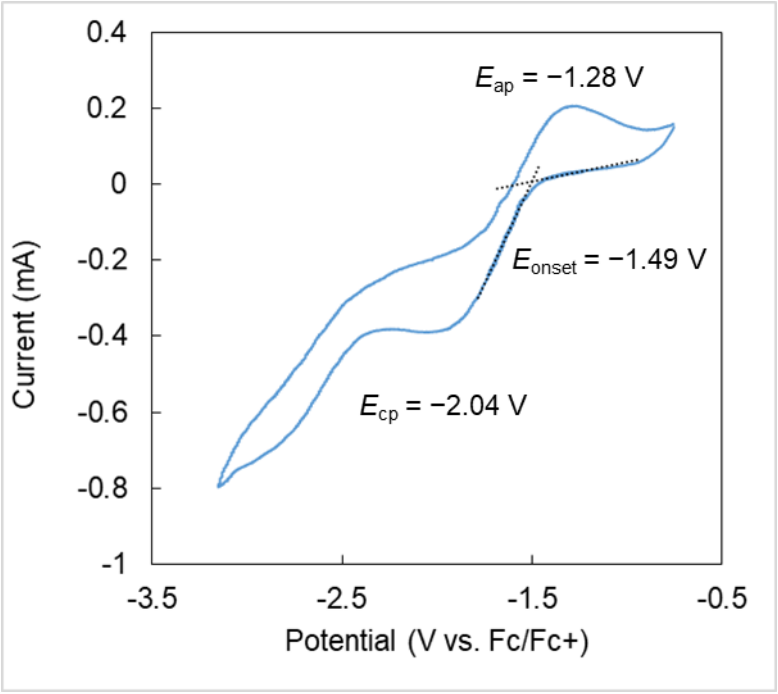


Figure S3. Cyclic voltammetric curve of **2** in a solution of nBu$_4$NPF$_6$/CH$_2$Cl$_2$ (2 mM). Working electrode: glassy carbon; counter electrode: Pt; reference electrode: Ag/Ag$^+$; T = room temperature; Scan rate: 100 mV·s^{-1} (vs. Fc$^{+/0}$).

4. NICS and AICD Calculations of 1 and 2.

Schleyer et al. proposed the NICS values which are a convenient and useful measure for the degree of local aromaticity/anti-aromaticity in polycyclic aromatic compounds.[11,12] The NICS values in the present work are the *zz* component of the chemical shift of a ghost atom 1 Å above the ring (NICS(1)$_{zz}$) obtained from NMR calculations at the B3LYP/6-311G(d, p) level of theory (GIAO method). The diatropic ring current induces magnetic shielding at the aromatic ring, which affords a negative NICS value. Conversely, the paratropic ring current results in deshielding at the anti-atomatic ring, giving a positive NICS value. To determine the coordination of ghost atoms for the NICS(1)$_{zz}$ value calculations, we used a Multiwfn application.[13] The calculated NICS values at each ring are summarized in Figures S4–S6. We also performed AICD calculations, which directly plot the induced ring currents, using the continuous set of gauge transformation (CSGT) method at the B3LYP/6-311G(d, p) level of theory.[14,15] The results of the contributions of the π-electrons in the systems are displayed in the AICD plots. An external magnetic field oriented perpendicular to the molecular plane and pointing upward was applied. The AICD plots are displayed in Figures S7–S9.

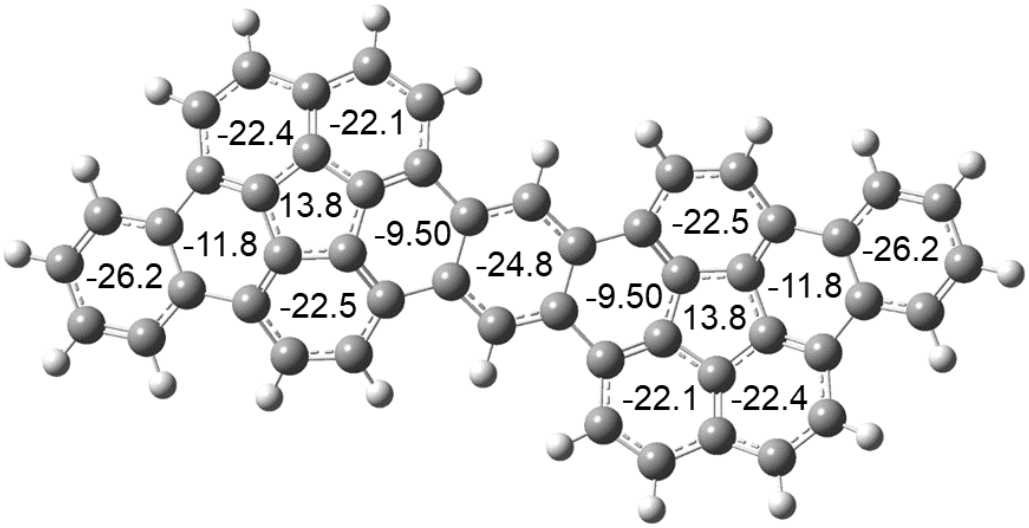


Figure S4. NICS(1)$_{zz}$ values of the model of *anti*-**1**.

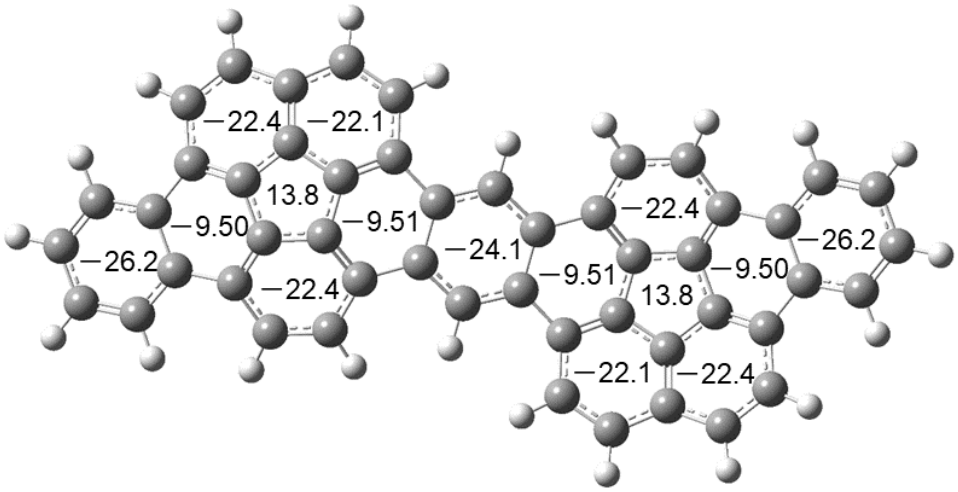


Figure S5. NICS(1)$_{zz}$ values of the model of *syn*-**1**.

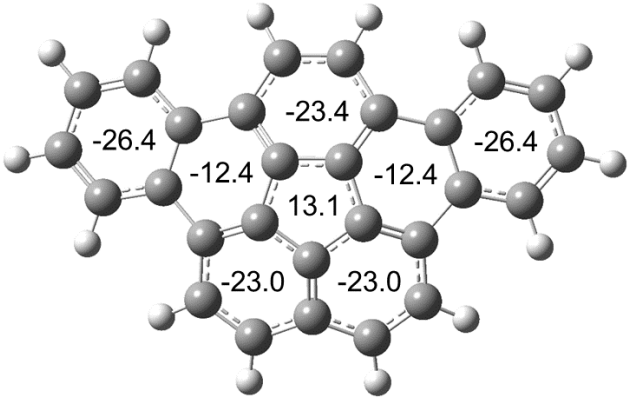


Figure S6. NICS(1)$_{zz}$ values of the model of **2**.

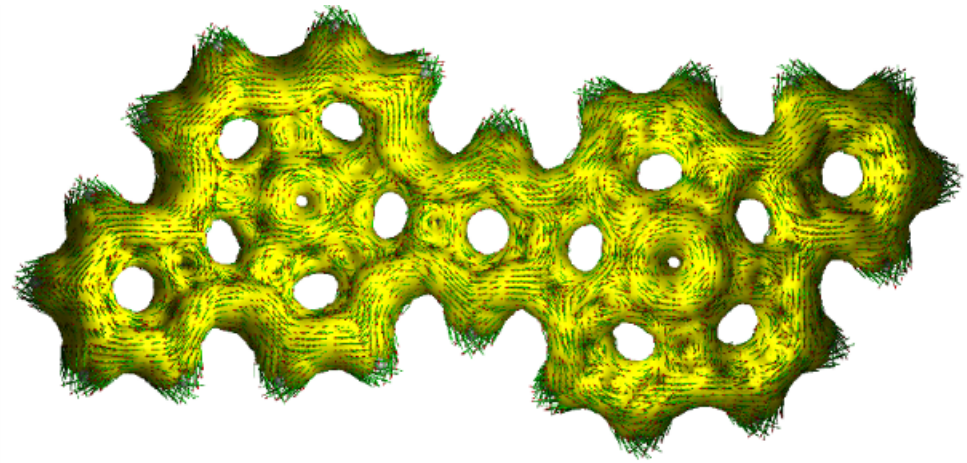


Figure S7. AICD image of the model of *anti*-**1** (isovalue = 0.03).

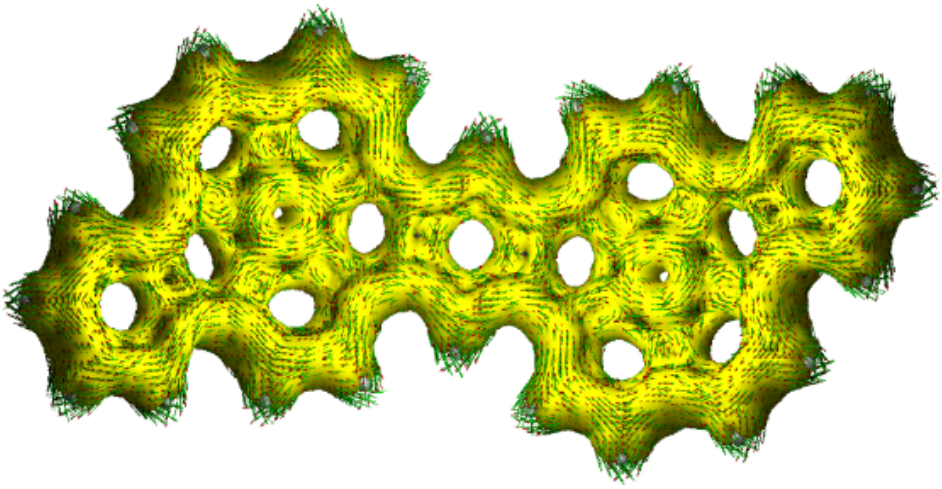


Figure S8. AICD image of the model of *syn*-**1** (isovalue = 0.03).

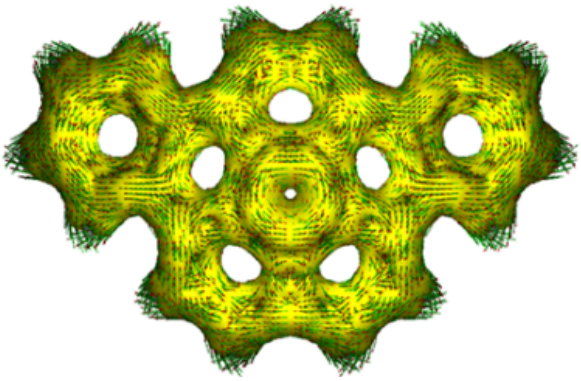


Figure S9. AICD image of the model of **2** (isovalue = 0.035).

5. VT NMR Spectra of 1 and 2 in CD_2Cl_2 and $CDCl_3$.

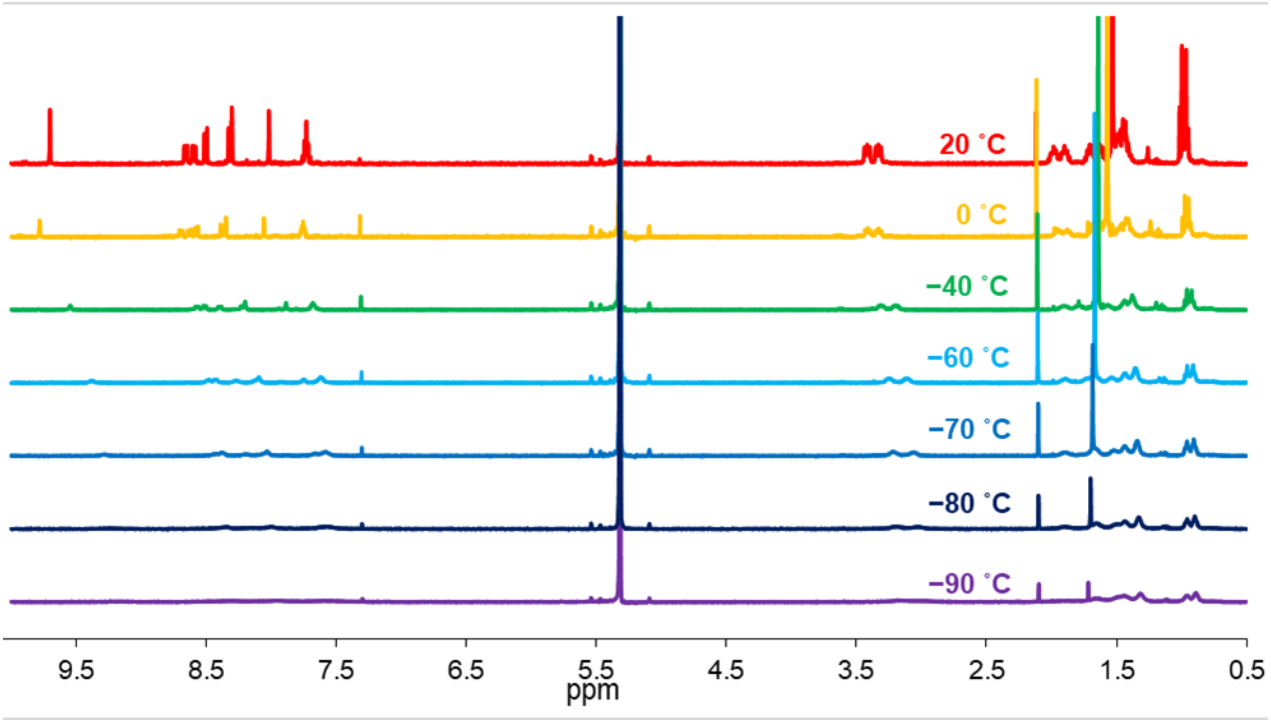


Figure S10. Variable Temperature (VT) ^{1}H NMR (400 MHz) spectra of **1** in CD_2Cl_2 recorded from –90 to 20 °C

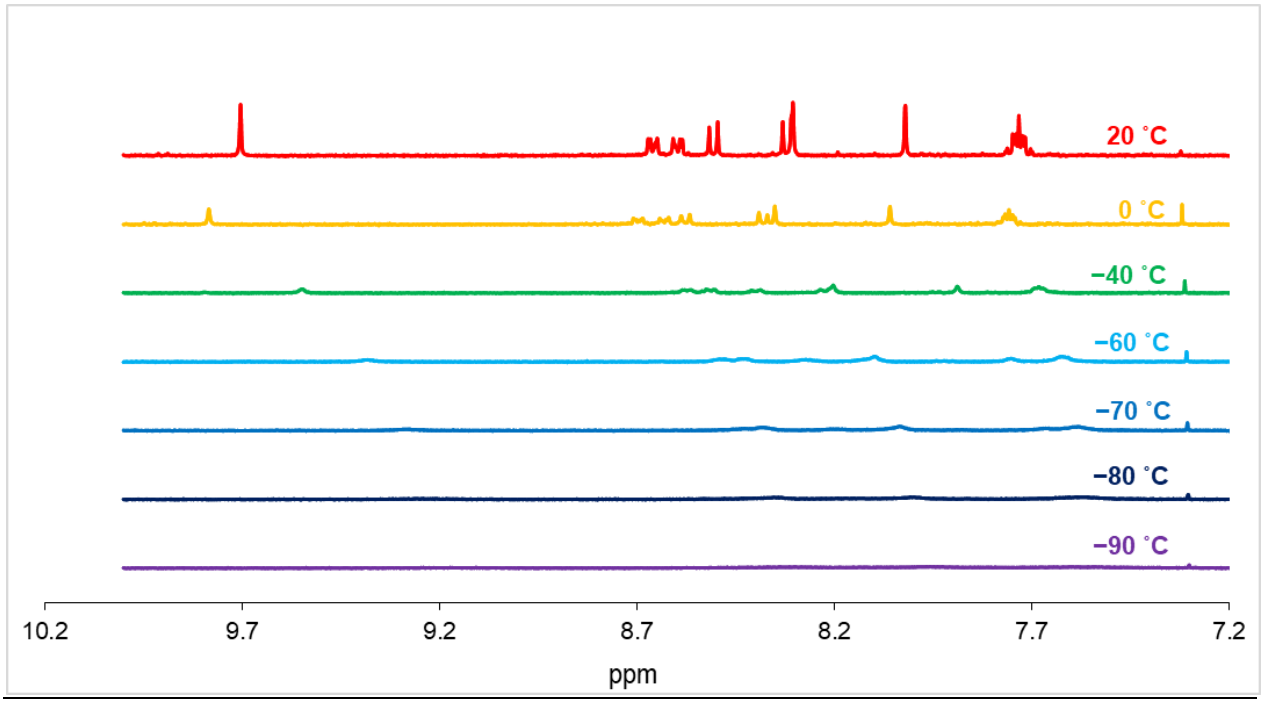


Figure S11. Partial VT ^{1}H NMR (400 MHz) spectra of **1** in CD_2Cl_2 recorded from –90 to 20 °C

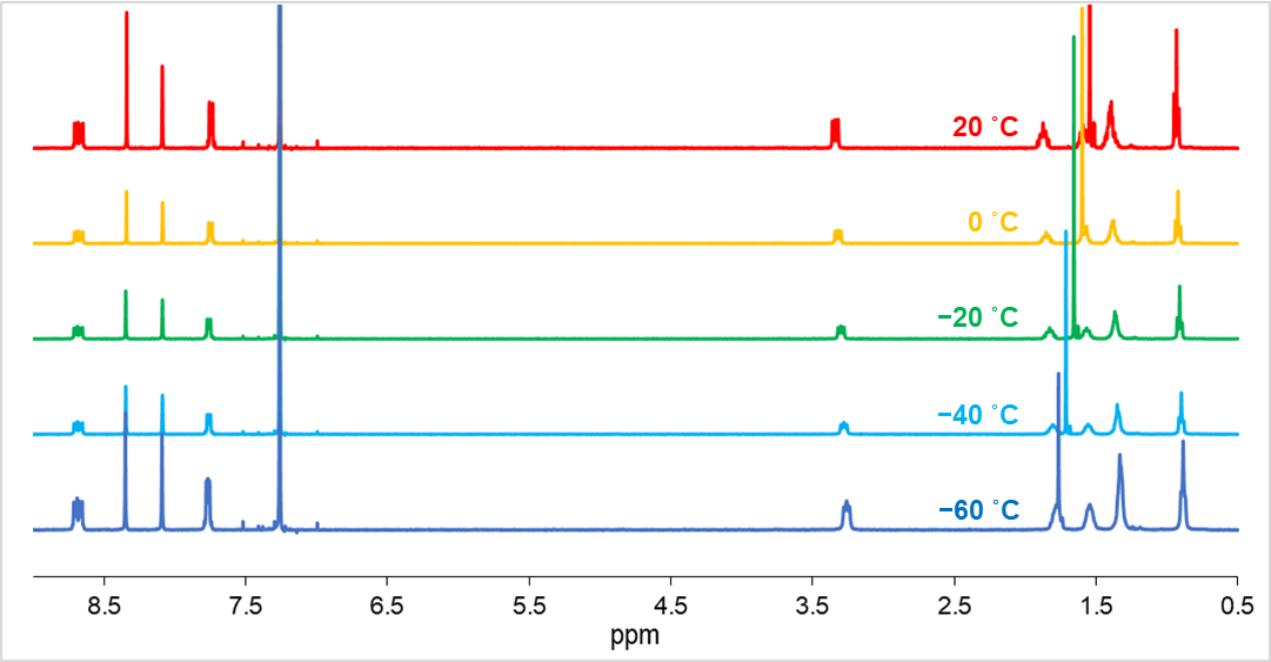


Figure S12. Variable Temperature (VT) ^{1}H NMR (400 MHz) spectra of **2** in $CDCl_3$ recorded from –60 to 20 °C

6. Optimization of *syn*- and *anti*-Geometries of 1 and 2.

All quantum chemical calculations were performed using the Gaussian 16 program package.[16] For the calculations of single molecules, we employed model compounds of **1** and **2** in which the hexyl groups are replaced with hydrogen atoms to reduce computational costs. *Syn*- and *anti*-geometries of the model compounds of **1** as well as **2** were optimized with the C_s, C_1, and C_1 symmetry constraints at the B3LYP/6-311G(d,p) level of theory. The absence of imaginary frequencies was confirmed by vibrational-frequency calculations for all optimized geometries. The zero-point-corrected energy (ZPE) values confirm a negligible energy difference between the *syn*- and *anti*-geometries of the model of **1** (0.1 kcal/mol, Figure S13). Moreover, a transition state with one imaginary frequency in a bowl-to-bowl inversion process was also calculated. One corannulene unit adopts a planar geometry at the transition state. The activation energy barrier is estimated to be 6.8 kcal/mol.

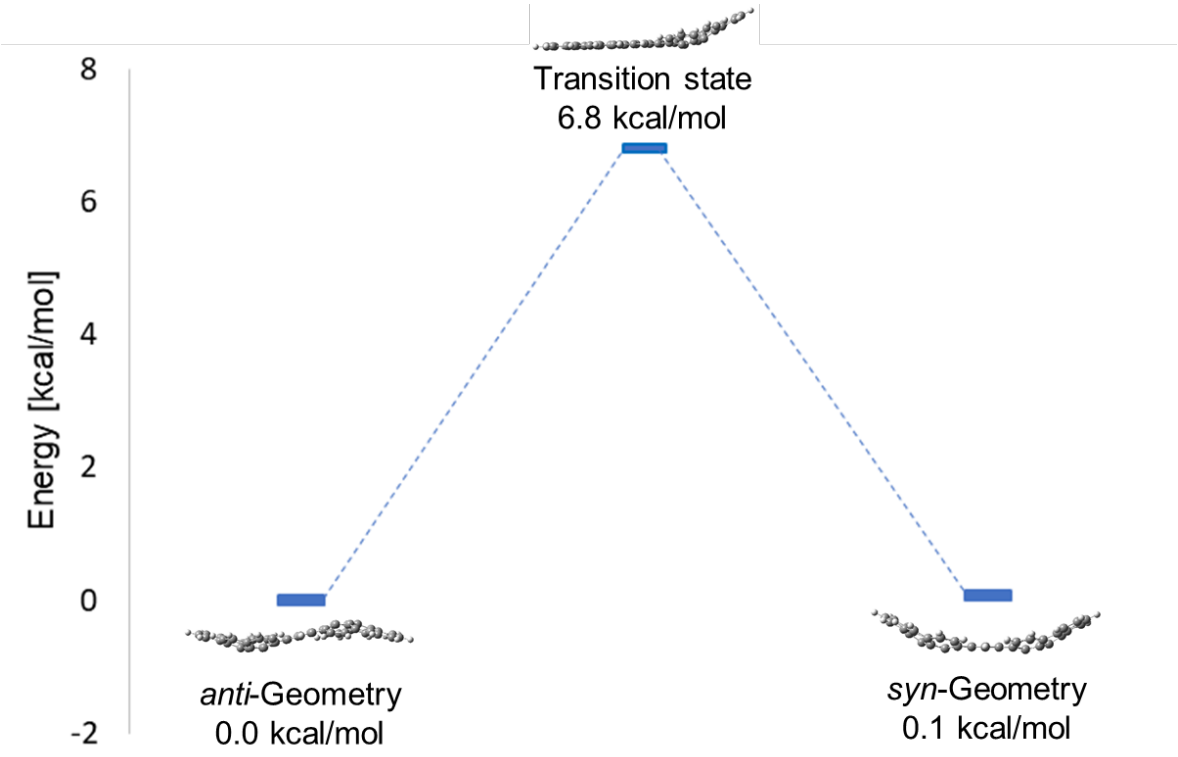


Figure S13. Bowl to bowl inversion of **1** through a transition state having one planar corannulene unit.

7. Self-Associations of 1 and 2 in $CDCl_3$.

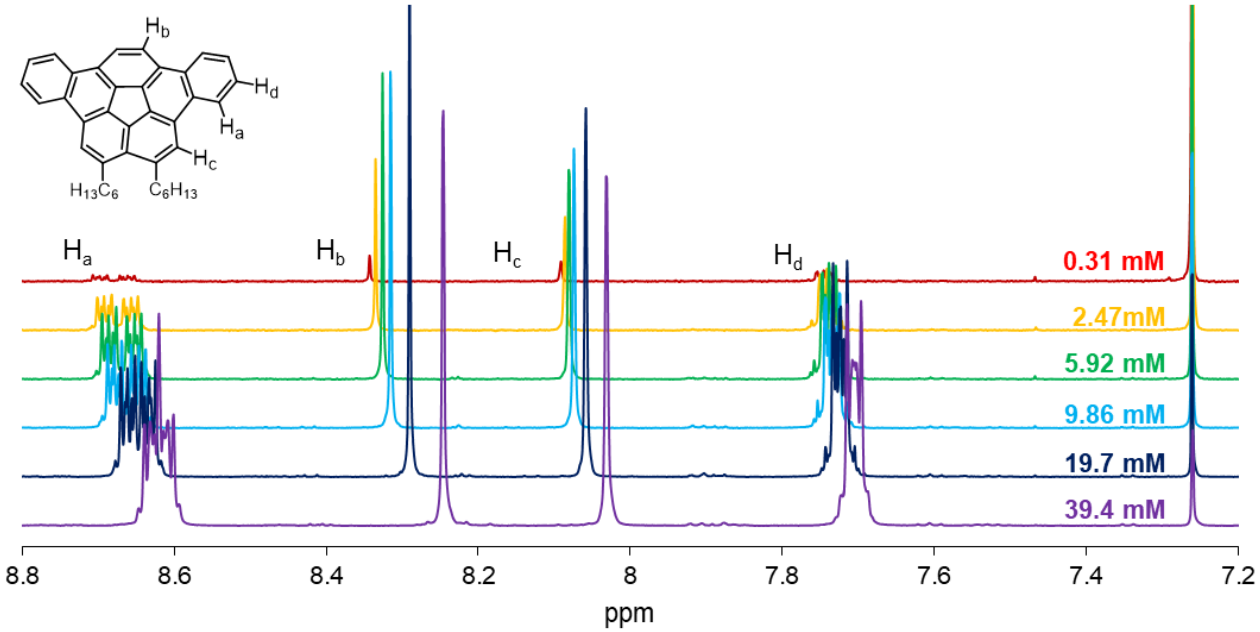


Figure 14. ^{1}H NMR (500 MHz) spectra of **2** at different solute concentrations in $CDCl_3$ at 25 °C. The signals of the aromatic hydrogens are slightly shifted to a low-magnetic field upon dilution.

Table S3. ^{1}H NMR dilution data of **1** in $CDCl_3$, calculated chemical shifts for monomer and dimer, and calculated association constants at 25 °C

concentration (mM)	Ha (ppm)
8.41	9.28
5.44	9.399
2.45	9.593
0.849	9.761
0.289	9.853
0.131	9.885
0.0410	9.908
calculated chemical shift for monomer (ppm)	9.910 ± 0.001
calculated chemical shift for dimer (ppm)	8.380 ± 0.018
association constants (M^{-1})	1.4×10^2

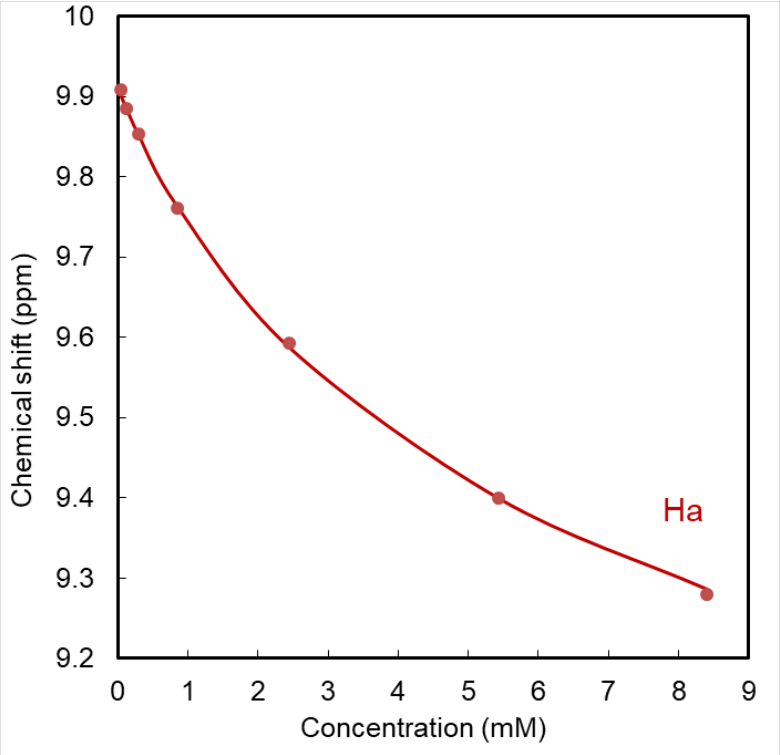


Figure S15. Concentration dependence of ^{1}H NMR chemical shifts for aromatic proton Ha of **1** in $CDCl_3$ at 25 °C. Red (Ha) line is curve fitting based on a monomer-dimer model.

Table S4. ^{1}H NMR dilution data of **2** in $CDCl_3$, calculated chemical shifts for monomer and dimer, and calculated association constants at 25 °C.

concentration (mM)	Hb (ppm)
39.4	8.246
19.7	8.291
11.8	8.310
9.86	8.316
5.92	8.326
4.93	8.328
2.47	8.335
1.23	8.340
0.616	8.342
0.308	8.343
calculated chemical shift for monomer (ppm)	8.344 ± 0.000
calculated chemical shift for dimer (ppm)	7.367 ± 0.45
association constants (M^{-1})	3.1 ± 0.2

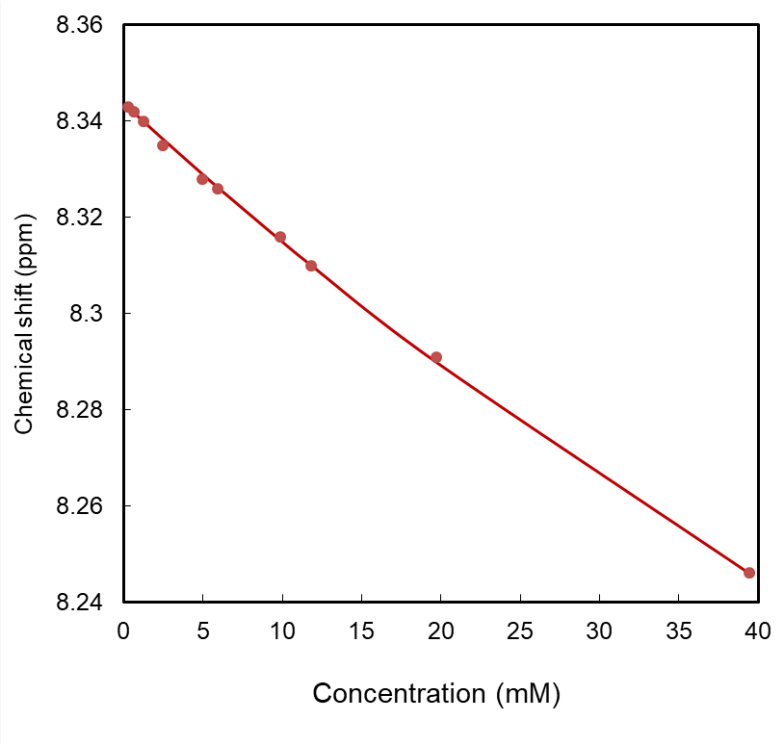


Figure S16. Concentration dependence of ^{1}H NMR chemical shifts for aromatic proton Hb of **2** in $CDCl_3$ at 25 °C. Red (Hb) line is curve fitting based on a monomer-dimer model.

8. Concentration-Dependent UV-vis and Emission Spectra of 1 in $CHCl_3$.

To address the interaction mode of the π-core of **1**, we performed the concentration-dependent UV-vis absorption and emission measurements in $CHCl_3$ at room temperature (Figure S17). In the absorption measurements, no changes in the absorption maxima were observed by changing the concentration of **1**. This indicates that molecule of **1** adopts various interaction modes in solution. The emission spectra showed the attenuated luminescence upon increasing the solute concentration. Moreover, the relative intensities in the first and second maxima (424 nm and 444 nm) changed at concentrations. The intestines of the second maxima are larger than those of the first ones at the highest and second-highest concentrations, implying the intermolecular energy transfer.

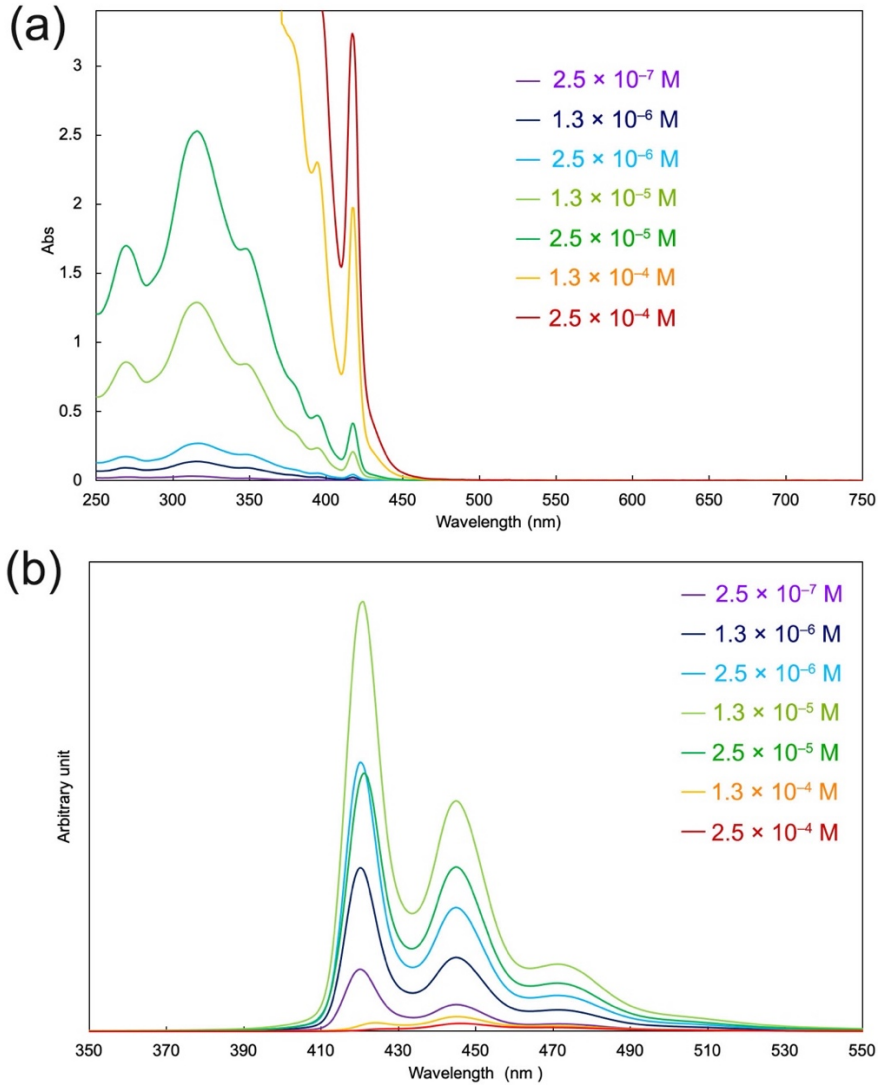


Figure S17. Concentration-dependent UV-vis and emission spectra of **1** in $CDCl_3$ at room temperature.

9. Dynamic Light Scattering Measurement of 1 in $CHCl_3$.

We performed the dynamic light scattering (DLS) measurement of a solution of **1** in $CHCl_3$ (1.5×10^{-4} M) at room temperature with a Zeta-potential & Particle size Analyzer, ELSZ (Otsuka Electronics) using a quartz cell (optical path of 10 mm). A representative particle distribution with the hydrodynamic diameter is shown in Figure S18. Small particles of a mean hydrodynamic diameter of 6 ± 7 nm from the 5 measurements were recorded.

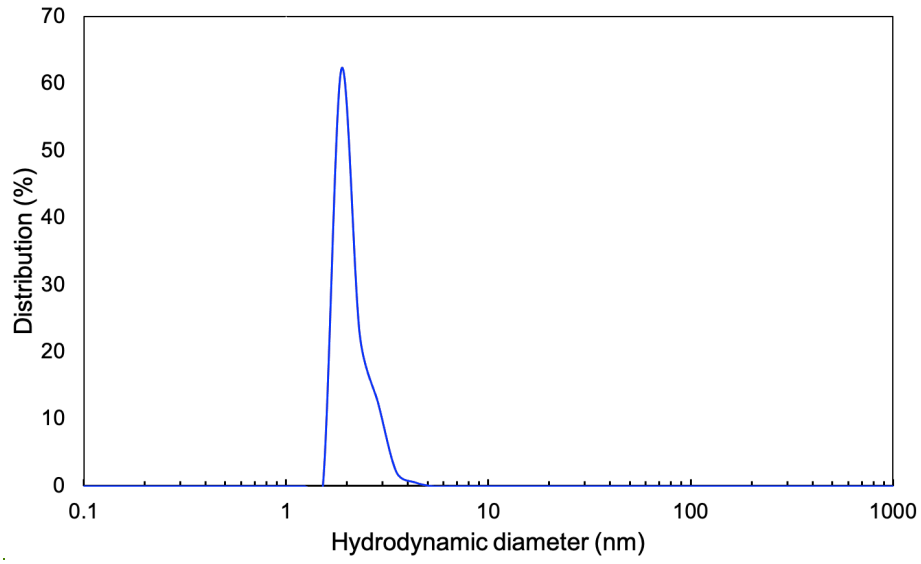


Figure S18. Representative DLS profile of a solution of **1** in $CHCl_3$ at room temperature.

10. Details of X-Ray Single Crystal Analysis.

Single crystals of **1** and **2** suitable for X-ray diffraction study were grown from EtOH/CH_2Cl_2 and hexane/CH_3CN, that are subjected to data collection. X-ray crystallography was performed on a Rigaku Mercury charge-coupled device (CCD) diffractometer at 173 K with graphite monochromated Mo-*K*α radiation (γ = 0.71075 Å) up to $2\theta_{max}$ = 60.6°. All calculations were performed by using the CrystalStructure crystallographic software package,[17] and structural refinements were made by using the SHELXL Version 2014/7 program.[18] The structures were solved by direct methods and expanded by using Fourier techniques. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using riding model and included in the structure factor calculations. The crystallographic data are summarized in Tables S5 and S6. The crystallographic data have been deposited to the Cambridge Crystallographic Data Center: Deposition numbers CCDC-2131853 for **1** and CCDC-2131864 for **2**. Copies of the data can be obtained free of charge via http://www.ccdc.cam.ac.uk/conts/retrieving.html (or from Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge, CB2 1EZ, UK; Fax+44 1223 336033; e-mail: deposit@ccdc.cam.ac.uk).

The atom numberings are shown in Figures S19 and S20. Other structural parameters, bond lengths and POAV angles, are summarized in Figures S21–S23.

The shortest intermolecular carbon-carbon distances are summarized in Tables S7 and S8. To visualize noncovalent intermolecular interactions in the crystal packing structures, we performed noncovalent interaction (NCI) analysis[19] at the B3LYP/6-31G(d,p) level of theory with Grimme's dispersion correction method D3[20] with Becke-Johnson damping[21] (D3BJ) (Figures 3d, 4d, S25 and S26). Basis set superposition error (BSSE) was corrected for all calculations using the counterpoise method.[22,23] This analysis visualizes the regions showing van der Waals interactions as green-colored isosurface, and the regions showing attractive or repulsive forces as a blue- or a red-colored isosurface, respectively. The isosurface values of all NCI plots were 0.60 a.u. The calculations for the NCI analysis were carried out with a Multiwfn program (ver. 3.8).[13] The visualization of NCI isosurfaces was performed using a VMD program (ver. 1.9.3).[24] The 2D reduced density gradient vs. sign(λ_2)ρ

plots (Figure S27) were visualized using Gnuplot 5.4.[25]

Table S5. Crystal Data and Structure Analysis Results for **1**.

Identification code	**1**
Empirical Formula	$C_{74}H_{70}$
Formula weight	959.37
Temperature	173 K
Wavelength	0.71073 Å
Crystal system	triclinic
Space group	*P-1*
Unit cell dimensions	a = 12.4769 (4) Å
	b = 14.4138 (5) Å
	c = 16.7423 (5) Å
	γ = 74.243°
Volume	V = 2612.52 (16) Å^3
Z	2
Density	1.219 g/cm^3
Absorption coefficient	0.684 cm^{-1}
F(000)	1028
Crustal size	0.250 × 0.050 × 0.050 mm^3
Reflections collected	32935
Independent reflections	13584 (R_{int} = 0.0466)
Absorption correction	empirical
Refinement method	full-matrix least-squares refinement on F_2
Data / restraints / parameters	13584 / 0 / 861
Goodness-of-fit	1.011
Final R indices [I>2sigma(I)]	$R1$ = 0.0631, $wR2$ = 0.1539
R indices (all data)	$R1$ = 0.1343, $wR2$ = 0.1539
Lardest diff. peak and hole	0.28 and –0.25 e. Å^3

Table S6. Crystal Data and Structure Analysis Results for **2**.

Identification code	**2**
Empirical Formula	$C_{40}H_{38}$
Formula weight	518.74
Temperature	173 K
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	$P\,2_1/c$
Unit cell dimensions	a = 9.5637 (3) Å
	b = 12.6304 (3) Å
	c = 23.2406 (6) Å
	γ = 92.682 (2)°
Volume	V = 2804.24 (13) Å^3
Z	4
Density	1.229 g/cm^3
Absorption coefficient	0.689 cm^{-1}
F(000)	1112
Crustal size	0.200 × 0.100 × 0.100 mm^3
Reflections collected	34268
Independent reflections	7568 (R_{int} = 0.0398)
Absorption correction	empirical
Refinement method	full-matrix least-squares refinement on F_2
Data / restraints / parameters	7568 / 0 / 363
Goodness-of-fit	1.026
Final R indices [I>2sigma(I)]	$R1$ = 0.0489, $wR2$ = 0.1312
R indices (all data)	$R1$ = 0.0704, $wR2$ = 0.1312
Largest diff. peak and hole	0.31 and –0.25 e. Å^3

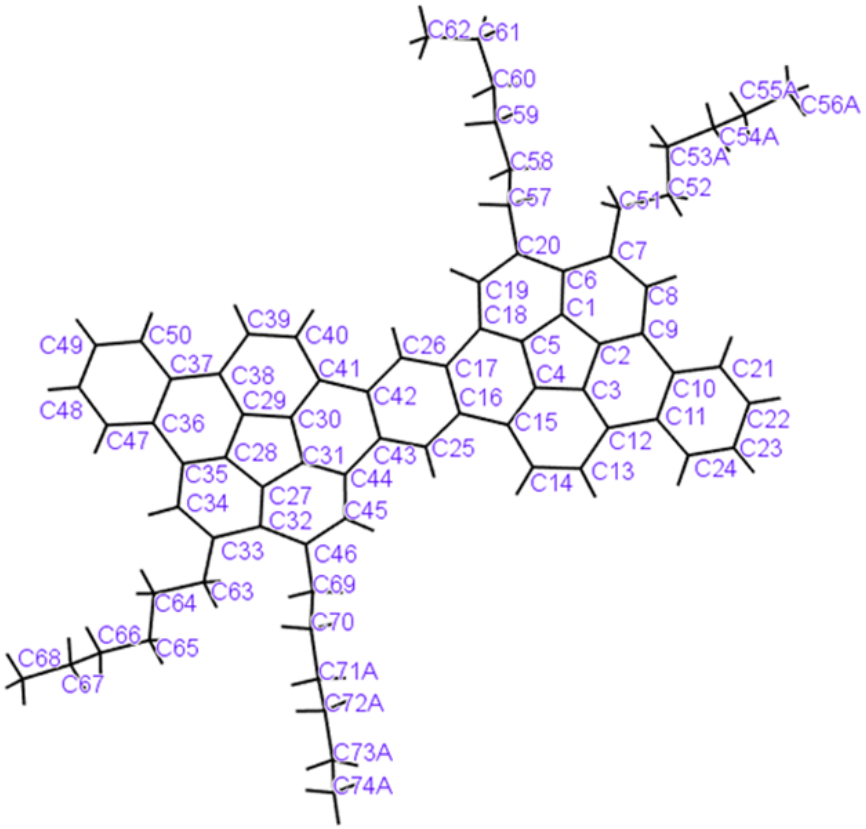


Figure S19. X-ray structure with atom numberings of **1**.

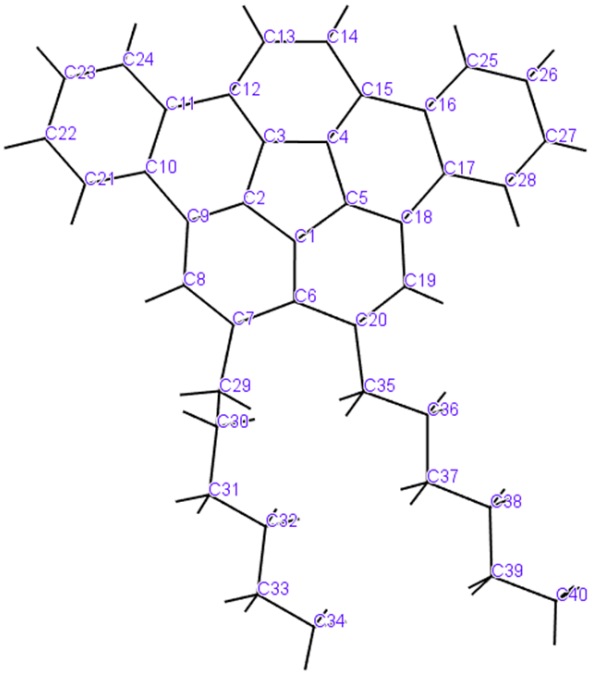


Figure S20. X-ray structure with atom numberings of **2**.

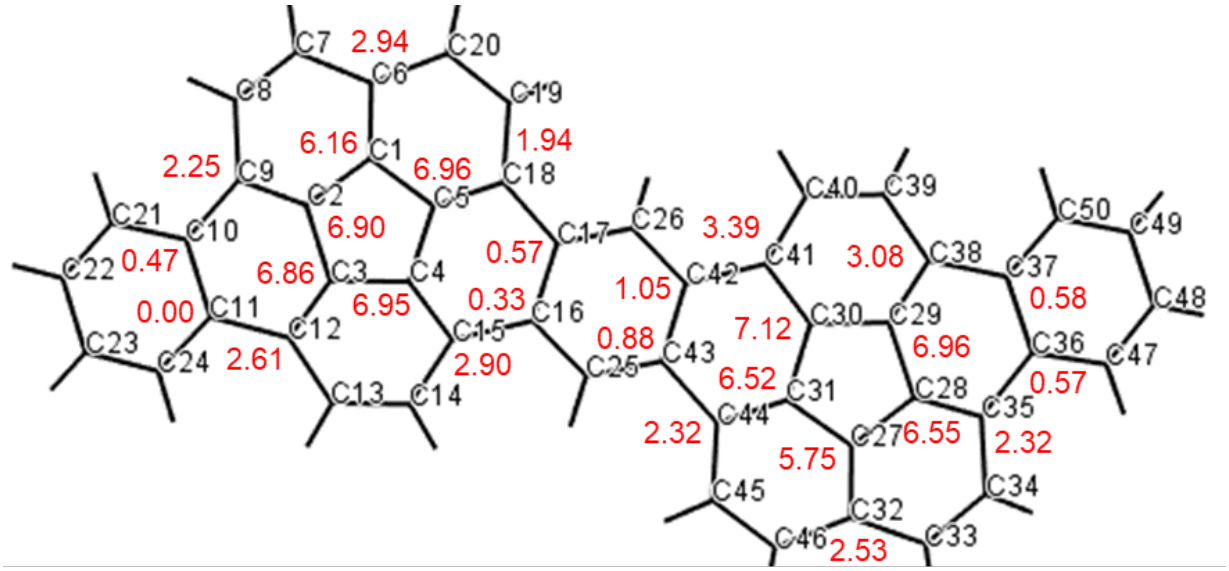


Figure S21. POAV pyramidalization angles (red numbers) of each quaternary carbon atom of **1**.

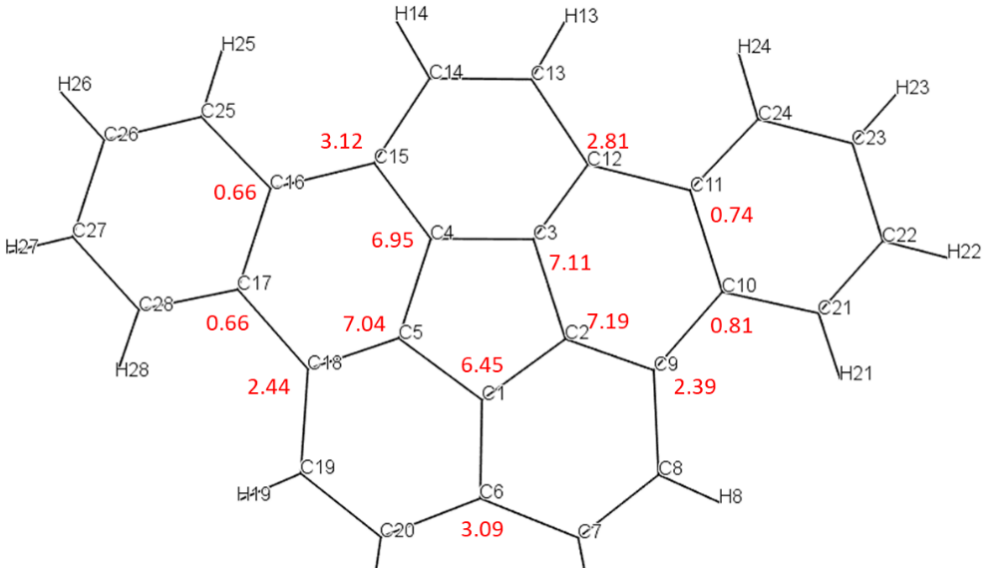


Figure S22. POAV pyramidalization angles (red numbers) of each quaternary carbon atom of **2**.

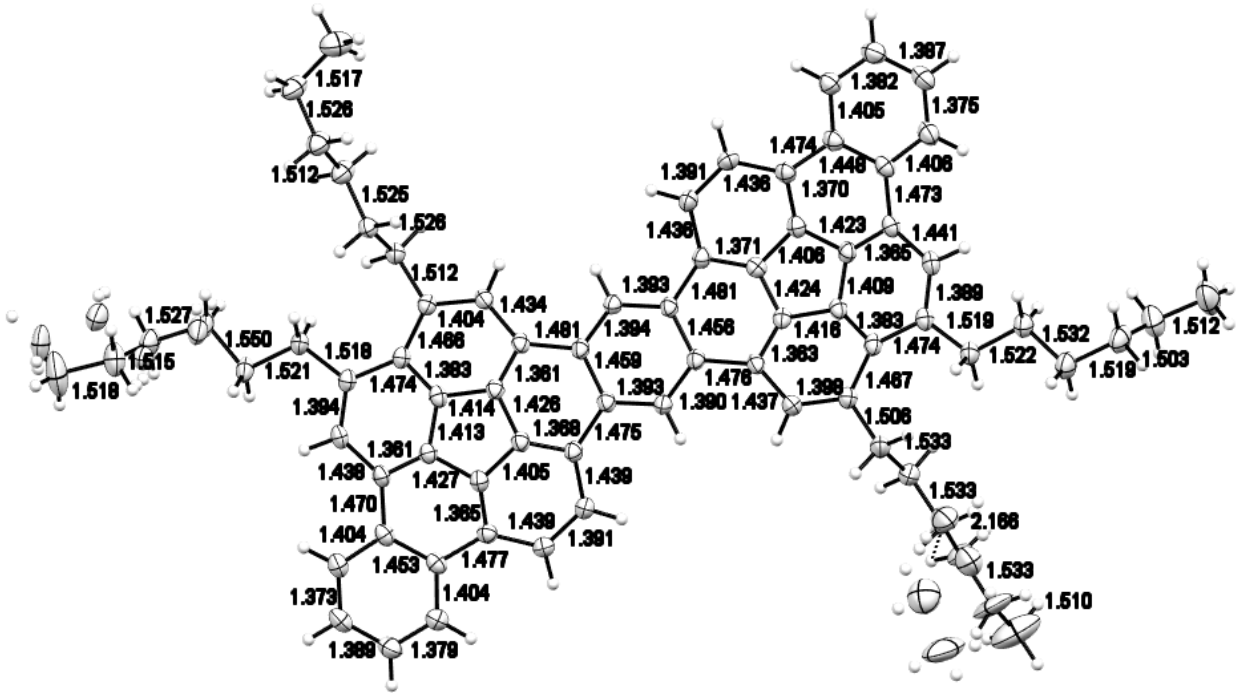


Figure S23. X-ray structure with carbon-carbon bond lengths of **1**.

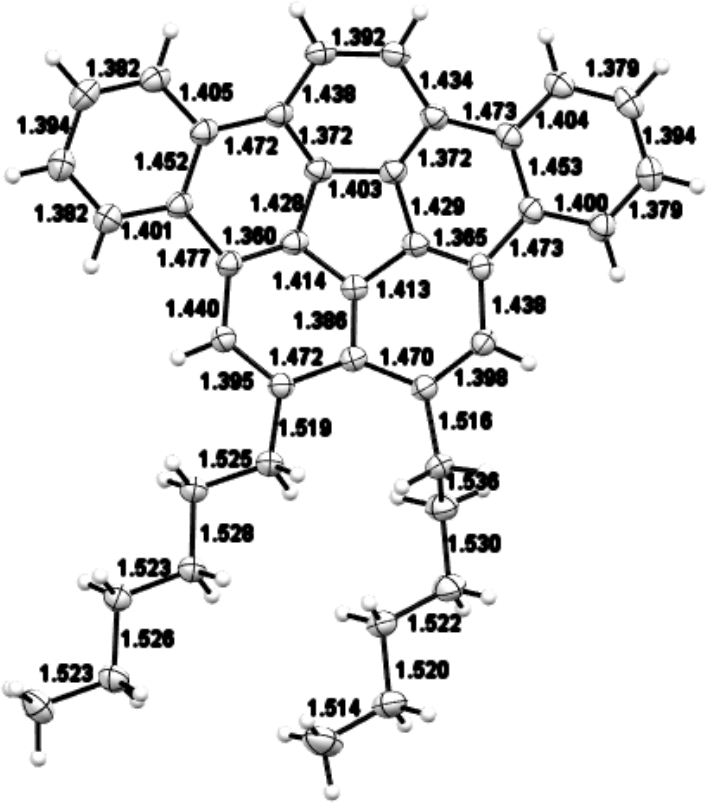


Figure S24. X-ray structure with carbon-carbon bond lengths of **2**.

Table S7. The Closest Interatomic Distances between Adjacent Molecules in Crystal Structure of **1**.

atom of molecule A	atom of molecule B	distance (Å)
C1	C30	3.63
C2	C29	3.72
C3	C39	3.98
C4	C40	3.96
C5	C30	3.70
C6	C31	3.55
C7	C28	3.27
C8	C28	3.42
C9	C29	3.58
C10	C37	3.62
C11	C38	3.86
C12	C39	3.73
C13	C39	3.85
C14	C40	3.87
C15	C40	3.75
C16	C41	3.94
C17	C42	3.55
C18	C41	3.57
C19	C43	3.7
C20	C20	3.18
C21	C50	3.59
C22	C50	3.58
C23	C50	3.74
C24	C50	3.89
C25	C26	4.13
C26	C26	3.45
C27	C7	3.55
C28	C7	3.27
C29	C9	3.58
C30	C18	3.6
C31	C20	3.18
C32	C51	3.9
C33	C51	4.04
C34	C52	3.79
C35	C8	3.75
C36	C8	3.98

Table S7 (continued). The Closest Interatomic Distances between Adjacent Molecules in Crystal Structure of **1**.

C37	C10	3.62
C38	C9	3.65
C39	C12	3.73
C40	C15	3.75
C41	C18	3.57
C42	C17	3.55
C43	C19	3.7
C44	C19	3.61
C45	C57	3.8
C46	C57	3.96
C47	C21	4.29
C48	C22	4.14
C49	C22	3.56
C50	C22	3.58

Table S8. The Closest Interatomic Distances between Adjacent Molecules in Crystal Structure of **2**.

atom of molecule A	atom of molecule B	distance (Å)
C1	C38	3.48
C2	C37	3.55
C3	C22	3.76
C4	C22	3.49
C5	C39	3.48
C6	C23	3.32
C7	C36	4.2
C8	C36	4.05
C9	C36	3.96
C10	C17	4.1
C11	C32	3.81
C12	C33	3.94
C13	C36	3.69
C14	C38	3.75
C15	C22	3.57
C16	C23	3.63
C17	C21	3.59
C18	C22	3.52
C19	C24	3.7
C20	C24	3.47
C21	C17	3.57
C22	C5	3.47
C23	C6	3.32
C24	C19	3.69
C25	C24	3.32
C26	C11	3.63
C27	C23	3.78
C28	C23	3.54

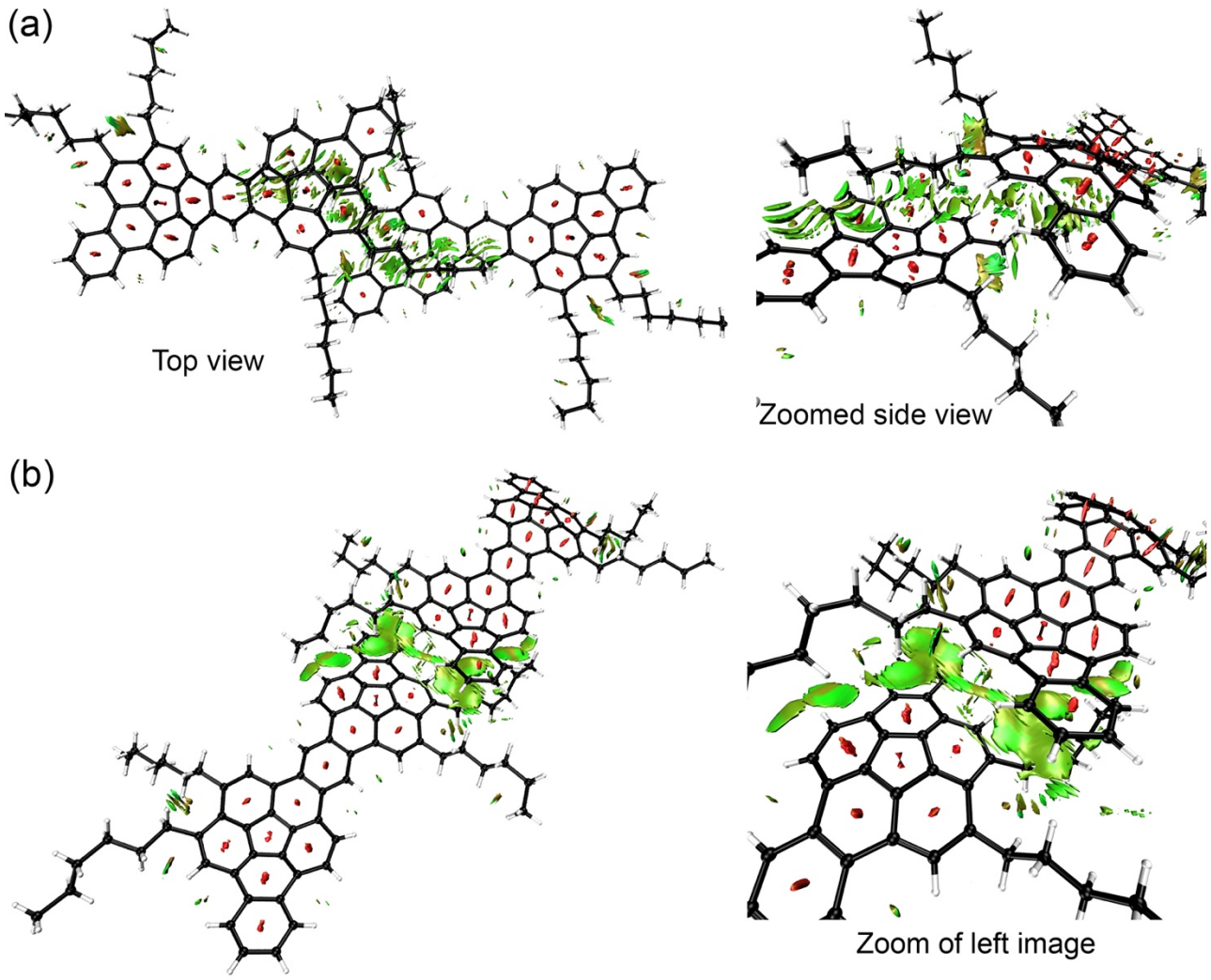


Figure S25. Non-covalent interaction (NCI) plots of the two molecules of **1** in the crystal structure (isovalue: 0.60). (a) (C-H)-π interactions between the hexyl groups and corannulene units. (b) (C-H)-π interactions between the methylene units of the hexyl chains and peripheral fused benzene rings.

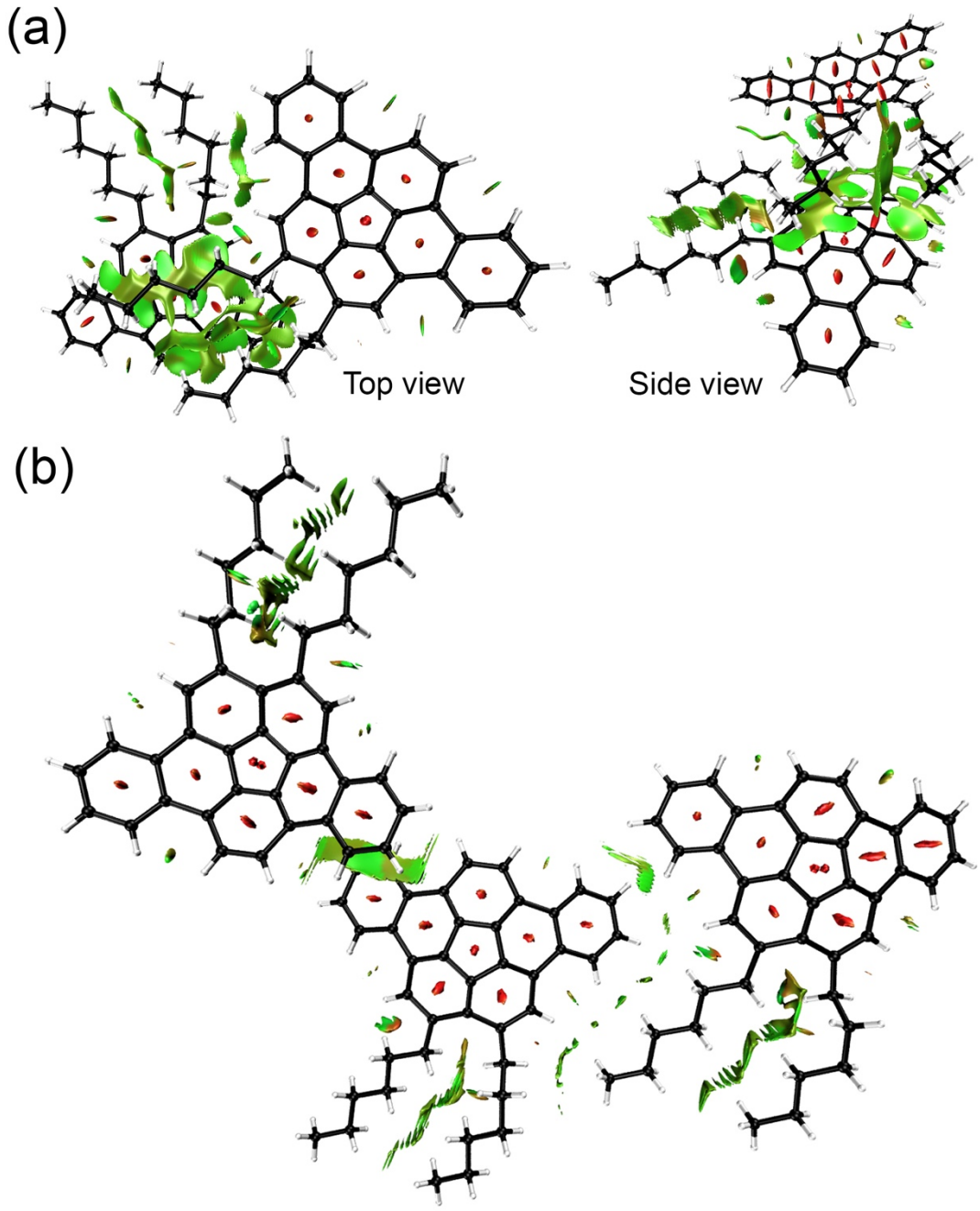


Figure S26. Non-covalent interaction (NCI) plots of the two or three molecules of **2** in the crystal structure (isovalue: 0.60). (a) (C-H)-π interactions between the hexyl groups and corannulene units. (b) π-π interactions between the peripheral fused benzene rings.

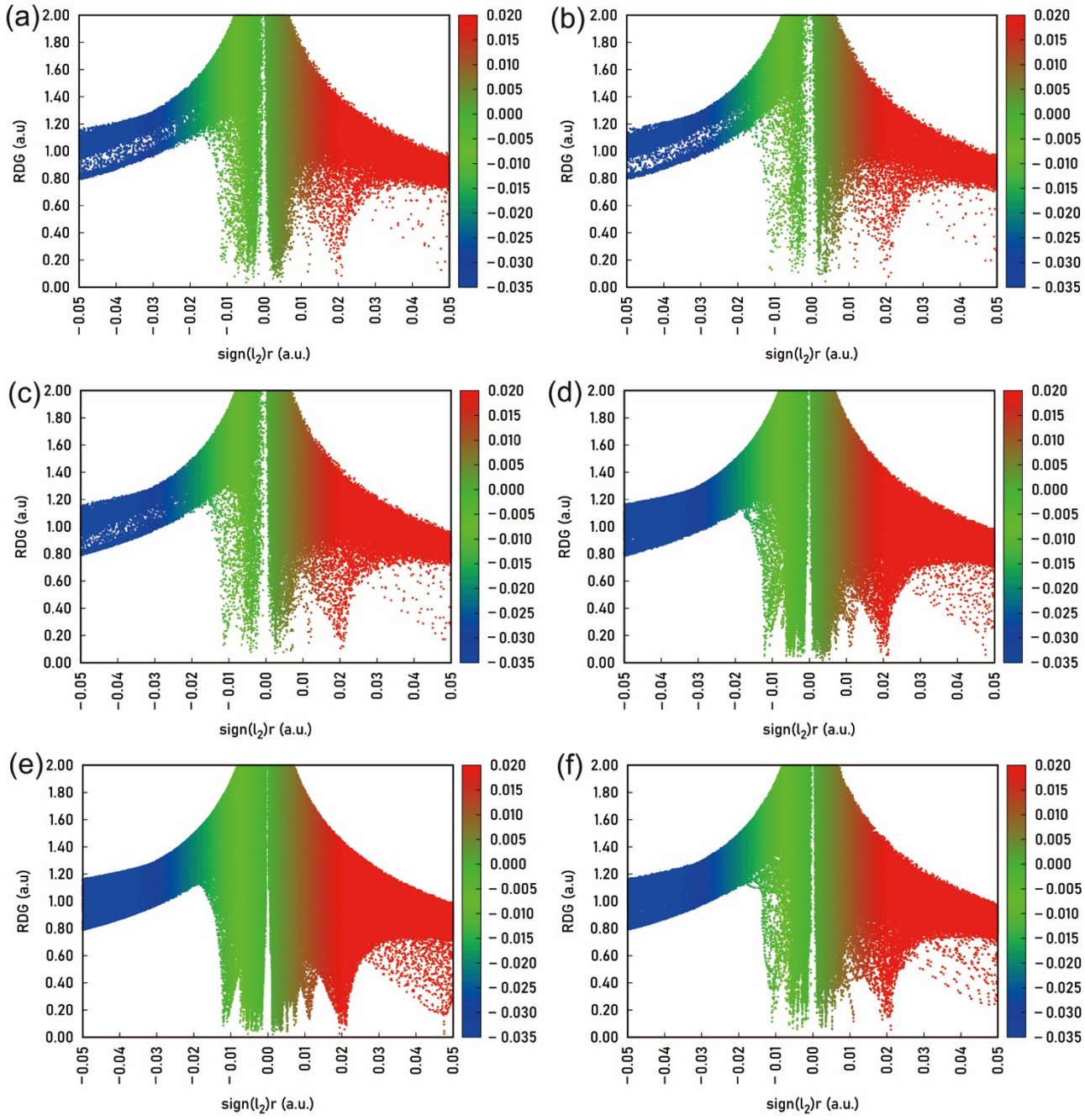


Figure S27. The 2D reduced density gradient vs. sign(λ_2)ρ plots of the NCI plots of (a) Figure 3d (main text), (b) Figure S25a, (c) Figure S25b, (d) Figure 4d (main text), (e) Figure S26a, and (f) Figure S26b.

11. Details of Interaction Energy Calculations.

To estimate intermolecular interaction energies, the geometry optimization of the model compounds of **1** and **2** that have methyl groups instead of the hexyl groups were performed by DFT calculations with B97D/cc-pvdz level of theory for the dimers (Figure 5) with different configurations. For all geometries, no symmetric constraint was applied. Basis set superposition error (BSSE) was corrected for all calculations using the counterpoise method.[22,23] The energies of intermolecular interactions (E_{inter}) were calculated by the following equation.

E_{inter} = (total energy of dimer) – (total energy of monomer) × 2

12. ^{1}H and/or ^{13}C{^{1}H} NMR Spectra of All Compounds

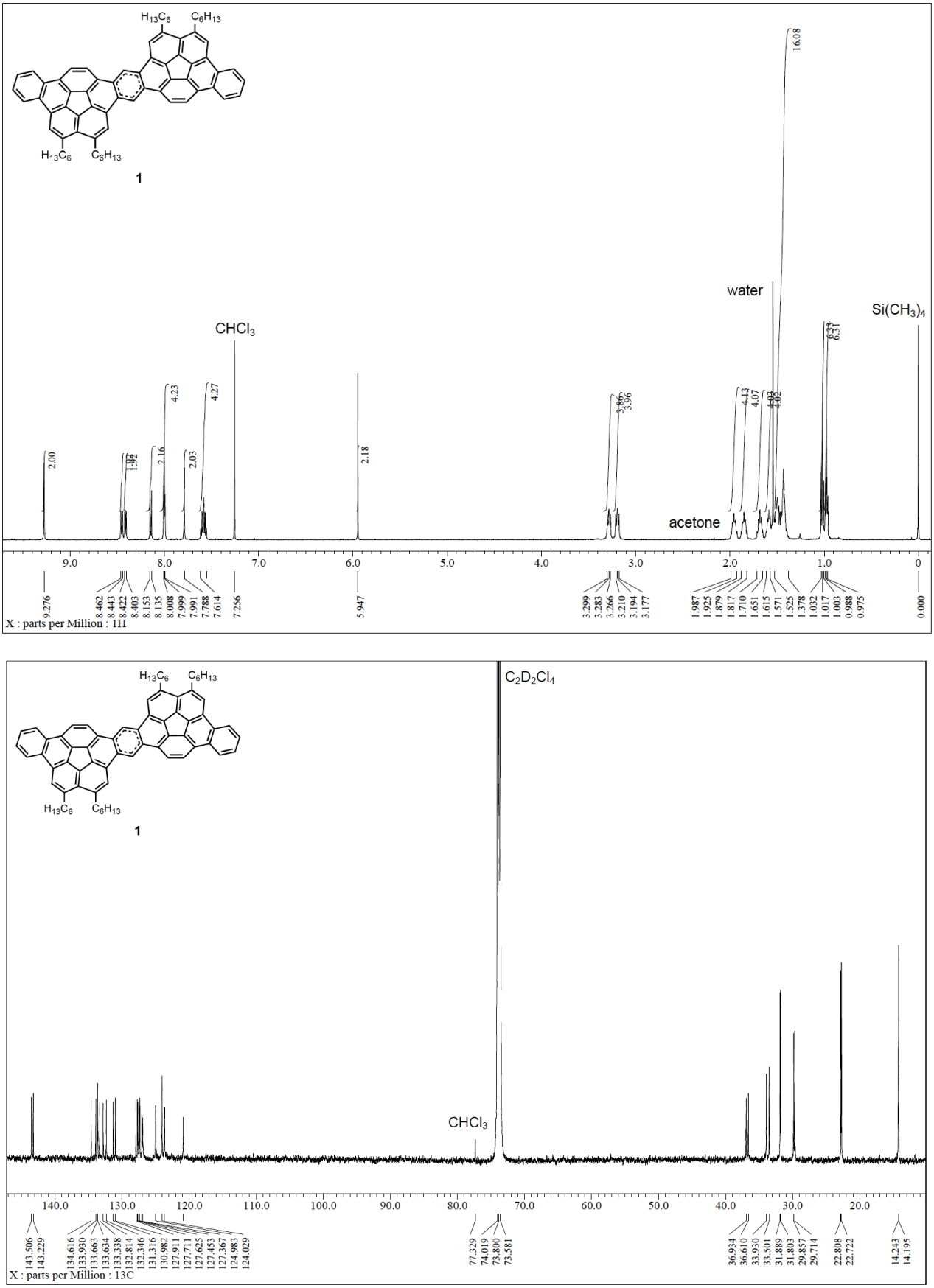
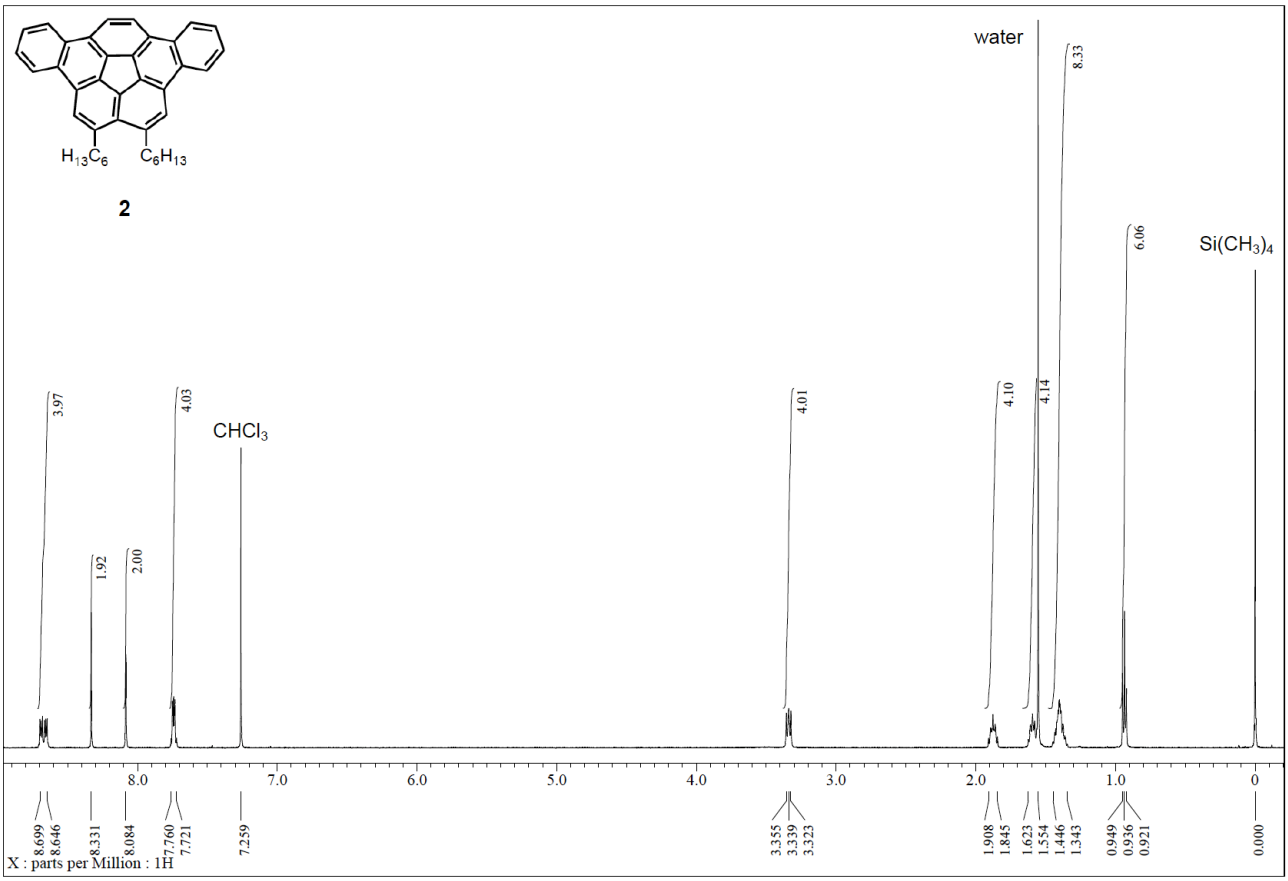


Figure S28. ^{1}H (top, 500 MHz) and ^{13}C{^{1}H} NMR (bottom, 126 MHz) NMR spectra of compound **1** in $CDCl_3$ (^{1}H) and CD_4Cl_2 (^{13}C) at 25.0 °C (^{1}H) and 24.9 °C (^{13}C).



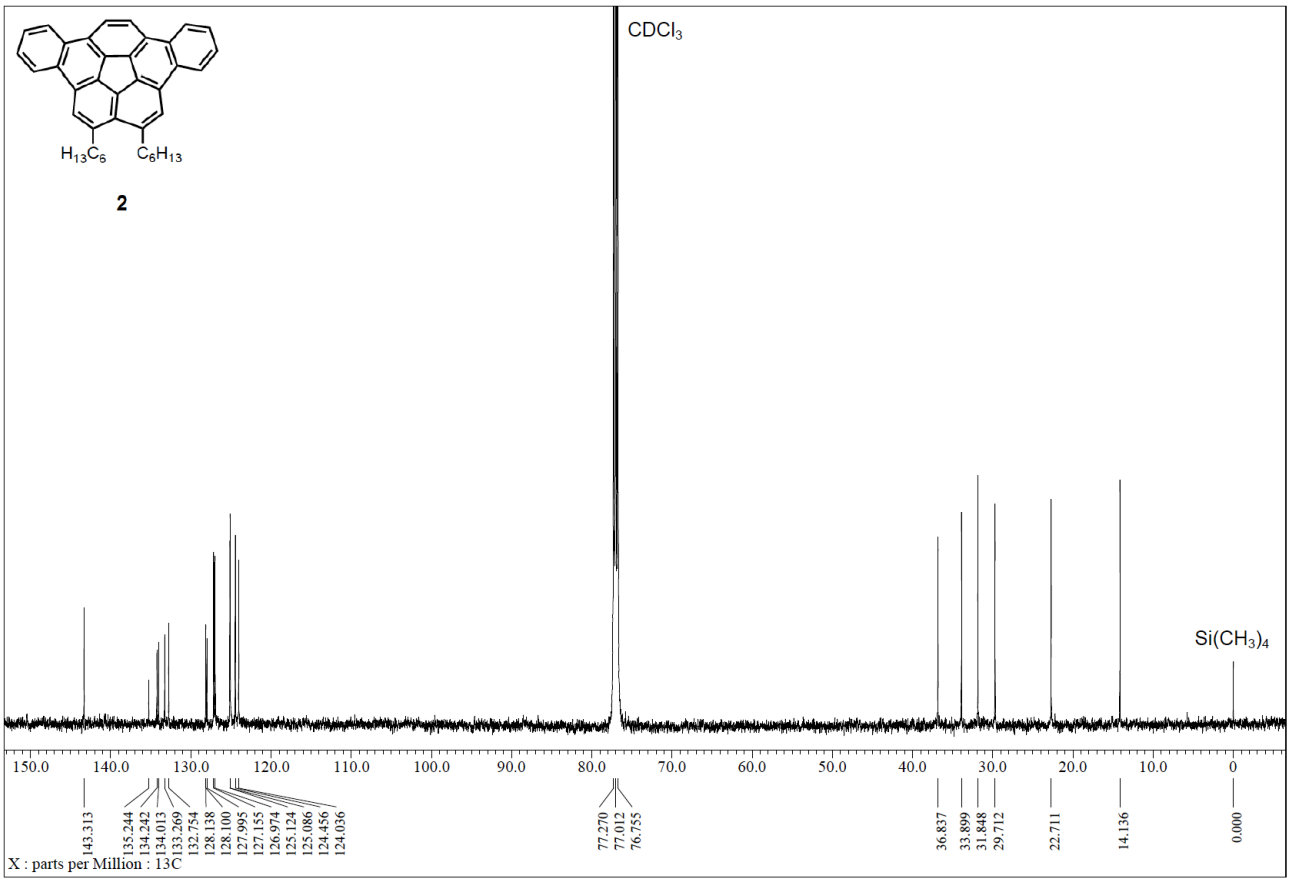
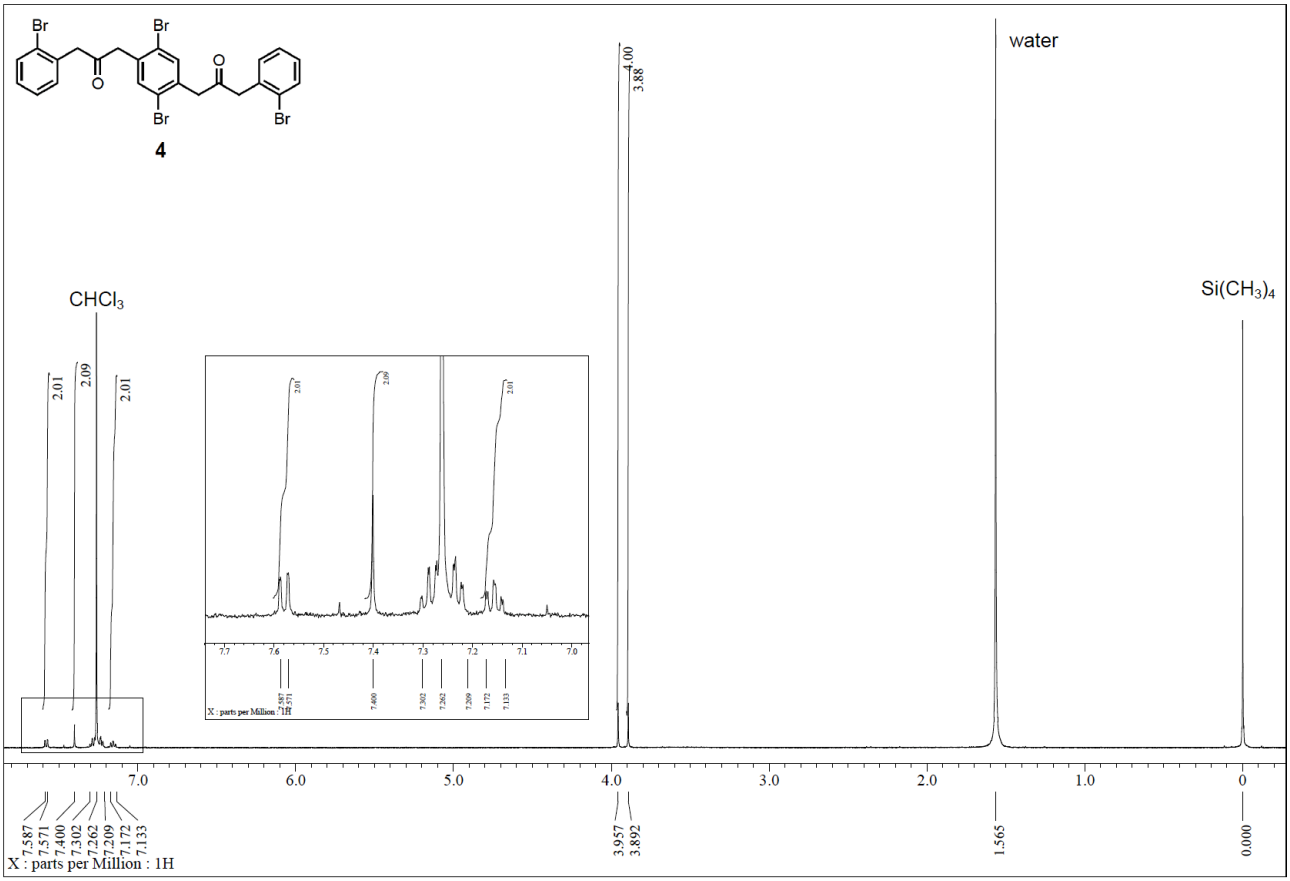


Figure S29. ^{1}H (top, 500 MHz) and $^{13}C\{^{1}H\}$ NMR (bottom, 126 MHz) NMR spectra of compound **2** in $CDCl_3$ at 23.1 °C (^{1}H) and 21.4 °C (^{13}C).



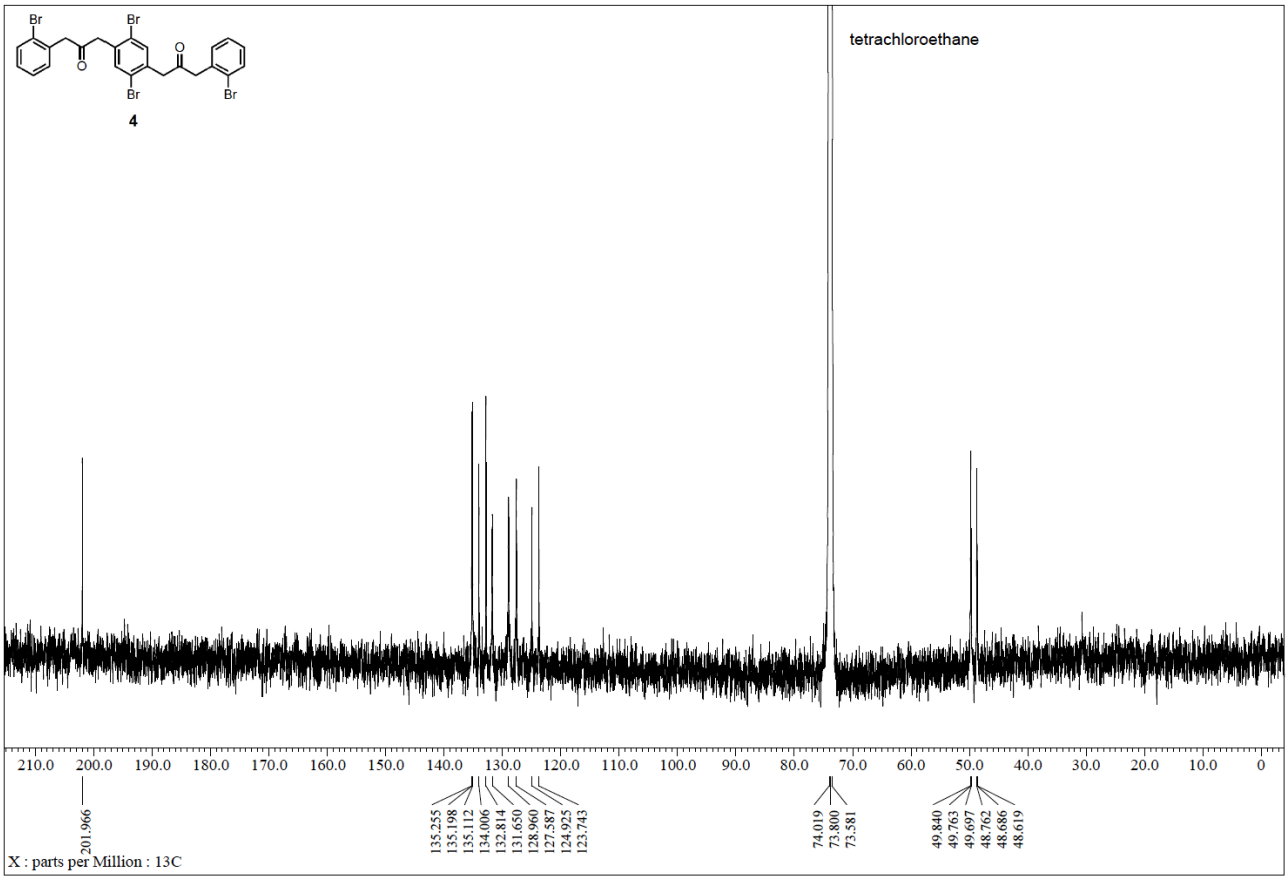


Figure S30. ^{1}H (top, 500 MHz) and ^{13}C{^{1}H} NMR (bottom, 126 MHz) NMR spectra of compound **4** in $CDCl_3$ and 1,1,2,2-tetrachloroethane-d_2 at 23.8 °C (^{1}H) and 60.0 °C (^{13}C).

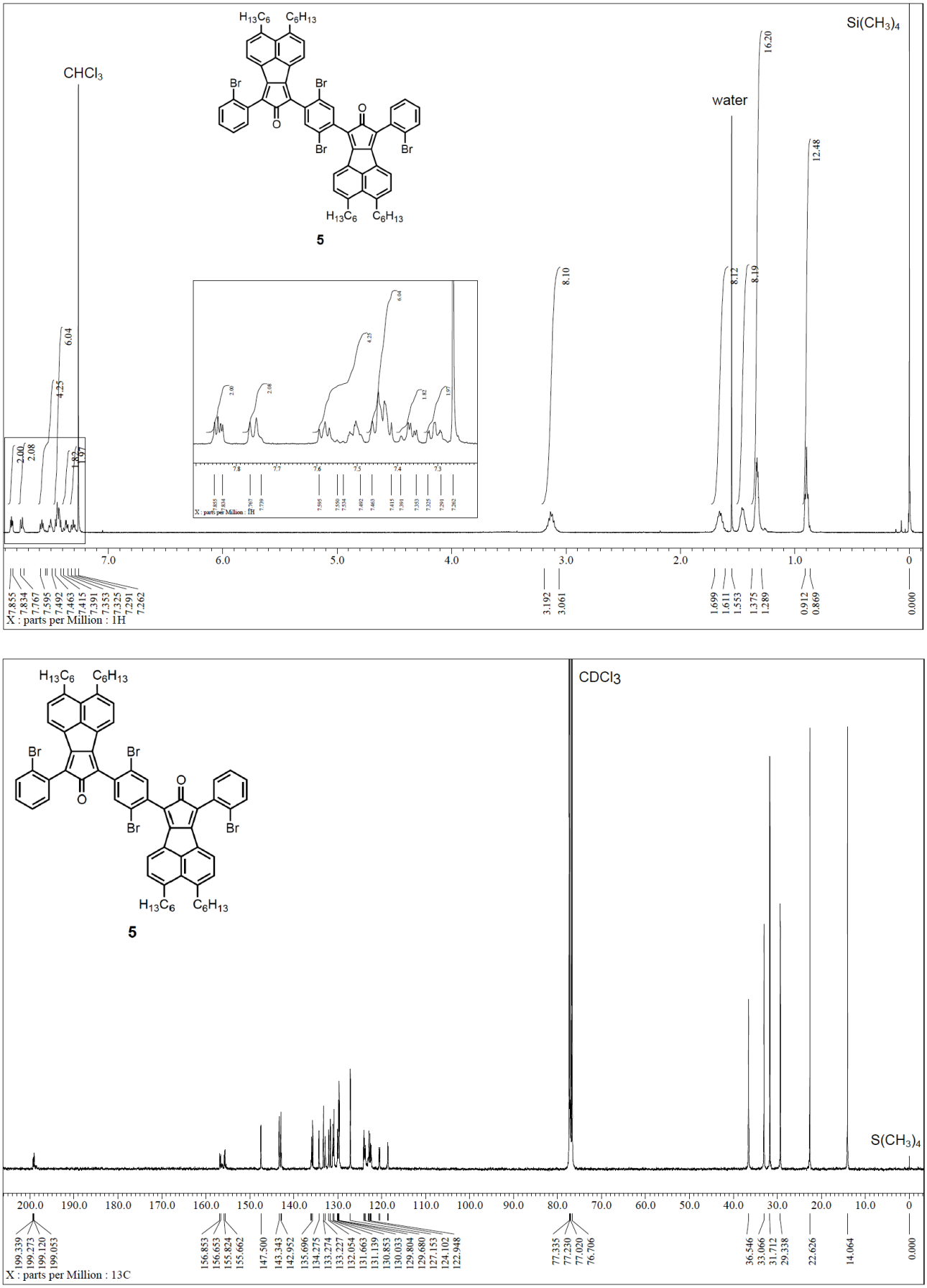
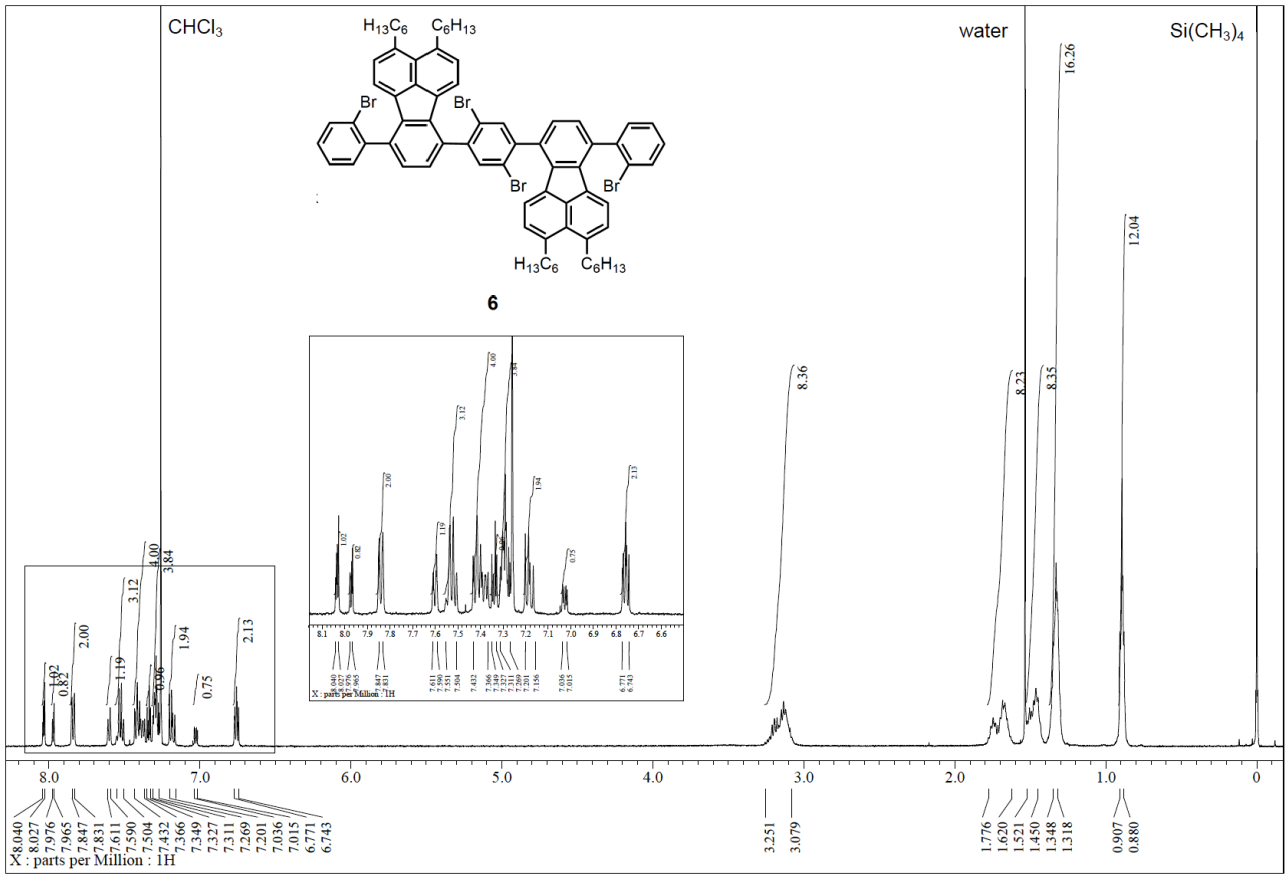


Figure S31. ^{1}H (top, 500 MHz) and ^{13}C{^{1}H} NMR (bottom, 101 MHz) NMR spectra of compound **5** in $CDCl_3$ at 18.3 °C (^{1}H) and 25.0 °C (^{13}C).



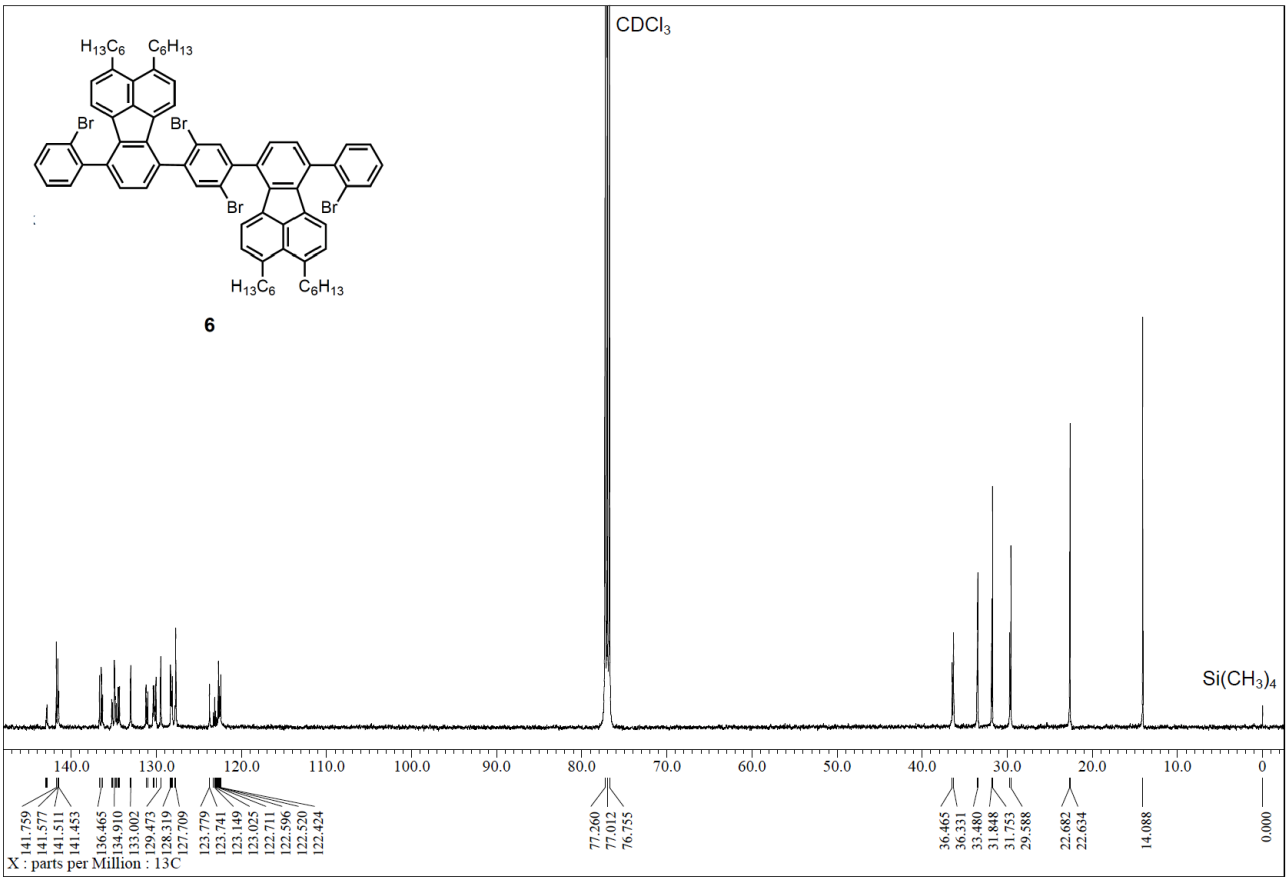
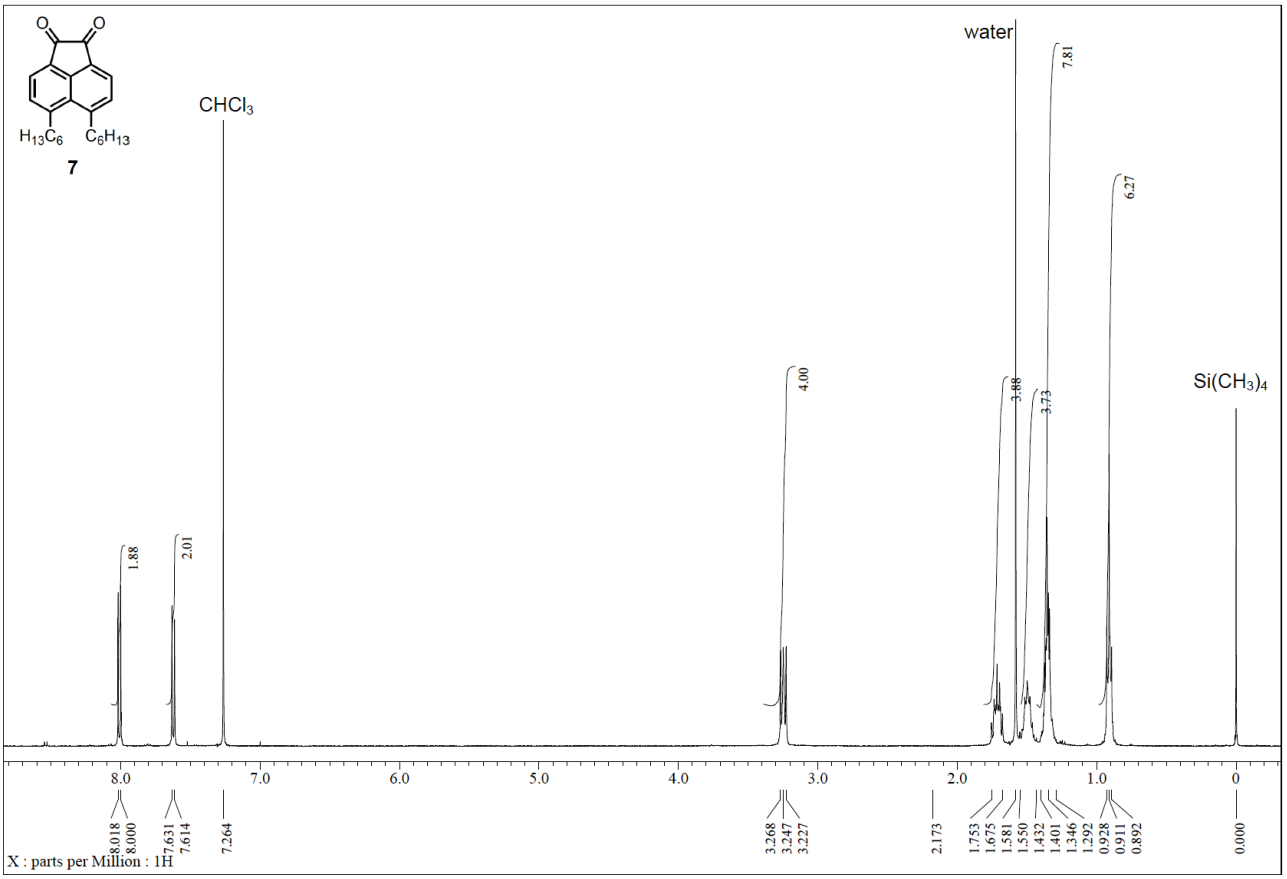


Figure S32. ^{1}H (top, 500 MHz) and $^{13}C\{^{1}H\}$ NMR (bottom, 126 MHz) NMR spectra of compound **6** in $CDCl_3$ at 25.0 °C (^{1}H) and 21.4 °C (^{13}C).



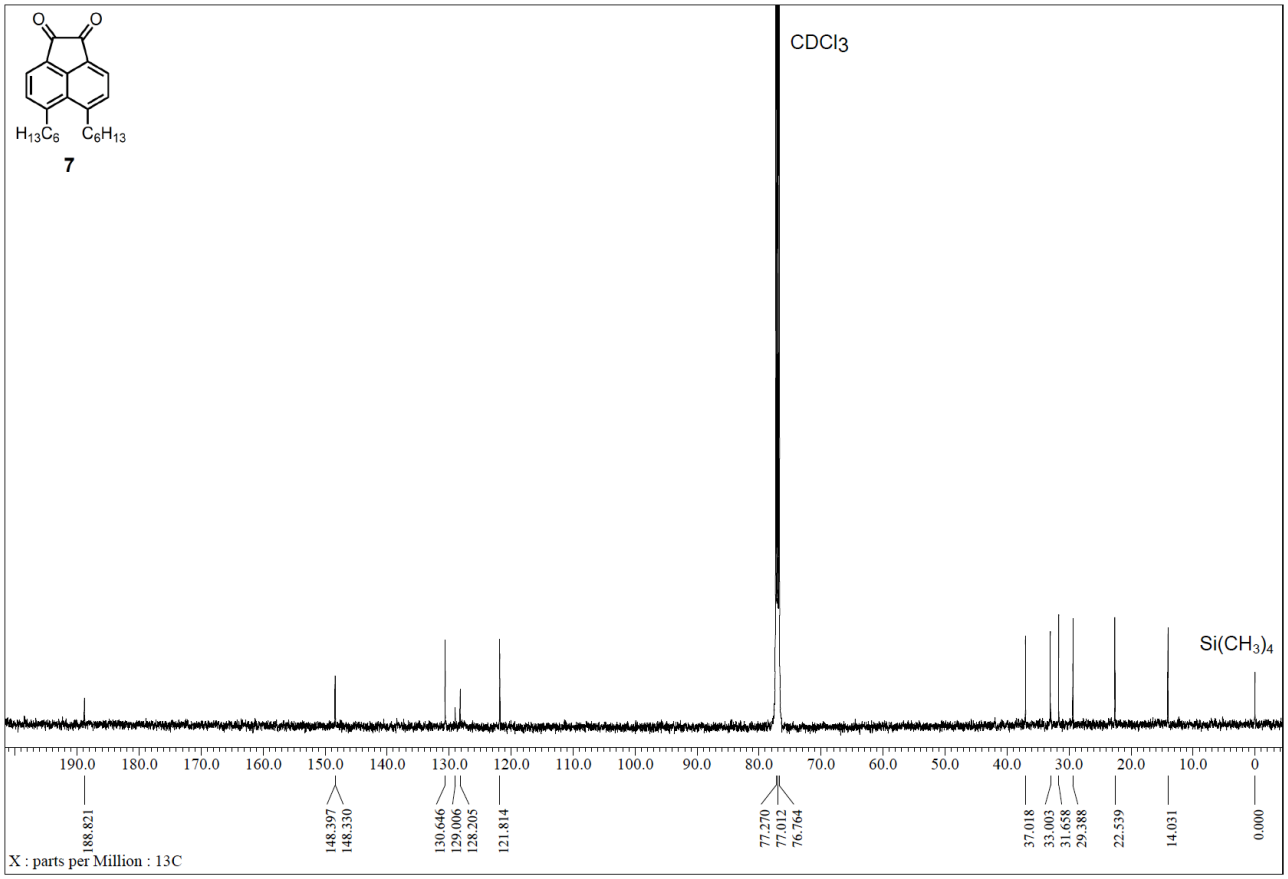
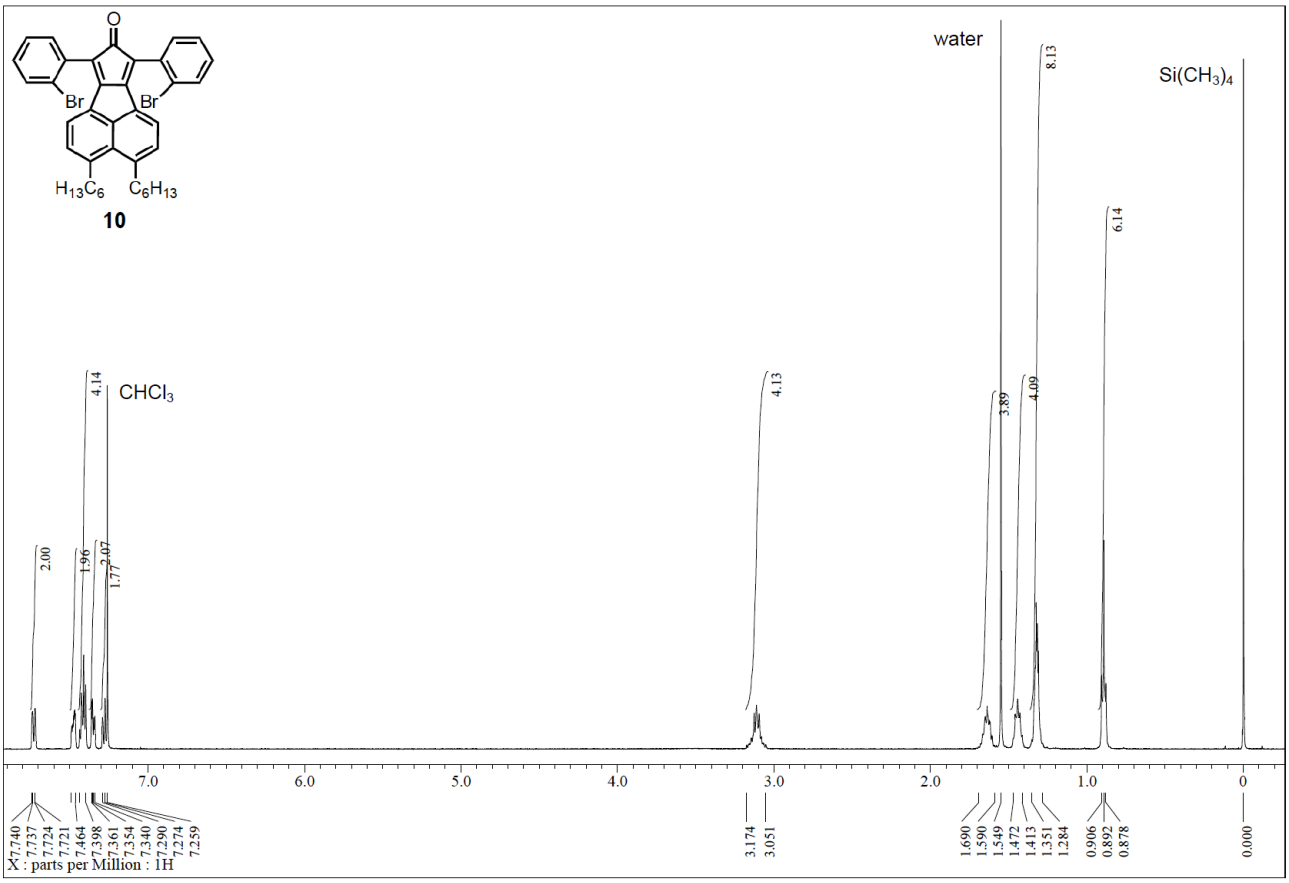


Figure S33. ^{1}H (top, 400 MHz) and ^{13}C{^{1}H} NMR (bottom, 126 MHz) NMR spectra of compound **7** in $CDCl_3$ at 23.6 °C (^{1}H) and 25.5 °C (^{13}C).



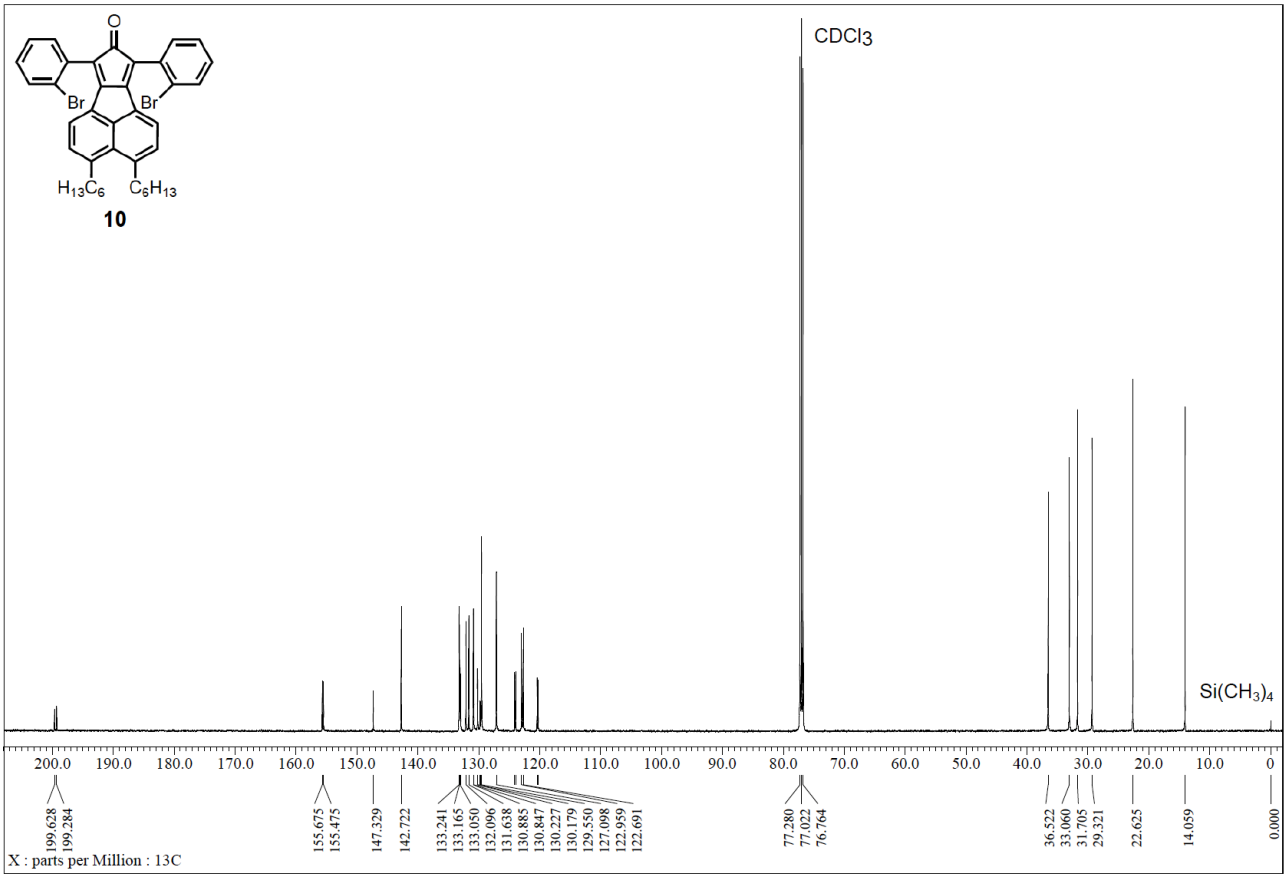
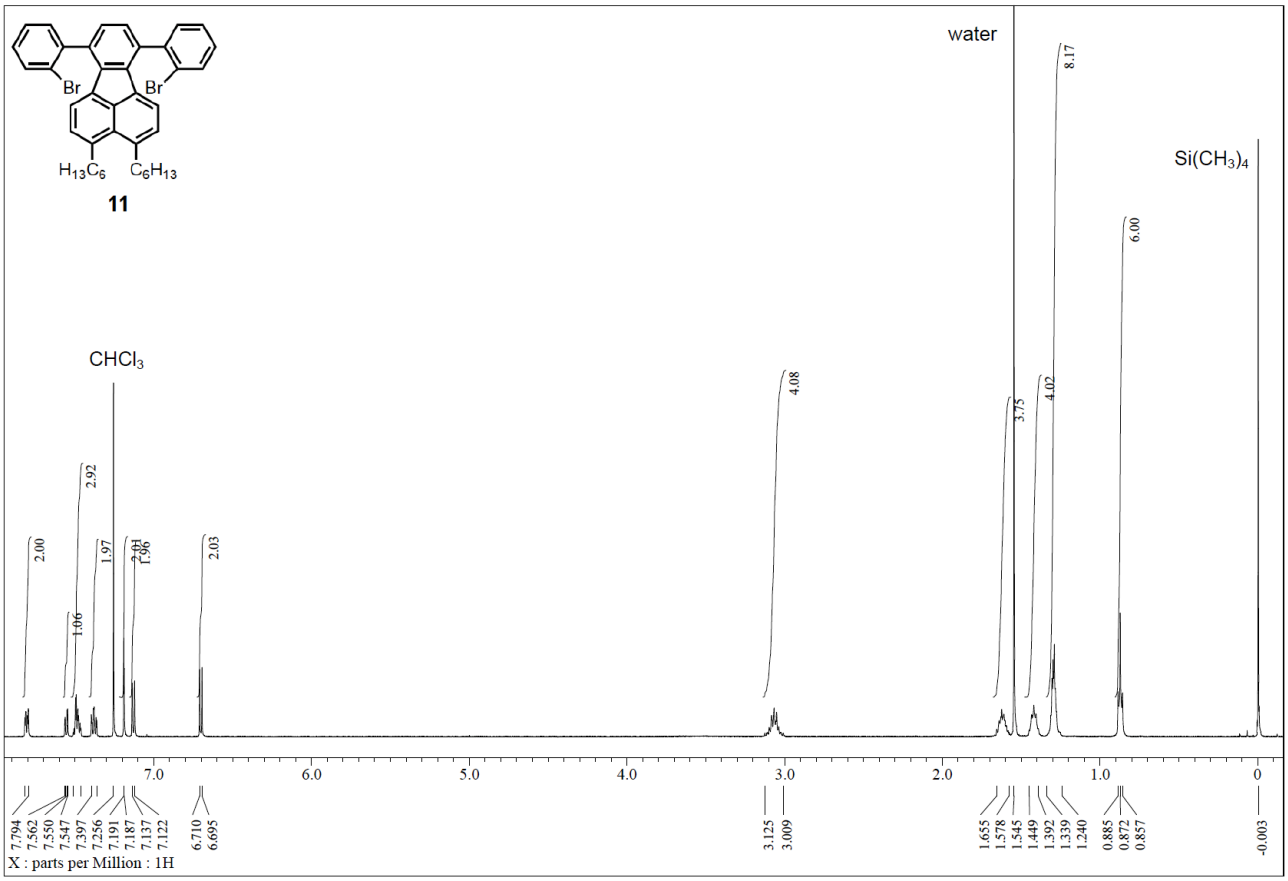


Figure S34. ^{1}H (top, 500 MHz) and $^{13}C\{^{1}H\}$ NMR (bottom, 126 MHz) NMR spectra of compound **10** in $CDCl_3$ at 25.0 °C.



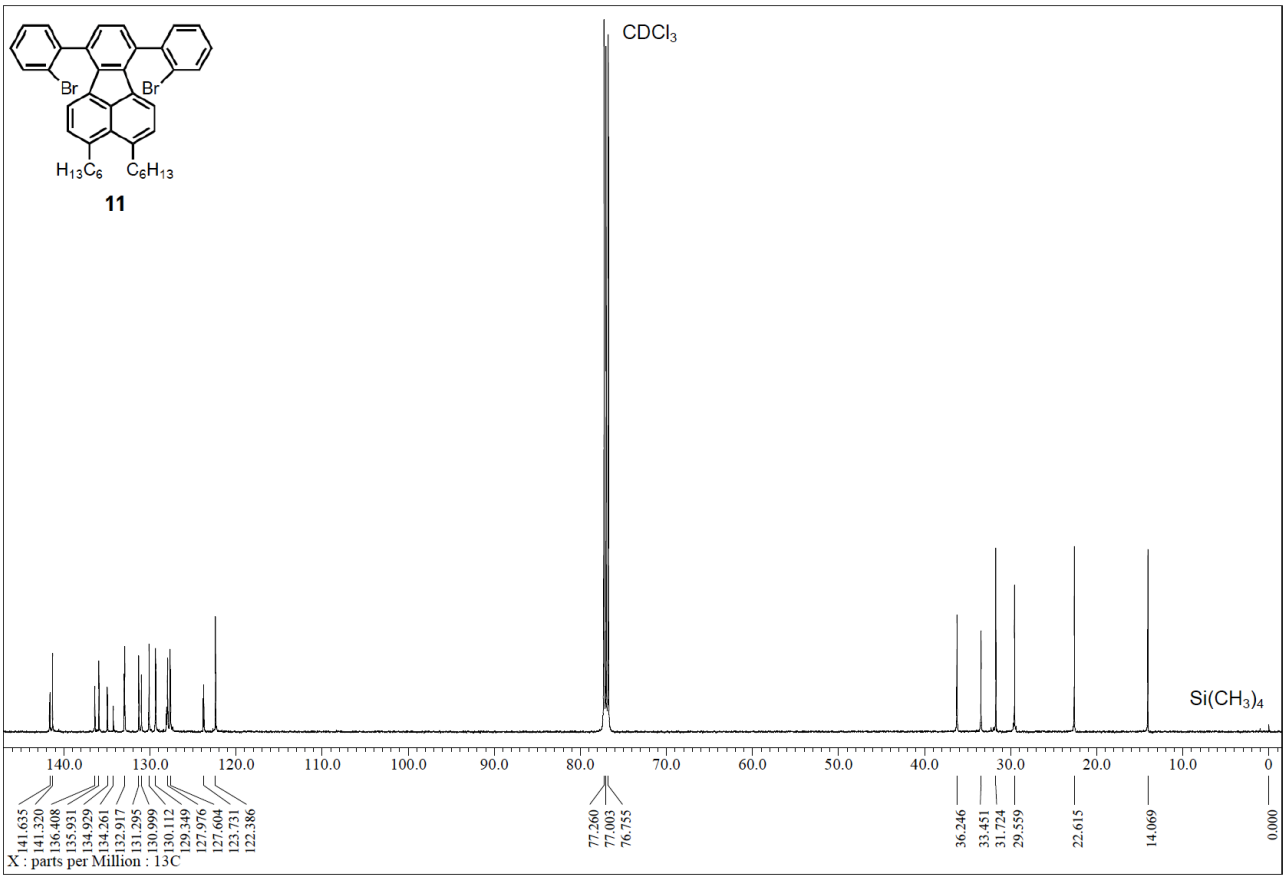


Figure S35. ^{1}H (top, 500 MHz) and $^{13}C\{^{1}H\}$ NMR (bottom, 126 MHz) NMR spectra of compound **11** in $CDCl_3$ at 25.0 °C (^{1}H) and 21.2 °C (^{13}C).

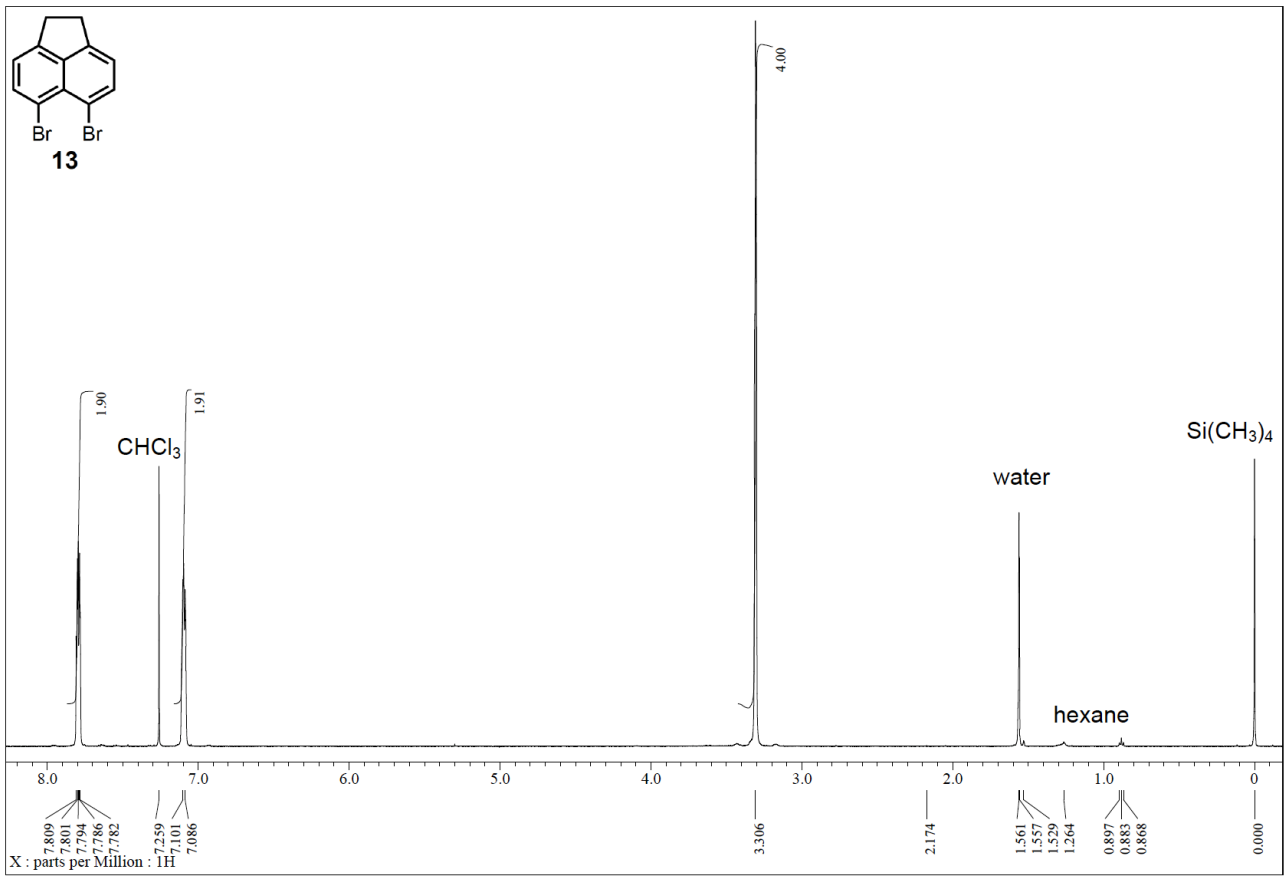


Figure S34. ^{1}H (500 MHz) NMR spectrum of compound **13** in $CDCl_3$ at 18.9 °C.

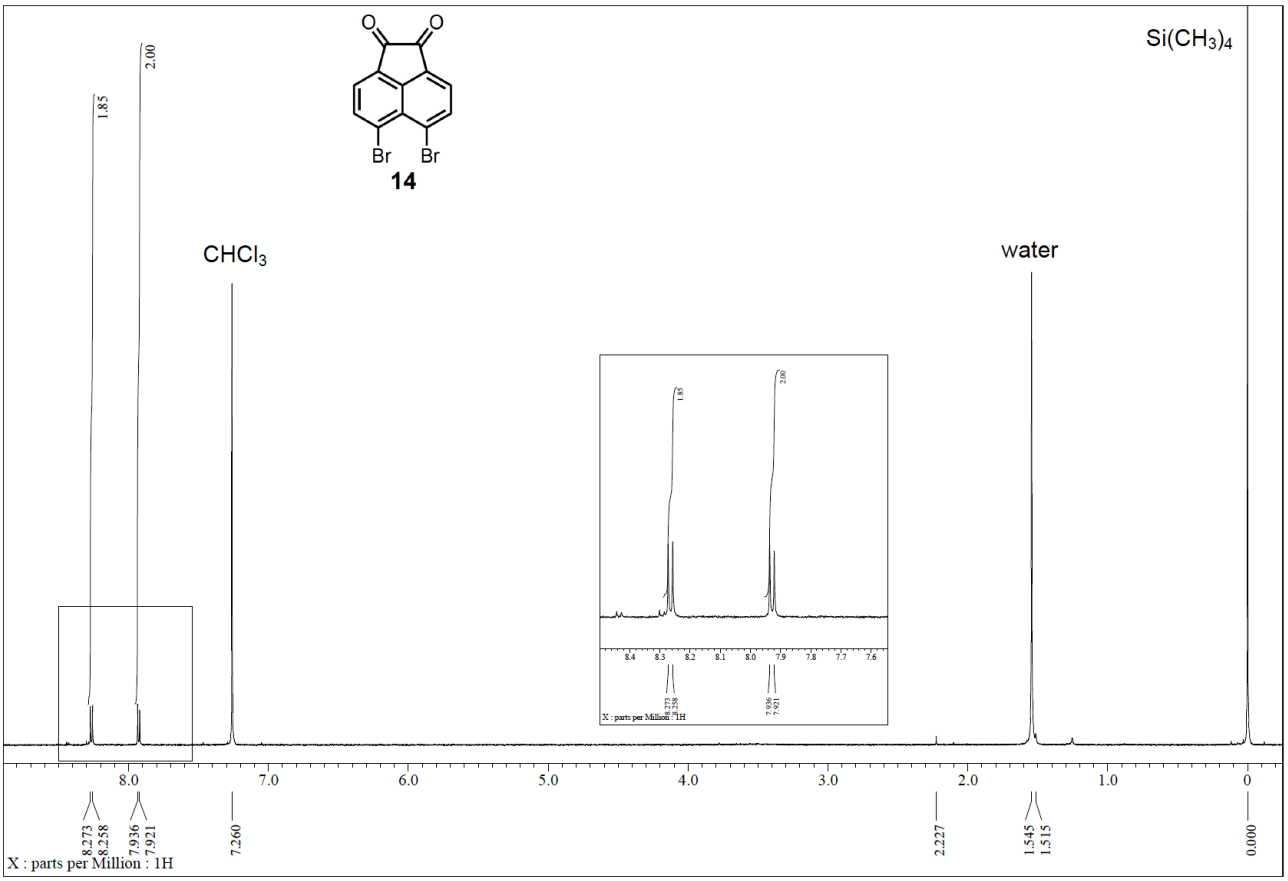


Figure S36. ^{1}H (500 MHz) NMR spectrum of compound **14** in $CDCl_3$ at 25.0 °C.

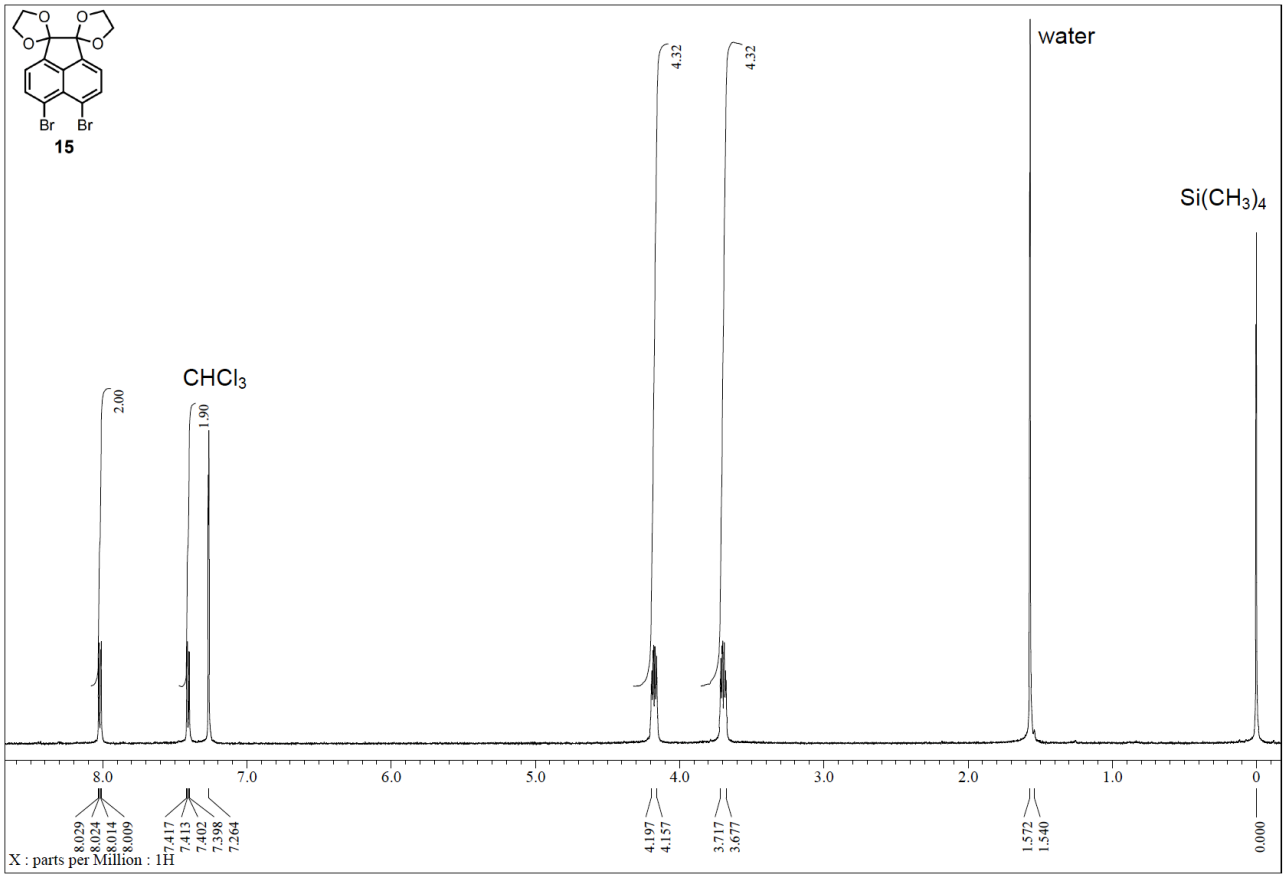


Figure S37. ^{1}H (top, 500 MHz) NMR spectrum of compound **15** in $CDCl_3$ at 17.6 °C.

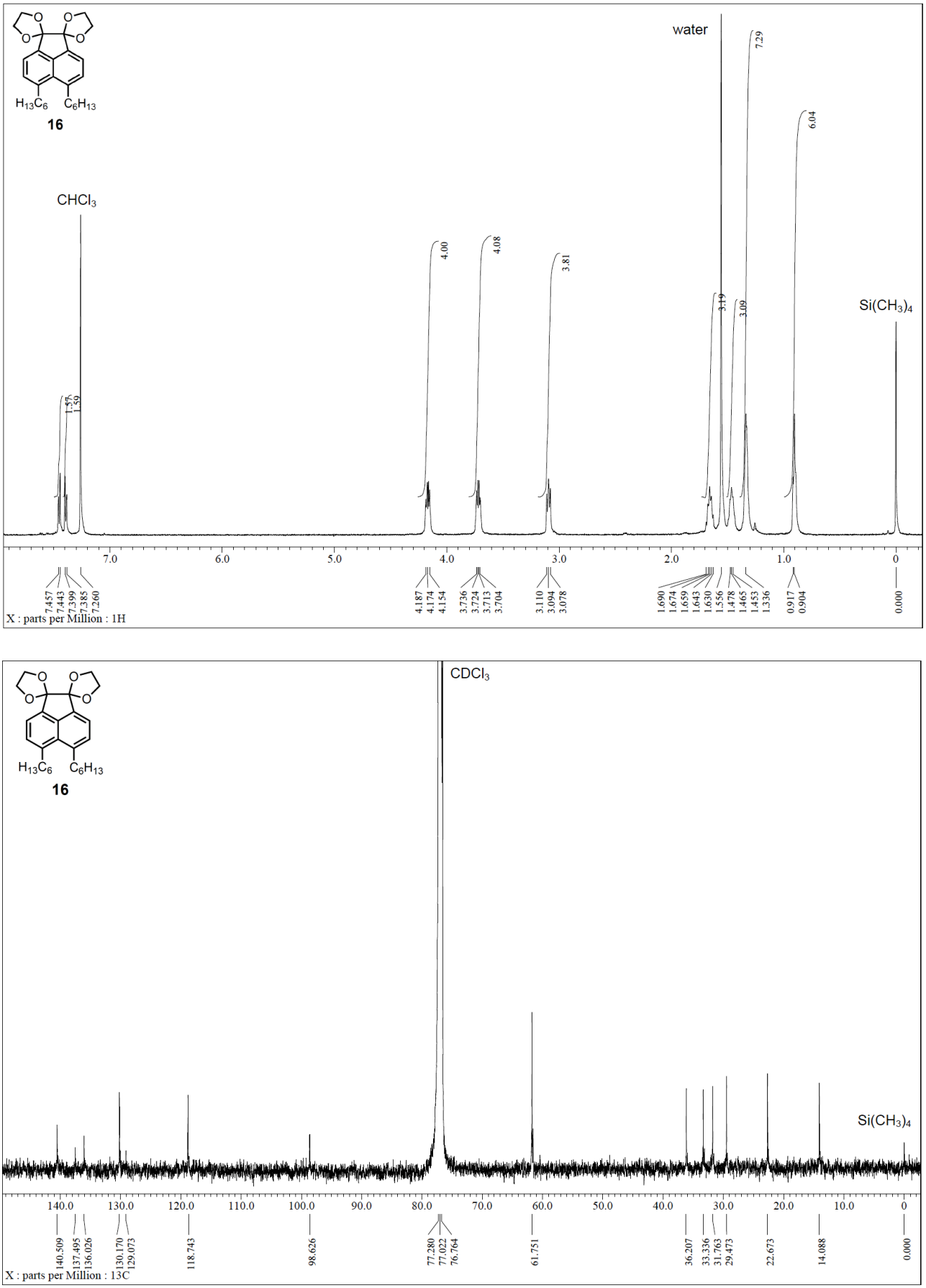


Figure S38. ^{1}H (top, 500 MHz) and ^{13}C{^{1}H} NMR (bottom, 126 MHz) NMR spectra of compound **16** in $CDCl_3$ at 25.1 °C (^{1}H) and 24.4 °C (^{13}C).

13. Cartesian Coordinates of All Optimized Geometries

The model of *anti*-1

Symbol	X	Y	Z
C	2.192018	1.848076	0.458013
C	2.341711	3.224146	0.053758
C	3.580037	3.851679	-0.00039
C	4.798034	3.161488	0.337494
C	4.602035	1.903776	0.884394
C	3.342157	1.27157	0.937508
C	1.075146	0.910194	0.247543
C	6.162869	3.434366	-0.03451
C	7.141033	2.448623	-0.01069
C	6.859947	1.09232	0.39315
C	5.600191	0.906175	0.906541
C	4.951083	-0.36266	0.971869
C	3.561389	-0.13896	0.990997
C	2.639658	-1.0692	0.568652
C	1.295341	-0.52661	0.303453
C	3.202594	-2.35081	0.255504
C	4.579017	-2.57238	0.23672
C	5.523846	-1.53321	0.528267
C	6.961139	-1.43925	0.220041
C	7.618263	-0.14719	0.152057
C	0.209196	-1.36657	0.05366
C	0.373108	-2.43702	0.096114
H	-1.07515	-0.91019	-0.24754
H	-1.29534	0.526608	-0.30345
H	-0.2092	1.36657	-0.05366
H	-0.37311	2.437023	-0.09611
C	7.722805	-2.58653	-0.05975
C	7.24421	-3.55756	-0.00289
C	9.065884	-2.51137	-0.38759
C	9.625266	-3.41801	-0.58818
C	8.980736	-0.11227	-0.19089
C	9.483599	0.846966	-0.23672
C	9.69892	-1.26641	-0.45365
C	10.75132	-1.20319	-0.7058
C	4.926199	-3.54279	-0.10039
C	2.559987	-3.16188	-0.06886
C	8.123233	2.704659	-0.39229

C	1.481137	3.777668	-0.30541
C	-6.85995	-1.09232	-0.39315
C	-7.14103	-2.44862	0.010686
C	-6.16287	-3.43437	0.034512
C	-4.79803	-3.16149	-0.33749
C	-4.60204	-1.90378	-0.88439
C	-5.60019	-0.90618	-0.90654
C	-7.61826	0.14719	-0.15206
H	-3.58004	-3.85168	0.000385
C	-2.34171	-3.22415	-0.05376
H	-2.19202	-1.84808	-0.45801
C	-3.34216	-1.27157	-0.93751
H	-3.56139	0.138964	-0.991
C	-4.95108	0.362662	-0.97187
H	-5.52385	1.533207	-0.52827
H	-6.96114	1.439252	-0.22004
H	-4.57902	2.572384	-0.23672
H	-3.20259	2.350806	-0.2555
H	-2.63966	1.069196	-0.56865
H	-7.72281	2.586525	0.059751
H	-7.24421	3.557555	0.002889
C	-9.06588	2.511366	0.387588
H	-9.62527	3.418014	0.588181
C	-9.69892	1.266411	0.453649
H	-10.7513	1.203189	0.705803
C	-8.98074	0.112272	0.190889
H	-9.4836	-0.84697	0.236721
C	-2.55999	3.16188	0.068863
H	-4.9262	3.542792	0.100387
H	-1.48114	-3.77767	0.305411
H	-8.12323	-2.70466	0.392294
C	-6.42599	-4.41069	0.42874
H	-3.62764	-4.86213	0.393523
C	3.62764	4.862132	-0.39352
H	6.425991	4.410689	-0.42874

Zero-point correction= 0.547924 (Hartree/Particle)

Thermal Correction to Energy= 0.578349

Thermal Correction to Enthalpy= 0.579294

Thermal Correction to Gibbs Free Energy= 0.488962

Sum of electronic and zero-point energies= -1918.509377

Sum of electronic and thermal Energies = -1918.478952

Sum of electronic and thermal Enthalpy = -1918.478008

Sum of electronic and thermal Free Energy Correction= -1918.568339

The model of *syn*-1

Symbol	X	Y	Z
C	2.694851	-1.08258	-0.82022
C	3.169426	-2.36493	-0.38684
C	4.507097	-2.59173	-0.0655
C	5.497723	-1.55747	-0.14617
C	5.041743	-0.38697	-0.70912
C	3.691282	-0.15809	-1.03375
C	1.327776	-0.53324	-0.85623
C	6.832881	-1.46725	0.469364
C	7.465288	-0.17721	0.674443
C	6.784339	1.063913	0.267548
C	5.666939	0.879663	-0.50872
C	4.693267	1.881172	-0.71091
C	3.47266	1.253468	-1.03635
C	2.24826	1.837191	-0.82428
C	1.107787	0.904666	-0.8568
C	2.312688	3.215443	-0.40506
C	3.511941	3.83857	-0.08312
C	4.770891	3.141446	-0.14099
C	6.022189	3.411172	0.520272
C	6.9767	2.421462	0.716609
C	-1.10779	-0.90467	-0.85679
C	-1.32778	0.533236	-0.85623
H	3.477338	4.851778	0.304301
H	1.397052	3.774976	-0.2485
H	4.767409	-3.56226	0.342187
H	2.467564	-3.17242	-0.20988
C	-6.78434	-1.06391	0.267586
C	-6.9767	-2.42146	0.716659
C	-6.02219	-3.41117	0.520325
C	-4.77089	-3.14145	-0.14094
C	-4.69327	-1.88118	-0.71087
C	-5.66694	-0.87967	-0.50868
C	-7.46529	0.177216	0.674474

C	-3.51194	-3.83857	-0.08308
C	-2.31269	-3.21545	-0.40502
C	-2.24826	-1.8372	-0.82425
C	-3.47267	-1.25348	-1.03633
C	-3.69129	0.158085	-1.03373
C	-5.04175	0.386964	-0.70911
C	-5.49772	1.557472	-0.14616
C	-6.83288	1.467251	0.469382
C	-4.5071	2.591729	-0.06551
C	-3.16943	2.364926	-0.38685
C	-2.69486	1.082577	-0.82022
C	-7.50925	2.615841	0.914083
H	-7.05037	3.585421	0.757453
C	-8.74813	2.544004	1.528194
H	-9.24567	3.451743	1.850103
C	-9.35706	1.301127	1.726493
H	-10.3288	1.240492	2.20303
C	-8.71942	0.145646	1.307866
H	-9.20456	-0.81193	1.458934
H	-2.46757	3.172421	-0.2099
H	-4.76741	3.562259	0.342178
H	-1.39705	-3.77498	-0.24847
H	-3.47734	-4.85178	0.304354
H	-6.19753	-4.38894	0.957498
H	-7.85257	-2.67603	1.303143
C	8.719429	-0.14564	1.30783
H	9.204563	0.811937	1.458889
C	7.509258	-2.61583	0.914072
H	7.050374	-3.58542	0.757452
C	8.748137	-2.54399	1.528177
H	9.24568	-3.45173	1.850092
C	9.357067	-1.30111	1.726464
H	10.32885	-1.24048	2.202997
H	7.85258	2.676038	1.303088
H	6.197538	4.388944	0.957436
C	0.209103	-1.36768	-0.84969
H	0.372984	-2.43892	-0.86608
C	-0.20911	1.367674	-0.8497
H	-0.37299	2.438911	-0.8661

Zero-point correction= 0.547965 (Hartree/Particle)

Thermal Correction to Energy= 0.578385

Thermal Correction to Enthalpy= 0.579329

Thermal Correction to Gibbs Free Energy= 0.488968

Sum of electronic and zero-point energies= -1918.509199

Sum of electronic and thermal Energies = -1918.478779

Sum of electronic and thermal Enthalpy = -1918.477835

Sum of electronic and thermal Free Energy Correction= -1918.568196

Transition state (with one imaginary frequency) of the model of 1

Symbol	X	Y	Z
C	2.291932	-1.85514	-0.58895
C	2.396324	-3.22543	-0.1516
C	3.620932	-3.84446	0.065174
C	4.868638	-3.15086	-0.12666
C	4.736828	-1.90143	-0.71023
C	3.490534	-1.27774	-0.92882
C	1.154145	-0.92134	-0.53026
C	6.177398	-3.41047	0.416876
C	7.146264	-2.41897	0.502552
C	6.911655	-1.06968	0.048755
C	5.725242	-0.89794	-0.62068
C	5.083391	0.36579	-0.78338
C	3.708022	0.132919	-0.97317
C	2.736024	1.06239	-0.68178
C	1.372531	0.5141	-0.57765
C	3.249346	2.351787	-0.31852
C	4.61141	2.582331	-0.1306
C	5.590399	1.545421	-0.28727
C	6.978127	1.464515	0.199845
C	7.627829	0.177606	0.36649
C	0.258613	1.351377	-0.47781
H	0.421657	2.422339	-0.5226
C	-1.05379	0.901258	-0.34141
C	-1.27564	-0.55655	-0.29209
C	-0.15694	-1.38278	-0.38597
H	-0.31934	-2.4544	-0.35856
C	7.693183	2.620011	0.557841
H	7.220842	3.587179	0.428798
C	8.984985	2.55753	1.052173

H	9.510455	3.47017	1.309306
C	8.936724	0.155687	0.877798
H	9.434491	-0.79966	0.998814
C	9.610764	1.317593	1.213239
H	10.62359	1.264266	1.595929
H	4.909124	3.559405	0.233502
H	2.567283	3.162953	-0.08886
H	8.07411	-2.66403	1.007488
H	6.393613	-4.38018	0.853693
H	3.623791	-4.84988	0.473804
H	1.500086	-3.78	0.103664
C	-6.93189	1.097935	0.220264
C	-7.23279	2.521264	0.222297
C	-6.24968	3.514262	0.108254
C	-4.8349	3.210804	-0.02285
C	-4.61693	1.857286	-0.01846
C	-5.59813	0.872473	0.095133
C	-7.70239	-0.16575	0.319469
C	-3.58729	3.942161	-0.15704
C	-2.34177	3.306944	-0.26501
C	-2.18148	1.861813	-0.25267
C	-3.37691	1.229342	-0.12599
C	-3.59134	-0.16422	-0.07848
C	-4.95921	-0.38274	0.057642
C	-5.56562	-1.59926	0.140385
C	-7.0374	-1.47802	0.280633
C	-4.60053	-2.67497	0.068302
C	-3.21804	-2.45427	-0.06943
C	-2.63667	-1.13173	-0.15111
C	-7.84406	-2.62202	0.381134
H	-7.36563	-3.59487	0.353668
C	-9.22177	-2.54848	0.513185
H	-9.80663	-3.4582	0.587524
C	-9.85262	-1.30327	0.550002
H	-10.9299	-1.24071	0.653088
C	-9.09922	-0.14394	0.454387
H	-9.60011	0.817465	0.484105
H	-2.58571	-3.33464	-0.11381
H	-4.92695	-3.70822	0.119624
H	-1.47282	3.949267	-0.36155

H	-3.59431	5.027177	-0.17741
H	-6.58348	4.546807	0.120884
H	-8.25959	2.85886	0.31524

Zero-point correction= 0.547334 (Hartree/Particle)

Thermal Correction to Energy= 0.577191

Thermal Correction to Enthalpy= 0.578135

Thermal Correction to Gibbs Free Energy= 0.489233

Sum of electronic and zero-point energies= -1918.499159

Sum of electronic and thermal Energies = -1918.469302

Sum of electronic and thermal Enthalpy = -1918.468358

Sum of electronic and thermal Free Energy Correction= -1918.55726

The model of compound 2

Symbol	X	Y	Z
C	-1.25079	0.207356	2.36476
C	-2.62756	-0.21849	2.431254
C	-3.44381	-0.27057	1.308587
C	-2.96259	0.092336	0.000000
C	-1.69925	0.660068	0000000
C	-0.87431	0.710784	1.143952
C	-0.14416	-0.00403	3.313519
C	-3.44381	-0.27057	-1.30859
C	-2.62756	-0.21849	-2.43125
C	-1.25079	0.207356	-2.36476
C	-0.87431	0.710784	-1.14395
C	0.480492	0.791751	-0.70422
C	0.480492	0.791751	0.70422
C	1.551388	0.374676	1.461067
C	1.234811	0.079587	2.869104
C	2.732809	0.092163	0.696941
C	2.732809	0.092163	-0.69694
C	1.551388	0.374676	-1.46107
C	1.234811	0.079587	-2.8691
C	-0.14416	-0.00403	-3.31352
C	2.25051	-0.17235	3.806967
H	3.284286	-0.10363	3.487929
C	1.967864	-0.48734	5.125263

H	2.777046	-0.66616	5.824149
C	0.639242	-0.56841	5.553351
H	0.413387	-0.8105	6.585603
C	-0.3899	-0.33335	4.65757
H	-1.41612	-0.39063	5.002165
C	2.25051	-0.17235	-3.80697
H	3.284286	-0.10363	-3.48793
C	1.967864	-0.48734	-5.12526
H	2.777046	-0.66616	-5.82415
C	-0.3899	-0.33335	-4.65757
H	-1.41612	-0.39063	-5.00217
C	0.639242	-0.56841	-5.55335
H	0.413387	-0.8105	-6.5856
H	3.641295	-0.22229	-1.19865
H	3.641295	-0.22229	1.198653
H	-3.03086	-0.59471	-3.36494
H	-3.03086	-0.59471	3.364938
H	-4.44301	-0.67999	-1.41776
H	-4.44301	-0.67999	1.417756

Zero-point correction= 0.324347 (Hartree/Particle)

Thermal Correction to Energy= 0.341472

Thermal Correction to Enthalpy= 0.342416

Thermal Correction to Gibbs Free Energy= 0.280858

Sum of electronic and zero-point energies= -1075.358696

Sum of electronic and thermal Energies = -1075.341571

Sum of electronic and thermal Enthalpy = -1075.340627

Sum of electronic and thermal Free Energy Correction= --1075.402185

Parallel stacked dimers of the *anti*-geometry of the model of 1

Symbol	X	Y	Z
C	2.106717	1.921693	-1.22065
C	2.263068	3.331215	-1.48753
C	3.509788	3.986169	-1.52445
C	4.744941	3.232624	-1.30027
C	4.536157	1.924087	-0.84539
C	3.265684	1.295935	-0.79698
C	0.975882	1.020614	-1.49945
C	6.134566	3.519411	-1.66073
C	7.083331	2.479578	-1.71562
C	6.780295	1.100754	-1.41773
C	5.51678	0.901446	-0.89079
C	4.853601	-0.36443	-0.87554
C	3.461037	-0.12015	-0.81988
C	2.509952	-1.0134	-1.29665
C	1.174671	-0.43163	-1.52698
C	3.047647	-2.28668	-1.70686
C	4.431967	-2.52909	-1.76528
C	5.402467	-1.52075	-1.41805
C	6.830453	-1.4229	-1.7749
C	7.513073	-0.12847	-1.76936
C	0.068992	-1.24216	-1.83037
H	0.20983	-2.32869	-1.83036
C	-1.21052	-0.73912	-2.11883
C	-1.40419	0.714922	-2.1157
C	-0.30067	1.525237	-1.80281
H	-0.44688	2.610807	-1.78251
C	7.557773	-2.55831	-2.19905
H	7.055955	-3.53203	-2.19371
C	8.893004	-2.47171	-2.59772
H	9.429493	-3.37633	-2.90819
C	8.86612	-0.0798	-2.18009
H	9.38146	0.888141	-2.17334
C	9.552936	-1.22625	-2.58653
H	10.60363	-1.15578	-2.89332
H	4.767315	-3.48796	-2.17909
H	2.373839	-3.0681	-2.07954

H	8.086082	2.744167	-2.07521
H	1.382033	3.928981	-1.75509
C	-7.0106	-0.79116	-2.01545
C	-7.30619	-2.15428	-1.64631
C	-6.36381	-3.19906	-1.69468
C	-4.98805	-2.93905	-2.12043
C	-4.78914	-1.65141	-2.63575
C	-5.76382	-0.6213	-2.59248
C	-7.72747	0.457731	-1.70134
C	-3.74819	-3.68666	-1.89946
C	-2.50244	-3.04025	-2.00166
C	-2.34893	-1.64711	-2.33885
C	-3.51808	-1.03181	-2.74903
C	-3.7058	0.386612	-2.76047
C	-5.09442	0.639544	-2.66924
C	-5.62354	1.824053	-2.17077
C	-7.04138	1.748064	-1.7725
C	-4.63982	2.847744	-1.914
C	-3.26001	2.594618	-1.99634
C	-2.73922	1.29643	-2.34924
C	-7.75465	2.906361	-1.38437
H	-7.24057	3.87349	-1.42054
C	-9.08405	2.846727	-0.96403
H	-9.60479	3.763947	-0.66699
C	-9.74683	1.604485	-0.90401
H	-10.7894	1.553396	-0.56796
C	-9.07088	0.435699	-1.25939
H	-9.58658	-0.53003	-1.20162
H	-2.57616	3.386338	-1.66957
H	-4.95742	3.823762	-1.52942
H	-1.61735	-3.62654	-1.7243
H	-8.28793	-2.39358	-1.21962
C	6.585257	4.911902	-2.05488
H	6.104638	5.246897	-2.99409
H	6.323902	5.659136	-1.28136
H	7.67941	4.941652	-2.20582
C	3.52667	5.460728	-1.87294
H	4.09895	6.046033	-1.1284

H	4.000538	5.644659	-2.85624
H	2.499299	5.865484	-1.91304
C	-6.79159	-4.56204	-1.19505
H	-6.59498	-5.3517	-1.94464
H	-6.23677	-4.84402	-0.28113
H	-7.86962	-4.57274	-0.95409
C	-3.75475	-5.13887	-1.47103
H	-4.16664	-5.25706	-0.45263
H	-4.37299	-5.75942	-2.1462
H	-2.72876	-5.54924	-1.46701
C	2.569617	1.207097	2.326719
C	2.935537	2.592808	2.148377
C	4.264696	3.059727	2.156488
C	5.378788	2.121987	2.325121
C	4.974475	0.828892	2.675054
C	3.625246	0.393081	2.697061
C	1.318861	0.489262	2.011084
C	6.801613	2.22213	1.990412
C	7.581505	1.057988	1.837478
C	7.071649	-0.28053	2.019617
C	5.791788	-0.32274	2.543709
C	4.948004	-1.47279	2.489941
C	3.609618	-1.03206	2.586154
C	2.531102	-1.7603	2.10267
C	1.293839	-0.97712	1.928025
C	2.871254	-3.08348	1.642314
C	4.205123	-3.52214	1.546384
C	5.317301	-2.67628	1.902348
C	6.745025	-2.77084	1.545045
C	7.607698	-1.58787	1.593119
C	0.074014	-1.60394	1.62556
H	0.053205	-2.69893	1.582812
C	-1.12021	-0.9056	1.375226
C	-1.08106	0.558338	1.394966
C	0.134539	1.185385	1.720584
H	0.161288	2.280087	1.746181
C	7.305251	-3.99015	1.096914
H	6.663603	-4.87887	1.064258

C	8.644228	-4.08773	0.713039
H	9.049001	-5.05056	0.378074
C	8.951453	-1.72266	1.173004
H	9.596048	-0.83677	1.189173
C	9.470262	-2.94593	0.746341
H	10.51751	-3.01411	0.429834
H	4.389134	-4.49992	1.085031
H	2.086913	-3.74177	1.249205
H	8.611695	1.197777	1.48694
H	2.157844	3.327685	1.907297
C	-6.85478	-0.00628	1.507057
C	-7.36956	-1.29458	1.8977
C	-6.60852	-2.47878	1.877453
C	-5.21137	-2.45273	1.438464
C	-4.81036	-1.22974	0.879825
C	-5.60382	-0.05188	0.914615
C	-7.35436	1.341997	1.827402
C	-4.10846	-3.37927	1.697521
C	-2.77328	-2.95366	1.558759
C	-2.39638	-1.6163	1.173709
C	-3.45378	-0.82686	0.754188
C	-3.40728	0.604221	0.738578
C	-4.73521	1.080858	0.834769
C	-5.06013	2.334467	1.342625
C	-6.46867	2.50094	1.739757
C	-3.92562	3.181022	1.609709
C	-2.60505	2.704355	1.524082
C	-2.30616	1.342089	1.161052
C	-6.98158	3.767372	2.109765
H	-6.32204	4.640609	2.039649
C	-8.29815	3.928391	2.546666
H	-8.66694	4.925192	2.817845
C	-9.15045	2.808109	2.638537
H	-10.1858	2.929836	2.979344
C	-8.67704	1.542959	2.285782
H	-9.34658	0.677554	2.346802
H	-1.79669	3.372975	1.844857
H	-4.08058	4.197937	1.991089

H	-1.99243	-3.66615	1.854661
H	-8.38031	-1.36232	2.32011
C	7.457884	3.557996	1.713288
H	7.043246	4.024949	0.801634
H	7.299713	4.2665	2.548149
H	8.545743	3.436063	1.562861
C	4.502803	4.529573	1.888106
H	5.135721	4.987341	2.671688
H	5.021752	4.675885	0.922877
H	3.546676	5.081063	1.844006
C	-7.25844	-3.73784	2.41661
H	-7.1633	-4.58271	1.711108
H	-6.79359	-4.06038	3.368151
H	-8.33372	-3.57021	2.608059
C	-4.34921	-4.77944	2.227103
H	-4.75769	-4.75865	3.256152
H	-5.07971	-5.33495	1.60985
H	-3.40775	-5.35717	2.249502

Parallel stacked dimers of the *syn*-geometries of the model of 1

Symbol	X	Y	Z
C	-2.40468	1.399842	-2.65087
C	-2.78118	2.728112	-2.23319
C	-4.11897	3.079806	-1.96299
C	-5.20352	2.136048	-2.0885
C	-4.82364	0.915009	-2.63047
C	-3.48399	0.562656	-2.89836
C	-1.09394	0.720072	-2.67269
C	-6.57878	2.162169	-1.55224
C	-7.34626	0.922268	-1.3985
C	-6.76672	-0.37811	-1.79082
C	-5.57253	-0.291	-2.48136
C	-4.68886	-1.38763	-2.64364
C	-3.4011	-0.86355	-2.91197
C	-2.2344	-1.5709	-2.68943
C	-1.00942	-0.747	-2.69277
C	-2.45318	-2.95444	-2.3409
C	-3.72509	-3.50752	-2.08201

C	-4.92685	-2.67049	-2.13955
C	-6.27463	-2.84012	-1.58774
C	-7.1279	-1.7298	-1.42696
C	1.37989	0.857676	-2.67689
C	1.464807	-0.60672	-2.70032
H	-1.58887	-3.61478	-2.19336
H	-4.31027	4.077858	-1.55182
H	-2.00467	3.47296	-2.01918
C	7.071037	0.461514	-1.54907
C	7.40349	1.794147	-1.10356
C	6.561156	2.909082	-1.27504
C	5.255583	2.76087	-1.92305
C	5.052582	1.501396	-2.50001
C	5.928593	0.398828	-2.32694
C	7.628764	-0.84708	-1.15782
C	4.051775	3.595163	-1.89015
C	2.797426	3.049235	-2.22549
C	2.602797	1.67996	-2.63387
C	3.779273	0.984876	-2.84963
C	3.863697	-0.4425	-2.87922
C	5.191279	-0.80354	-2.55727
C	5.539139	-2.03614	-2.01773
C	6.875335	-2.08008	-1.39443
C	4.45196	-2.98174	-1.96068
C	3.129866	-2.62178	-2.28019
C	2.775415	-1.28398	-2.68371
C	7.432675	-3.29972	-0.94758
H	6.869348	-4.22469	-1.11822
C	8.669494	-3.3515	-0.30064
H	9.071404	-4.31441	0.035287
C	9.391369	-2.16497	-0.06714
H	10.35428	-2.20014	0.454837
C	8.869555	-0.93949	-0.48672
H	9.429514	-0.01699	-0.2945
H	2.342189	-3.36497	-2.10705
H	4.623995	-3.98554	-1.55518
H	1.923409	3.69799	-2.08622
H	8.317081	1.95203	-0.5176

C	-8.62503	0.997876	-0.79984
H	-9.19332	0.070523	-0.66452
C	-7.16525	3.369314	-1.10823
H	-6.59302	4.298102	-1.21784
C	-8.43987	3.403964	-0.53772
H	-8.86318	4.357566	-0.2012
C	-9.17289	2.211626	-0.3796
H	-10.1637	2.232312	0.088051
H	-8.07913	-1.91158	-0.912
C	0.10561	1.449816	-2.64709
H	0.043706	2.543881	-2.62877
C	0.265041	-1.33842	-2.68849
H	0.326684	-2.43261	-2.70265
C	7.002032	4.228601	-0.68025
H	6.980961	5.041028	-1.43111
H	6.333328	4.532858	0.145351
H	8.026383	4.154627	-0.27359
C	4.093852	5.033768	-1.42177
H	4.363403	5.099905	-0.35265
H	4.844475	5.621063	-1.98338
H	3.108493	5.516951	-1.55054
C	-3.79488	-4.96273	-1.67195
H	-4.13786	-5.06705	-0.62715
H	-4.50436	-5.52778	-2.30569
H	-2.80235	-5.44192	-1.75212
C	-6.75438	-4.18219	-1.07931
H	-6.66665	-4.96632	-1.8548
H	-6.15291	-4.51337	-0.21243
H	-7.8088	-4.12645	-0.75504
C	-2.73859	1.306378	0.848525
C	-3.08018	2.632552	1.300781
C	-4.39188	2.984833	1.668862
C	-5.47758	2.036972	1.624811
C	-5.1428	0.818586	1.049015
C	-3.83033	0.468487	0.664385
C	-1.42829	0.635116	0.781224
C	-6.80119	2.068935	2.271764
C	-7.55817	0.834594	2.484263

C	-7.00005	-0.46585	2.070935
C	-5.86914	-0.38756	1.279667
C	-4.99752	-1.48368	1.062262
C	-3.74266	-0.96065	0.663752
C	-2.55867	-1.65496	0.829337
C	-1.33933	-0.82936	0.764458
C	-2.73358	-3.02536	1.245889
C	-3.97137	-3.57515	1.63299
C	-5.18022	-2.74877	1.632567
C	-6.47623	-2.91614	2.295064
C	-7.32583	-1.80825	2.491685
C	1.044426	0.781576	0.777027
C	1.132633	-0.68081	0.746041
H	-1.85223	-3.67177	1.346572
H	-4.55634	3.98575	2.086927
H	-2.28845	3.376839	1.451713
C	6.686184	0.365355	2.094505
C	6.999641	1.684454	2.585899
C	6.155907	2.799986	2.421401
C	4.880316	2.663644	1.71541
C	4.709925	1.426005	1.077891
C	5.580269	0.319292	1.262868
C	7.227767	-0.94456	2.495678
C	3.67073	3.487453	1.74851
C	2.436348	2.953501	1.332264
C	2.266557	1.601267	0.861173
C	3.452529	0.915758	0.662135
C	3.538604	-0.51348	0.615689
C	4.852563	-0.87973	0.987402
C	5.173296	-2.11327	1.544268
C	6.477209	-2.16932	2.227252
C	4.08425	-3.05692	1.564053
C	2.775749	-2.69094	1.202252
C	2.443246	-1.35271	0.783307
C	7.008577	-3.39515	2.692869
H	6.452723	-4.31738	2.48698
C	8.220291	-3.45845	3.383064
H	8.608408	-4.42732	3.720164

C	8.946331	-2.27605	3.639731
H	9.900667	-2.32121	4.178442
C	8.448265	-1.04635	3.205281
H	9.016685	-0.13003	3.403998
H	1.978761	-3.43212	1.34009
H	4.243098	-4.06515	1.966223
H	1.551759	3.589935	1.463872
H	7.897528	1.82952	3.200564
C	-8.81204	0.919641	3.134831
H	-9.38437	-0.0026	3.291404
C	-7.3591	3.283402	2.734267
H	-6.79835	4.211097	2.57063
C	-8.60517	3.330293	3.363078
H	-9.01437	4.291663	3.696788
C	-9.33811	2.141113	3.562238
H	-10.3187	2.173727	4.052521
H	-8.24386	-1.98518	3.067235
C	-0.23142	1.369935	0.796556
H	-0.29713	2.463757	0.805029
C	-0.06403	-1.41678	0.751111
H	0.000792	-2.51032	0.723657
C	6.57653	4.102795	3.072097
H	6.553257	4.94398	2.354248
H	5.905678	4.377473	3.908518
H	7.602736	4.025101	3.474227
C	3.674105	4.891237	2.321791
H	3.869069	4.883283	3.411847
H	4.458646	5.522604	1.864873
H	2.698761	5.383333	2.156688
C	-3.98622	-5.00748	2.129126
H	-4.22193	-5.06038	3.20965
H	-4.75141	-5.61444	1.608984
H	-3.00325	-5.48719	1.973075
C	-6.91984	-4.25564	2.84778
H	-6.88179	-5.04504	2.073189
H	-6.27066	-4.59206	3.678781
H	-7.95513	-4.19901	3.229667

Dimer of the *anti*-geometry of the model of 1 through the concave-convex interaction at one corannulene unit

Symbol	X	Y	Z
C	4.74554	-2.34465	0.573578
C	4.741948	-3.78566	0.661299
C	5.878176	-4.58793	0.42013
C	7.160058	-3.97141	0.062874
C	7.070181	-2.59817	-0.1987
C	5.911069	-1.82	0.046114
C	3.794761	-1.34072	1.085256
C	8.538519	-4.46643	0.142439
C	9.622103	-3.56343	0.142183
C	9.474064	-2.12812	0.051106
C	8.181063	-1.71429	-0.21815
C	7.705668	-0.38765	0.026812
C	6.304664	-0.45473	0.190692
C	5.566906	0.490155	0.89089
C	4.201623	0.058497	1.243135
C	6.32895	1.642132	1.304956
C	7.728519	1.708109	1.150027
C	8.488101	0.629861	0.561888
C	9.930041	0.319414	0.637981
C	10.41639	-1.04126	0.387205
C	3.250156	0.975641	1.720815
H	3.545638	2.026132	1.813599
C	1.922792	0.630851	2.022374
C	1.517426	-0.77553	1.87544
C	2.478471	-1.69578	1.425711
H	2.173688	-2.74001	1.297633
C	10.87229	1.307646	1.011501
H	10.51434	2.327077	1.198346
C	12.23398	1.019245	1.135157
H	12.9372	1.811866	1.417969
C	11.80146	-1.29541	0.532371
H	12.1697	-2.31108	0.345006
C	12.70163	-0.28973	0.894194
H	13.76978	-0.51942	0.988802
H	8.249181	2.573653	1.577924

H	5.833485	2.46093	1.840844
H	10.62112	-3.99193	0.29456
H	3.836893	-4.30079	1.008558
C	-3.84449	1.476427	2.349664
C	-3.96591	2.89568	2.115095
C	-2.87553	3.793016	2.141028
C	-1.52077	3.314981	2.429015
C	-1.47247	1.966492	2.801623
C	-2.58262	1.088031	2.75927
C	-4.76956	0.360587	2.071398
C	-0.19745	3.910638	2.211453
C	0.954306	3.099311	2.182756
C	0.931534	1.666696	2.370679
C	-0.29692	1.175368	2.768855
C	-0.6841	-0.19692	2.658412
C	-2.09474	-0.25084	2.661709
C	-2.82935	-1.30188	2.127946
C	-4.26734	-1.01111	1.95416
C	-2.01918	-2.40748	1.676955
C	-0.61016	-2.35047	1.66193
C	0.118959	-1.18664	2.106985
C	-5.19469	-2.03714	1.665055
H	-4.82668	-3.06489	1.572729
C	-6.55858	-1.7759	1.512942
H	-7.25214	-2.59406	1.296014
C	-7.0406	-0.45863	1.628782
H	-8.10711	-0.2513	1.49699
C	-6.15304	0.585451	1.896857
H	-6.53033	1.60953	1.981201
H	-0.06895	-3.19177	1.212447
H	-2.50056	-3.2933	1.244156
H	1.897836	3.592612	1.920767
H	-4.93968	3.305713	1.819417
C	8.84425	-5.9411	0.313492
H	8.47145	-6.3236	1.283298
H	8.362345	-6.54908	-0.47517
H	9.933123	-6.12379	0.273828
C	5.743656	-6.08416	0.622505

H	6.113962	-6.6476	-0.25449
H	6.330558	-6.43082	1.494971
H	4.688456	-6.36364	0.79349
C	-3.14106	5.237498	1.767384
H	-2.76257	5.936286	2.536723
H	-2.63463	5.506707	0.819741
H	-4.22388	5.418754	1.639059
C	-0.02704	5.393995	1.959269
H	-0.50565	5.700446	1.011716
H	-0.4859	5.993511	2.768924
H	1.043291	5.65909	1.894074
C	-5.60163	1.264246	-1.3331
C	-6.17854	2.475768	-0.80567
C	-7.546	2.622907	-0.50308
C	-8.4748	1.510849	-0.72033
C	-7.91491	0.433902	-1.42252
C	-6.5336	0.318899	-1.72343
C	-4.20378	0.801363	-1.3331
C	-9.79162	1.22259	-0.14574
C	-10.3046	-0.09085	-0.16147
C	-9.60764	-1.21806	-0.73624
C	-8.46509	-0.87565	-1.43956
C	-7.41991	-1.8023	-1.7468
C	-6.22537	-1.06492	-1.91379
C	-4.96196	-1.60823	-1.71477
C	-3.88733	-0.61865	-1.51764
C	-4.95745	-3.0363	-1.51396
C	-6.14535	-3.77333	-1.35722
C	-7.44353	-3.14402	-1.38188
C	-8.73524	-3.61716	-0.84832
C	-9.80169	-2.66608	-0.52465
C	-2.54091	-1.01128	-1.44697
H	-2.30231	-2.07202	-1.57777
C	-1.47809	-0.11602	-1.24008
C	-1.79596	1.308874	-1.06602
C	-3.14533	1.695502	-1.10382
H	-3.38228	2.753996	-0.95646
C	-8.95239	-4.98747	-0.5657

H	-8.15819	-5.70366	-0.80757
C	-10.1467	-5.44381	-0.00224
H	-10.2844	-6.51365	0.195512
C	-10.9937	-3.16624	0.052917
H	-11.7953	-2.45868	0.29533
C	-11.1737	-4.52786	0.308805
H	-12.1132	-4.88226	0.749634
H	-6.05899	-4.83774	-1.10614
H	-4.00549	-3.56343	-1.37598
H	-11.2527	-0.25714	0.365728
H	-5.51712	3.305869	-0.52962
C	3.929327	1.911961	-2.0093
C	4.630798	0.766914	-2.5409
C	4.115974	-0.54716	-2.52485
C	2.792367	-0.81792	-1.95975
C	2.222137	0.283121	-1.31981
C	2.770642	1.585919	-1.33102
C	4.134272	3.361777	-2.20184
C	1.876526	-1.95562	-2.07902
C	0.507926	-1.80764	-1.76625
C	-0.07875	-0.57671	-1.28746
C	0.853779	0.395239	-0.98287
C	0.547057	1.777635	-0.80739
C	1.732832	2.513332	-1.01982
C	1.754224	3.850963	-1.38972
C	3.059489	4.317199	-1.90326
C	0.450555	4.47279	-1.39775
C	-0.73229	3.737631	-1.18275
C	-0.72301	2.313793	-0.94552
C	3.295978	5.689024	-2.15938
H	2.497099	6.407148	-1.93788
C	4.514705	6.145652	-2.66928
H	4.666053	7.217334	-2.84688
C	5.548564	5.227944	-2.95052
H	6.507722	5.58307	-3.34639
C	5.350944	3.863347	-2.72238
H	6.157546	3.152981	-2.93892
H	-1.68815	4.264845	-1.29057

H	0.352193	5.533333	-1.66128
H	-0.13822	-2.67401	-1.95837
H	5.59802	0.910584	-3.03853
C	-10.6034	2.290009	0.560799
H	-10.0961	2.647717	1.477572
H	-10.7573	3.175117	-0.08448
H	-11.5945	1.899576	0.853644
C	-7.98579	3.917711	0.150431
H	-8.86356	4.357045	-0.35851
H	-8.27673	3.760806	1.208047
H	-7.1687	4.661492	0.132963
C	4.939897	-1.64152	-3.16943
H	5.073255	-2.49778	-2.4847
H	4.451861	-2.02708	-4.08625
H	5.941482	-1.26747	-3.44633
C	2.356534	-3.30094	-2.58191
H	2.709825	-3.24476	-3.62927
H	3.208391	-3.66696	-1.97729
H	1.546479	-4.05146	-2.53552

Dimer of the *anti*- geometry of the model of 1 through the concave-concave interaction at one corannulene

Symbol	X	Y	Z
C	4.648642	2.439288	-1.20172
C	4.486611	3.792672	-0.72245
C	3.256404	4.482771	-0.7263
C	2.040683	3.829496	-1.22044
C	2.277523	2.597261	-1.84333
C	3.531602	1.93323	-1.84215
C	5.71816	1.452982	-0.94882
C	0.620767	4.108308	-0.98842
C	-0.34962	3.112143	-1.21774
C	-0.04053	1.781393	-1.68306
C	1.277253	1.6183	-2.07129
C	1.910687	0.345008	-2.19995
C	3.303067	0.537682	-2.05917
C	4.174179	-0.46482	-1.65166
C	5.484362	0.018857	-1.17343

C	3.565341	-1.76989	-1.5539
C	2.177445	-1.96043	-1.69701
C	1.27379	-0.86369	-1.94605
C	-0.18631	-0.76557	-1.76527
C	-0.83538	0.540763	-1.63606
C	6.517595	-0.87833	-0.84898
H	6.343769	-1.94748	-1.01587
C	7.758676	-0.48227	-0.31866
C	7.991933	0.949715	-0.09379
C	6.960715	1.848199	-0.42106
H	7.133349	2.91688	-0.25013
C	-0.98905	-1.92353	-1.65571
H	-0.50843	-2.90375	-1.74023
C	-2.36546	-1.84496	-1.43961
H	-2.95904	-2.7591	-1.3444
C	-2.23018	0.577817	-1.41083
H	-2.71911	1.551118	-1.30295
C	-2.98969	-0.58874	-1.31711
H	-4.06707	-0.52747	-1.13457
H	1.775326	-2.96366	-1.51343
H	4.174086	-2.6362	-1.26564
H	-1.38302	3.353371	-0.94072
H	5.338138	4.303965	-0.25518
C	13.50065	-0.82547	0.547587
C	13.81774	-2.15182	0.072212
C	12.85029	-3.14495	-0.18207
C	11.42634	-2.86052	0.020679
C	11.17709	-1.63652	0.658491
C	12.17612	-0.6602	0.917904
C	14.30067	0.41472	0.513761
C	10.2251	-3.5044	-0.51885
C	8.997414	-2.81179	-0.54533
C	8.824755	-1.46724	-0.04941
C	9.924019	-0.96921	0.630487
C	10.15049	0.42714	0.855245
C	11.54144	0.617009	1.032605
C	12.18616	1.823022	0.77566
C	13.65136	1.722789	0.626015

C	11.2961	2.91744	0.471199
C	9.91216	2.728384	0.293723
C	9.295892	1.428518	0.406437
C	14.4586	2.881602	0.52793
H	13.97824	3.863395	0.614592
C	15.84074	2.802553	0.338634
H	16.43751	3.720548	0.27685
C	16.46604	1.542514	0.230408
H	17.55084	1.476625	0.083913
C	15.70148	0.375926	0.312533
H	16.19216	-0.60104	0.229615
H	9.316016	3.588363	-0.03558
H	11.70592	3.915202	0.271896
H	8.158182	-3.31179	-1.04582
H	14.85635	-2.39624	-0.18508
C	0.153337	5.424143	-0.3994
H	0.515188	5.555211	0.639748
H	0.529512	6.288798	-0.97715
H	-0.95033	5.475483	-0.3814
C	3.222605	5.870755	-0.11857
H	2.753438	6.601679	-0.80343
H	2.634201	5.890279	0.819406
H	4.243427	6.222233	0.11582
C	13.32701	-4.46843	-0.74681
H	12.93349	-5.3227	-0.16483
H	12.98959	-4.61091	-1.79156
H	14.4304	-4.52323	-0.73791
C	10.27069	-4.88584	-1.14106
H	10.88163	-4.8969	-2.06425
H	10.71941	-5.62596	-0.45244
H	9.254625	-5.23037	-1.40471
C	-8.82499	1.467016	0.04958
C	-8.99786	2.811483	0.545637
C	-10.2256	3.503921	0.519175
C	-11.4268	2.859931	-0.0205
C	-11.1773	1.636053	-0.65846
C	-9.92413	0.968916	-0.63046
C	-7.75879	0.482158	0.318792

C	-12.8508	3.144136	0.182152
C	-13.8181	2.150907	-0.07235
C	-13.5007	0.82466	-0.54784
C	-12.1762	0.659624	-0.91808
C	-11.5413	-0.61749	-1.03288
C	-10.1504	-0.42745	-0.85539
C	-9.29569	-1.42875	-0.40663
C	-7.99183	-0.94983	0.093747
C	-9.91179	-2.72872	-0.29411
C	-11.2957	-2.91795	-0.47171
C	-12.1859	-1.82362	-0.77612
C	-13.6511	-1.72361	-0.62658
C	-14.3006	-0.41565	-0.51423
C	-6.96052	-1.84821	0.42099
H	-7.13299	-2.9169	0.249919
C	-5.71805	-1.45288	0.948879
C	-5.48448	-0.01875	1.173683
C	-6.5178	0.878332	0.849247
H	-6.34414	1.947494	1.016257
C	-14.4582	-2.88255	-0.52869
H	-13.9777	-3.86426	-0.61543
C	-15.8403	-2.80372	-0.3395
H	-16.437	-3.7218	-0.27787
C	-15.7014	-0.37707	-0.31311
H	-16.1923	0.599813	-0.23012
C	-16.4658	-1.54378	-0.23118
H	-17.5507	-1.47806	-0.08476
H	-11.7054	-3.91579	-0.27255
H	-9.31555	-3.58865	0.035145
H	-14.8567	2.39516	0.184869
H	-8.15873	3.311537	1.046225
C	0.040665	-1.7806	1.683407
C	0.34999	-3.11128	1.218042
C	-0.62026	-4.10752	0.988486
C	-2.04024	-3.8289	1.220343
C	-2.27729	-2.59679	1.84341
C	-1.27717	-1.61771	2.071536
C	0.835329	-0.53985	1.636484

C	-3.25586	-4.48228	0.726075
C	-4.48616	-3.79235	0.722268
C	-4.6484	-2.43905	1.201713
C	-3.53147	-1.93293	1.842262
C	-3.30313	-0.53737	2.059446
C	-1.91078	-0.34451	2.200271
C	-1.27405	0.864314	1.946536
C	0.186055	0.766397	1.765666
C	-2.1779	1.96098	1.697739
C	-3.56576	1.77024	1.554548
C	-4.17438	0.465054	1.652024
C	0.988585	1.924461	1.655832
H	0.507819	2.904624	1.740241
C	2.364974	1.846106	1.439488
H	2.958299	2.760342	1.343674
C	2.989415	0.589983	1.31718
H	4.066788	0.528859	1.134495
C	2.230126	-0.5767	1.411201
H	2.71923	-1.54992	1.30342
H	-4.17465	2.636534	1.266566
H	-1.77602	2.964448	1.514819
H	-5.33761	-4.3037	0.254922
H	1.3835	-3.3525	0.941395
C	-13.3278	4.467491	0.746948
H	-12.9906	4.609877	1.791796
H	-12.9342	5.321887	0.165174
H	-14.4312	4.522163	0.737816
C	-10.2714	4.88531	1.141494
H	-10.7202	5.62543	0.452915
H	-10.8824	4.896227	2.064667
H	-9.25539	5.229927	1.405191
C	-0.15252	-5.42329	0.399555
H	-0.52857	-6.28799	0.97733
H	-0.51425	-5.55451	-0.63961
H	0.951158	-5.47441	0.381664
C	-3.22189	-5.87014	0.118065
H	-2.63378	-5.88927	-0.82011
H	-2.75234	-6.60111	0.802594

H	-4.2427	-6.22181	-0.11611

Dimer of the *syn*-geometry of model of 1 through the concave-concave interaction at one corannulene

Symbol	X	Y	Z
C	8.94998	-0.232	1.336421
C	9.834503	0.813176	0.880745
C	11.07068	0.53209	0.268221
C	11.53121	-0.81913	0.056518
C	10.73307	-1.79368	0.647453
C	9.491045	-1.51122	1.263807
C	7.504929	-0.18792	1.635917
C	12.55854	-1.33665	-0.8686
C	12.5404	-2.7384	-1.29285
C	11.49407	-3.65722	-0.80268
C	10.71353	-3.16179	0.22893
C	9.454572	-3.72018	0.57775
C	8.701921	-2.70599	1.226898
C	7.317466	-2.71136	1.269198
C	6.697817	-1.4138	1.6029
C	6.717528	-3.93272	0.787282
C	7.440493	-4.96224	0.151115
C	8.88347	-4.82629	-0.0683
C	9.785548	-5.49364	-1.01189
C	11.02318	-4.90876	-1.3482
C	5.469372	1.136736	2.142172
C	4.661219	-0.09072	2.108617
H	5.627845	-4.05351	0.840139
H	11.64238	1.374088	-0.14097
H	9.507092	1.859556	0.916567
C	0.26713	3.72296	1.904
C	0.599341	5.094904	1.603122
C	1.902608	5.623353	1.692573
C	3.02061	4.77518	2.116174
C	2.624887	3.515369	2.584296
C	1.302031	3.013383	2.486463
C	-0.90895	2.917738	1.529446
C	4.469321	4.909695	1.939616

C	5.310453	3.783018	2.054193
C	4.832747	2.452372	2.352267
C	3.495961	2.401666	2.705337
C	2.708417	1.207457	2.669109
C	1.3546	1.587153	2.532123
C	0.376794	0.761312	1.990766
C	-0.85646	1.454993	1.575246
C	0.823501	-0.58691	1.737748
C	2.172256	-0.9673	1.873872
C	3.195688	-0.03252	2.275817
C	-1.99783	0.731867	1.1603
H	-1.96344	-0.36233	1.186579
C	-3.15536	1.375373	0.720003
H	-4.0215	0.787494	0.400367
C	-3.20199	2.781872	0.668193
H	-4.09953	3.28686	0.29888
C	-2.0937	3.5313	1.063574
H	-2.13143	4.623932	1.008522
H	2.451132	-1.98313	1.566878
H	0.120577	-1.32473	1.33265
H	6.372651	3.934365	1.822571
H	-0.17705	5.754788	1.198863
C	13.51271	-3.16925	-2.22732
H	13.50412	-4.2181	-2.54662
C	13.5484	-0.48453	-1.41461
H	13.56862	0.564923	-1.0977
C	14.49807	-0.94941	-2.32806
H	15.25729	-0.26415	-2.72389
C	14.48034	-2.29959	-2.73687
H	15.22537	-2.66846	-3.45203
H	11.61143	-5.41033	-2.12733
C	6.850184	1.029139	1.896656
H	7.452688	1.944278	1.922905
C	5.31441	-1.30513	1.832945
H	4.712492	-2.2207	1.80861
C	2.113723	7.054379	1.239975
H	2.66265	7.647061	1.995149
H	2.708507	7.102245	0.306037

H	1.145495	7.551613	1.049188
C	5.102908	6.228216	1.543038
H	4.78002	6.547883	0.533237
H	4.819439	7.039521	2.239469
H	6.204792	6.148461	1.536029
C	6.663346	-6.1569	-0.36507
H	6.656323	-6.1916	-1.47159
H	7.106655	-7.1091	-0.01859
H	5.613923	-6.11938	-0.0216
C	9.393713	-6.77571	-1.71939
H	9.086058	-7.55778	-1.00032
H	8.538993	-6.61792	-2.40512
H	10.23719	-7.16728	-2.31585
C	-8.94991	-0.23193	-1.3369
C	-9.83468	0.813184	-0.88157
C	-11.071	0.532013	-0.26944
C	-11.5315	-0.81924	-0.05782
C	-10.7331	-1.79375	-0.64844
C	-9.49088	-1.5112	-1.26439
C	-7.50477	-0.18774	-1.63594
C	-12.5591	-1.33681	0.866985
C	-12.541	-2.73854	1.29131
C	-11.4944	-3.65728	0.801539
C	-10.7135	-3.16183	-0.22983
C	-9.45442	-3.72011	-0.5782
C	-8.70165	-2.70589	-1.22716
C	-7.31718	-2.71113	-1.26901
C	-6.69756	-1.41353	-1.60259
C	-6.71729	-3.9324	-0.78683
C	-7.44036	-4.96195	-0.15083
C	-8.88342	-4.82614	0.068108
C	-9.78576	-5.49353	1.011431
C	-11.0236	-4.90875	1.347284
C	-5.46918	1.137091	-2.14164
C	-4.66091	-0.09031	-2.10777
H	-5.62757	-4.05309	-0.83933
H	-11.6429	1.373976	0.139524
H	-9.50735	1.859593	-0.91733

C	-0.26696	3.72398	-1.90314
C	-0.5993	5.096135	-1.6031
C	-1.90262	5.624416	-1.69276
C	-3.02067	4.775856	-2.11563
C	-2.62479	3.515901	-2.58317
C	-1.30191	3.014079	-2.48508
C	0.909248	2.918894	-1.52861
C	-4.46941	4.910253	-1.93925
C	-5.31048	3.783486	-2.05385
C	-4.83264	2.45281	-2.35163
C	-3.49573	2.402139	-2.70418
C	-2.7081	1.208018	-2.66763
C	-1.35437	1.587863	-2.53043
C	-0.37652	0.762179	-1.98895
C	0.856685	1.45611	-1.5737
C	-0.82313	-0.58609	-1.73601
C	-2.17182	-0.96666	-1.87241
C	-3.19532	-0.03202	-2.27453
C	1.998051	0.733118	-1.15849
H	1.963528	-0.36108	-1.18404
C	3.155758	1.376779	-0.71894
H	4.02192	0.789023	-0.39914
C	3.202641	2.783322	-0.66825
H	4.100615	3.288273	-0.29992
C	2.094284	3.532634	-1.06363
H	2.132119	4.62532	-1.00938
H	-2.4506	-1.98255	-1.56552
H	-0.12019	-1.32384	-1.33082
H	-6.37271	3.934835	-1.82242
H	0.177181	5.756514	-1.19979
C	-13.5136	-3.16943	2.225472
H	-13.505	-4.21826	2.544822
C	-13.5492	-0.48475	1.412613
H	-13.5694	0.564684	1.09564
C	-14.4992	-0.94967	2.325762
H	-15.2586	-0.26447	2.721297
C	-14.4814	-2.29983	2.734644
H	-15.2267	-2.66873	3.449566

H	-11.612	-5.41034	2.126234
C	-6.85005	1.029374	-1.89654
H	-7.45262	1.944462	-1.923
C	-5.31408	-1.30475	-1.83221
H	-4.71208	-2.22026	-1.8076
C	-2.11374	7.056046	-1.24199
H	-2.66236	7.64769	-1.9982
H	-2.70879	7.105304	-0.30833
H	-1.1455	7.553426	-1.05162
C	-5.10308	6.228702	-1.54257
H	-4.77985	6.548395	-0.53289
H	-4.81998	7.040057	-2.23909
H	-6.20495	6.148782	-1.53516
C	-6.66325	-6.15652	0.365659
H	-6.65652	-6.19113	1.472183
H	-7.10639	-7.10878	0.019121
H	-5.61374	-6.11893	0.022463
C	-9.39406	-6.77553	1.719114
H	-9.08607	-7.5576	1.000176
H	-8.53962	-6.61765	2.405158
H	-10.2377	-7.16716	2.315262

Parallel stacked dimer of the model of 2

Symbol	X	Y	Z
C	-2.13733	1.030063	2.177782
C	-1.98371	2.445254	1.939715
C	-0.74207	3.110365	1.950756
C	0.497761	2.369772	2.196854
C	0.288531	1.044481	2.594673
C	-0.97657	0.403901	2.59538
C	-3.25468	0.119779	1.866728
C	1.898901	2.68103	1.900537
C	2.8589	1.651765	1.832958
C	2.558488	0.257804	2.058179
C	1.279873	0.031929	2.534993
C	0.625994	-1.23674	2.487768
C	-0.76817	-1.00743	2.526355
C	-1.70347	-1.90356	2.025214
C	-3.04008	-1.32628	1.786509
C	-1.14435	-3.17058	1.620189
C	0.243341	-3.39875	1.581744
C	1.198648	-2.38104	1.947591
C	2.637514	-2.26203	1.645824
C	3.307812	-0.96077	1.697475
C	-4.13192	-2.14441	1.412755
H	-3.97309	-3.22584	1.336482
C	-5.39305	-1.6115	1.14327
H	-6.21588	-2.27547	0.854985
C	-5.60072	-0.21956	1.225113
H	-6.58949	0.20292	1.008563
C	-4.5431	0.623592	1.571589
H	-4.70529	1.706487	1.625241
C	3.393088	-3.38677	1.239881
H	2.894568	-4.36232	1.196107
C	4.746677	-3.2846	0.910632
H	5.305297	-4.17915	0.608935
C	4.674387	-0.89535	1.338553
H	5.175468	0.078748	1.36098
C	5.39064	-2.03144	0.959687
H	6.448998	-1.94437	0.68837

H	0.592839	-4.34775	1.158793
H	-1.80155	-3.95325	1.222893
H	3.867256	1.938069	1.508882
H	-2.85851	3.038481	1.646667
C	-0.72527	4.580157	1.592981
H	-0.18651	5.179467	2.35066
H	-0.21172	4.744152	0.627824
H	-1.75318	4.975308	1.50428
C	2.34587	4.089291	1.569084
H	1.901652	4.433917	0.616995
H	2.041429	4.807482	2.353554
H	3.44498	4.136308	1.464532
C	-2.54824	0.550691	-1.36439
C	-2.86405	1.934303	-1.62486
C	-1.90722	2.967723	-1.62221
C	-0.49789	2.669376	-1.35823
C	-0.2714	1.363681	-0.9029
C	-1.26025	0.34511	-0.90157
C	-3.30037	-0.67341	-1.69034
C	0.723386	3.403971	-1.68863
C	1.969307	2.745585	-1.69895
C	2.138032	1.346467	-1.39673
C	0.995963	0.72846	-0.91845
C	0.793624	-0.68635	-0.94722
C	-0.6009	-0.92219	-0.94127
C	-1.18028	-2.07158	-1.46419
C	-2.62583	-1.97083	-1.73164
C	-0.23468	-3.08357	-1.86472
C	1.152009	-2.84918	-1.87091
C	1.714513	-1.58054	-1.47991
C	3.041473	-1.00767	-1.76877
C	3.255083	0.438374	-1.7138
C	-3.38413	-3.10942	-2.09429
H	-2.8843	-4.08523	-2.11824
C	-4.74178	-3.0191	-2.41117
H	-5.30217	-3.92263	-2.681
C	-5.3878	-1.76583	-2.38483
H	-6.45359	-1.69002	-2.63227

C	-4.67143	-0.62058	-2.03148
H	-5.18126	0.348665	-1.99761
C	4.122734	-1.8281	-2.16348
H	3.969397	-2.91211	-2.19957
C	5.375412	-1.29617	-2.47645
H	6.195913	-1.96404	-2.76558
C	4.537783	0.941227	-2.03571
H	4.703606	2.024186	-1.98659
C	5.587311	0.09594	-2.40571
H	6.572223	0.516798	-2.64232
H	1.803756	-3.63173	-2.27828
H	-0.59534	-4.03821	-2.26758
H	2.834913	3.329454	-2.0376
H	-3.88685	2.206909	-1.91529
C	-2.37452	4.367363	-1.9679
H	-2.04496	5.101575	-1.20915
H	-1.9685	4.708227	-2.93968
H	-3.47705	4.407488	-2.03081
C	0.691382	4.85546	-2.12594
H	0.163608	4.976025	-3.09185
H	0.162283	5.496152	-1.3956
H	1.716055	5.249854	-2.25059

Antiparallel stacked dimer of the model of 2

Symbol	X	Y	Z
C	2.088033	0.492468	2.242258
C	2.186523	-0.92847	2.473026
C	1.074857	-1.76307	2.70638
C	-0.28109	-1.20901	2.708601
C	-0.31818	0.189848	2.667502
C	0.821769	1.00847	2.455501
C	3.045316	1.427878	1.621474
C	-1.58944	-1.84054	2.509232
C	-2.70056	-1.07025	2.110772
C	-2.65177	0.356523	1.899444
C	-1.46053	0.94216	2.291229
C	-1.02626	2.22577	1.839446
C	0.383669	2.265532	1.938623

C	1.178012	3.110311	1.173991
C	2.597608	2.720591	1.098801
C	0.434555	4.085918	0.413136
C	-0.96823	4.050519	0.320142
C	-1.75445	3.032832	0.975097
C	-3.12856	2.56937	0.71144
C	-3.56905	1.247131	1.162911
C	3.545281	3.543849	0.447071
H	3.213555	4.510808	0.050966
C	4.879029	3.156269	0.296839
H	5.588883	3.822192	-0.20913
C	5.308118	1.908285	0.794189
H	6.351608	1.594185	0.672185
C	4.400199	1.065569	1.43895
H	4.73682	0.091327	1.810192
C	-4.02724	3.35023	-0.05227
H	-3.70029	4.339261	-0.39413
C	-5.30768	2.894678	-0.37706
H	-5.98156	3.528927	-0.96598
C	-4.86922	0.818158	0.808142
H	-5.19838	-0.17541	1.131305
C	-5.73077	1.620627	0.05589
H	-6.73417	1.257138	-0.1974
H	-1.45551	4.769121	-0.34938
H	0.969176	4.829254	-0.19014
H	-3.62066	-1.61842	1.875148
H	3.160253	-1.42335	2.372355
C	1.324109	-3.25034	2.830263
H	0.83084	-3.67235	3.725494
H	0.930182	-3.79187	1.950046
H	2.406539	-3.46112	2.896022
C	-1.776	-3.33678	2.633048
H	-1.19975	-3.87574	1.858332
H	-1.42748	-3.70631	3.615889
H	-2.83954	-3.60961	2.513816
C	-2.17656	-0.36369	-1.37276
C	-2.33659	0.90961	-2.02899
C	-1.27707	1.810211	-2.252

C	0.081515	1.484268	-1.81262
C	0.157422	0.333962	-1.01903
C	-0.92756	-0.55529	-0.81299
C	-3.0514	-1.55079	-1.35332
C	1.38775	2.003287	-2.2249
C	2.56062	1.260411	-1.9875
C	2.572427	-0.02711	-1.33837
C	1.353892	-0.39476	-0.79941
C	1.008299	-1.74331	-0.48273
C	-0.40015	-1.8421	-0.48976
C	-1.08123	-3.03383	-0.69789
C	-2.51198	-2.87015	-1.01621
C	-0.23155	-4.19865	-0.75586
C	1.174947	-4.09965	-0.74653
C	1.852977	-2.82767	-0.67897
C	3.250341	-2.46459	-0.98487
C	3.604183	-1.08097	-1.31167
C	-3.38945	-3.97979	-1.04071
H	-2.99067	-4.96802	-0.78161
C	-4.74171	-3.84204	-1.36712
H	-5.39761	-4.72113	-1.36469
C	-5.25945	-2.57194	-1.6978
H	-6.32012	-2.45964	-1.95389
C	-4.42084	-1.45383	-1.69469
H	-4.82757	-0.46596	-1.93613
C	4.273561	-3.4424	-1.01303
H	4.013851	-4.47872	-0.7652
C	5.594825	-3.11694	-1.33197
H	6.365442	-3.89739	-1.33391
C	4.94989	-0.79299	-1.6402
H	5.217718	0.243689	-1.87277
C	5.934579	-1.78427	-1.64786
H	6.971025	-1.52452	-1.89574
H	1.754049	-5.02128	-0.88409
H	-0.67452	-5.19172	-0.90193
H	3.497629	1.67272	-2.38053
H	-3.31705	1.184959	-2.43533
C	-1.58103	3.075679	-3.0258

H	-1.19427	3.968402	-2.50272
H	-1.11118	3.062061	-4.0287
H	-2.67046	3.197582	-3.16186
C	1.5206	3.311305	-2.9759
H	1.050197	3.258393	-3.9767
H	1.02299	4.135387	-2.43245
H	2.583971	3.577916	-3.1133

Dimer of the model of 2 through the concave-concave interaction

Symbol	X	Y	Z
C	3.293226	-1.62538	1.373844
C	4.224546	-0.56277	1.235541
C	3.561795	0.662186	1.555754
C	2.225528	0.354135	1.897685
C	2.060815	-1.06014	1.788966
C	3.409671	-2.86033	0.723611
C	4.690406	-3.04388	0.033432
C	5.589707	-1.96598	-0.1022
H	6.487974	-2.14553	-0.70698
C	5.340571	-0.64206	0.421504
C	5.951879	0.657109	0.076966
C	5.272558	1.914589	0.406163
C	3.962164	1.906882	1.085734
C	1.179954	1.26335	1.798727
C	0.839427	-1.67368	1.57453
C	2.156681	-3.61876	0.67186
C	7.17211	0.722185	-0.6381
H	7.683824	-0.21532	-0.88596
C	7.73742	1.940436	-1.02353
H	8.688067	1.954127	-1.57002
C	7.084033	3.150065	-0.70711
C	5.052229	-4.35496	-0.63545
H	4.37954	-4.57757	-1.48661
H	6.087026	-4.32668	-1.02146
H	3.486685	-1.55844	-1.88303
C	1.326065	-1.46475	-1.88016
H	1.20719	-2.5506	-1.95657
C	2.93125	2.916399	1.143759

H	3.1527	3.942193	0.823171
C	1.600852	2.608056	1.486481
H	0.853657	3.40719	1.414448
C	-0.16571	0.660302	1.814248
H	7.524701	4.108697	-1.00633
C	5.873773	3.127154	-0.00903
H	5.37108	4.070364	0.235853
C	-1.32652	1.463672	1.879997
H	-1.20791	2.54955	1.956384
C	1.646631	1.311113	-1.6602
H	1.778802	2.393183	-1.562
C	2.767971	0.484163	-1.73285
H	3.771979	0.917626	-1.68805
C	2.606189	-0.91012	-1.84485
C	-0.33366	-0.79004	1.701217
C	0.945876	-3.02661	1.083835
H	0.031177	-3.61331	0.93528
C	-1.64639	-1.31226	1.659985
H	-1.77829	-2.39437	1.561744
C	2.092983	-5.01263	0.080349
H	2.325111	-5.00478	-1.00314
H	2.822973	-5.69397	0.55568
C	-1.60159	-2.60839	-1.48637
H	-0.85461	-3.40773	-1.41448
C	-2.93205	-2.91639	-1.14358
H	-3.15374	-3.94213	-0.82299
C	-5.27312	-1.91397	-0.40603
C	-5.87464	-3.12636	0.009219
H	-5.37218	-4.06971	-0.23561
C	-7.08492	-3.14894	0.707286
H	-7.52583	-4.10745	1.006546
C	-7.73801	-1.93914	1.023642
H	-8.68867	-1.95257	1.57011
C	-2.60651	0.90873	1.844634
H	-3.48716	1.556841	1.882768
C	-2.76794	-0.48559	1.732608
H	-3.77184	-0.91929	1.687754
C	-3.2929	1.62546	-1.37384

C	-2.06064	1.059898	-1.78895
C	-2.22571	-0.35433	-1.89762
C	-3.56204	-0.66204	-1.55565
C	-4.22449	0.563097	-1.23549
C	-3.40904	2.860465	-0.72365
C	-2.15586	3.61857	-0.67191
C	-0.9452	3.026128	-1.08393
H	-0.03036	3.612601	-0.93539
C	-0.83909	1.673152	-1.5746
C	0.333768	0.789212	-1.70135
C	0.165454	-0.66109	-1.81433
C	-1.18036	-1.2638	-1.79869
C	-3.96272	-1.90662	-1.08558
C	-5.95213	-0.6563	-0.07689
C	-5.34051	0.642703	-0.42148
C	-5.58931	1.966716	0.102166
H	-6.48751	2.146512	0.706969
C	-4.68972	3.044368	-0.03348
C	-7.17239	-0.72104	0.638173
H	-7.68387	0.216597	0.885985
C	-2.09183	5.012434	-0.08038
H	-2.32373	5.004652	1.003175
H	-1.08319	5.445847	-0.20642
C	-5.05112	4.355546	0.635436
H	-4.37805	4.578169	1.486296
H	-4.96693	5.205608	-0.0672
H	4.96787	-5.2051	0.067066
H	1.08439	-5.44621	0.206178
H	-6.08577	4.327444	1.021845
H	-2.8218	5.693888	-0.55554

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