Supporting Information for

Facile Photochemical Synthesis of 5,10-Disubstituted [5]Helicenes by Removing Molecular Orbital Degeneracy

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Contents

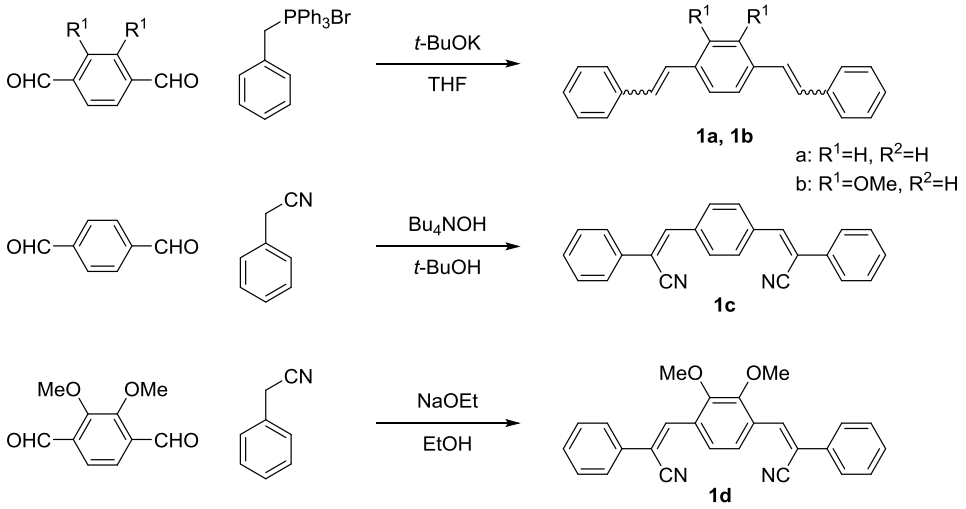
1. Synthesis of Materials

General. Unless specifically mentioned, reagents and solvents were obtained from commercial suppliers and used without further purification. All reactions were monitored by thin-layer chromatography carried out on 0.2 mm Merck silica gel plates (60F-254). Column chromatography was performed on silica gel (Nakalai Tesque, 70-230 mesh) or on a Biotage Instrument (Isolera One) with a SNAP flash silica gel cartridge (KP-Sil). Photoirradiation was performed using USHIO 500 W super-high-pressure mercury lamp. Final products were purified by the HPLC (Kanto chemical, Mightysil Si 60 250–20, 5 μm). ^{1}H and ^{13}C NMR spectra were recorded on a JEOL JMN-A500 instrument at room temperature unless otherwise noted. Proton and carbon chemical shifts were reported in ppm downfield from tetramethylsilane (TMS). Mass spectra were obtained by a Thermo Scientific Exactive mass spectrometer (ESI-Orbitrap) and a Thermo Scientific LTQ orbitrapXL mass spectrometer (MALDI-Orbitrap). Dithranol was used as the matrix of MALDI. Ethanol was refluxed in the presence of magnesium and iodine, and then distilled. Toluene was dried over calcium hydride and distilled before use.

Benzylcyanide and terephthalaldehyde (**7c**) are commercially available. Compounds 1,4-distyrylbenzene (**1a**)[S1] and 1,4-distyryl-2,3-dimethoxybenzene (**1b**)[S2] were prepared by a modified procedure.[S3] Compound 1,4-bis(2-cyano-2-phenylethenyl)benzene (**1c**)[S4], 7,8-dibromo[5]helicene[S5] and 2,3-dimethoxyterephthalaldehyde (**7d**)[S3] were prepared according to the literature. [5]helicene (**2a**)[S6] and benzo[*ghi*]perylene (**3a**)[S7] are known compounds.

Syntheses of the compounds

Scheme S1. Synthesis of **1a**–**d**.

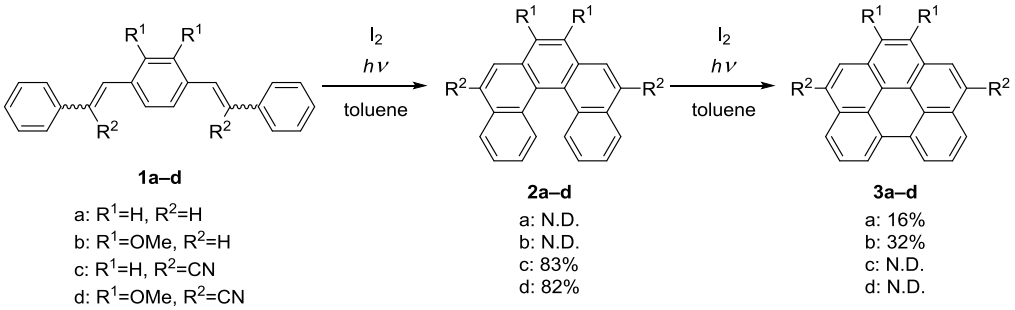


*Synthesis of 1,4-bis(2-cyano-2-phenylethenyl)-2,3-dimethoxybenzene (**1d**).*

To a solution of 1,4-diformyl-2,3-dimethoxybenzene (390 mg, 2.0 mmol) and benzyl cyanide (730 mg, 6.2 mmol) in dry ethanol (20 mL) was added sodium ethoxide (410 mg, 6.0 mmol). The reaction mixture was refluxed for 2.5 h. After cooling to room temperature, precipitates were filtered and washed with cold ethanol to give **1d** as an orange solid (360 mg, 0.92 mmol). To collect remaining product in solution, the filtrate was evaporated and the mixture was dissolved in dichloromethane. The resulting mixture was washed with brine, dried over $MgSO_4$, filtrated, and evaporated. The crude product was purified by silica gel column chromatography (hexane/dichloromethane = 50/50) to yield **1d** (32 mg, 0.081mmol) as an orange solid (combined yield: 50%).

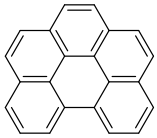
^{1}H NMR ($CDCl_3$, 500 MHz) δ 3.93 (6H, s), 7.50-7.41 (6H, m), 7.74-7.72 (4H, m), 7.89 (2H, s), 8.09 (2H, s); ^{13}C NMR ($CDCl_3$, 500 MHz) δ 61.5, 113.6, 117.6, 123.3, 126.1, 129.1, 129.5, 130.6, 134.3, 135.3, 152.0; MALDI HRMS (*m*/*z*) $[M]^+$ calcd. for $C_{26}H_{20}N_2O_2^+$: 392.1519; found: 392.1504.

Scheme S2. Photoreaction of **1a**–**d**.

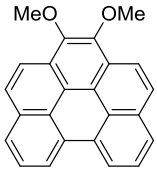


*General procedure of photoreaction of 1,4-distyrylbenzene **1a**–**d**.*

A round-bottom quartz flask was charged with 1,4-distyrylbenzene (0.15 mmol), iodine (39 mg, 0.15 mmol) and toluene (45 mL). The solution was stirred and irradiated by super-high-pressure mercury lamp (500 W) through a sharp-cut filter UV-29 for 36 h. The mixture was washed with aq. $Na_2S_2O_3$ and water, dried over $MgSO_4$, filtered, and concentrated *in vacuo*. The crude product was purified by silica gel column chromatography (hexane/dichloromethane) to afford a helicene derivative or a benzo[*ghi*]perylene derivative.

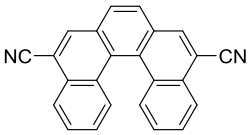


Benzo[*ghi*]perylene (3a).[S8] Prepared as above from **1a** (43 mg, 0.15 mmol) to give **3a** (6.6 mg, 0.024 mmol, 16%) as a colorless solid after silica gel column chromatography (hexane/dichloromethane = 75/25).



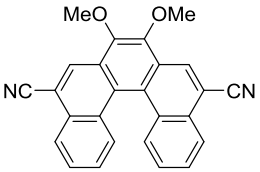
11,12-Dimethoxybenzo[*ghi*]perylene (3b). Prepared as above from **1b** (50 mg, 0.15 mmol) to give **3b** (15 mg, 0.045 mmol, 31%) as a yellow solid after silica gel column chromatography (hexane/dichloromethane =50/50).

^{1}H NMR ($CDCl_3$, 500 MHz) δ 4.26 (6H, s), 7.96 (2H, t, *J* = 7.6 Hz), 8.11 (2H, d, *J* = 8.9 Hz), 8.17 (2H, d, *J* = 7.7 Hz), 8.45 (2H, d, *J* = 8.9 Hz), 8.96 (2H, d, *J* = 7.7 Hz); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 61.8, 120.8, 121.0, 121.7, 124.8, 125.7, 125.9, 126.5, 127.6, 130.1, 131.7, 145.7; MALDI HRMS (*m*/*z*) $[M]^+$ calcd. for $C_{24}H_{16}O_2^+$: 336.1145; found: 336.1133.



5,10-Dicyano[5]helicene (2c). Prepared as above from **1c** (49 mg, 0.15 mmol) to give **2c** (41 mg, 0.13 mmol, 83%) as a yellow solid after silica gel column chromatography (hexane/dichloromethane = 25/75).

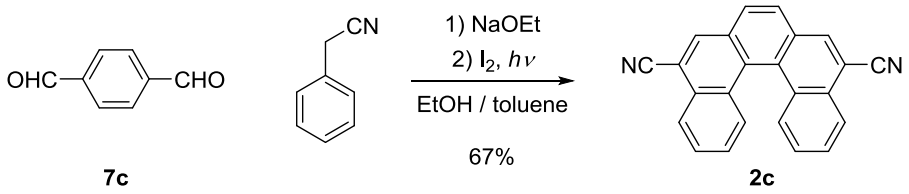
^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.42 (2H, t, *J* = 7.3 Hz), 7.73 (2H, t, *J* = 7.5 Hz), 7.98 (2H, s), 8.43–8.38 (6H, m); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 111.1, 117.4, 125.5, 126.5, 128.1, 128.6, 129.0, 129.1, 129.9, 130.3, 131.8, 134.0; MALDI HRMS (*m*/*z*) $[M]^+$ calcd. for $C_{24}H_{12}N_2^+$: 328.0995; found: 328.0985.



5,10-Dicyano-7,8-dimethoxy[5]helicene (2d). Prepared as above from **1d** (59 mg, 0.15 mmol) to give **2d** (48 mg, 0.13 mmol, 82%) as a yellow solid after silica gel column chromatography (hexane/dichloromethane = 25/75).

^{1}H NMR ($CDCl_3$, 500 MHz) δ 4.17 (6H, s), 7.38 (2H, t, *J* = 7.7 Hz), 7.69 (2H, t, *J* = 7.5 Hz), 8.31 (2H, d, *J* = 8.6 Hz), 8.37 (2H, d, *J* = 8.3 Hz) 8.80 (2H, s); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 61.4, 110.9, 117.7, 125.3, 126.0, 126.5, 128.1, 128.2, 128.5, 129.0, 129.4, 130.2, 144.9; MALDI HRMS (*m*/*z*) $[M]^+$ calcd. for $C_{26}H_{16}N_2O_2^+$: 388.1206; found: 388.1195.

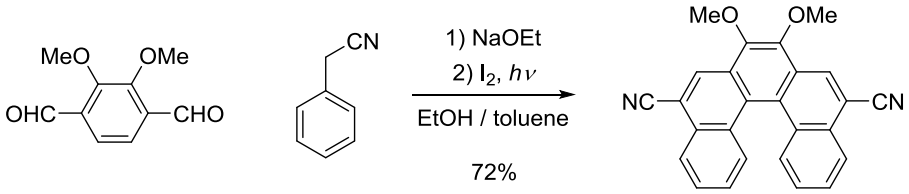
*One-pot synthesis of **2c**.*



7c **2c**

A round-bottom quartz flask was charged with terephthalaldehyde (**7c**) (19 mg, 0.15 mmol), benzyl cyanide (58 mg, 0.50 mmol), sodium ethoxide (30 mg, 0.44 mmol) and ethanol (2 mL). The mixture was stirred for 4 h at 50 °C and cooled to room temperature. After addition of iodine (39 mg, 0.15 mmol) and toluene (43 mL), the mixture was irradiated by super-high-pressure mercury lamp (500 W, without UV cut filter) for 64 h. The mixture was washed with aq. $Na_2S_2O_3$ and water, dried over $MgSO_4$, filtered, and concentrated *in vacuo*. The crude product was purified by silica gel column chromatography (hexane/dichloromethane = 75/25–25/75) to afford compound **2c** (33 mg, 0.10 mmol, 67%) as a yellow solid.

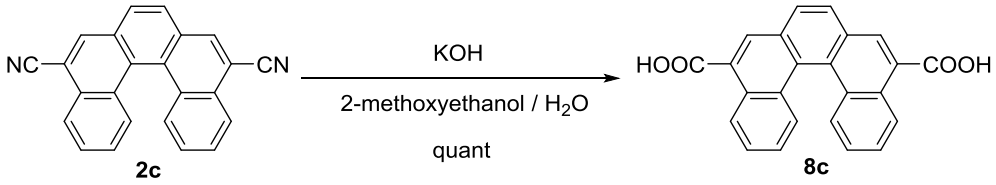
*One-pot synthesis of **2d**.*



7d **2d**

A round-bottom quartz flask was charged with 2,3-dimethoxyterephtalaldehyde (**7d**) (29 mg, 0.15 mmol), benzyl cyanide (50 mg, 0.43 mmol), sodium ethoxide (30 mg, 0.44 mmol) and ethanol (2 mL). The mixture was stirred for 4 h at 50 °C and cooled to room temperature. After addition of iodine (39 mg, 0.15 mmol) and toluene (43 mL), the mixture was irradiated by super-high-pressure mercury lamp (500 W, without UV cut filter) for 60 h. The mixture was washed with aq. $Na_2S_2O_3$ and water, dried over $MgSO_4$, filtered, and concentrated *in vacuo*. The crude product was purified by silica gel column chromatography (hexane/dichloromethane = 50/50–0/100) to afford compound **2d** (42 mg, 0.11 mmol, 72%) as a yellow solid.

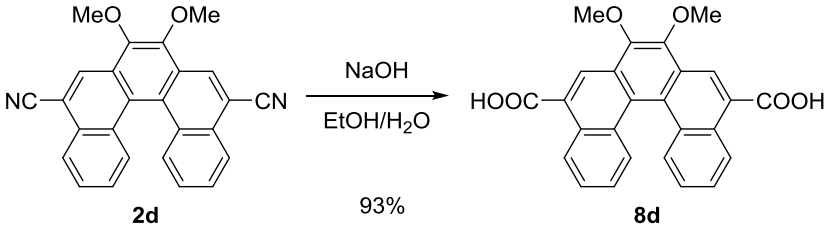
*Synthesis of [5]helicene-5,10-dicarboxylic acid (**8c**).*



To a suspension of **2c** (34 mg, 0.10 mmol) in 2-methoxyethanol (3 mL) was added aq. KOH (12 M, 1 mL). The mixture was refluxed for 24 h. After cooling to room temperature, the solution was acidified by 1 N HCl. The precipitate was filtrated, washed with water and dissolved in NaOH (1 M, 5 mL). 1 N HCl (15 mL) was added to the solution and the precipitate was filtered to afford **8c** (38 mg, 0.10 mmol, quant) as a brown solid.

^{1}H NMR (DMSO-d_6, 500 MHz) δ 7.36 (2H, t, J = 7.8 Hz), 7.66 (2H, t, J = 7.8 Hz), 8.25 (2H, s), 8.32 (2H, d, J = 8.6 Hz), 8.71 (2H, s), 8.87 (2H, d, J = 8.6Hz); ^{13}C NMR (DMSO-d_6, 126 MHz) δ 125.1, 125.8, 127.5, 127.8, 128.1, 128.48, 128.51, 129.2, 130.4, 130.6, 131.4, 168.2; ESI HRMS (*m*/*z*) $[M-H]^-$ calcd. for $C_{24}H_{13}O_4^-$: 365.0819; found: 365.0819.

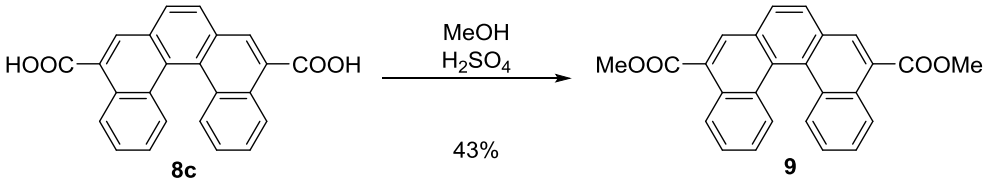
*Synthesis of 7,8-dimethoxy[5]helicene-5,10-dicarboxylic acid (**8d**).*



To a suspension of **2d** (150 mg, 0.39 mmol) in ethanol (8 mL) was added aq. NaOH (10 M, 8 mL). The mixture was refluxed for 25 h. After cooling to room temperature, the solution was acidified by 1 N HCl. The precipitate was filtrated to afford **8d** (160 mg, 0.36 mmol, 93%) as a pale yellow powder.

^{1}H NMR (DMSO-d_6, 500 MHz) δ 4.13 (6H, s), 7.35 (2H, t, J = 8 Hz), 7.63 (2H, t, J = 8 Hz), 8.21 (2H, d, J = 9 Hz), 8.84 (2H, d, J = 9Hz), 8.86 (2H, s); ^{13}C NMR (DMSO-d_6, 126 MHz) δ 61.3, 123.5, 125.28, 125.31, 125.8, 127.3, 127.5, 128.4, 128.6, 128.6, 130.6, 144.8, 168.3; MALDI HRMS (*m*/*z*) $[M]^+$ calcd. for $C_{26}H_{18}O_6^+$: 426.1098; found: 426.1085.

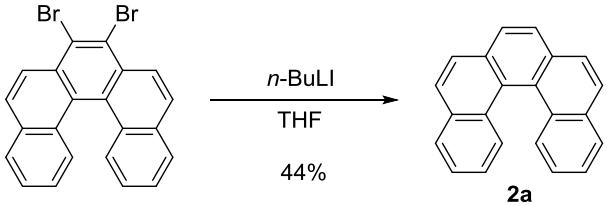
*Synthesis of dimethyl [5]helicene-5,10-dicarboxylate (**9**).*



8c **9**

A seal tube was charged with **8c** (160 mg, 0.40 mmol), dry methanol (2 mL) and sulfonic acid (0.2 mL). The suspension was stirred at 70°C for 30 h. The suspension was evaporated and diluted with ethyl acetate. The organic layer was washed with aq. $NaHCO_3$ and brine, dried over $MgSO_4$, filtered, and concentrated in *vacuo*. The crude product was purified by silica gel column chromatography (toluene) to afford **9** as a yellow solid (67 mg, 0.17 mmol, 43%)
^{1}H NMR ($CDCl_3$, 500 MHz) δ 4.12 (6H, s), 7.28 (2H, t, *J* = 7.5 Hz), 7.60 (2H, t, *J* = 7.5 Hz), 7.96 (2H, s), 8.43 (2H, d, *J* = 8.5 Hz), 8.60 (2H, s), 8.87 (2H, d, *J* = 8.9Hz); ^{13}C NMR ($CDCl_3$, 45 °C, 126 MHz) δ 52.3, 125.1, 125.8, 127.5, 127.6, 128.2, 129.3, 129.7, 131.0, 131.5, 131.7, 167.7; MALDI HRMS (*m*/*z*) $[M]^+$ calcd. for $C_{26}H_{18}O_4^+$: 394.1200; found: 394.1192.

*Synthesis of [5]helicene (**2a**).*

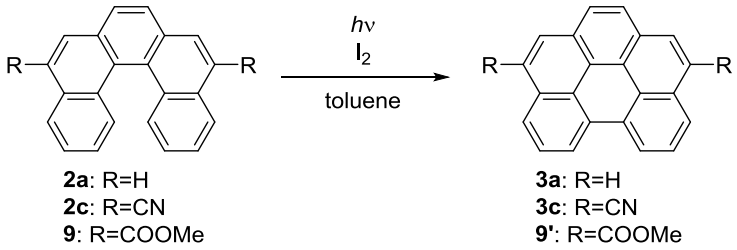


2a

To a solution of 7,8-dibromo[5]helicene (60 mg, 0.14 mmol) in dry THF (6 mL) was slowly added *n*-BuLi (1.6 M in hexanes, 0.3 mL, 0.5 mmol) at −78 °C under nitrogen atmosphere. The mixture was stirred at −78 °C for 40 min and water (0.2 mL, 10 mmol) was added. After warming up to the room temperature, water and ether were added to the mixture. The mixture was extracted with Et_2O and combined organic layers were washed with water, dried over $MgSO_4$, filtered, and evaporated. The crude product was purified by silica gel column chromatography (hexane/dichloromethane = 80/20) to give **2a** as a colorless solid (17 mg, 0.061 mmol, 44%).

2. Photoirradiation Experiment

*Photoreaction of **2a**, **2c**, and **9**.*



2a: R=H
2c: R=CN
9: R=COOMe

3a: R=H
3c: R=CN
9': R=COOMe

A round-bottom quartz flask was charged with [5]helicene (0.050 mmol), iodine (39 mg, 0.15 mmol) and toluene (45 mL). The solution was stirred and irradiated by super-high-pressure mercury lamp (500 W) through a sharp-cut filter UV-29. The small amount (0.2 mL) of reaction mixture was sampled at a fixed irradiation time in order to check the ratio between [5]helicene derivative and benzo[*ghi*]perylene by ^{1}H NMR. The plot was shown in Figure S2.

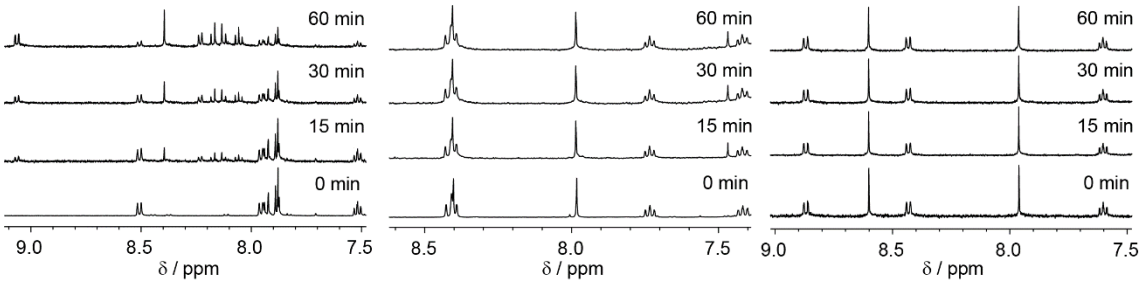


Figure S1. ^{1}H NMR spectra of (a) **2a**, (b) **2c**, and (c) **9** during the photochemical reaction.

Table S1. Fractions of [5]helicene derivatives upon the photochemical reaction

time/min	Fraction of a [5]helicene derivative [a]		
	2a	**2c**	**9**
0	1.00	1.00	1.00
15	0.76	1.00	1.00
30	0.54	1.00	1.00
60	0.27	1.00	1.00

[a] Fraction of a [5]helicene derivative was derived from ^{1}H NMR.

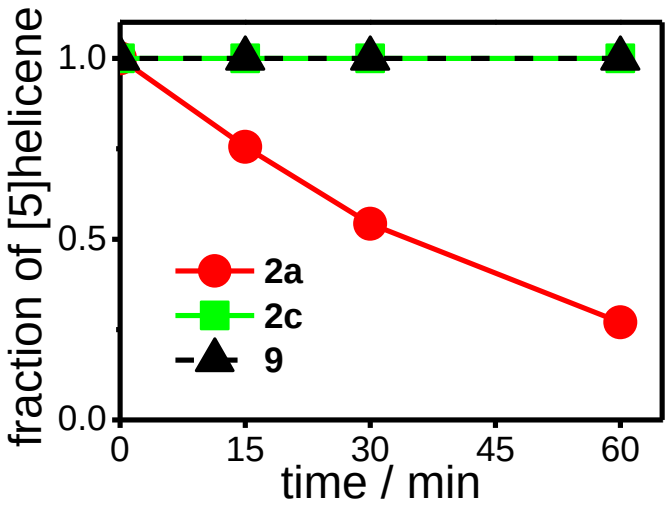


Figure S2. The plot of fraction of **2a**, **2c** and **9** upon the photochemical reaction.

3. Supporting Data

Theoretical calculation. The geometrical optimization was carried out at the RB3LYP/6-31g(d) level of theory. Convergence at a local minimum structure was confirmed by no imaginary frequencies on frequency analysis. Successively the optimized local minimum structures were subjected to TD-DFT calculations to obtain 10 excited states from the lowest energy transition at the identical level of theory.

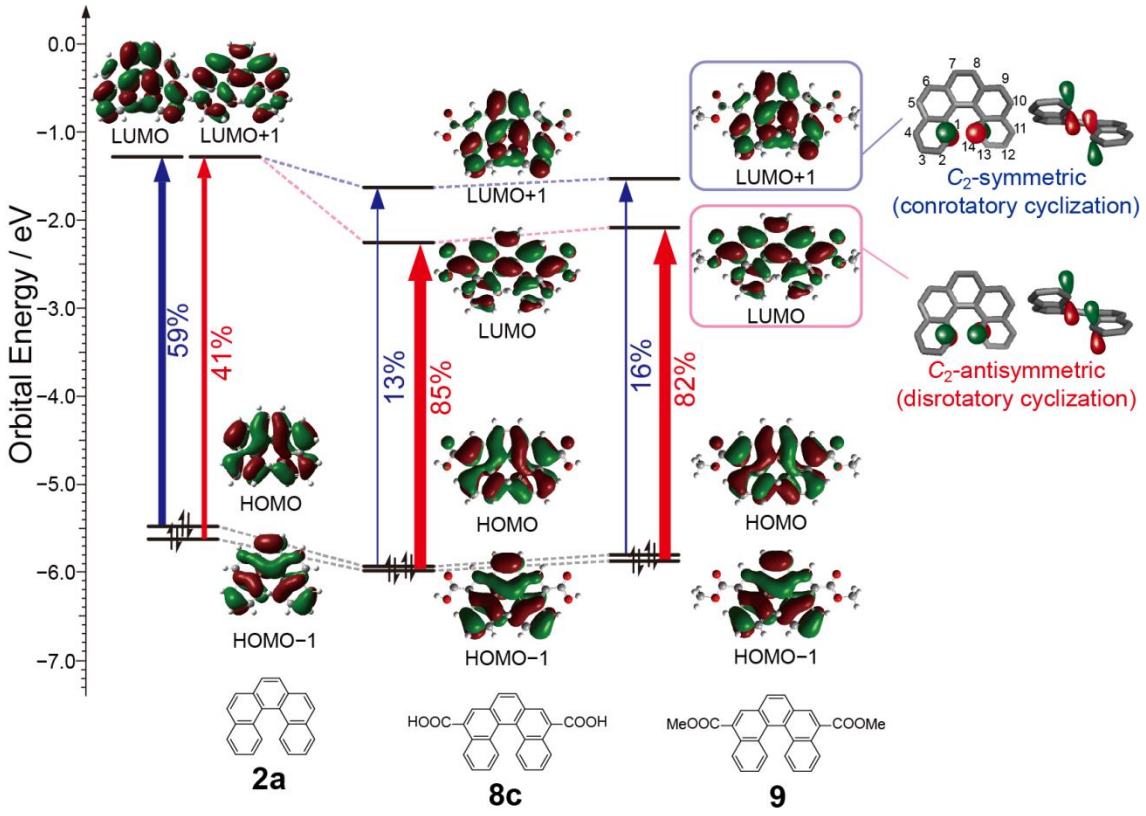


Figure S3. Orbital correlation diagram of **2a**, **8c** and **9** calculated at the RB3LYP/6-31g(d) level of theory. The transitions in blue arrows represent the transition to the symmetry-allowed orbital and those in red arrows represent the transition to the symmetry-forbidden orbital for conrotatory cyclization.

^{1}H and ^{13}C NMR spectra of the compounds

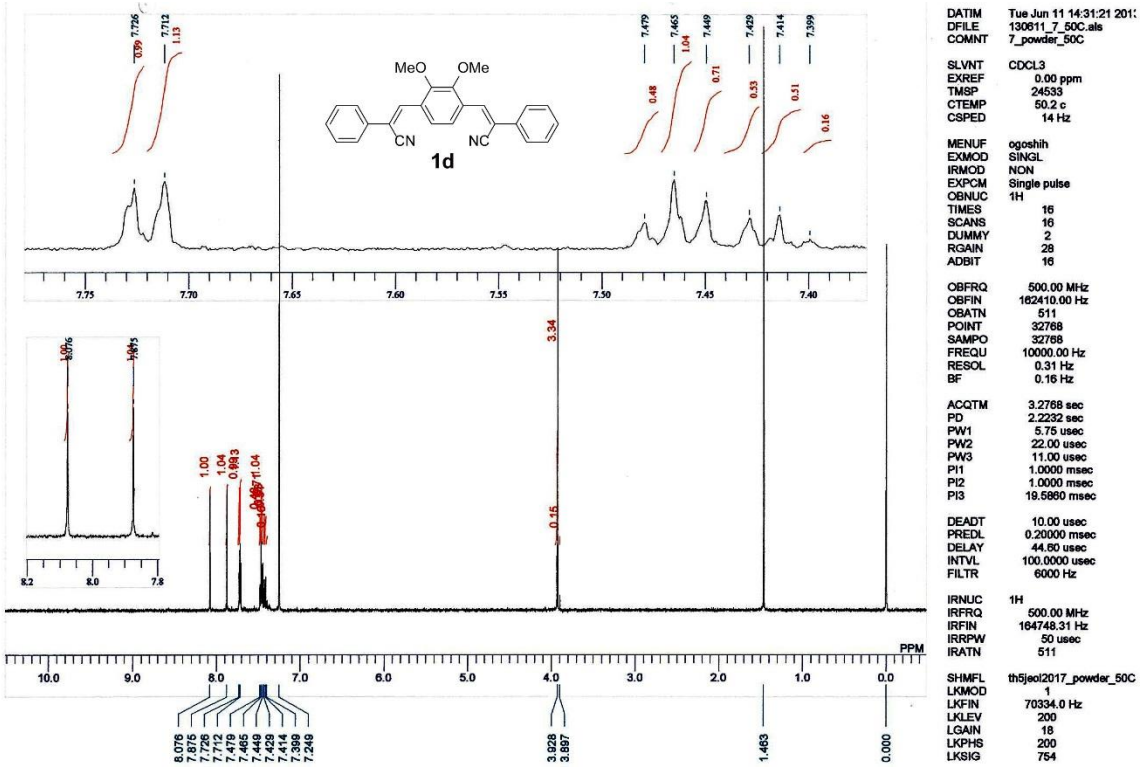


Figure S4. ^{1}H NMR spectrum of **1d** (500 MHz, $CDCl_3$) at room temperature.

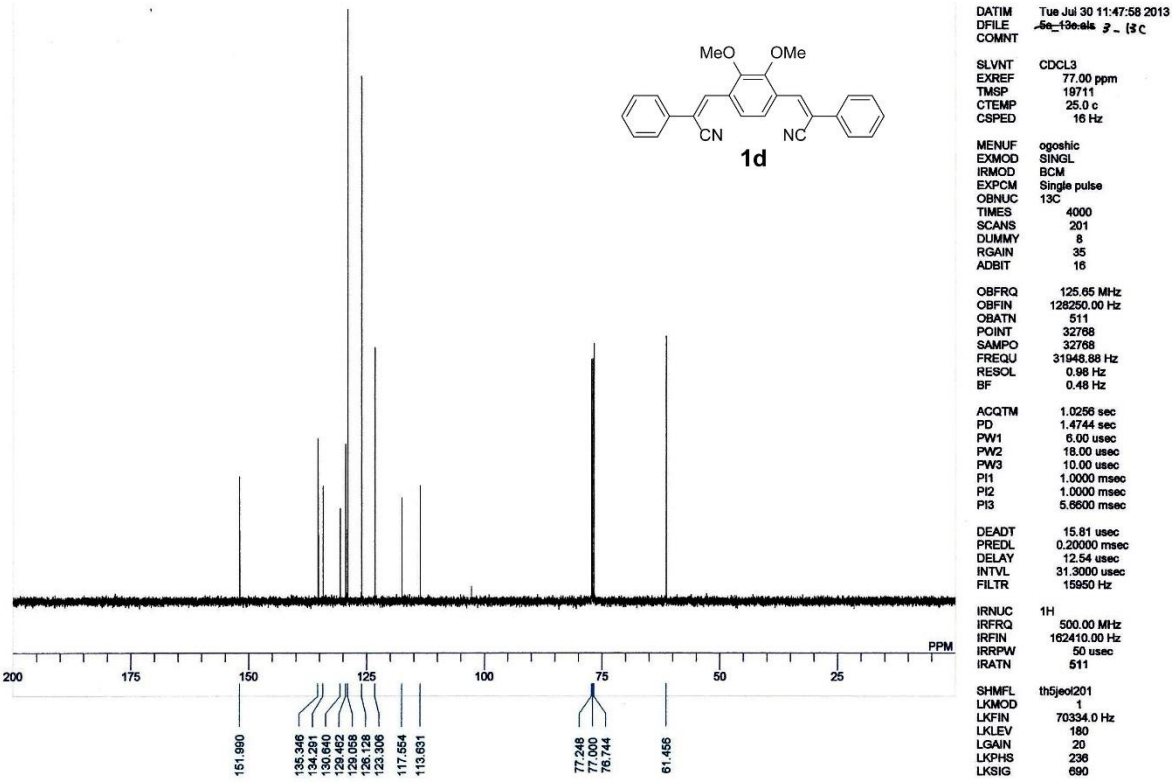


Figure S5 ^{13}C NMR spectrum of **1d** (126 MHz, $CDCl_3$) at room temperature.

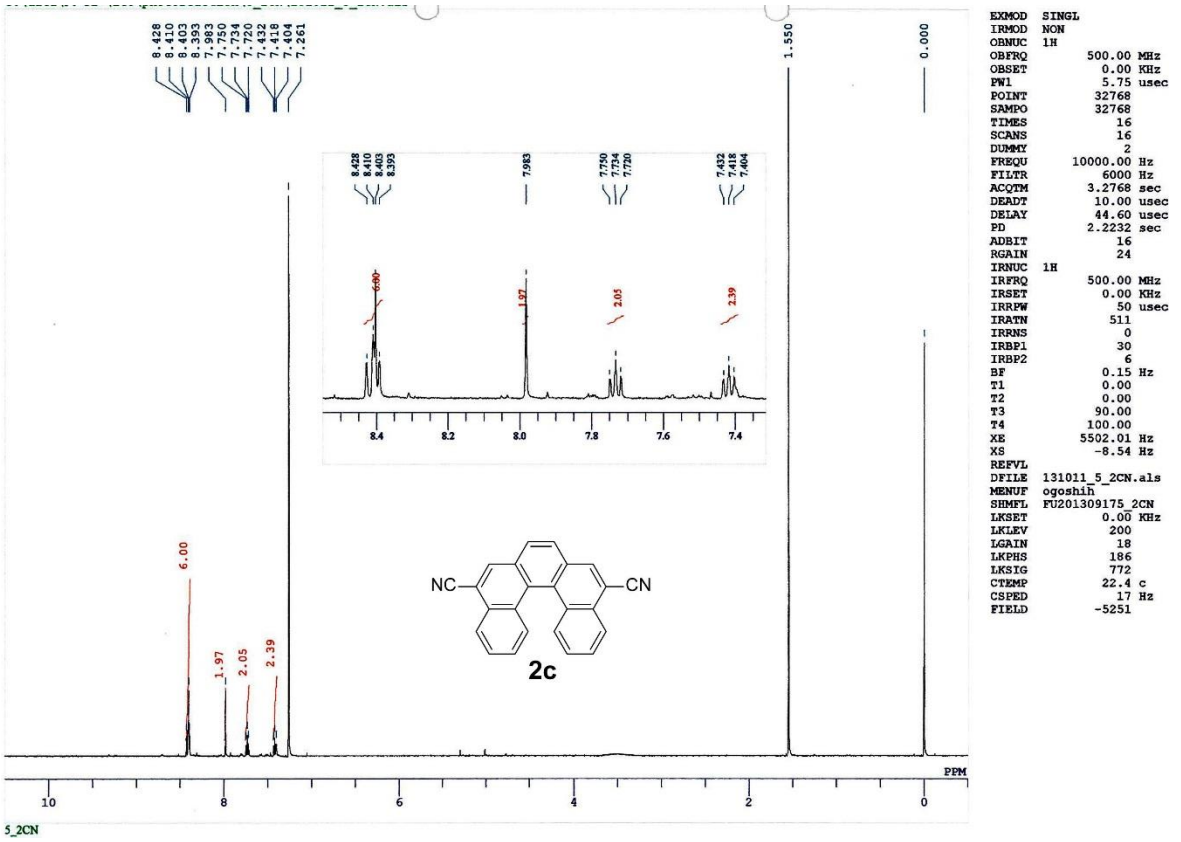


Figure S6. ^{1}H NMR spectrum of **2c** (500 MHz, $CDCl_3$) at room temperature.

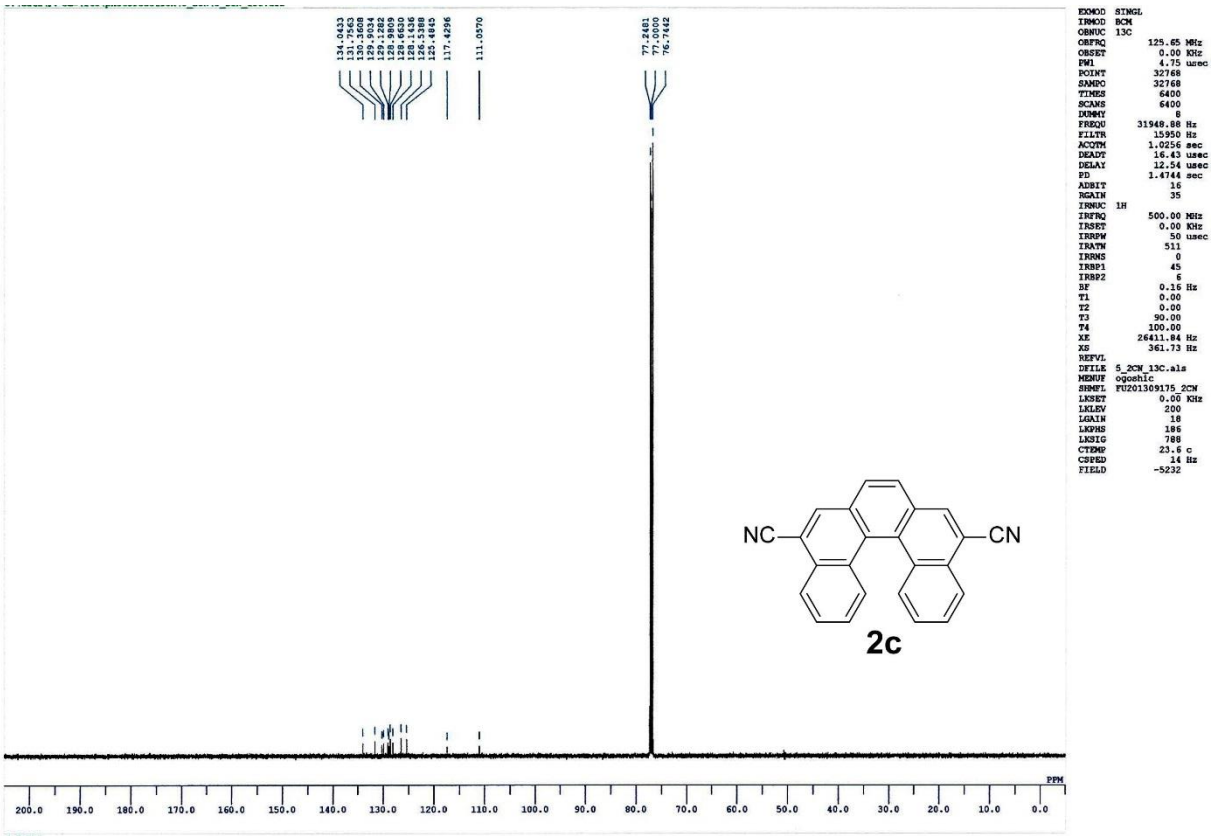


Figure S7. ^{13}C NMR spectrum of **2c** (126 MHz, $CDCl_3$) at room temperature.

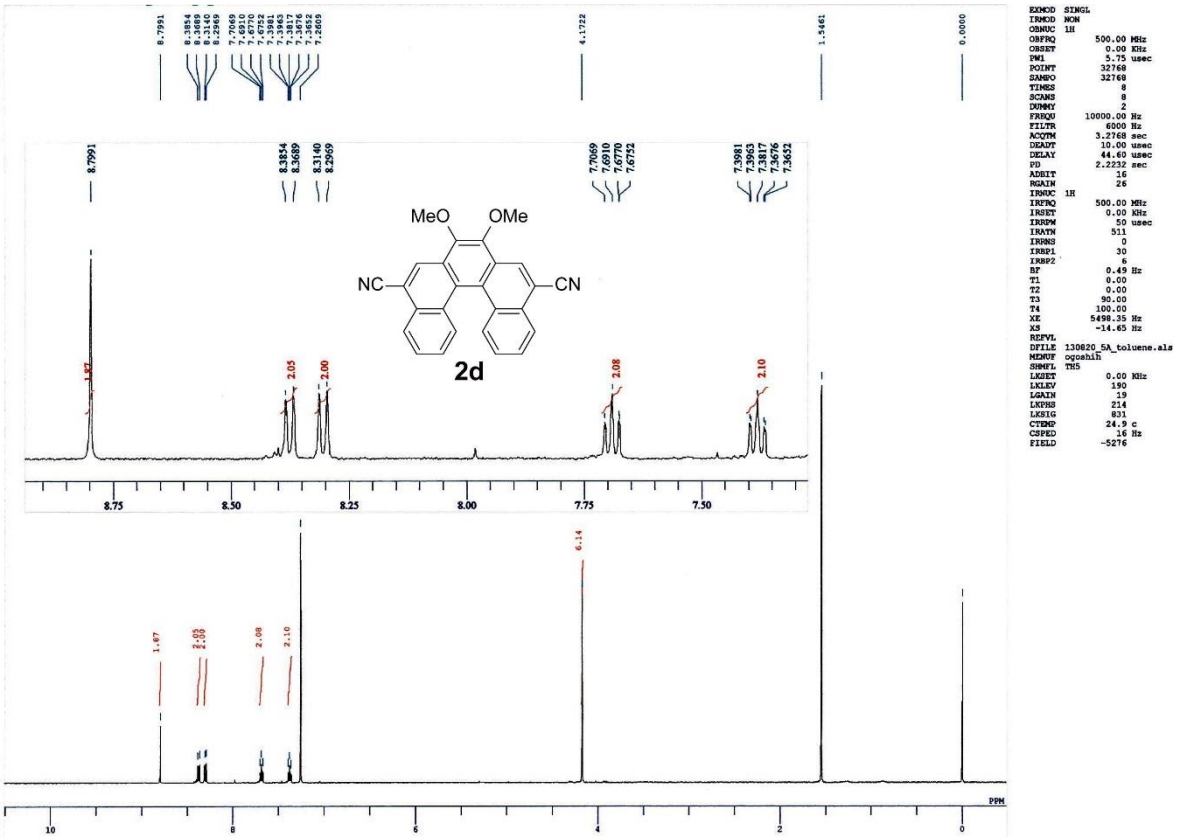


Figure S8. ^{1}H NMR spectrum of **2d** (500 MHz, $CDCl_3$) at room temperature.

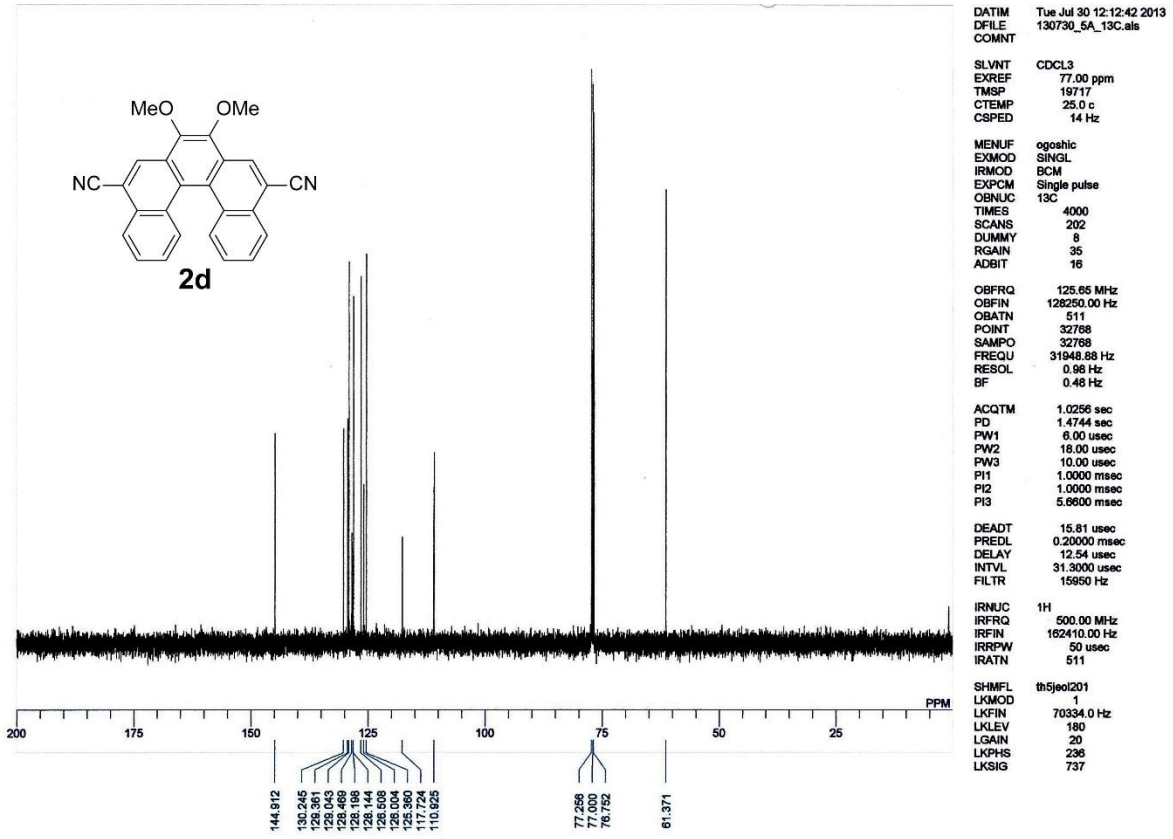


Figure S9. ^{13}C NMR spectrum of **2d** (126 MHz, $CDCl_3$) at room temperature.

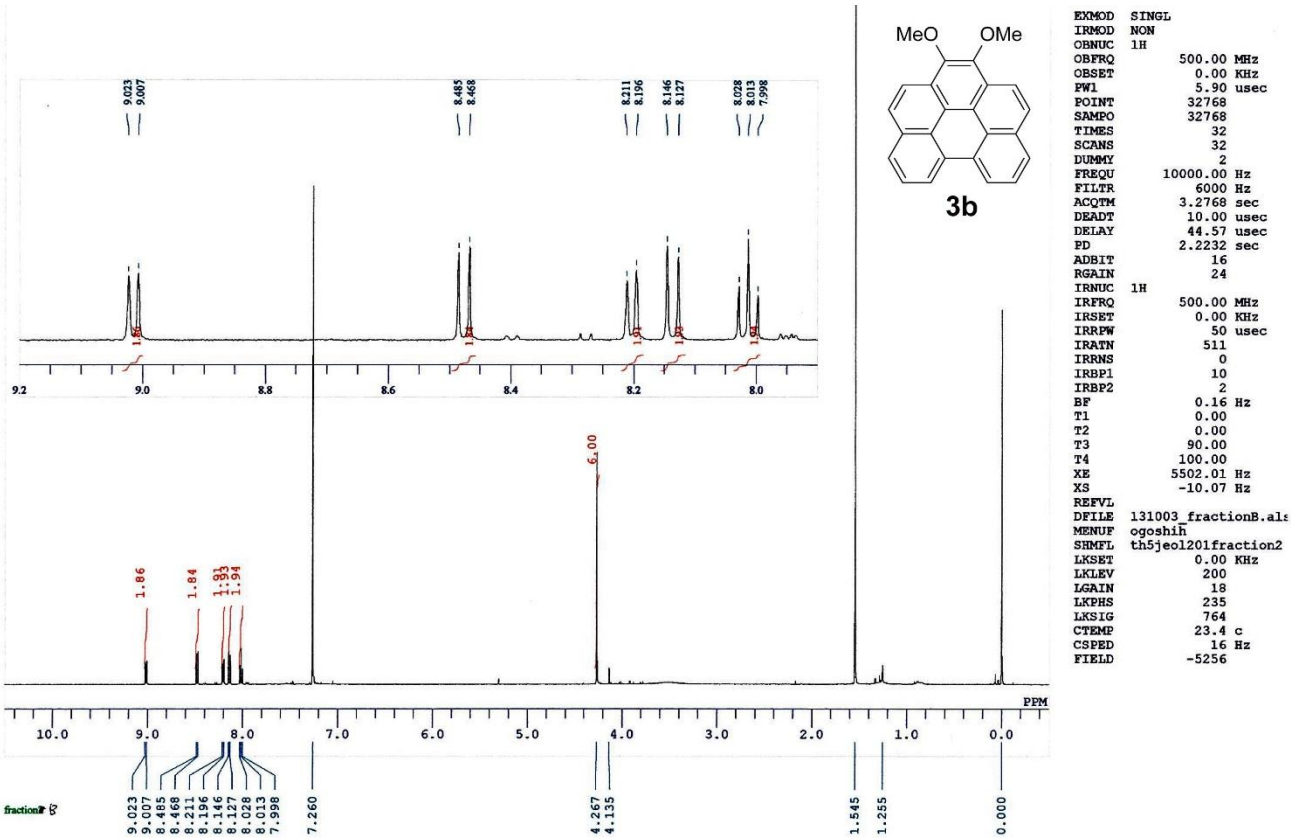


Figure S10. ^{1}H NMR spectrum of **3b** (500 MHz, $CDCl_3$) at room temperature.

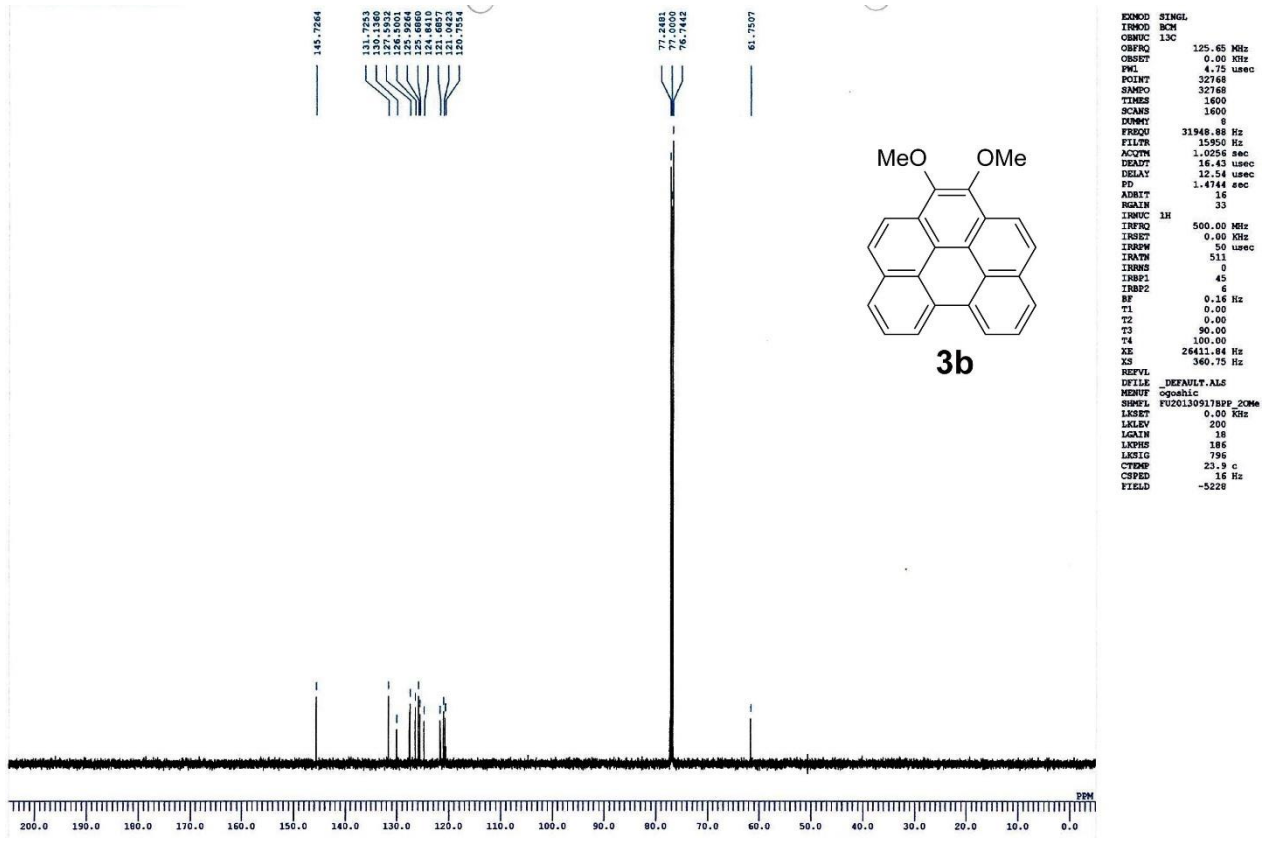


Figure S11. ^{13}C NMR spectrum of **3b** (126 MHz, $CDCl_3$) at room temperature.

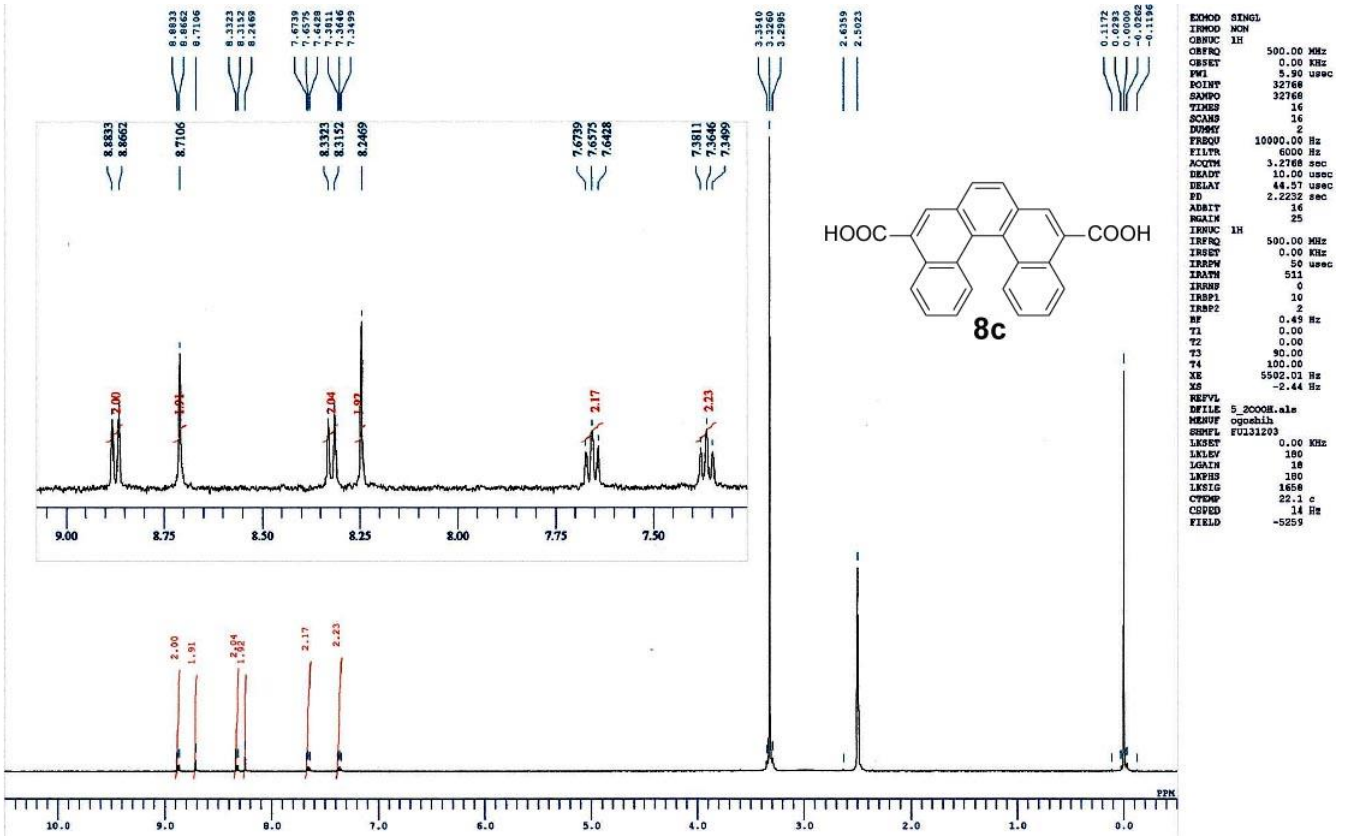


Figure S12. ^{1}H NMR spectrum of **8c** (126 MHz, $CDCl_3$) at room temperature.

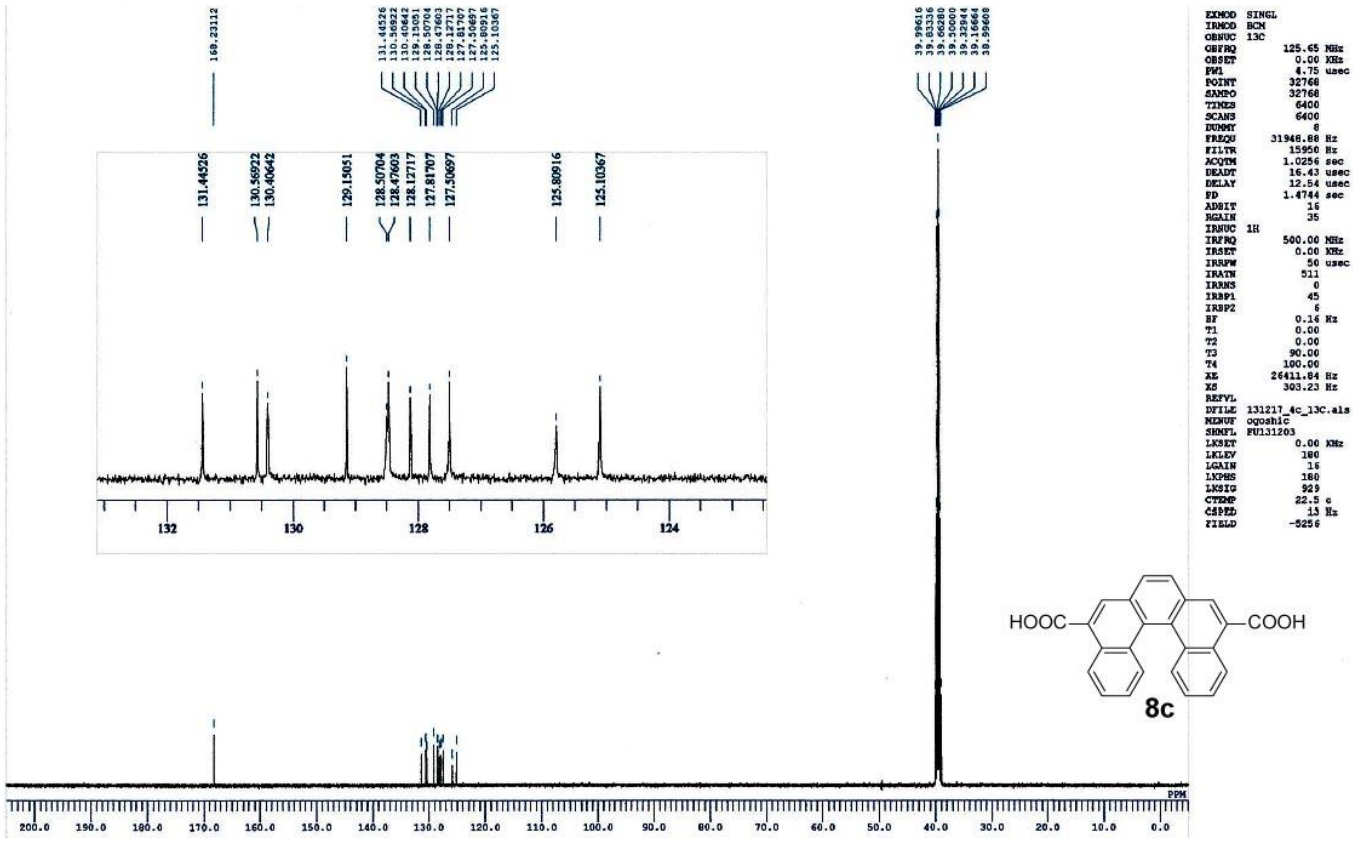


Figure S13. ^{13}C NMR spectrum of **8c** (126 MHz, $CDCl_3$) at room temperature.

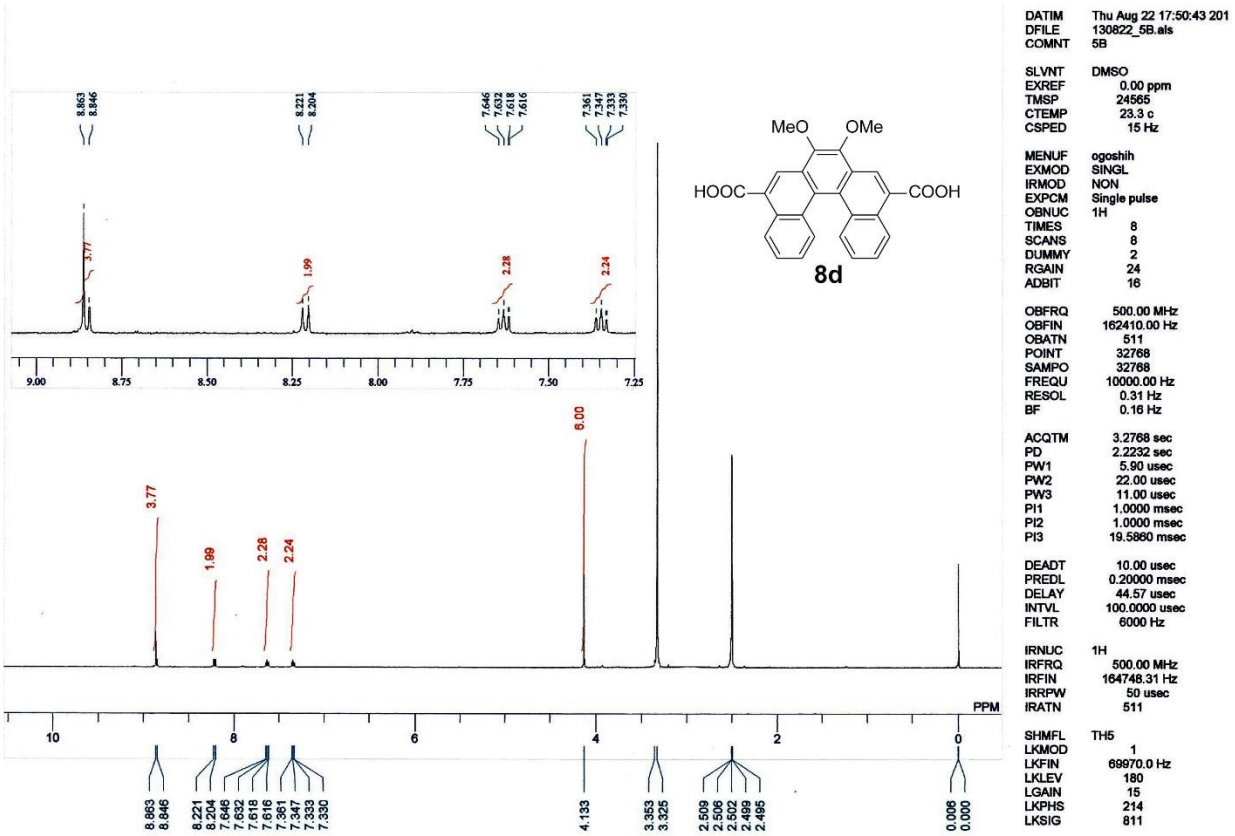


Figure S14. ^{1}H NMR spectrum of **8d** (500 MHz, $CDCl_3$) at room temperature.

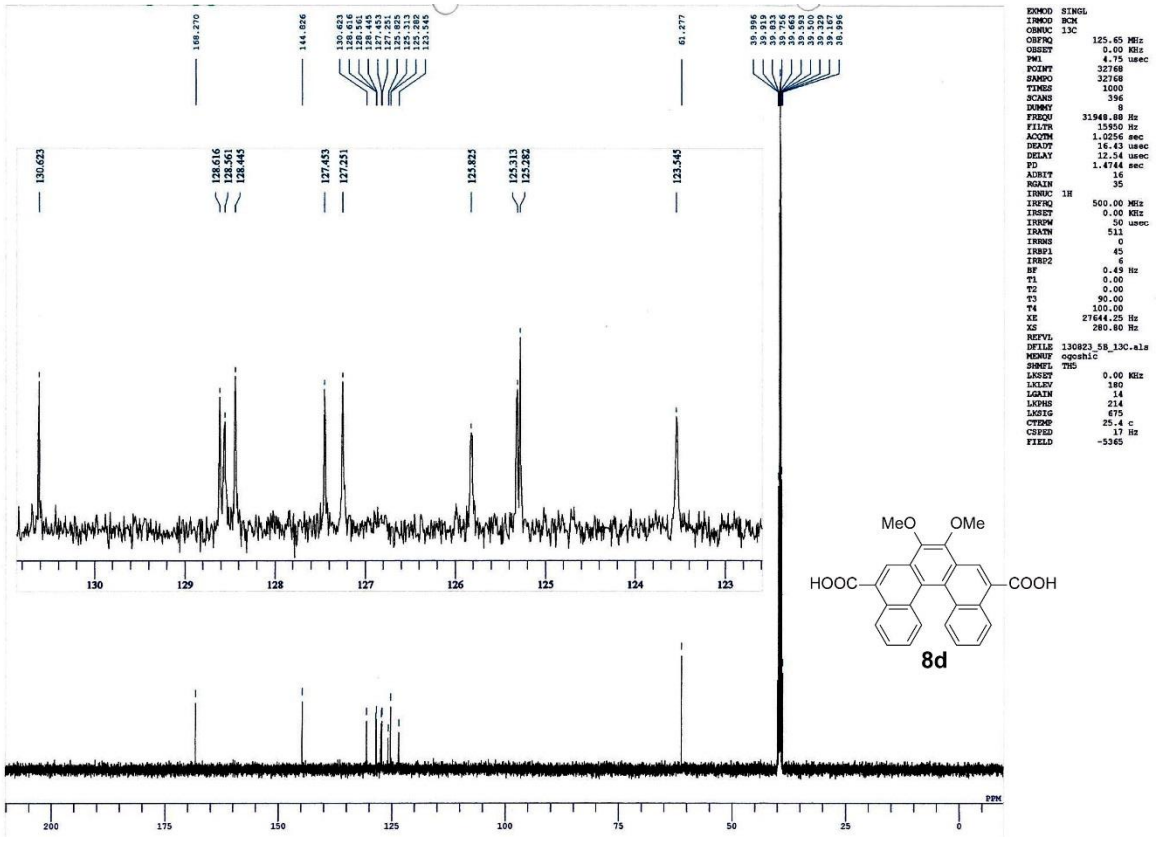


Figure S15. ^{13}C NMR spectrum of **8d** (126 MHz, $CDCl_3$) at room temperature.

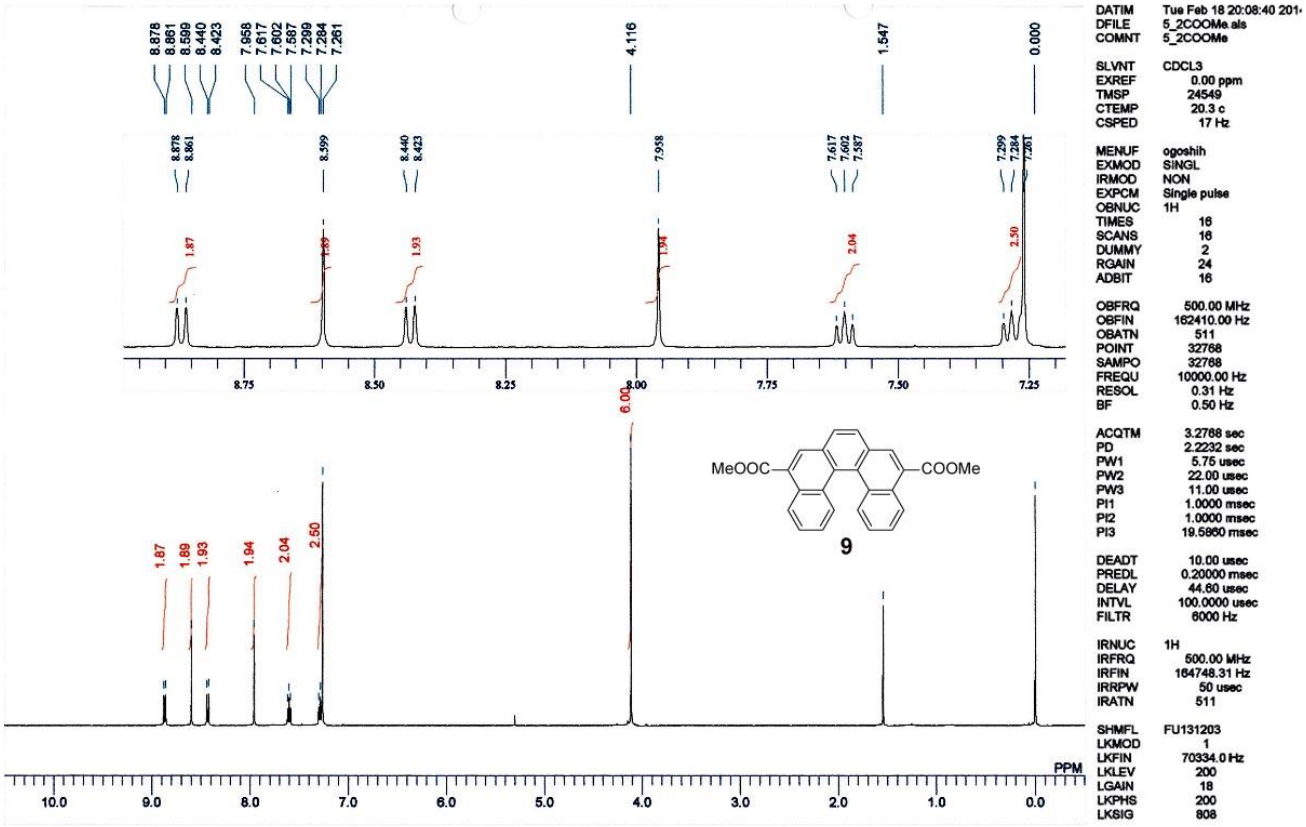


Figure S16. ^{1}H NMR spectrum of **9** (500 MHz, $CDCl_3$) at room temperature.

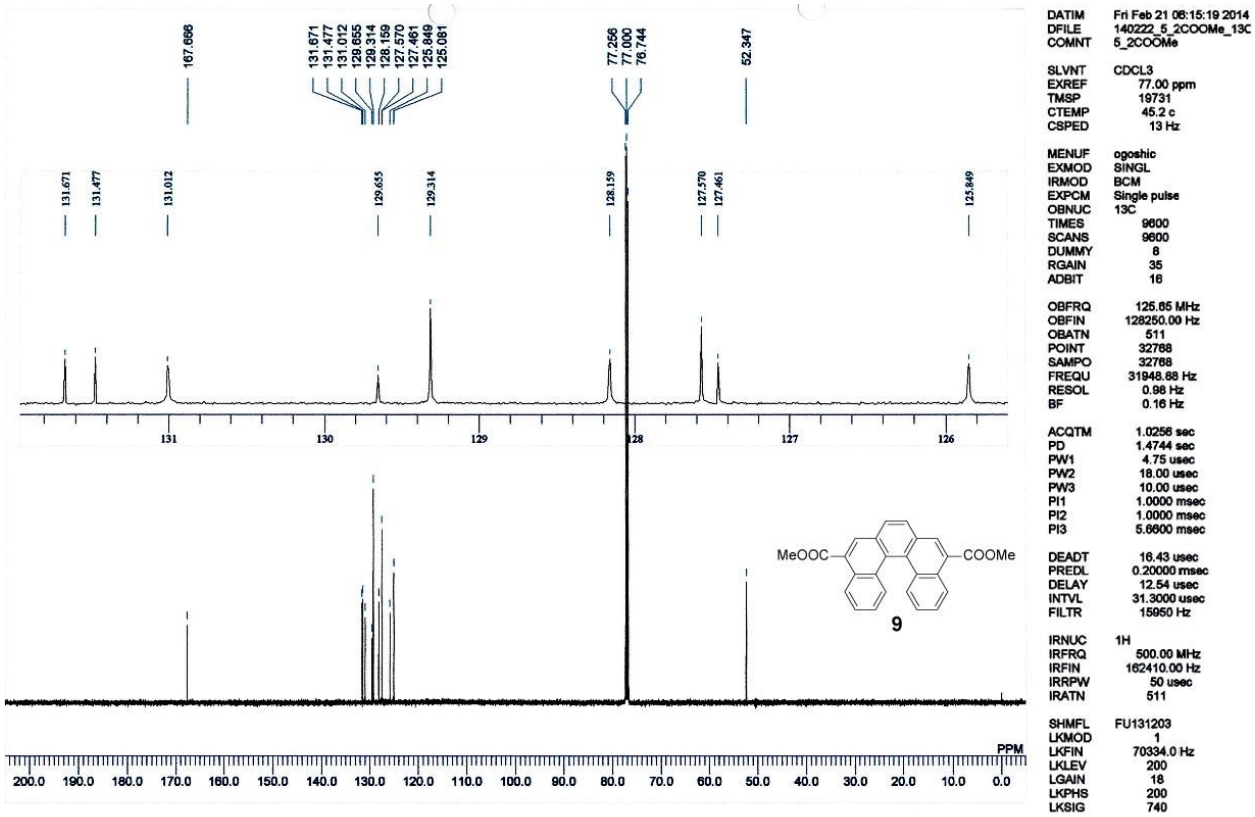


Figure S17. ^{13}C NMR spectrum of **9** (126 MHz, $CDCl_3$) at 45 °C.

Calculated excited states by TD-DFT (RB3LYP/6-31g(d) level of theory)

Table S2. Calculated excited states of 2a

States	Main Contributions (|C| > 0.2)	Excitation Energy in eV (nm)	Oscillator Strength (UV)	R_{length} (CD)
1	0.45 (72→75) + 0.54 (73→74)	3.40 (364)	0.0010	−2.07
2	−0.44 (72→74) + 0.54 (73→75)	3.64 (341)	0.0130	−1.76
3	0.53 (72→74) + 0.41 (73→75)	3.93 (316)	0.3557	356.26
4	0.52 (72→75) − 0.43 (73→74)	4.06 (306)	0.0714	−98.25
5	0.56 (71→74) − 0.37 (72→76)	4.12 (301)	0.0280	4.51
6	0.57 (71→75) + 0.40 (73→76)	4.22 (294)	0.0046	−5.85
7	0.33 (70→74) − 0.32 (71→75) + 0.50 (73→76)	4.46 (278)	0.0844	−44.72
8	0.35 (71→74) + 0.53 (72→76) + 0.21 (73→77)	4.60 (269)	0.3231	5.49
9	0.53 (70→75) + 0.20 (72→76) − 0.41 (73→77)	4.72 (263)	0.0001	−0.41
10	0.47 (70→74) + 0.47 (72→77)	4.81 (258)	0.0355	−12.44

Table S3. Calculated excited states of 2b

States	Main Contributions (|C| > 0.2)	Excitation Energy in eV (nm)	Oscillator Strength (UV)	R_{length} (CD)
1	0.46 (88→91) + 0.54 (89→90)	3.33 (372)	0.0015	0.05
2	−0.49 (88→90) + 0.50 (89→91)	3.56 (348)	0.0022	2.77
3	0.47 (88→90) + 0.47 (89→91)	3.86 (321)	0.3951	323.51
4	0.53 (88→91) − 0.44 (89→90)	3.96 (313)	0.1261	−131.21
5	0.53 (87→91) + 0.43 (89→92)	4.09 (303)	0.0029	4.40
6	0.61 (87→90) − 0.35 (88→92)	4.18 (296)	0.0048	−3.94
7	0.27 (86→91) + 0.29 (87→90) + 0.55 (88→92)	4.41 (281)	0.0785	−25.66
8	−0.40 (87→91) + 0.51 (89→92)	4.47 (277)	0.2833	−29.10
9	0.52 (86→90) − 0.43 (88→93)	4.67 (265)	0.0208	−1.23
10	0.47 (86→91) + 0.49 (89→93)	4.75 (261)	0.0071	−3.38

Table S4. Calculated excited states of 2c

States	Main CI coefficient (|C| > 0.2)	Excitation Energy in eV (nm)	Oscillator Strength (UV)	R_{length} (CD)
1	0.63 (84→86) − 0.30 (85→87)	3.14 (395)	0.0095	−7.50
2	0.67 (85→86)	3.32 (373)	0.2674	18.16
3	0.57 (83→86) + 0.35 (85→87)	3.70 (335)	0.0000	−0.48
4	0.67 (84→87)	3.83 (324)	0.2933	259.86
5	−0.36 (83→86) + 0.23 (84→86) + 0.52 (85→87)	3.92 (316)	0.1111	−112.94
6	−0.27 (82→86) + 0.49 (83→87) + 0.40 (84→88)	4.06 (306)	0.0063	8.37
7	0.61 (82→86) + 0.26 (84→88)	4.34 (286)	0.0056	12.28
8	−0.26 (82→87) + 0.62 (85→88)	4.36 (284)	0.0575	−27.28
9	−0.43 (83→87) + 0.49 (84→88)	4.44 (279)	0.2793	9.57
10	0.49 (82→87) − 0.45 (84→89)	4.79 (259)	0.0300	−12.95

Table S5. Calculated excited states of 2d

States	Main CI coefficient (|C| > 0.2)	Excitation Energy in eV (nm)	Oscillator Strength (UV)	R_{length} (CD)
1	−0.23 (100→103) + 0.66 (101→102)	2.97 (417)	0.0268	−17.25
2	0.66 (100→102) + 0.23 (101→103)	3.28 (378)	0.2234	14.94
3	0.65 (99→102) − 0.22 (100→103)	3.68 (337)	0.0042	2.52
4	−0.20 (100→102) + 0.65 (101→103)	3.74 (331)	0.3567	232.43
5	0.22 (99→102) + 0.62 (100→103) + 0.21 (101→102)	3.87 (320)	0.1325	−113.95
6	0.20 (98→102) − 0.42 (99→103) + 0.50 (101→104)	4.01 (309)	0.0277	−3.89
7	0.56 (98→102) − 0.37 (101→104)	4.24 (293)	0.0578	13.23
8	0.20 (98→103) + 0.63 (100→104) +	4.31 (288)	0.0467	−8.66
9	0.31 (98→102) + 0.52 (99→103) + 0.24 (101→104)	4.38 (283)	0.1859	−2.15
10	0.70 (97→102)	4.53 (274)	0.0010	−5.91

Table S6. Calculated excited states of 4

States	Main CI coefficient (|C| > 0.2)	Excitation Energy in eV (nm)	Oscillator Strength (UV)	R_{length} (CD)
1	0.69 (107→108)	2.67 (464)	0.0108	−19.97
2	0.68 (106→108)	2.90 (428)	0.1353	10.78
3	0.68 (107→109)	3.20 (388)	0.1032	−8.38
4	0.61 (105→108) + 0.33 (106→109)	3.29 (377)	0.0099	−2.82
5	−0.30 (105→108) + 0.60 (106→109)	3.44 (360)	0.0933	−35.88
6	0.32 (102→109) + 0.56 (103→108) + 0.26 (104→108)	3.60 (344)	0.0001	3.00
7	0.60 (102→108) + 0.33 (103→109)	3.64 (341)	0.0006	12.41
8	0.23 (104→108) + 0.65 (107→110)	3.77 (329)	0.1571	112.55
9	−0.21 (103→108) + 0.50 (104→108) −0.36 (105→109) + −0.21 (107→110)	3.83 (324)	0.0536	86.95
10	0.65 (106→110)	3.89 (319)	0.0572	−72.60

Table S7. Calculated excited states of 5

States	Main CI coefficient (|C| > 0.2)	Excitation Energy in eV (nm)	Oscillator Strength (UV)	R_{length} (CD)
1	0.41 (72→75) + 0.56 (73→74)	3.43 (361)	0.0041	−1.82
2	0.55 (72→74) − 0.42 (73→75)	3.65 (340)	0.0111	−1.36
3	0.39 (72→74) + 0.53 (73→75)	3.96 (313)	0.3442	332.30
4	−0.39 (71→74) + 0.43 (72→75) − 0.33 (73→74)	4.03 (308)	0.0285	−49.91
5	0.29 (70→74) − 0.34 (71→74) + 0.43 (71→75) − 0.22 (73→76)	4.12 (301)	0.0395	22.72
6	0.41 (71→74) + 0.31 (71→75) 0.29 (72→75) − 0.20 (73→74)	4.19 (296)	0.0758	−94.05
7	0.33 (69→74) + 0.50 (70→74)	4.23 (293)	0.0182	14.17
8	0.56 (70→75) − 0.31 (72→76) + 0.22 (73→76)	4.53 (274)	0.0158	0.11
9	0.43 (69→75) + 0.21 (70→75) + 0.44 (72→76)	4.62 (268)	0.0306	−2.62
10	0.23 (69→74) − 0.25 (71→75) + 0.24 (72→76) + 0.51 (73→76)	4.64 (267)	0.2089	−3.97

Table S8. Calculated excited states of 6

States	Main CI coefficient (|C| > 0.2)	Excitation Energy in eV (nm)	Oscillator Strength (UV)	R_{length} (CD)
1	0.50 (72→74) − 0.49 (73→75)	3.41 (364)	0.0004	1.05
2	0.36 (72→75) + 0.59 (73→74)	3.60 (344)	0.0317	2.86
3	0.57 (72→75) − 0.33 (73→74)	3.90 (318)	0.2775	275.27
4	0.44 (72→74) + 0.44 (73→75)	3.97 (312)	0.0541	−58.97
5	0.41 (70→74) − 0.23 (71→74) + 0.35 (71→75) − 0.26 (72→76)	4.19 (296)	0.0013	2.19
6	0.28 (70→74) − 0.28 (71→74) − 0.30 (71→75) + 0.21 (72→76) + 0.34 (73→76)	4.27 (291)	0.0553	51.92
7	0.29 (70→74) + 0.33 (71→74) + 0.35 (72→76) − 0.34 (73→76)	4.30 (288)	0.0198	−5.41
8	−0.35 (70→75) + 0.37 (71→74) + 0.38 (73→76)	4.42 (281)	0.0613	−28.56
9	0.32 (70→74) + 0.52 (70→75)	4.48 (277)	0.0276	−35.86
10	0.44 (71→75) + 0.41 (72→76)	4.58 (270)	0.3271	−5.15

Table S9. Calculated excited states of 8c

States	Main Contributions (|C| > 0.2)	Excitation Energy in eV (nm)	Oscillator Strength (UV)	R_{length} (CD)
1	0.65 (94→96) + 0.26 (95→97)	3.09 (401)	0.0136	−10.09
2	0.68 (95→96)	3.27 (379)	0.2699	5.92
3	0.64 (93→96) − 0.24 (95→97)	3.64 (341)	0.0032	2.54
4	0.68 (94→97)	3.83 (324)	0.2718	245.50
5	0.24 (93→96) − 0.23 (94→96) + 0.60 (95→97)	3.90 (318)	0.1003	−114.79
6	0.34 (92→96) + 0.49 (93→97) + 0.34 (94→98)	4.04 (307)	0.0009	--0.72
7	0.59 (92→96) − 0.25 (93→97) − 0.25 (94→98)	4.27 (290)	0.0101	10.97
8	−0.26 (92→97) + 0.63 (95→98)	4.37 (284)	0.0323	−13.08
9	−0.38 (93→97) + 0.53 (94→98)	4.39 (282)	0.2099	17.81
10	0.65 (90→96)	4.51 (275)	0.0017	−12.03

Table S10. Calculated excited states of 9

States	Main Contributions (|C| > 0.2)	Excitation Energy in eV (nm)	Oscillator Strength (UV)	R_{length} (CD)
1	0.64 (102→104) − 0.29 (103→105)	3.14 (395)	0.0109	-7.84
2	0.68 (103→104)	3.30 (375)	0.2968	-2.55
3	0.62 (101→104) + 0.28 (103→105)	3.69 (336)	0.0005	2.01
4	0.67 (102→105)	3.84 (323)	0.3019	237.11
5	−0.29 (101→104) + 0.24 (102→104) + 0.57 (103→105)	3.91 (317)	0.1020	-117.20
6	0.29 (100→104) + 0.52 (101→105) + 0.34 (102→106)	4.06 (306)	0.0029	0.00
7	0.61 (100→104) − 0.23 (101→105) − 0.22 (102→106)	4.32 (287)	0.0142	7.26
8	0.27 (100→105) + 0.62 (103→106)	4.38 (283)	0.0353	-10.02
9	− 0.16 (99→104) − 0.37 (101→105)	4.43 (280)	0.2467	17.38
10	0.66 (98→104)	4.52 (274)	0.0022	-14.16

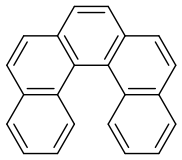
Table S11. Calculated excited states of (*cis*,*cis*)-**1a**

States	Main Contributions (|C| > 0.2)	Excitation Energy in eV (nm)	Oscillator Strength (UV)	R_{length} (CD)
1	0.70 (75→76)	3.47 (357)	0.6542	−540.84
2	0.56 (74→76) + 0.41 (75→77)	4.07 (304)	0.0066	15.12
3	−0.38 (74→76) + 0.42 (75→77) + 0.35 (75→78)	4.33 (286)	0.1224	446.10
4	0.46 (73→76) − 0.37 (75→77) + 0.29 (75→78)	4.38 (283)	0.0438	166.75
5	0.58 (72→76) + 0.33 (75→79)	4.58 (271)	0.0017	2.01
6	0.55 (71→76) − 0.22 (73→76) + 0.31 (75→80)	4.65 (267)	0.0012	−1.27
7	−0.41 (73→76) + 0.50 (75→78)	4.88 (254)	0.1726	−58.78
8	0.57 (70→76) + 0.30 (75→81)	4.91 (253)	0.0040	−12.03
9	−0.21 (70→76) − 0.35 (72→76) + 0.55 (75→79)	4.94 (251)	0.0519	84.47
10	0.63 (74→77) − 0.28 (75→81)	5.07 (245)	0.0552	−186.84

Table S12. Calculated excited states of (*cis*,*cis*)**-1c**

States	Main Contributions (|C| > 0.2)	Excitation Energy in eV (nm)	Oscillator Strength (UV)	R_{length} (CD)
1	0.70 (87→88)	3.20 (388)	0.7093	0.00
2	0.66 (86→88)	3.77 (329)	0.0437	0.00
3	0.67 (85→88)	3.98 (312)	0.0147	0.00
4	0.70 (84→88)	4.03 (308)	0.0039	0.00
5	0.23 (82→88) + 0.57 (87→89)	4.22 (294)	0.1293	0.00
6	0.59 (82→88) − 0.29 (87→89)	4.26 (291)	0.0058	0.00
7	0.68 (83→88)	4.37 (284)	0.1941	0.00
8	0.53 (81→88) − 0.37 (87→90) − 0.20 (87→93)	4.83 (257)	0.0101	0.00
9	0.32 (81→88) − 0.24 (84→89) + 0.43 (87→90) − 0.24 (87→94)	4.94 (251)	0.1041	0.00
10	0.66 (86→89)	4.95 (250)	0.0002	0.00

Cartesian coordinate [Å] of optimized structure (2a)



2a

1	C	1.367749	2.021028	0.328058
2	C	0.723667	0.781498	0.054639
3	C	-0.723667	0.781498	-0.054639
4	C	-1.367749	2.021028	-0.328058
5	C	-0.650226	3.244761	-0.207560
6	C	0.650226	3.244761	0.207560
7	C	-1.588873	-0.370163	0.186872
8	C	-2.968833	-0.303677	-0.186899
9	C	-3.509849	0.921236	-0.687382
10	C	-2.752485	2.052059	-0.689299
11	C	-1.169972	-1.521350	0.903959
12	C	-2.022640	-2.582152	1.138566
13	C	-3.350494	-2.551604	0.667514
14	C	-3.812462	-1.421747	0.026990
15	C	2.752485	2.052059	0.689299
16	C	3.509849	0.921236	0.687382
17	C	2.968833	-0.303677	0.186899
18	C	1.588873	-0.370163	-0.186872
19	C	3.812462	-1.421747	-0.026990
20	C	3.350494	-2.551604	-0.667514
21	C	2.022640	-2.582152	-1.138566
22	C	1.169972	-1.521350	-0.903959
23	H	-1.177307	4.177584	-0.391577
24	H	1.177307	4.177584	0.391577
25	H	-4.554957	0.948931	-0.985643
26	H	-3.185867	3.009021	-0.969828
27	H	-0.162014	-1.562518	1.296310
28	H	-1.666236	-3.440931	1.700985
29	H	-4.011929	-3.396387	0.839265
30	H	-4.849552	-1.355049	-0.293677
31	H	3.185867	3.009021	0.969828
32	H	4.554957	0.948931	0.985643
33	H	4.849552	-1.355049	0.293677
34	H	4.011929	-3.396387	-0.839265
35	H	1.666236	-3.440931	-1.700985
36	H	0.162014	-1.562518	-1.296310

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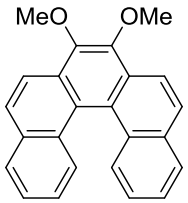
# of imaginary frequencies = 0

Cartesian coordinate [Å] of optimized structure (2b)



2b

1	C	2.370686	-0.654313	0.209239
2	C	1.139702	-1.367144	0.345420
3	C	-0.096941	-0.721996	0.067424
4	C	-0.096941	0.721996	-0.067424
5	C	1.139702	1.367144	-0.345420
6	C	2.370686	0.654313	-0.209239
7	C	-1.249758	1.589526	0.161151
8	C	-1.187638	2.962400	-0.236843
9	C	0.035266	3.493477	-0.751143
10	C	1.171019	2.743172	-0.738951
11	C	-2.398628	1.180459	0.887628
12	C	-3.461053	2.034807	1.108861
13	C	-3.434898	3.354220	0.614389
14	C	-2.307055	3.807317	-0.036011
15	C	1.171019	-2.743172	0.738951
16	C	0.035266	-3.493477	0.751143
17	C	-1.187638	-2.962400	0.236843
18	C	-1.249758	-1.589526	-0.161151
19	C	-2.307055	-3.807317	0.036011
20	C	-3.434898	-3.354220	-0.614389
21	C	-3.461053	-2.034807	-1.108861
22	C	-2.398628	-1.180459	-0.887628
23	O	3.551667	-1.314759	0.476910
24	C	4.289339	-1.709937	-0.687712
25	O	3.551667	1.314759	-0.476910
26	C	4.289339	1.709937	0.687712
27	H	0.059307	4.530498	-1.077225
28	H	2.125238	3.161006	-1.038739
29	H	-2.436799	0.179672	1.298099
30	H	-4.317737	1.686288	1.679408
31	H	-4.281114	4.016428	0.775843
32	H	-2.243016	4.838519	-0.375729
33	H	2.125238	-3.161006	1.038739
34	H	0.059307	-4.530498	1.077225
35	H	-2.243016	-4.838519	0.375729
36	H	-4.281114	-4.016428	-0.775842
37	H	-4.317737	-1.686288	-1.679408
38	H	-2.436799	-0.179672	-1.298099
39	H	5.179575	-2.226751	-0.321561
40	H	3.698129	-2.395850	-1.307390
41	H	4.582836	-0.837820	-1.280179
42	H	4.582836	0.837820	1.280179
43	H	5.179575	2.226751	0.321561
44	H	3.698129	2.395850	1.307390

B3LYP/6-31g(d)
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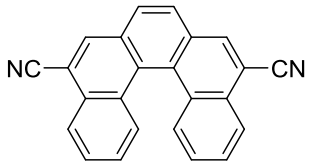
# of imaginary frequencies = 0

Cartesian coordinate [Å] of optimized structure (2c)

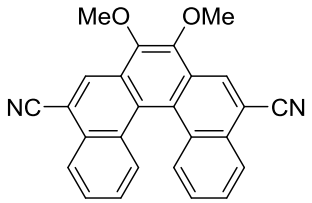


2c

1	C	1.391335	-1.882540	-0.167413
2	C	0.723624	-0.641325	0.032235
3	C	-0.723624	-0.641325	-0.032235
4	C	-1.391335	-1.882540	0.167413
5	C	-0.668985	-3.110337	0.132080
6	C	0.668985	-3.110337	-0.132080
7	C	2.799690	-1.911968	-0.378761
8	C	3.559669	-0.773596	-0.296155
9	C	2.965959	0.461405	0.157639
10	C	1.554160	0.509326	0.377193
11	C	-1.554160	0.509326	-0.377193
12	C	-2.965959	0.461405	-0.157639
13	C	-3.559669	-0.773596	0.296155
14	C	-2.799690	-1.911968	0.378761
15	C	-1.043908	1.649871	-1.049321
16	C	-1.853060	2.717109	-1.384029
17	C	-3.223405	2.702038	-1.060840
18	C	-3.770370	1.583370	-0.468339
19	C	3.770370	1.583370	0.468339
20	C	3.223405	2.702038	1.060840
21	C	1.853060	2.717109	1.384029
22	C	1.043908	1.649871	1.049321
23	C	-4.962957	-0.839400	0.576237
24	N	-6.102728	-0.887304	0.806965
25	C	4.962957	-0.839400	-0.576237
26	N	6.102728	-0.887304	-0.806966
27	H	-1.214981	-4.041290	0.256913
28	H	1.214981	-4.041290	-0.256912
29	H	3.269601	-2.860645	-0.619909
30	H	-3.269601	-2.860645	0.619909
31	H	0.002077	1.676443	-1.325564
32	H	-1.427963	3.567580	-1.909411
33	H	-3.853845	3.550934	-1.308846
34	H	-4.835929	1.534392	-0.265395
35	H	4.835929	1.534392	0.265395
36	H	3.853845	3.550933	1.308846
37	H	1.427963	3.567580	1.909411
38	H	-0.002077	1.676443	1.325564

B3LYP/6-31g(d)
Int = Ultrafine
E = -1031.2923865 hartree
# of imaginary frequencies = 0

Cartesian coordinate [Å] of optimized structure (2d)

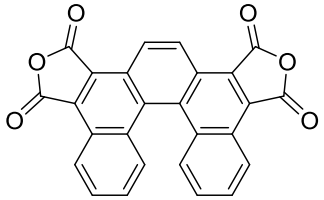


2d

1	C	-1.392171	1.126323	-0.175141
2	C	-0.723131	-0.113094	0.022767
3	C	0.723131	-0.113094	-0.022767
4	C	1.392171	1.126323	0.175141
5	C	0.675232	2.363789	0.126796
6	C	-0.675232	2.363789	-0.126796
7	C	-2.796359	1.157139	-0.412684
8	C	-3.552439	0.015385	-0.342797
9	C	-2.966032	-1.219008	0.121020
10	C	-1.557410	-1.264630	0.357517
11	C	1.557410	-1.264630	-0.357517
12	C	2.966032	-1.219008	-0.121020
13	C	3.552439	0.015385	0.342797
14	C	2.796359	1.157139	0.412684
15	C	-3.773027	-2.341415	0.422797
16	C	-3.232206	-3.459483	1.022189
17	C	-1.865855	-3.472385	1.361629
18	C	-1.053910	-2.404162	1.036400
19	C	1.053910	-2.404162	-1.036400
20	C	1.865855	-3.472385	-1.361628
21	C	3.232206	-3.459483	-1.022189
22	C	3.773027	-2.341415	-0.422797
23	O	1.372107	3.533098	0.314229
24	C	1.598017	4.303156	-0.879097
25	O	-1.372107	3.533098	-0.314229
26	C	-1.598017	4.303156	0.879097
27	C	4.950518	0.077879	0.649476
28	N	6.086504	0.120966	0.899308
29	C	-4.950518	0.077879	-0.649476
30	N	-6.086504	0.120966	-0.899308
31	H	-3.251126	2.105811	-0.670201
32	H	3.251126	2.105811	0.670201
33	H	-4.836052	-2.293292	0.206611
34	H	-3.864581	-4.308991	1.263134
35	H	-1.445772	-4.321809	1.892780
36	H	-0.011618	-2.429162	1.326272
37	H	0.011618	-2.429162	-1.326272
38	H	1.445772	-4.321809	-1.892780
39	H	3.864580	-4.308991	-1.263134
40	H	4.836052	-2.293292	-0.206611
41	H	2.165992	5.181152	-0.565473
42	H	2.185012	3.726551	-1.604100
43	H	0.650605	4.611223	-1.330699
44	H	-0.650605	4.611223	1.330699
45	H	-2.165992	5.181152	0.565473
46	H	-2.185013	3.726551	1.604100

B3LYP/6-31g(d)
Int = Ultrafine
E = -1260.32776266 hartree
# of imaginary frequencies = 0

Cartesian coordinate [Å] of optimized structure (4)

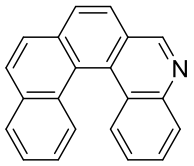


4

1	C	1.392286	-1.298311	-0.093570
2	C	0.720512	-0.049261	0.074692
3	C	-0.720512	-0.049261	-0.074692
4	C	-1.392286	-1.298311	0.093569
5	C	-0.675626	-2.528146	0.100103
6	C	0.675626	-2.528146	-0.100103
7	C	-1.513506	1.114562	-0.481269
8	C	-2.942090	1.105487	-0.342718
9	C	-3.540038	-0.116018	0.074692
10	C	-2.812122	-1.265387	0.213951
11	C	2.812122	-1.265387	-0.213951
12	C	3.540038	-0.116018	-0.074693
13	C	2.942090	1.105487	0.342718
14	C	1.513505	1.114562	0.481269
15	C	3.713072	2.235823	0.708843
16	C	3.105190	3.333542	1.280034
17	C	1.717569	3.313470	1.524949
18	C	0.945041	2.236207	1.135815
19	C	-0.945041	2.236207	-1.135815
20	C	-1.717569	3.313470	-1.524949
21	C	-3.105190	3.333542	-1.280034
22	C	-3.713072	2.235823	-0.708843
23	C	-4.969381	-0.448731	0.300213
24	O	-5.039656	-1.815783	0.569413
25	C	-3.758578	-2.369487	0.515768
26	C	3.758578	-2.369487	-0.515768
27	O	5.039656	-1.815783	-0.569413
28	C	4.969381	-0.448731	-0.300214
29	O	5.950789	0.243371	-0.280786
30	O	3.571903	-3.541905	-0.696319
31	O	-3.571903	-3.541905	0.696319
32	O	-5.950789	0.243371	0.280786
33	H	-1.231005	-3.452530	0.206806
34	H	1.231005	-3.452530	-0.206806
35	H	4.786649	2.198473	0.562667
36	H	3.698337	4.193996	1.575249
37	H	1.247178	4.148583	2.036280
38	H	-0.114204	2.243515	1.357097
39	H	0.114204	2.243515	-1.357097
40	H	-1.247178	4.148584	-2.036280
41	H	-3.698338	4.193996	-1.575249
42	H	-4.786649	2.198473	-0.562667

B3LYP/6-31g(d)
Int = Ultrafine
E = -1448.21394115 hartree
# of imaginary frequencies = 0

Cartesian coordinate [Å] of optimized structure (5)

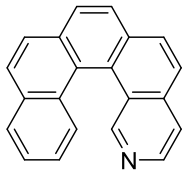


5

1	C	1.361560	2.019171	0.307282
2	C	0.735205	0.767055	0.046027
3	C	-0.710791	0.756228	-0.058226
4	C	-1.365611	1.986496	-0.320847
5	C	-0.672328	3.222582	-0.223160
6	C	0.632375	3.236773	0.179066
7	C	-1.595036	-0.378025	0.174957
8	C	-2.973222	-0.245961	-0.184675
9	N	-3.523533	0.923211	-0.665076
10	C	-2.757468	1.975603	-0.663206
11	C	2.746099	2.069728	0.668399
12	C	3.514373	0.946513	0.680880
13	C	2.988243	-0.292488	0.199273
14	C	1.609926	-0.380317	-0.174835
15	C	-1.214671	-1.560725	0.859367
16	C	-2.111481	-2.587994	1.079755
17	C	-3.441691	-2.489192	0.624159
18	C	-3.862821	-1.329311	0.009185
19	C	3.844889	-1.403641	0.004386
20	C	3.395371	-2.548847	-0.617723
21	C	2.068301	-2.602139	-1.088291
22	C	1.203159	-1.547183	-0.872283
23	H	-1.214143	4.145959	-0.411665
24	H	1.154258	4.174485	0.351539
25	H	-3.215448	2.920522	-0.962260
26	H	3.169748	3.034241	0.936796
27	H	4.558871	0.989832	0.979373
28	H	-0.204977	-1.652722	1.239008
29	H	-1.787338	-3.474043	1.618885
30	H	-4.136190	-3.308890	0.786483
31	H	-4.891038	-1.187490	-0.308374
32	H	4.880806	-1.320359	0.324580
33	H	4.065827	-3.389146	-0.775193
34	H	1.721946	-3.474284	-1.636046
35	H	0.196123	-1.606549	-1.264540

B3LYP/6-31g(d)
Int = Ultrafine
E = -862.847260329 hartree
# of imaginary frequencies = 0

Cartesian coordinate [Å] of optimized structure (6)

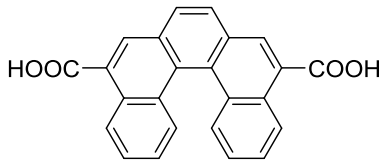


6

1	C	-1.336918	2.036498	-0.310012
2	C	-0.709561	0.786582	-0.043488
3	C	0.736551	0.770347	0.060957
4	C	1.402121	2.000300	0.326531
5	C	0.702081	3.233980	0.212738
6	C	-0.602224	3.250017	-0.190569
7	C	1.589213	-0.388151	-0.174357
8	C	2.969867	-0.343425	0.180913
9	C	3.538201	0.871148	0.674335
10	C	2.790921	2.009224	0.677401
11	C	-2.722455	2.087646	-0.665563
12	C	-3.492350	0.965480	-0.669458
13	C	-2.965194	-0.271301	-0.183431
14	C	-1.585924	-0.358679	0.187738
15	C	1.174769	-1.538532	-0.901373
16	N	1.931224	-2.593013	-1.155025
17	C	3.202188	-2.581049	-0.686778
18	C	3.758673	-1.494484	-0.050093
19	C	-3.821382	-1.382171	0.016307
20	C	-3.370769	-2.526475	0.638805
21	C	-2.042911	-2.579051	1.107180
22	C	-1.179067	-1.524262	0.887647
23	H	1.242153	4.159748	0.393994
24	H	-1.118855	4.189794	-0.368115
25	H	4.585406	0.885472	0.964525
26	H	3.238365	2.961396	0.952521
27	H	-3.145335	3.051491	-0.937874
28	H	-4.537744	1.007944	-0.964812
29	H	0.173804	-1.570018	-1.319778
30	H	3.787451	-3.478259	-0.877966
31	H	4.805902	-1.497048	0.241125
32	H	-4.857753	-1.299598	-0.302653
33	H	-4.040425	-3.367146	0.797460
34	H	-1.694399	-3.451053	1.653487
35	H	-0.172106	-1.583474	1.280682

B3LYP/6-31g(d)
Int = Ultrafine
E = -862.843940351 hartree
# of imaginary frequencies = 0

Cartesian coordinate [Å] of optimized structure (8c)

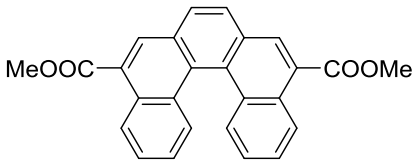


8c

1	C	1.396831	-1.776992	-0.077051
2	C	0.719893	-0.537227	0.075867
3	C	-0.719938	-0.537207	-0.075954
4	C	-1.396904	-1.776960	0.076915
5	C	-0.676606	-3.006318	0.087249
6	C	0.676502	-3.006331	-0.087428
7	C	-1.533301	0.608729	-0.472070
8	C	-2.961058	0.573139	-0.324674
9	C	-3.577766	-0.658829	0.123085
10	C	-2.812563	-1.792276	0.215031
11	C	2.812491	-1.792343	-0.215166
12	C	3.577715	-0.658914	-0.123176
13	C	2.961037	0.573047	0.324614
14	C	1.533285	0.608679	0.472015
15	C	3.716279	1.700892	0.737814
16	C	3.114041	2.792597	1.328951
17	C	1.726752	2.792314	1.555605
18	C	0.961753	1.724181	1.135660
19	C	-0.961718	1.724225	-1.135682
20	C	-1.726667	2.792397	-1.555613
21	C	-3.113958	2.792721	-1.328979
22	C	-3.716246	1.701025	-0.737873
23	C	-5.021389	-0.858788	0.447842
24	C	5.021349	-0.858822	-0.447907
25	O	5.689118	0.272893	-0.793247
26	O	5.574830	-1.941294	-0.465240
27	O	-5.574731	-1.941326	0.465446
28	O	-5.689103	0.272798	0.793707
29	H	-1.232429	-3.935607	0.176770
30	H	1.232302	-3.935631	-0.176983
31	H	-3.306207	-2.733360	0.436199
32	H	3.306115	-2.733431	-0.436360
33	H	4.789670	1.686962	0.610251
34	H	3.720493	3.635175	1.649757
35	H	1.255486	3.622767	2.073919
36	H	-0.100957	1.724954	1.340609
37	H	0.100995	1.724960	-1.340617
38	H	-1.255363	3.622842	-2.073903
39	H	-3.720376	3.635326	-1.649780
40	H	-4.789635	1.687141	-0.610341
41	H	6.595415	-0.022045	-1.004310
42	H	-6.595309	-0.022245	1.005016

B3LYP/6-31g(d)
Int = Ultrafine
E = -1223.93972191 hartree
# of imaginary frequencies = 0

Cartesian coordinate [Å] of optimized structure (9)

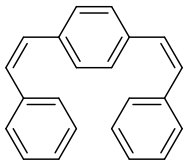


9

1	C	-1.399668	-1.783373	0.006050
2	C	-0.715293	-0.543981	-0.111374
3	C	0.715293	-0.543981	0.111374
4	C	1.399668	-1.783373	-0.006050
5	C	0.680223	-3.012259	-0.052525
6	C	-0.680223	-3.012259	0.052525
7	C	-2.821130	-1.799247	0.071661
8	C	-3.581102	-0.666433	-0.057008
9	C	-2.941555	0.565280	-0.471393
10	C	-1.508358	0.601883	-0.547058
11	C	1.508358	0.601883	0.547058
12	C	2.941554	0.565280	0.471393
13	C	3.581102	-0.666433	0.057008
14	C	2.821130	-1.799247	-0.071661
15	C	-3.675791	1.691729	-0.924365
16	C	-3.046396	2.783553	-1.485887
17	C	-1.649148	2.784869	-1.640952
18	C	-0.905381	1.717906	-1.181668
19	C	0.905381	1.717907	1.181668
20	C	1.649148	2.784869	1.640952
21	C	3.046396	2.783553	1.485887
22	C	3.675791	1.691729	0.924365
23	C	5.043182	-0.866686	-0.195715
24	O	5.597052	-1.947988	-0.142128
25	O	5.695254	0.262079	-0.560625
26	C	7.088314	0.087564	-0.870100
27	C	-5.043181	-0.866686	0.195715
28	O	-5.597052	-1.947988	0.142128
29	O	-5.695254	0.262079	0.560626
30	C	-7.088314	0.087565	0.870100
31	H	1.239626	-3.941807	-0.113119
32	H	-1.239626	-3.941807	0.113118
33	H	-3.324719	-2.741445	0.264057
34	H	3.324719	-2.741445	-0.264057
35	H	-4.754116	1.674716	-0.849961
36	H	-3.636776	3.624764	-1.838882
37	H	-1.152950	3.615451	-2.135335
38	H	0.166391	1.719679	-1.332417
39	H	-0.166391	1.719679	1.332416
40	H	1.152950	3.615451	2.135334
41	H	3.636776	3.624765	1.838881
42	H	4.754116	1.674716	0.849961
43	H	7.629528	-0.304409	-0.005109
44	H	7.209222	-0.604822	-1.707047
45	H	7.452330	1.080308	-1.136331
46	H	-7.209222	-0.604821	1.707047
47	H	-7.452329	1.080309	1.136332
48	H	-7.629528	-0.304408	0.005109

B3LYP/6-31g(d)
Int = Ultrafine
E = -1302.55279899 hartree
# of imaginary frequencies = 0

Cartesian coordinate [Å] of optimized structure (1a)

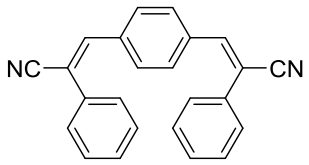


(*cis,cis*)-**1a**

1	C	1.309594	1.786360	-0.565351
2	C	0.633560	2.987797	-0.286052
3	C	-0.633557	2.987797	0.286053
4	C	-1.309591	1.786360	0.565350
5	C	-0.636950	0.582551	0.276233
6	C	0.636951	0.582551	-0.276235
7	C	2.634264	1.848771	-1.204056
8	C	3.690977	1.008550	-1.156776
9	C	3.945106	-0.190363	-0.337101
10	C	4.755389	-1.212125	-0.865372
11	C	-3.484037	-0.330760	-0.985078
12	C	-3.945106	-0.190362	0.337101
13	C	-3.690975	1.008550	1.156776
14	C	-2.634262	1.848771	1.204055
15	C	3.484037	-0.330760	0.985078
16	C	3.797493	-1.462626	1.733896
17	C	4.581545	-2.480531	1.184247
18	C	5.061995	-2.348987	-0.119682
19	C	-3.797495	-1.462625	-1.733896
20	C	-4.581549	-2.480529	-1.184246
21	C	-5.061998	-2.348984	0.119682
22	C	-4.755390	-1.212123	0.865372
23	H	1.120217	3.934544	-0.509640
24	H	-1.120213	3.934544	0.509643
25	H	-1.119845	-0.364007	0.494273
26	H	1.119846	-0.364007	-0.494277
27	H	2.765625	2.725541	-1.838905
28	H	4.516093	1.260058	-1.823659
29	H	5.141098	-1.110879	-1.877375
30	H	-2.888844	0.460515	-1.428680
31	H	-4.516091	1.260060	1.823660
32	H	-2.765622	2.725542	1.838905
33	H	2.888845	0.460515	1.428680
34	H	3.434882	-1.546729	2.755134
35	H	4.824210	-3.362196	1.771320
36	H	5.681808	-3.128693	-0.554752
37	H	-3.434884	-1.546729	-2.755133
38	H	-4.824215	-3.362194	-1.771319
39	H	-5.681812	-3.128689	0.554753
40	H	-5.141100	-1.110876	1.877375

B3LYP/6-31g(d)
Int = Ultrafine
E = -849.155849930 hartree
# of imaginary frequencies = 0

Cartesian coordinate [Å] of optimized structure (1c)



(*cis,cis*)-**1c**

1	C	1.423231	-1.874292	0.016385
2	C	0.693144	-0.808264	-0.551196
3	C	-0.693132	-0.808263	-0.551195
4	C	-1.423220	-1.874289	0.016386
5	C	-0.694072	-2.958253	0.542294
6	C	0.694083	-2.958254	0.542293
7	C	2.883877	-1.968194	0.010346
8	C	3.835546	-0.997927	-0.067444
9	C	3.654806	0.480490	-0.002863
10	C	4.329285	1.315937	-0.907152
11	C	-4.329290	1.315928	-0.907159
12	C	-3.654809	0.480488	-0.002866
13	C	-3.835539	-0.997930	-0.067443
14	C	-2.883866	-1.968192	0.010350
15	C	2.863653	1.063858	0.999940
16	C	2.730652	2.448554	1.077874
17	C	3.388411	3.271436	0.160389
18	C	4.189157	2.701073	-0.830524
19	C	-4.189170	2.701066	-0.830535
20	C	-3.388432	3.271436	0.160380
21	C	-2.730671	2.448562	1.077870
22	C	-2.863664	1.063864	0.999939
23	C	-5.197141	-1.442880	-0.191138
24	N	-6.305130	-1.782961	-0.305281
25	C	5.197149	-1.442871	-0.191144
26	N	6.305147	-1.782924	-0.305290
27	H	1.220303	0.014611	-1.019354
28	H	-1.220288	0.014613	-1.019354
29	H	-1.229592	-3.809709	0.954524
30	H	1.229601	-3.809712	0.954523
31	H	3.259177	-2.988804	0.061139
32	H	4.965421	0.876069	-1.670175
33	H	-4.965421	0.876055	-1.670184
34	H	-3.259163	-2.988803	0.061150
35	H	2.363054	0.427723	1.723319
36	H	2.120997	2.886191	1.863655
37	H	3.285738	4.351147	0.224606
38	H	4.711840	3.334122	-1.542065
39	H	-4.711854	3.334110	-1.542080
40	H	-3.285766	4.351148	0.224594
41	H	-2.121023	2.886204	1.863652
42	H	-2.363064	0.427734	1.723322

B3LYP/6-31g(d)
Int = Ultrafine
E = -1033.64063035 hartree
# of imaginary frequencies = 0

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