Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information for

An Oxanorbornene-Fused Nanocage Consisting of Hexaazatrinaphthylene and Pyrene Units

Liping Ye, Han Chen, Qian Miao*

Department of Chemistry, The Chinese University of Hong Kong, Shatin, New Territories, Hong Kong, China

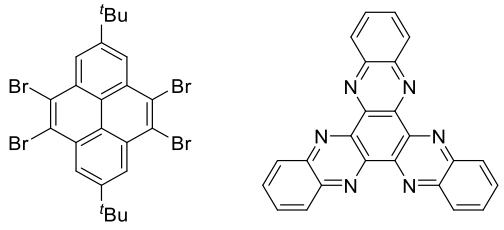
* email of the corresponding author: miaoqian@cuhk.edu.hk

Table of Contents

1. Synthesis
2. NMR spectra
3. High-resolution mass spectra
4. X-ray crystallography
5. Photophysical properties
6. Density functional theory (DFT) calculations
7. References

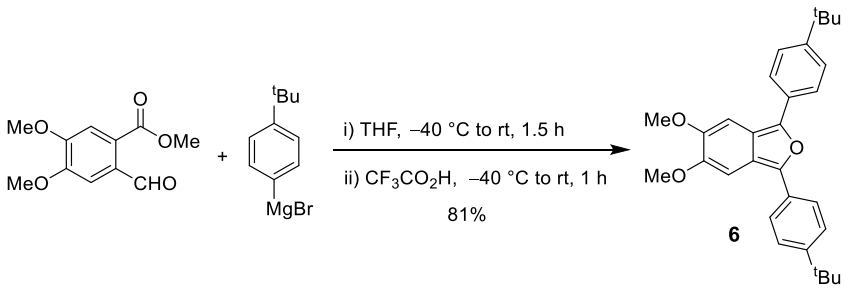
1. Synthesis

General: The reagents and starting materials employed were commercially available and used without any further purification or made following reported methods as indicated. Unless otherwise noted, all reaction were performed with dry solvents under an atmosphere of nitrogen in dried glassware with standard vacuum-line techniques. Anhydrous and oxygen-free toluene, THF and dichloromethane were purified by an Advanced Technology Pure-Solv PS-MD-4 system. Gel permeation chromatography (GPC) were performed on a JAI LC-9160 II NEXT automatic recycling preparative HPLC system with a UV/VIS detector. ^{1}H and ^{13}C NMR spectra were recorded on Brucker AVANCE III 400 NMR or AVANCE III HD 500 NMR spectrometers. Abbreviations: *s* = singlet, *d* = doublet, *t* = triplet, *m* = multiplet, *br* = broad. Chemical shift values (δ) are expressed in parts per million using residual solvent protons as an internal standard (^{1}H NMR, δ_H = 5.32 for CD_2Cl_2, δ_H = 7.26 for $CDCl_3$; ^{13}C NMR, δ_C = 53.84 for CD_2Cl_2, δ_C = 77.16 for $CDCl_3$). Mass spectra were recorded on a Bruker Autoflex speed MALDI-TOF spectrometer. Melting points, without correction, were measured using a Nikon Polarized Light Microscope ECLIPSE 50i POL equipped with an INTEC HCS302 heating stage.



5 HATN

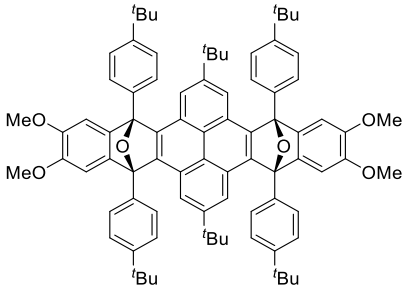
4,5,9,10-tetrabromo-2,7-di(t-butyl)pyrene (**5**) [1] and hexaazatrinaphthylene (HATN) [2] were synthesized following the reported procedures.



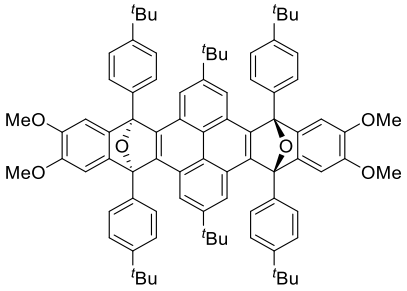
6

Compound 6: According to the reported procedure for preparing 1,3-diarylisobenzofuran,[3] to a stirred solution of magnesium (993 mg, 41.4 mmol) in dry THF (50 mL) under an atmosphere of N_2, 1-bromo-4-*tert*-butylbenzene (7.6 mL, 44.2 mmol) was added dropwise at room temperature. After stirring for 1.5 h, the resulting solution of 4-*tert*-butylphenylmagnesium bromide was cooled with a liquid nitrogen-acetonitrile bath. Into this cooled solution, a solution of methyl 2-formyl-4,5-dimethoxybenzoate (3.1 g, 13.8 mmol) in THF (50 mL) was added slowly, and the reaction mixture was then warmed to room temperature. After stirring at room temperature for 1.5 h, then mixture was cooled with a liquid nitrogen-acetonitrile bath again. Then CF_3CO_2H (5.1 mL) was added dropwise into the cooled mixture. The reaction mixture was stirred for 1 h when slowly warmed to room temperature, then quenched with sat. aq. $NaHCO_3$, extracted with ethyl acetate. The extracts were combined, washed with brine, dried over $MgSO_4$, and concentrated under a reduced pressure. The residue was purified by column chromatography on silica gel with hexane/ethyl acetate 8/1 (V/V) as eluent to afford 6 (4.909

g, 81%) as yellow solids. Melting point: 86−90 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.79 (d, *J* = 8.5 Hz, 4H), 7.51 (d, *J* = 8.6 Hz, 4H), 6.97 (s, 2H), 3.97 (s, 6H), 1.38 (s, 18H); ^{13}C NMR (126 MHz, $CDCl_3$) δ =150.5, 149.5, 142.4, 129.4, 126.0, 124.3, 118.3, 96.3, 55.9, 34.8, 31.4. HRMS (APCI): calcd. for $C_{30}H_{34}O_3$ ($[M+H]^+$): 443.25807, found: 443.25776.



syn-**7**

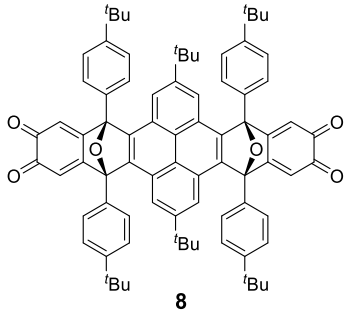


anti-**7**

Compounds *syn*-**7** and *anti*-**7**: According to the reported procedure for preparing a similar compound,[4] *n*-BuLi (2.2 mL of a 1.6 M solution in hexane, 3.42 mmol) was added to a stirred solution of **5** (715 mg, 1.14 mmol) and **6** (1.00 g, 2.28 mmol) in anhydrous THF (100 mL), which was cooled with a liquid nitrogen-ethyl acetate bath, under an atmosphere of N_2. The reaction mixture was stirred overnight when slowly warmed to room temperature, then quenched with H_2O, extracted with ethyl acetate. The extracts were combined, washed with brine, dried over $MgSO_4$, and concentrated under a reduced pressure. The residue was purified by column chromatography on silica gel with hexane/ethyl acetate 7/1 (V/V) as eluent to afford *syn*-**7** (26%) and *anti*-**7** (30%) as off-white solids separately.

syn-**7**: Melting point: not melt when heated up to 350 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.02 (d, *J* = 7.8 Hz, 8H), 7.73 (s, 4H), 7.56 (d, *J* = 8.6 Hz, 8H), 7.23 (s, 4H), 3.73 (s, 12H), 1.38 (s, 36H), 0.98 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.4, 150.4, 147.2, 146.2, 144.8, 132.4, 130.1, 126.5, 125.7, 122.0, 118.8, 108.2, 93.2, 56.6, 34.9, 31.4, 31.3. HRMS (MALDI-TOF): calcd. for $C_{84}H_{90}O_6$ ($[M]^+$): 1194.6732, found: 1194.6711.

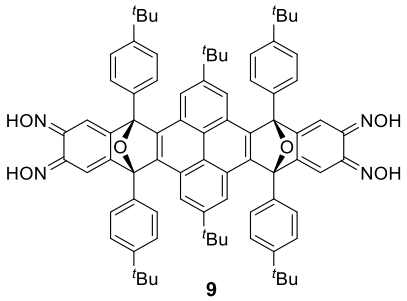
anti-**7**: Melting point: not melt when heated up to 350 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.03−7.92 (m, 8H), 7.77 (s, 4H), 7.53 (d, *J* = 7.8 Hz, 8H), 7.36 (s, 4H), 3.85 (s, 12H), 1.36 (s, 36H), 0.99 (s, 18H); ^{13}C NMR (126 MHz, $CDCl_3$) δ = 152.3, 150.0, 147.3, 146.2, 144.8, 132.8, 130.1, 126.0, 125.7, 121.9, 118.9, 108.4, 93.0, 56.7, 35.0, 34.9, 31.4, 31.3. HRMS (MALDI-TOF): calcd. for $C_{84}H_{90}O_6$ ($[M]^+$): 1194.6732, found: 1194.6767.



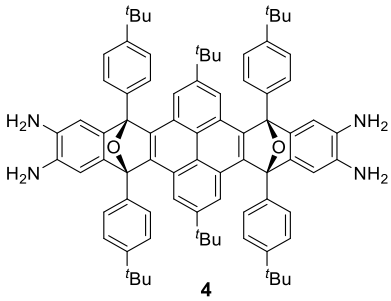
8

Compound **8**: To a stirred solution of *syn*-**7** (600 mg, 0.503 mmol) in acetonitrile (240 mL) under N_2 was added $Ce(NH_4)_2(NO_3)_6$ (1.376 g, 5.0 mmol) in 24 mL H_2O at 0 °C. The reaction mixture was stirred for 1 h when slowly warmed from 0 °C to room temperature. Then the mixture was dissolved in ethyl acetate and water. The organic layer was further washed with brine and dried with anhydrous $MgSO_4$, and concentrated under a reduced pressure. The

residue was purified by column chromatography on silica gel with hexane/ethyl acetate 7/1 (V/V) as eluent to afford **8** as red solids in a yield of 84%. Melting point: not melt when heated up to 350 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.89 (d, *J* = 8.0 Hz, 8H), 7.84 (s, 4H), 7.59 (d, *J* = 8.5 Hz, 8H), 6.73 (s, 4H), 1.38 (s, 36H), 0.96 (s, 18H); ^{13}C NMR (126 MHz, $CDCl_3$) δ = 178.4, 156.0, 154.0, 149.4, 142.6, 129.6, 128.3, 126.1, 125.8, 125.2, 121.8, 119.9, 89.7, 35.1, 35.0, 31.3, 31.0. HRMS (MALDI-TOF): calcd. for $C_{80}H_{78}O_6$ ($[M+H]^+$): 1135.5871, found: 1135.5877.



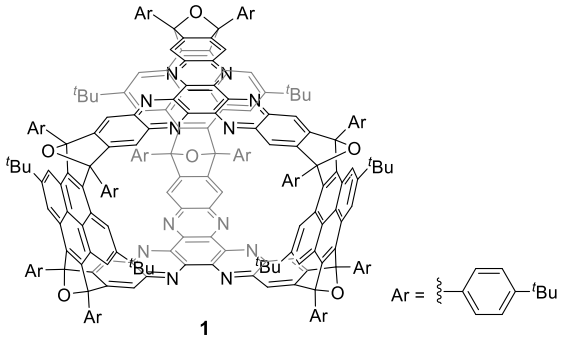
9



4

Compounds **9**: To a stirred solution of **8** (45 mg, 0.040 mmol) and hydroxylamine hydrochloride (40 mg, 0.576 mmol) in ethanol (10 mL) under N_2 was added pyridine (0.05 mL). The reaction mixture was stirred at reflux for 2 h. After cooled to room temperature, the mixture was concentrated under a reduced pressure. The residue was washed with an aquesous solution of 0.2 M HCl, then extracted with ethyl acetate. The extracts were combined, washed with brine, and dried over $MgSO_4$. The crude product of **9** (47 mg) was obtained as orange solids, used in the next step without further purifications.

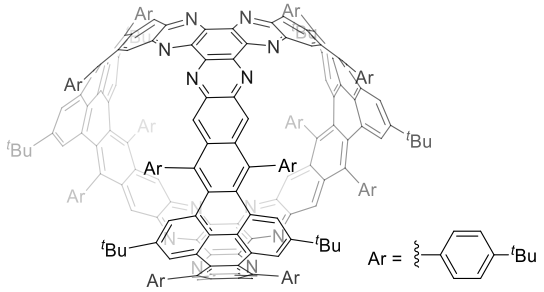
Compounds **4**: To a stirred mixture of **9** (47 mg of the above crude product) and Pd on carbon (Pd: 10%) (40 mg) in ethanol (10 mL) under N_2 was added hydrazine monohydrate (0.5 mL) in ethanol (1 mL). The mixture was stirred at 78 °C overnight. The hot reaction mixture was filtered through a pad of celite with ethyl acetate as eluent. The filtrate was washed with brine, dried over $MgSO_4$ and concentrated under a reduced pressure. Compound **4** (45 mg, 100% from **8**) was obtained as dark green solids, which were immediately used in the next step or kept in vacuum for further characterization due to its sensitivity to air. Melting point: not melt when heated up to 350 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.02 (d, *J* = 7.3 Hz, 8H), 7.67 (s, 4H), 7.54 (d, *J* = 8.24 Hz, 8H), 7.05 (s, 4H), 3.28 (br, 8H), 1.38 (s, 36H), 0.99 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.1, 150.1, 147.1, 144.0, 132.7, 130.5, 130.0, 126.3, 125.5, 121.9, 118.7, 112.9, 92.8, 34.9, 34.8, 31.4, 31.3. HRMS (APCI): calcd. for $C_{80}H_{86}N_4O_2$ ($[M+H]^+$): 1135.68235, found: 1135.68272.



1

Compound **1:** A solution of **4** (45 mg, 0.039 mmol) and cyclohexanehexone octahydrate (8 mg, 0.026 mmol) in acetic acid (20 mL) was stirred at 100 °C under an atomosphere of N_2 overnight, and cooled to room temperature, then quenched with H_2O and extracted with CH_2Cl_2. The

extracts were combined, washed with brine, dried over $MgSO_4$, and concentrated under a reduced pressure. The residue was purified by column chromatography on silica gel with hexane/dichloromethane/ethyl acetate 20/5/1 (V/V/V) as eluent to afford crude product. Then the crude product was purified by recycling preparative gel permeation chromatography using $CHCl_3$ as eluent to give 5.2 mg of **1** (11%) as orange solids. Melting point: not melt when heated up to 350 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.51 (s, 12H), 8.16−8.06 (m, 24H), 7.73 (s, 12H), 7.58 (d, J = 8.4 Hz, 24H), 1.41 (s, 108H), 0.93 (s, 54H); ^{13}C NMR (126 MHz, CD_2Cl_2) δ = 153.4, 153.3, 148.6, 148.3, 143.0, 142.6, 131.3, 130.3, 126.3, 126.2, 123.6, 121.7, 120.3, 92.4, 46.4, 35.2, 31.5, 31.2. HRMS (MALDI-TOF): calcd. for $C_{252}H_{234}N_{12}O_6$ ($[M+H]^+$): 3526.8513, found: 3526.8515.



10

Compound **10:** Hydrobromic acid (33 wt% solution in acetic acid) (13 μL, 0.076 mmol) was added to a solution of $SnCl_2$ (7 mg, 0.037 mmol) in THF (0.3 mL) at room temperature and the resulting solution was stirred at this temperature for 10 min under nitrogen atmosphere.[5] This solution was added into a solution of **1** (13 mg, 0.0037 mmol) in THF (5 mL) at room temperature, and the mixture was stirred overnight at this temperature. To the resulting mixture was added 10% aqueous NaOH solution, and the reaction mixture was extracted with CH_2Cl_2. The extracts were combined, washed with brine, dried over $MgSO_4$, and concentrated under a reduced pressure. This crude mixture was characterized with MALDI-TOF mass spectroscopy and used in the next step without purification. HRMS (MALDI-TOF): calcd. for $C_{252}H_{244}N_{12}$ ($[M]^+$): 3439.9522, found: 3439.9520.

A solution of above crude reduction product (4 mg) and *o*-chloranil (4.5 mg, 0.018 mmol) in 1,1,2,2-tetrachloroethane (5 mL) was stirred at 140 °C under N_2 for 1h. The system was cooled to room temperature, then quenched with H_2O, extracted with CH_2Cl_2, and concentrated under a reduced pressure to afford the crude product, from which compound **10** was identified with HRMS (MALDI-TOF): calcd. for $C_{252}H_{234}N_{12}$ ($[M+H]^+$): 3430.8818, found: 3430.8637.

2. NMR Spectra

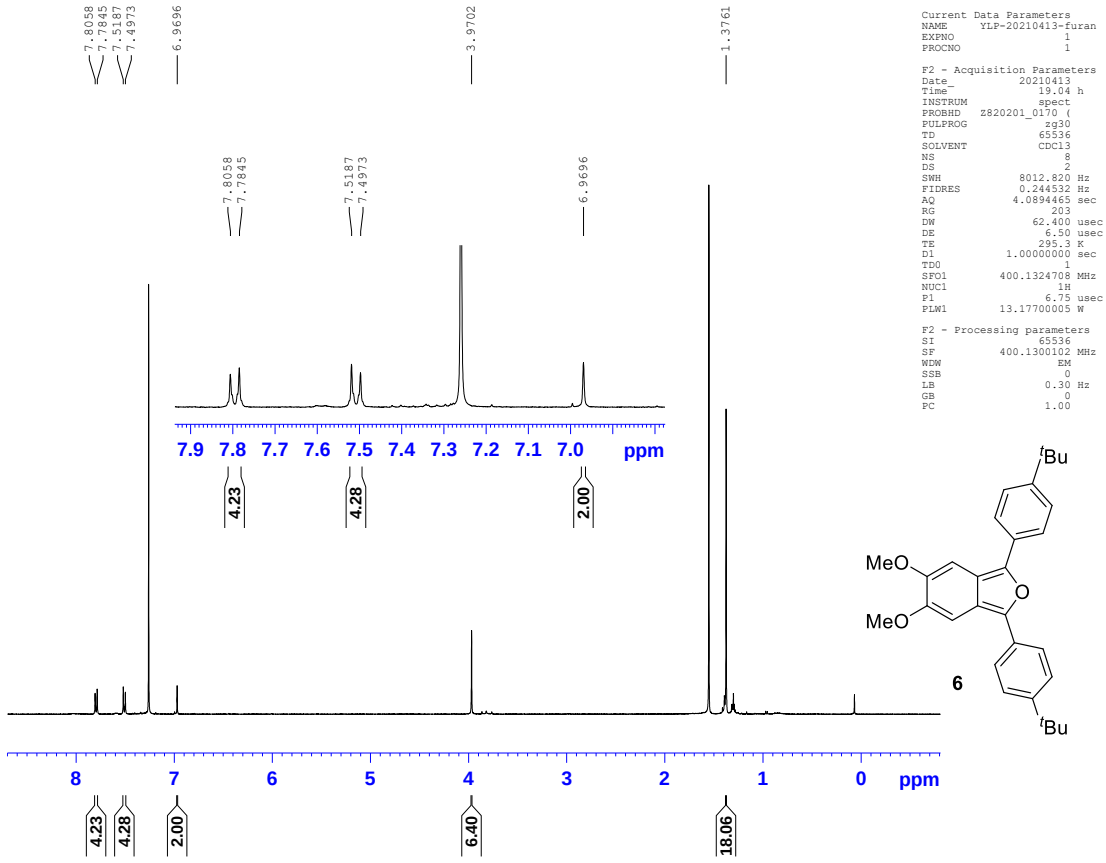


Figure S1. ^{1}H NMR spectrum of **6** in $CDCl_3$ at 294K.

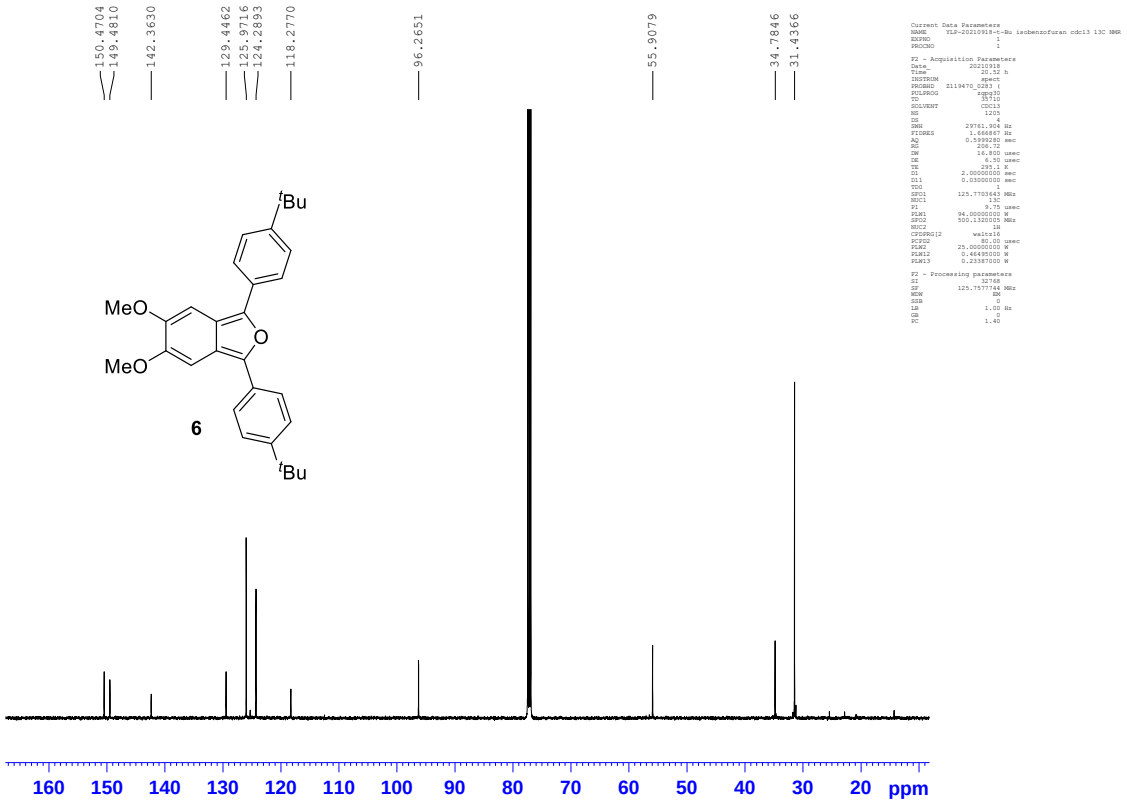


Figure S2. ^{13}C NMR spectrum of **6** in $CDCl_3$ at 294K.

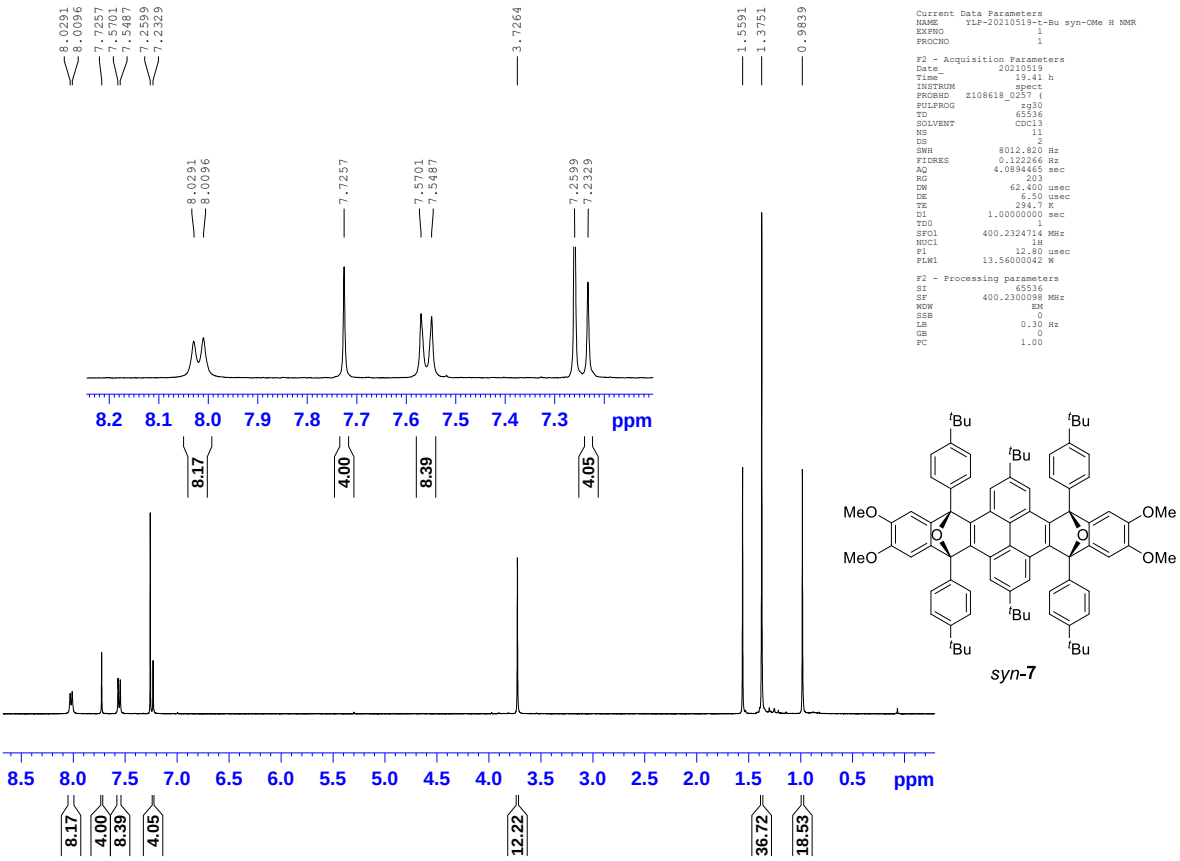


Figure S3. ^{1}H NMR spectrum of *syn*-**7** in $CDCl_3$ at 294K.

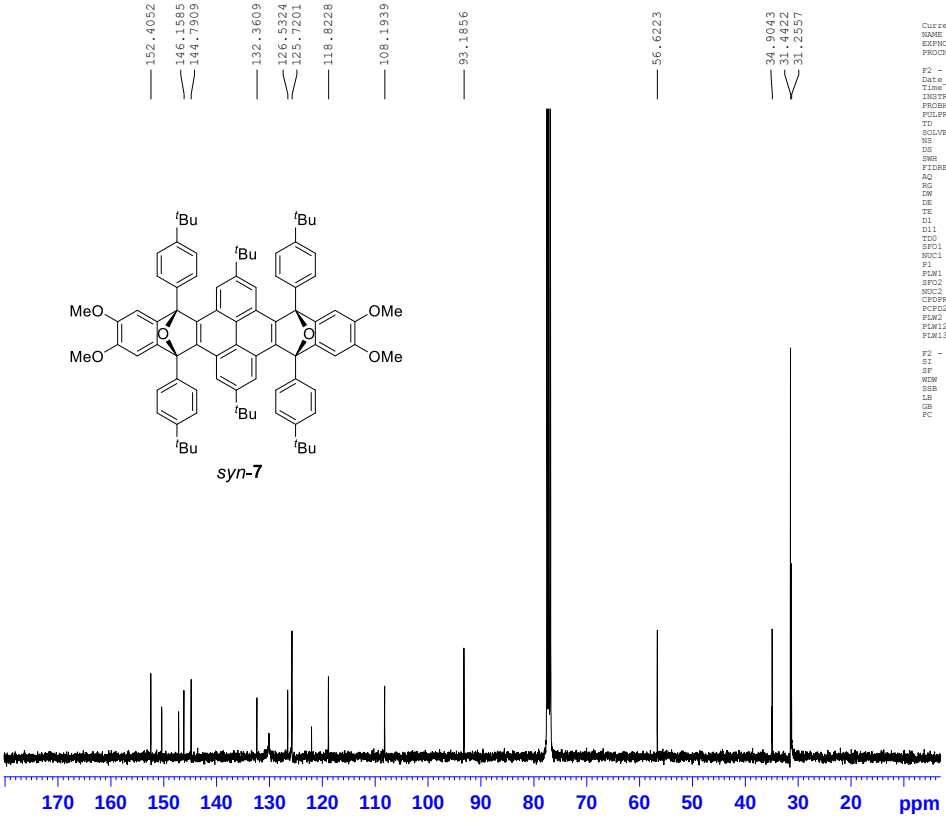


Figure S4. ^{13}C NMR spectrum of *syn*-**7** in $CDCl_3$ at 294K.

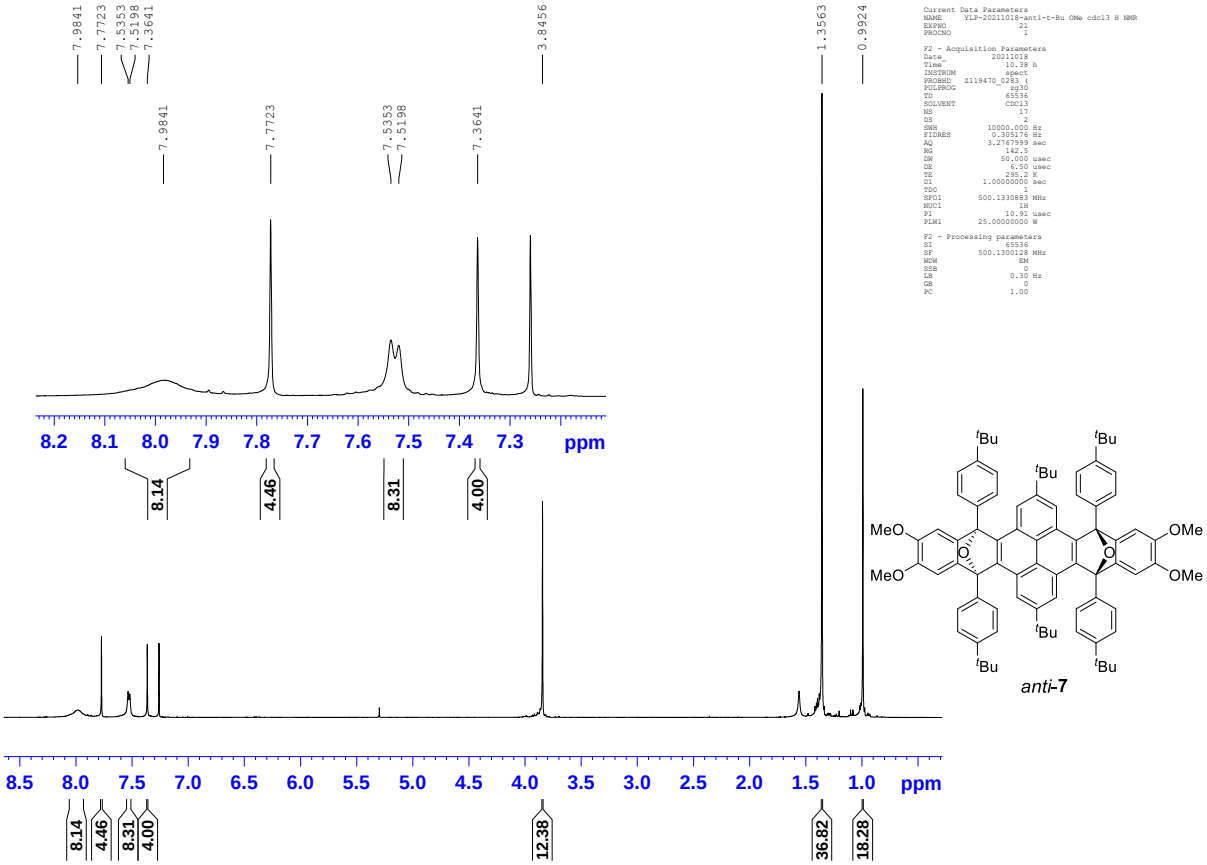


Figure S5. ^{1}H NMR spectrum of *anti*-**7** in $CDCl_3$ at 294K.

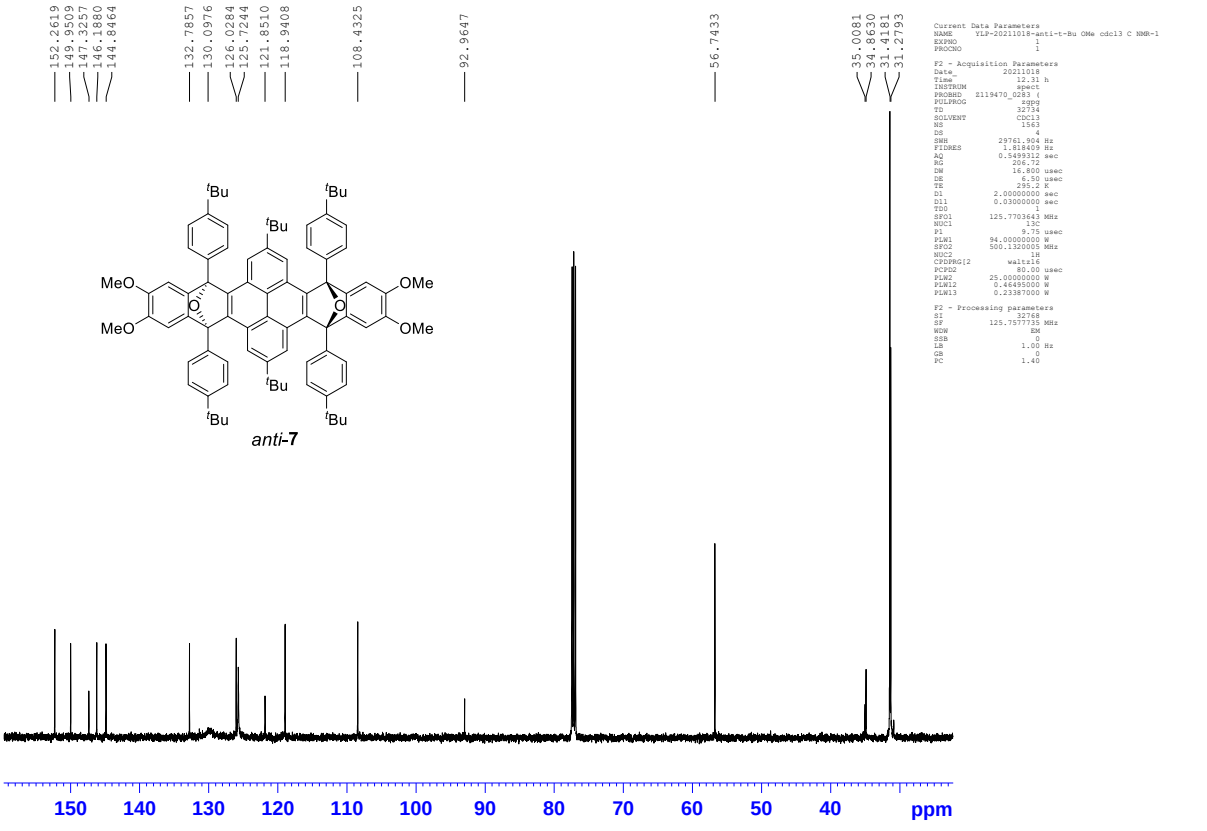


Figure S6. ^{13}C NMR spectrum of *anti*-**7** in $CDCl_3$ at 294K

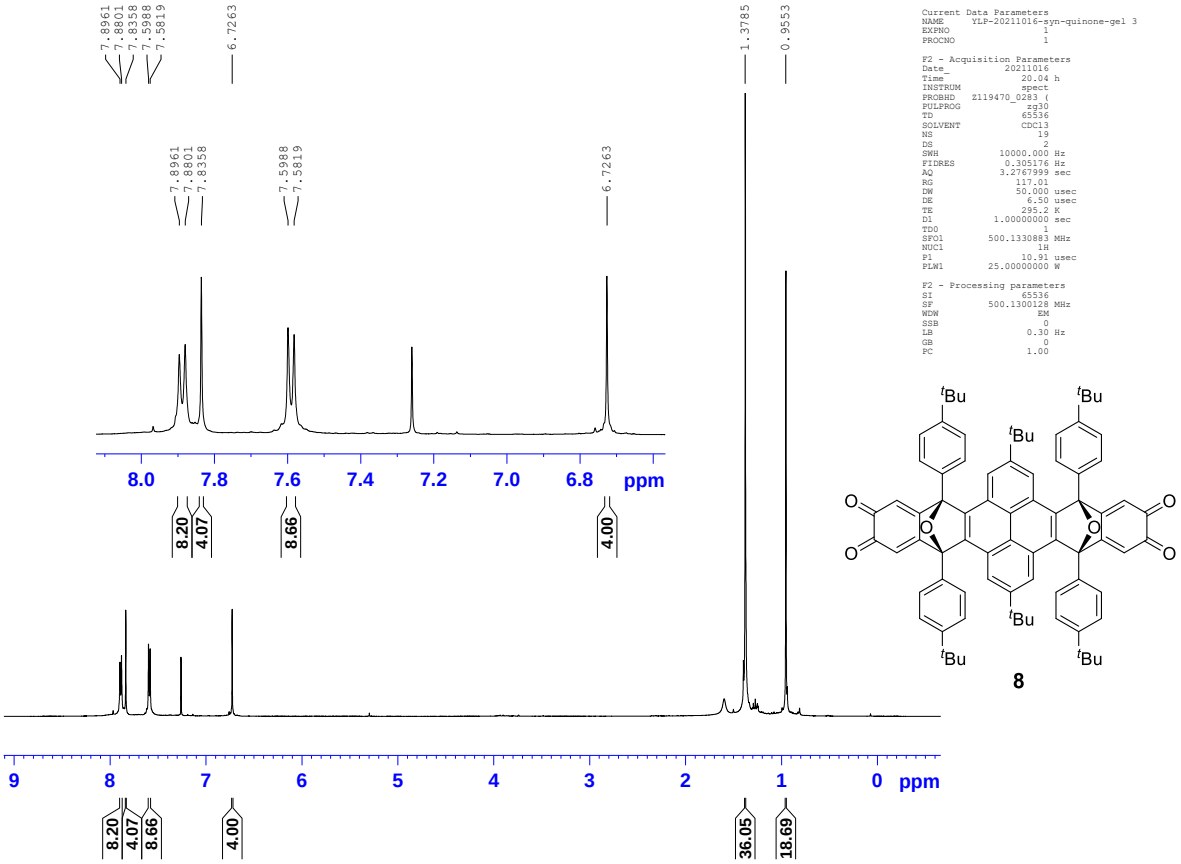


Figure S7. ^{1}H NMR spectrum of **8** in $CDCl_3$ at 294K.

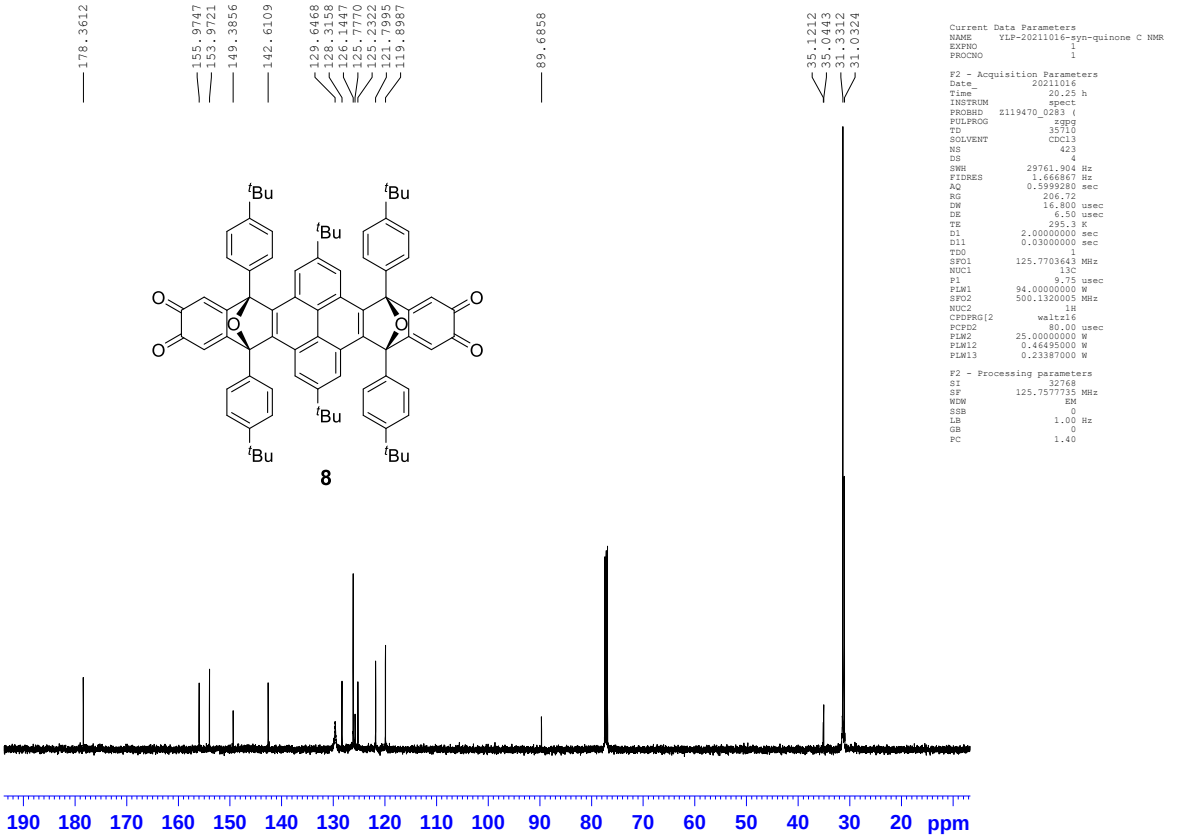


Figure S8. ^{13}C NMR spectrum of **8** in $CDCl_3$ at 294K.

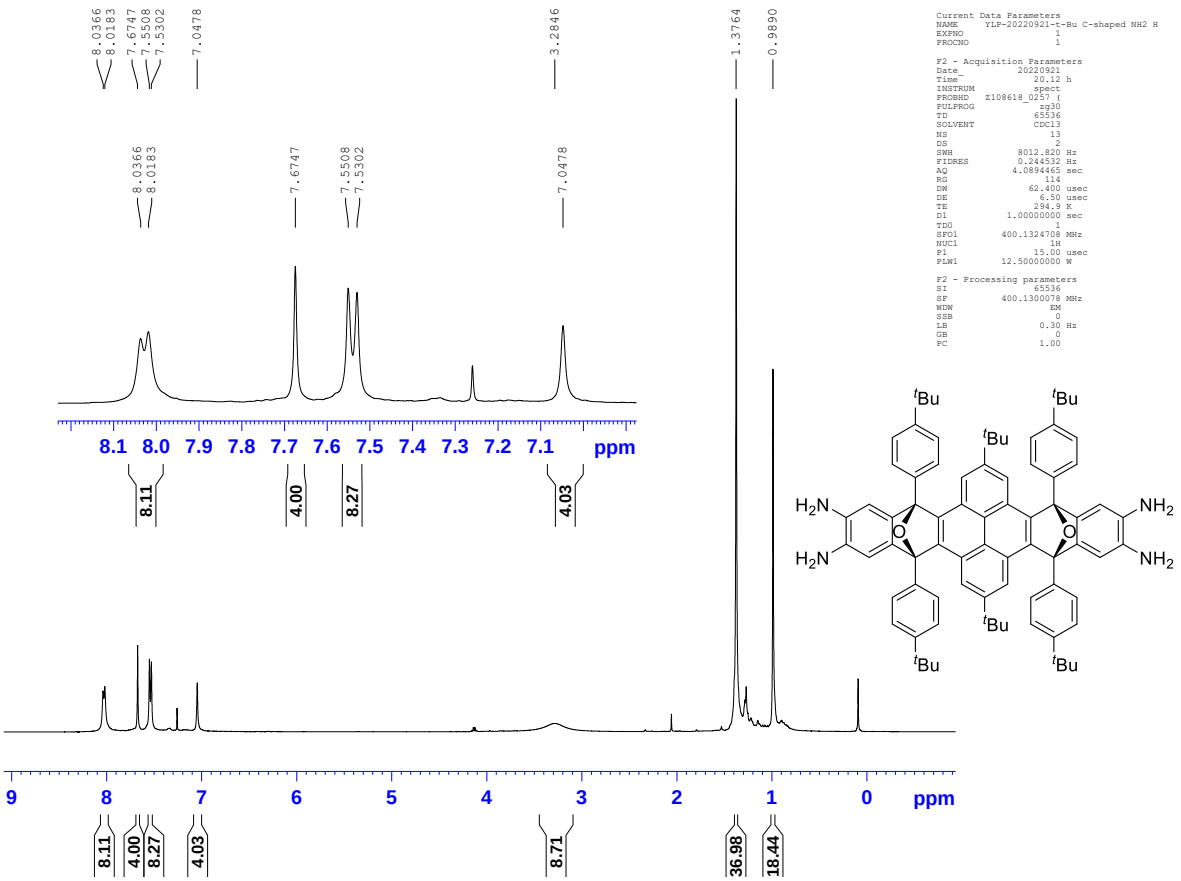


Figure S9. ^{1}H NMR spectrum of **4** in $CDCl_3$ at 294K.

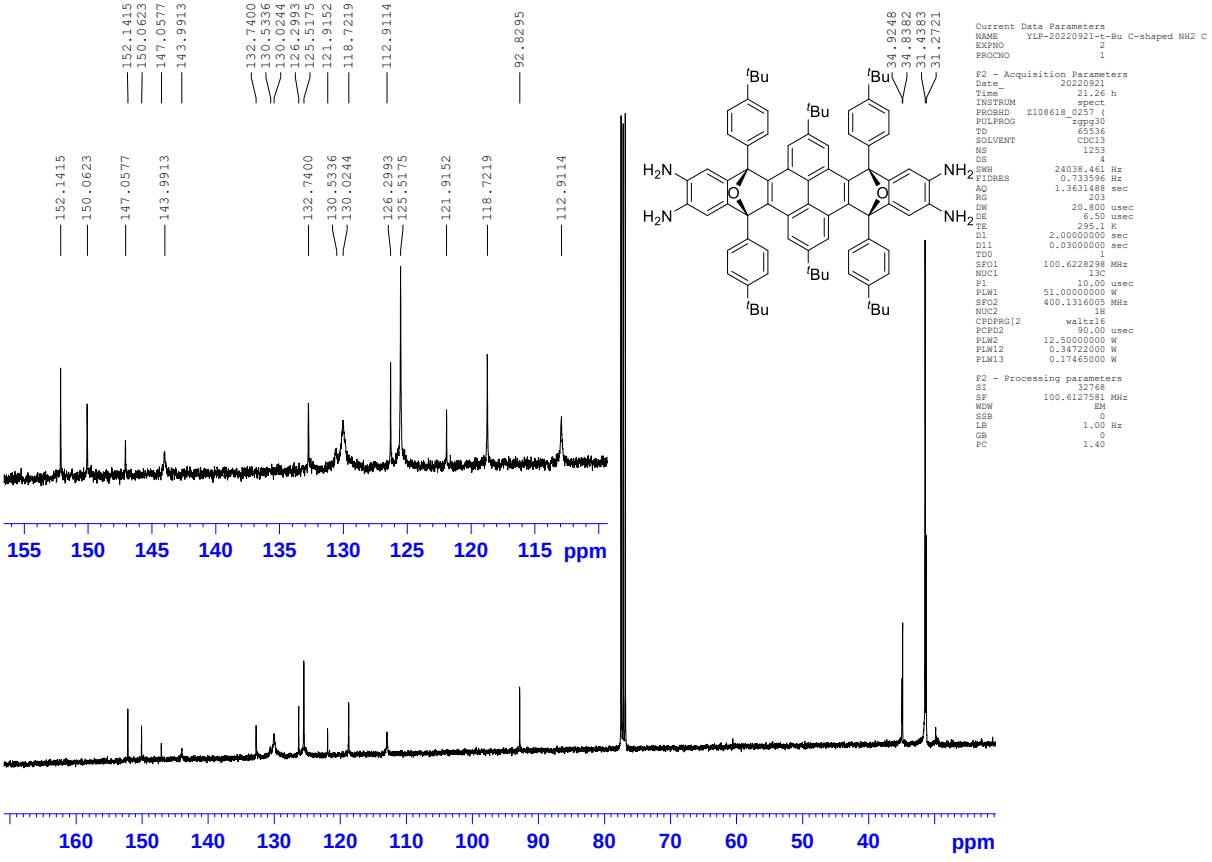


Figure S10. ^{13}C NMR spectrum of **4** in $CDCl_3$ at 294K.

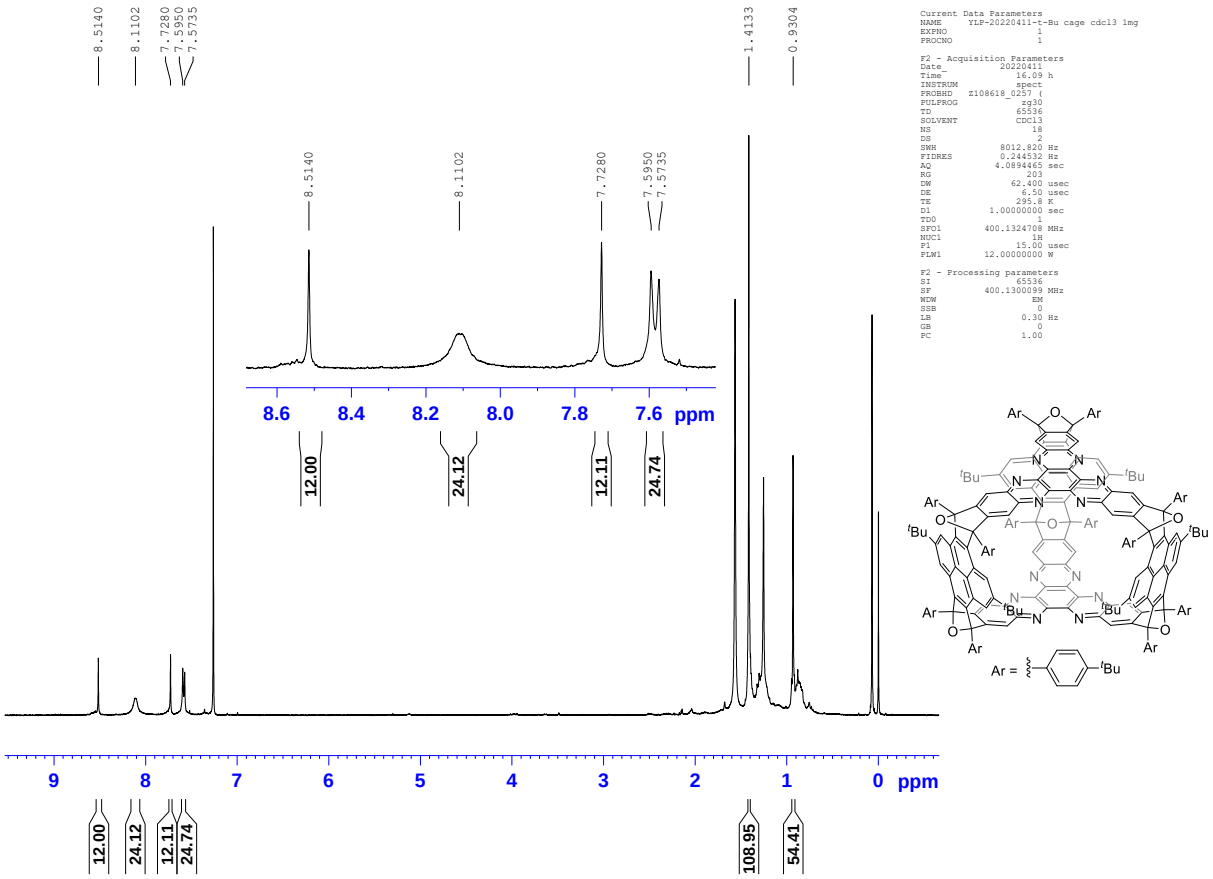


Figure S11. ^{1}H NMR spectrum of **1** in $CDCl_3$ at 294K.

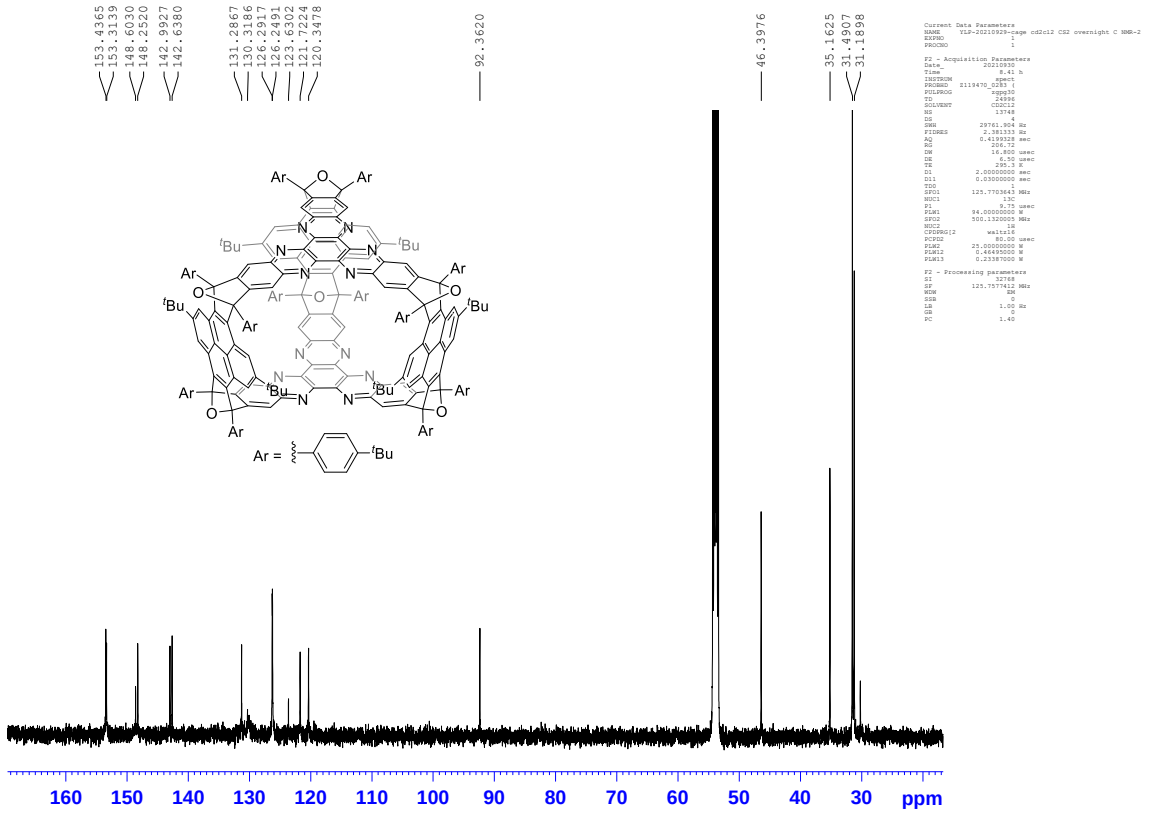


Figure S12. ^{13}C NMR spectrum of **1** in CD_2Cl_2 + CS_2 at 294K.

3. High-resolution mass spectra

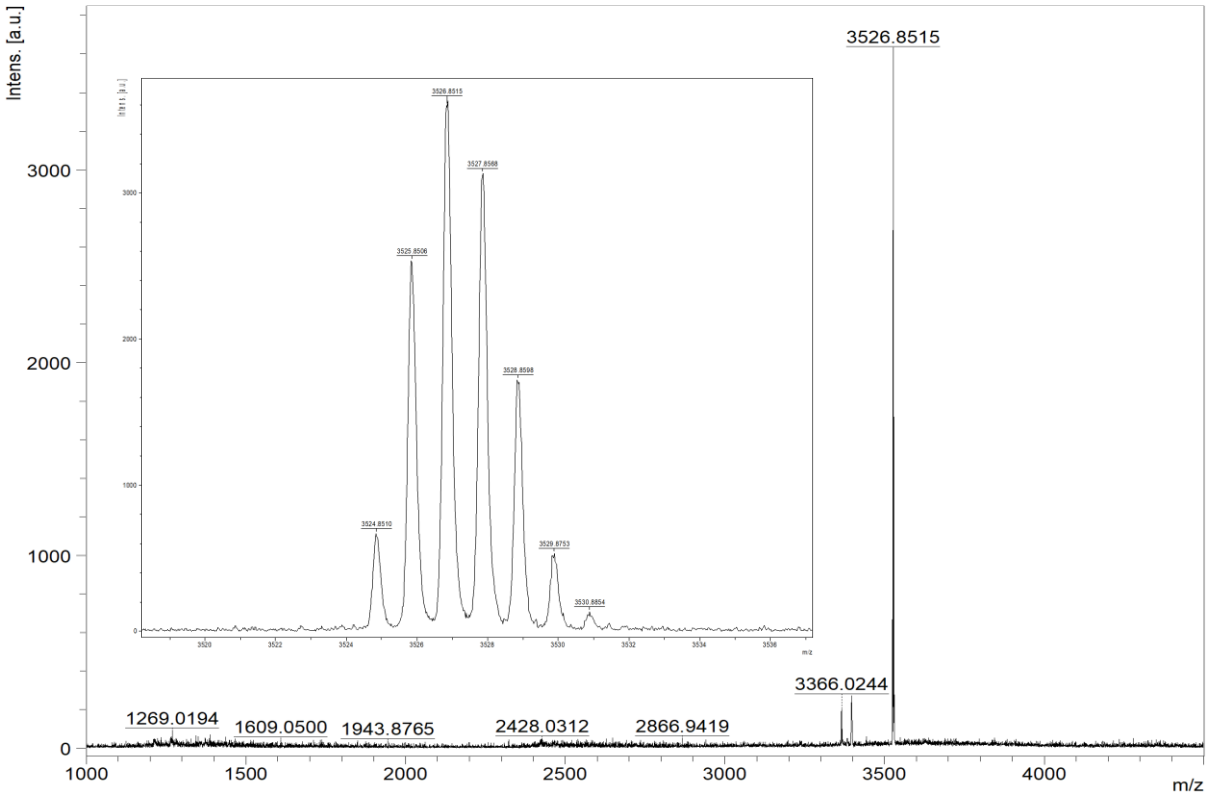


Figure S13. High resolution mass spectra (MALDI-TOF) of **1** ($C_{252}H_{234}N_{12}O_6$).

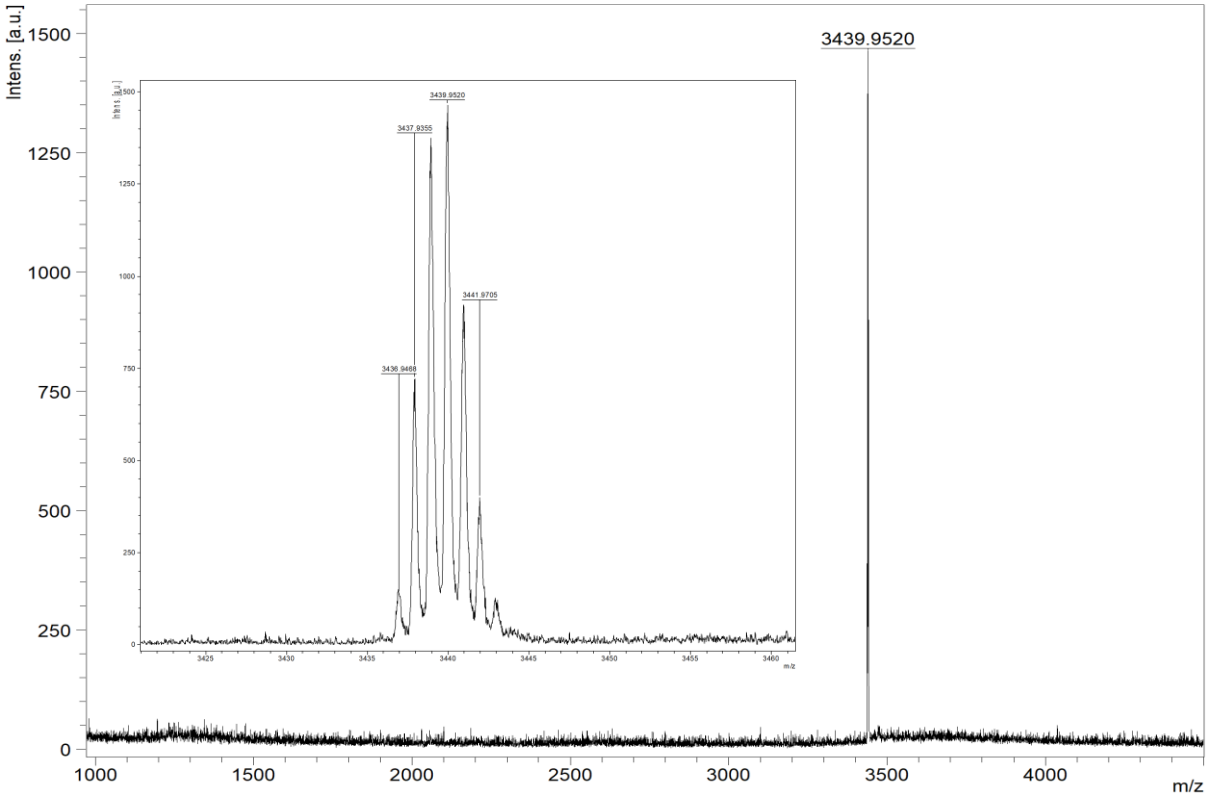


Figure S14. High resolution mass spectra (MALDI-TOF) of $C_{252}H_{244}N_{12}$, which was obtained by reduction of **1** with $SnCl_2$ in a solution of HBr in acetic acid.

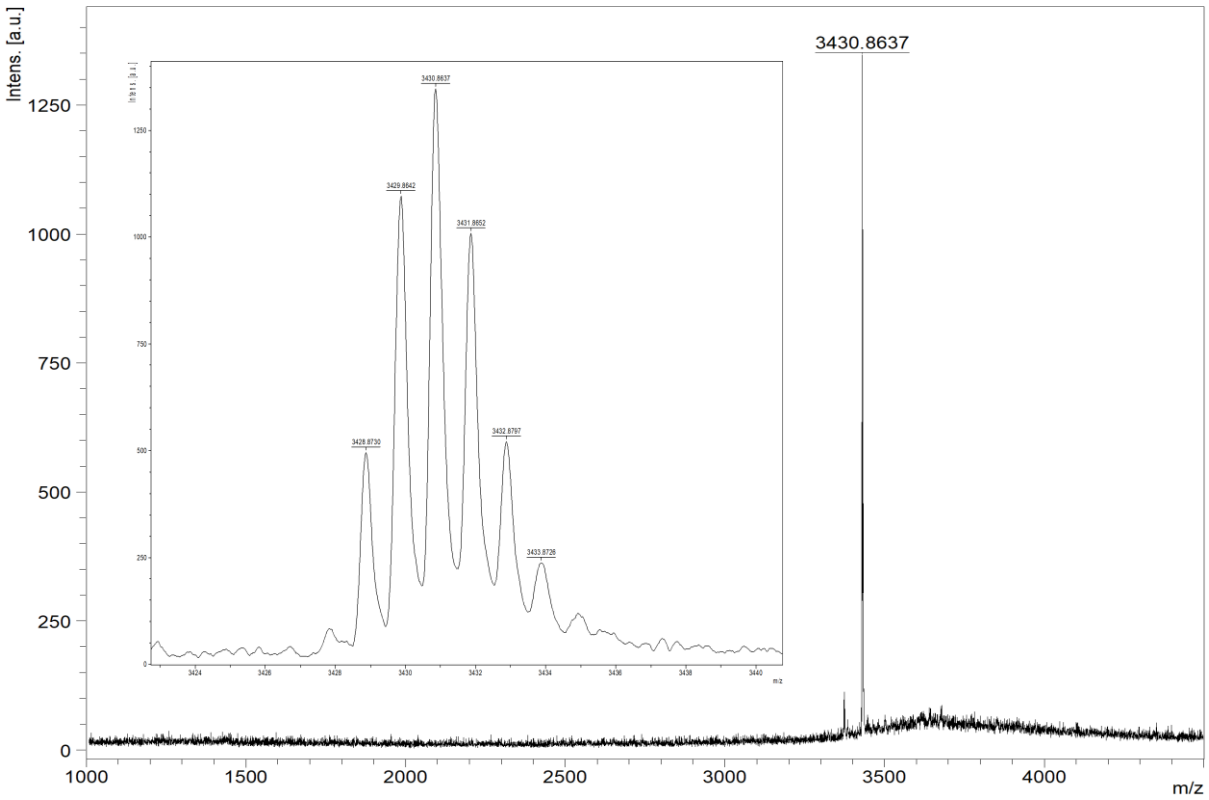


Figure S15. High resolution mass spectra (MALDI-TOF) of **10** (found as $C_{252}H_{235}N_{12}$ for $[\mathbf{10}+H]^+$).

4. X-ray crystallography

X-ray crystallography data were collected on a Bruker AXS Kappa ApexII Duo Diffractometer.

Table 1. Crystallographic Data

		1 • CH_2Cl_2
Crystallized from		CH_2Cl_2/*i*-PrOH
Empirical formula		$C_{253}H_{236}Cl_2N_{12}O_6$
Formula weight [g mol^{-1}]		3611.42
Crystal temp. [K]		173(2)
Wavelength		1.54178 Å
Crystal system		Triclinic
Space group		P-1
Unit cell parameters	*a* [Å]	24.932(2)
	b [Å]	27.812(2)
	c [Å]	28.879(3)
	α [°]	70.817(5)
	β [°]	66.129(5)
	γ [°]	63.469(5)
	V [Å^3]	16114(3)
Z		2
D_{calc} [g cm^{-3}]		0.744
Absorption coefficient [mm^{-1}]		0.488
F(000)		3840
Crystal size [mm^3]		0.50 x 0.40 x 0.30
Theta range for data collection		2.246 to 69.613°
Reflections collected		470260
Independent reflections		59412 [R(int) = 0.1979]
Completeness to theta = 25.242°		99.8 %
Absorption correction		multi-scan
Max. and min. transmission		0.7531 and 0.5052
Refinement method		Full-matrix least-squares on F^2
Data / restraints / parameters		59412 / 10163 / 2511
Goodness-of-fit on F^2		1.482
Final R indices [I>2sigma(I)]		R1 = 0.1988, wR2 = 0.4839
R indices (all data)		R1 = 0.2962, wR2 = 0.5537
Extinction coefficient		n/a
Largest diff. peak and hole		0.849 and -0.458 e.Å^{-3}

5. Photophysical properties

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

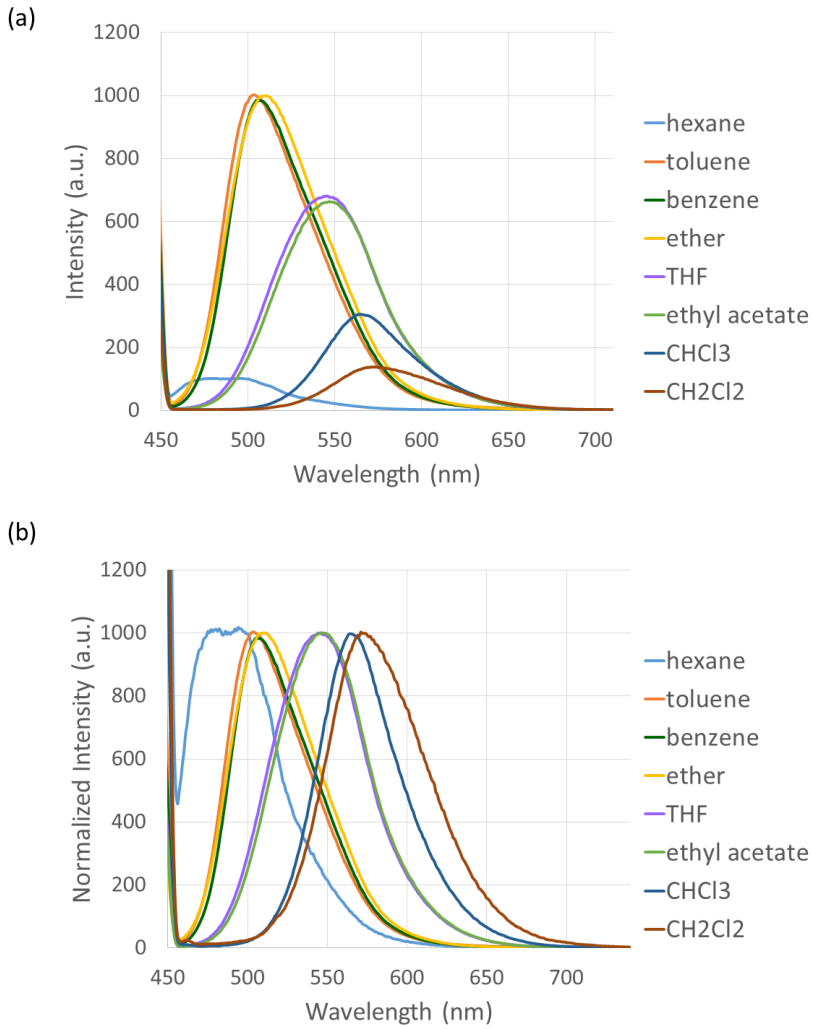


Figure S16. Photoluminescence spectra (a) and normalized photoluminescence spectra (b) of **1** in different solvents as excited at 447 nm. (The solutions of **1** except that in hexane had a concentration of 2×10^{-6} mol/L. Due to the low solubility of **1** in hexane, a saturated solution of **1** in hexane was filtered through a nylon syringe filter (0.45 um) before the spectrum was recorded.)

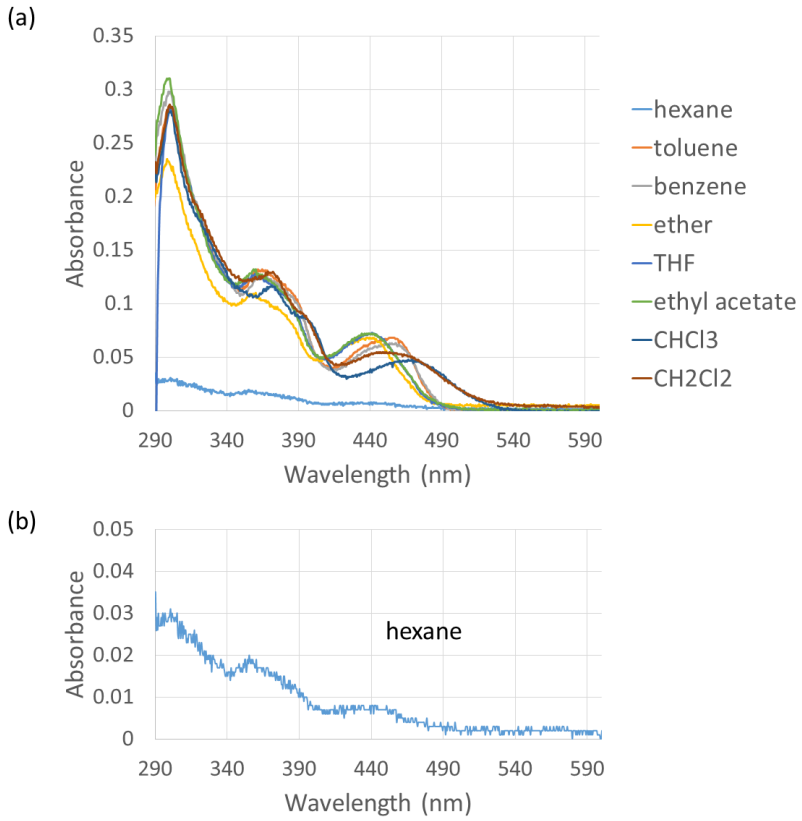


Figure S17. (a) UV-vis absorption spectra of **1** in different solvents. (b) UV-vis absorption spectrum of **1** in hexane. (The solutions of **1** except that in hexane had a concentration of 2×10^{-6} mol/L. Due to the low solubility of **1** in hexane, a saturated solution of **1** in hexane was filtered through a nylon syringe filter (0.45 um) before the spectrum was recorded.)

6. Density functional theory (DFT) calculations

All the DFT calculations were done by using Gaussian 09 program.[6]
The frontier molecular orbitals of **1** were calculated using simplified model molecule **1'**, in which all *t*-butyl groups were removed to reduce computational cost. Energy-minimized model of **1'** and their molecular orbitals were calculated at the B3LYP/6-31G(d) level of DFT. The fully optimized structure is confirmed as a true minimum by vibrational analysis with no imaginary frequency. The optimized structure **1'** has a total energy of −8021.770948 hartree.

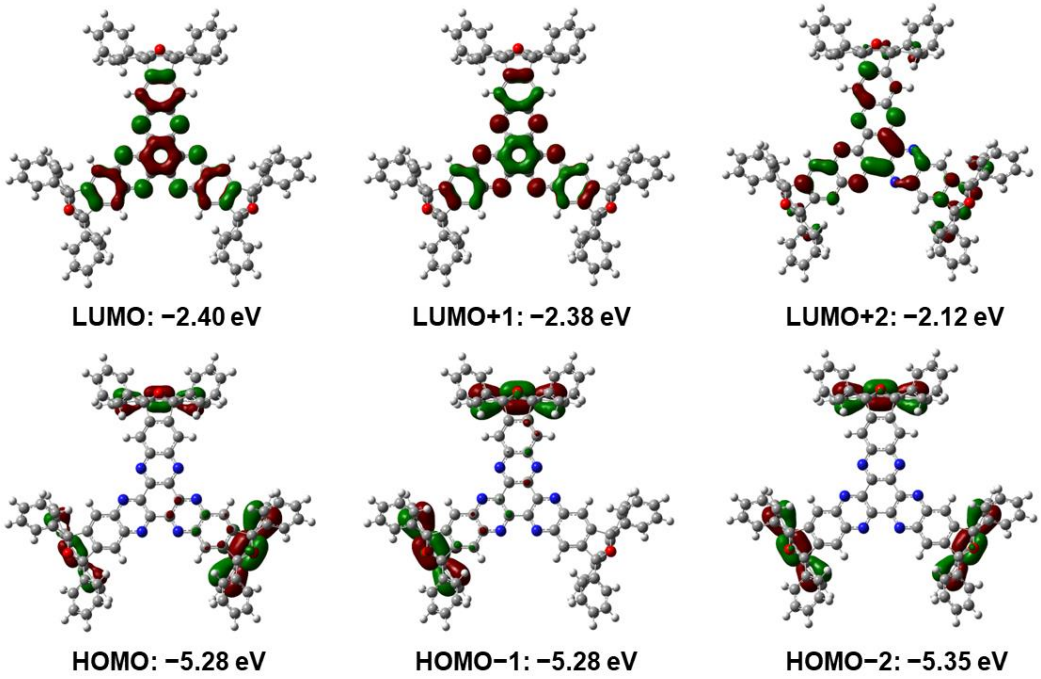


Figure S18. Frontier molecular orbitals of **1'** calculated at B3LYP/6-31G(d) level.

Optimized Cartesian coordinates

Molecule **1'** was calculated at B3LYP/6-31G(d) level

	X	Y	Z
C	-0.18518000	-7.94838700	1.20946600
C	-1.53431100	-7.55357500	1.23842900
C	-2.22540700	-7.31657300	-0.00000300
C	-1.53436700	-7.55355800	-1.23846900
C	-0.18523500	-7.94837000	-1.20957200
C	0.47762700	-8.12913000	-0.00006900
C	-2.26173100	-7.32249200	2.44996300
C	-3.52914000	-6.80282100	2.45000300
C	-4.20944400	-6.45678600	1.23849600

C	-3.55094500	-6.77308400	0.00003100
C	-4.20950000	-6.45676900	-1.23840000
C	-3.52925100	-6.80278800	-2.44994200
C	-2.26184200	-7.32245800	-2.44996700
C	-5.44756100	-5.79113800	1.20959600
C	-6.04661200	-5.45471000	0.00009700
C	-5.44761500	-5.79112100	-1.20943400
C	-3.83827000	-6.45171900	-3.93061200
C	-2.92311400	-5.23344700	-4.17340800
C	-1.59184400	-5.77927800	-4.17339000
C	-1.79535300	-7.28933800	-3.93062400
C	-1.79517700	-7.28939400	3.93060000
C	-1.59165500	-5.77933800	4.17337800
C	-2.92292500	-5.23350500	4.17346500
C	-3.83809200	-6.45177300	3.93069100
O	-3.06658400	-7.48024300	4.59992800
O	-3.06678900	-7.48017900	-4.59989800
C	-3.14343000	-3.88916400	-4.23539200
C	-0.49122200	-4.97660000	-4.23534300
C	-0.49102900	-4.97666100	4.23529100
C	-0.68251000	-3.55949100	4.31929000
C	-2.01199400	-3.01440900	4.31940700
C	-3.14323700	-3.88922300	4.23548000
C	-5.25034400	-6.49866000	-4.45803100
C	-0.82269000	-8.31412400	-4.45794900
C	-5.25014400	-6.49871800	4.45817100
C	-0.82249300	-8.31419100	4.45786600
C	-6.10250200	-7.52489500	-4.02386900
C	-7.38660400	-7.65197600	-4.54826200
C	-7.83757000	-6.75658100	-5.52146900
C	-6.99110800	-5.74461400	-5.97264000
C	-5.70190500	-5.62075400	-5.44979200
C	0.11461300	-8.00629200	-5.45038900
C	0.94582700	-8.99963200	-5.97297100
C	0.83891000	-10.31426900	-5.52082700

C	-0.11022900	-10.63498600	-4.54692200
C	-0.93558700	-9.64293800	-4.02283100
C	-5.70166200	-5.62082300	5.44996000
C	-6.99084300	-5.74468700	5.97286100
C	-7.83732500	-6.75664800	5.52171300
C	-7.38640300	-7.65203100	4.54847700
C	-6.10232200	-7.52494600	4.02403100
C	-0.93542100	-9.64299900	4.02273900
C	-0.11004200	-10.63505800	4.54677700
C	0.83914900	-10.31435800	5.52063600
C	0.94609700	-8.99972700	5.97279000
C	0.11486300	-8.00637600	5.45026200
C	-1.14212100	-0.89856400	4.38912700
C	0.18323000	-1.44191800	4.38902200
C	1.34948200	-0.54023000	4.38890700
C	1.15730600	0.87924100	4.38899100
C	-0.20669300	1.43841000	4.38897400
C	-1.33988800	0.56224900	4.38900400
C	-0.68270800	-3.55942900	-4.31931200
N	-2.21467000	-1.68424800	-4.36272300
C	-2.01219200	-3.01434800	-4.31935900
C	-6.79181900	4.13461500	1.20970700
C	-5.77510800	5.10535400	1.23863500
C	-5.22439500	5.58537400	0.00015900
C	-5.77516700	5.10537100	-1.23829700
C	-6.79187600	4.13463100	-1.20933500
C	-7.28002600	3.65121500	0.00019400
C	-5.21104300	5.61955800	2.45014300
C	-4.12739600	6.45750200	2.45006200
C	-3.48774200	6.87385200	1.23854800
C	-4.09102500	6.46173700	0.00013900
C	-3.48780000	6.87387000	-1.23829400
C	-4.12751100	6.45753600	-2.44978200
C	-5.21115800	5.61959100	-2.44982400
C	-2.29210400	7.61309900	1.20961300

C	-1.70124600	7.96365000	0.00009300
C	-2.29216200	7.61311600	-1.20940500
C	-3.66876300	6.54952500	-3.93036600
C	-3.07106900	5.14790100	-4.17295900
C	-4.20931900	4.26777600	-4.17295700
C	-5.41548600	5.19893200	-3.93051000
C	-5.41530100	5.19888000	3.93083300
C	-4.20912500	4.26771800	4.17320800
C	-3.07087400	5.14784200	4.17317100
C	-3.66857700	6.54947000	3.93062500
O	-4.94485300	6.39539500	4.60007600
O	-4.94507100	6.39545800	-4.59975900
C	-1.79664800	4.66670400	-4.23463400
C	-1.60446500	3.24963100	-4.31856800
C	-2.74118400	2.37070600	-4.31853700
C	-4.06429000	2.91328800	-4.23461500
C	-4.06409300	2.91322800	4.23483800
C	-2.74098300	2.37064500	4.31869400
C	-1.60426400	3.24957000	4.31868800
C	-1.79645000	4.66664400	4.23478400
C	-3.00364500	7.79603700	-4.45774300
C	-6.78909100	4.86886400	-4.45833400
C	-3.00343000	7.79597200	4.45798800
C	-6.78888300	4.86880800	4.45871700
C	-3.46632900	9.04696700	-4.02308300
C	-2.93471000	10.22278900	-4.54736700
C	-1.93421000	10.16605900	-5.52101800
C	-1.48107200	8.92719900	-5.97270600
C	-2.01798500	7.74856400	-5.44992300
C	-6.99072400	3.90335400	-5.45097400
C	-8.26633000	3.68039100	-5.97429700
C	-9.35154400	4.43036400	-5.52263900
C	-9.15514400	5.41251600	-4.54846100
C	-7.88357300	5.63109800	-4.02369100
C	-2.01773300	7.74847800	5.45013100

C	-1.48079000	8.92710200	5.97290900
C	-1.93393400	10.16597200	5.52125300
C	-2.93447000	10.22272200	4.54764000
C	-3.46611900	9.04691100	4.02336100
C	-7.88338100	5.63105600	4.02414000
C	-9.15492800	5.41247100	4.54896500
C	-9.35128800	4.43030100	5.52313300
C	-8.26605700	3.68031400	5.97472700
C	-6.99047400	3.90328000	5.45134800
C	6.97640700	3.81398500	1.20938500
C	7.30871800	2.44812700	1.23827900
C	7.44893800	1.73116300	-0.00015700
C	7.30866000	2.44814600	-1.23857500
C	6.97635000	3.81400300	-1.20964600
C	6.80177800	4.47847500	-0.00012100
C	7.47234200	1.70261000	2.44977000
C	7.65609800	0.34516900	2.44978500
C	7.69648200	-0.41701900	1.23827200
C	7.64106400	0.31146100	-0.00017200
C	7.69642400	-0.41700000	-1.23863000
C	7.65598200	0.34520600	-2.45012900
C	7.47222600	1.70264600	-2.45008600
C	7.73896800	-1.82208200	1.20933500
C	7.74716100	-2.50906000	-0.00019600
C	7.73891400	-1.82206300	-1.20971800
C	7.50651600	-0.09781900	-3.93081000
C	5.99384100	0.08544600	-4.17344900
C	5.80080400	1.51127700	-4.17350700
C	7.21026500	2.09018700	-3.93071700
C	7.21044800	2.09012700	3.93041900
C	5.80099700	1.51121600	4.17326200
C	5.99403400	0.08538400	4.17317600
C	7.50669800	-0.09787800	3.93046600
O	8.01150400	1.08456700	4.59970500
O	8.01129200	1.08463700	-4.60005300

C	4.93986300	-0.77758900	-4.23503300
C	3.61657300	-0.23545300	-4.31899600
C	3.42379300	1.18843200	-4.31908800
C	4.55526500	2.06294800	-4.23515400
C	4.55546000	2.06288600	4.23497200
C	3.42399300	1.18836800	4.31894700
C	3.61677300	-0.23551700	4.31882900
C	4.94005900	-0.77765100	4.23479900
C	8.25360900	-1.29700400	-4.45819700
C	7.61154200	3.44496200	-4.45788400
C	8.25380800	-1.29707200	4.45780600
C	7.61175100	3.44489400	4.45758900
C	9.56845600	-1.52127600	-4.02381600
C	10.32109400	-2.56955800	-4.54792100
C	9.77167900	-3.40810800	-5.52116400
C	8.47202300	-3.18163300	-5.97254400
C	7.71958900	-2.12738000	-5.44992000
C	6.87553600	4.10396500	-5.44896600
C	7.32048500	5.32045700	-5.97140100
C	8.51352300	5.88392600	-5.52053400
C	9.26655300	5.22113700	-4.54796700
C	8.81978200	4.01040700	-4.02397400
C	7.71983500	-2.12743300	5.44956800
C	8.47228400	-3.18169400	5.97215400
C	9.77191000	-3.40819200	5.52069700
C	10.32127800	-2.56965900	4.54741400
C	9.56862500	-1.52136800	4.02334700
C	8.81997500	4.01034100	4.02363900
C	9.26677100	5.22106200	4.54763100
C	8.51378300	5.88384100	5.52023700
C	7.32076100	5.32036900	5.97114500
C	6.87578700	4.10388500	5.44871100
N	-2.21446900	-1.68430900	4.36280000
N	0.39539500	-2.75430200	4.36258500
N	-2.58254900	1.03459600	4.36234600

N	-0.35108100	2.75996300	4.36229900
N	-2.58275100	1.03465800	-4.36221700
N	-0.35128400	2.76002600	-4.36224300
N	2.18772700	1.71922500	4.36246800
N	2.56615800	-1.07599200	4.36226100
N	2.56595600	-1.07592800	-4.36239200
N	2.18752500	1.71928900	-4.36254700
N	0.39519500	-2.75423900	-4.36264500
C	1.15710300	0.87930500	-4.38903300
C	1.34927900	-0.54016600	-4.38897700
C	0.18302800	-1.44185500	-4.38905200
C	-1.14232400	-0.89850100	-4.38908900
C	-1.34009100	0.56231200	-4.38893700
C	-0.20689600	1.43847300	-4.38894500
H	0.34572100	-8.10460700	2.14049500
H	0.34562400	-8.10457800	-2.14062700
H	1.52474900	-8.41876100	-0.00009500
H	-5.93542200	-5.52990000	2.14062100
H	-6.99582000	-4.92616600	0.00012200
H	-5.93551900	-5.52986900	-2.14043300
H	-4.12989400	-3.43910200	-4.19612100
H	0.52723000	-5.34864100	-4.19596800
H	0.52742100	-5.34870100	4.19586100
H	-4.12970200	-3.43916000	4.19626100
H	-5.75092500	-8.22500700	-3.27185400
H	-8.03475200	-8.45123400	-4.19906900
H	-8.84036500	-6.85274000	-5.92909700
H	-7.32759400	-5.05177100	-6.73911800
H	-5.04299800	-4.84783900	-5.82951600
H	0.18747000	-6.99352000	-5.83085200
H	1.67137500	-8.74272900	-6.73999500
H	1.48561100	-11.08679000	-5.92825200
H	-0.20917900	-11.65897200	-4.19691600
H	-1.67693700	-9.89446100	-3.27022100
H	-5.04273800	-4.84791400	5.82966600

H	-7.32729600	-5.05185300	6.73936200
H	-8.84010400	-6.85281000	5.92938300
H	-8.03456600	-8.45128300	4.19930100
H	-5.75077800	-8.22504900	3.27199200
H	-1.67681100	-9.89450900	3.27016500
H	-0.20901700	-11.65904000	4.19676400
H	1.48586600	-11.08688800	5.92802000
H	1.67168500	-8.74283800	6.73978000
H	0.18774500	-6.99360900	5.83073500
H	-7.19269600	3.75305400	2.14071700
H	-7.19279700	3.75308300	-2.14033100
H	-8.05470100	2.88948400	0.00020800
H	-1.82187400	7.90485800	2.14064900
H	-0.76881800	8.52126100	0.00007400
H	-1.82197500	7.90488900	-2.14045900
H	-0.91376000	5.29611500	-4.19525300
H	-4.89561300	2.21717700	-4.19529900
H	-4.89541700	2.21711900	4.19554900
H	-0.91356400	5.29605600	4.19537500
H	-4.24818400	9.09226000	-3.27078500
H	-3.30281200	11.18357800	-4.19775500
H	-1.51639800	11.08275300	-5.92858900
H	-0.71316100	8.87249900	-6.73956000
H	-1.67819400	6.79164300	-5.83019000
H	-6.14989200	3.33396500	-5.83116300
H	-8.40627600	2.92373500	-6.74152100
H	-10.34371800	4.25673400	-5.93061900
H	-9.99258800	6.01024600	-4.19882100
H	-7.73099800	6.39877900	-3.27090800
H	-1.67793400	6.79154900	5.83037200
H	-0.71285100	8.87238500	6.73973400
H	-1.51610000	11.08265700	5.92882000
H	-3.30257600	11.18351800	4.19805400
H	-4.24800200	9.09222000	3.27109300
H	-7.73083600	6.39875100	3.27136500

H	-9.99238600	6.01021200	4.19937600
H	-10.34344400	4.25666900	5.93115600
H	-8.40597200	2.92364500	6.74194300
H	-6.14962800	3.33388000	5.83148800
H	6.84646700	4.35188700	2.14043100
H	6.84636700	4.35191900	-2.14067800
H	6.52938200	5.53021400	-0.00010700
H	7.75645500	-2.37518900	2.14038100
H	7.76393900	-3.59537200	-0.00020500
H	7.75635800	-2.37515600	-2.14077300
H	5.04342100	-1.85690500	-4.19545300
H	4.36805000	3.13092200	-4.19552800
H	4.36824300	3.13086000	4.19536800
H	5.04361700	-1.85696700	4.19520400
H	9.99857200	-0.86645500	-3.27180300
H	11.33734600	-2.73077500	-4.19851500
H	10.35676700	-4.22826500	-5.92862000
H	8.04063600	-3.81972300	-6.73902300
H	6.72075600	-1.94370600	-5.82986100
H	5.96123400	3.66163700	-5.82863000
H	6.73461700	5.82126300	-6.73736200
H	8.85943100	6.83020600	-5.92785200
H	10.20366300	5.64643800	-4.19898700
H	9.40890400	3.49316400	-3.27251300
H	6.72102700	-1.94374100	5.82956500
H	8.04093400	-3.81977100	6.73866400
H	10.35700900	-4.22835500	5.92812400
H	11.33750600	-2.73089400	4.19794700
H	9.99870600	-0.86656000	3.27130400
H	9.40906600	3.49310700	3.27214700
H	10.20386900	5.64636400	4.19861900
H	8.85971000	6.83011300	5.92755400
H	6.73492600	5.82116600	6.73713600
H	5.96149900	3.66155500	5.82840600

Molecule **2** was calculated at B3LYP/6-31G(d,p) level

	X	Y	Z
C	6.27682800	-1.64619800	3.45176100
C	5.25333600	-1.88081600	4.41095700
C	4.59240900	-3.16915900	4.41091600
C	4.99910900	-4.13732500	3.45184600
C	4.99398900	-4.13604500	-3.46019000
C	4.58593100	-3.16755400	-4.41835000
C	5.24689100	-1.87924200	-4.41894400
C	6.27175900	-1.64493900	-3.46114000
C	4.71195900	-0.82542100	5.16236300
C	3.41912400	-3.34519100	5.16187200
C	3.41158500	-3.34334200	-5.16770500
C	2.77823400	-2.23828600	-5.74845900
C	3.43717600	-0.95427600	-5.74934100
C	4.70447100	-0.82360000	-5.16926500
C	1.46243400	0.06412300	-6.31113100
C	0.79901100	-1.22858900	-6.31010700
C	-0.68278000	-1.30185100	-6.30917800
C	-1.47053100	-0.08094500	-6.30937900
C	-0.79315300	1.23893600	-6.30989300
C	0.65807600	1.31069700	-6.31081300
C	2.78654300	-2.24031200	5.74381500
N	2.76760300	0.17033600	6.10360200
C	3.44547100	-0.95628900	5.74416700
C	-1.70825700	6.25431900	3.45901700
C	-0.99285600	5.48470400	4.41737200
C	0.45335800	5.55620900	4.41637000
C	1.08803200	6.39256100	3.45703700
C	1.08301800	6.39380100	-3.45643100
C	0.44697000	5.55777700	-4.41513800
C	-0.99924300	5.48626000	-4.41407500
C	-1.71326500	6.25553500	-3.45441600
C	-1.63595500	4.48796400	5.16870500

C	-0.88931300	3.45600200	5.74937900
C	0.55214700	3.52726800	5.74833700
C	1.19262200	4.62778100	5.16675300
C	1.18515900	4.62961500	-5.16690600
C	0.54385600	3.52928700	-5.74793300
C	-0.89760200	3.45800600	-5.74691500
C	-1.64341600	4.48976800	-5.16482100
C	-6.08362600	-2.25521500	-3.45278900
C	-6.07863500	-2.25637100	3.46059200
C	-4.56665400	-4.60836300	-3.45341000
C	-4.56167700	-4.60952200	3.45823000
C	-4.25107400	-3.60622600	4.41711500
C	-5.03582900	-2.38931900	4.41848300
C	-5.04218500	-2.38782200	-4.41220500
C	-4.25743000	-3.60472900	-4.41239300
C	-3.06509700	-3.66569600	5.16641100
C	-2.54379500	-2.50384800	5.74779100
C	-3.32620000	-1.29108200	5.74945600
C	-4.60020300	-1.28573300	5.16939100
C	-4.60763700	-1.28396100	-5.16332800
C	-3.33446600	-1.28909200	-5.74521300
C	-2.55206500	-2.50186200	-5.74512500
C	-3.07253300	-3.66392600	-5.16342400
N	2.75880900	0.17247500	-6.10748300
N	1.46705500	-2.34469400	-6.10549200
N	1.29100900	2.44717800	-6.10679300
N	-1.53485400	2.30745700	-6.10496700
N	1.29980600	2.44502700	6.10573000
N	-1.52605500	2.30532700	6.10793500
N	-2.77103300	-0.10097200	-6.10421500
N	-1.23723100	-2.47842000	-6.10383800
N	-1.22844500	-2.48054400	6.10461200
N	-2.76224500	-0.10309900	6.10809200
N	1.47586800	-2.34684200	6.10262400
C	-1.46144800	-0.08315000	6.31140200

C	-0.67369300	-1.30405500	6.30960900
C	0.80809600	-1.23079400	6.30849800
C	1.47150600	0.06190300	6.30901200
C	0.66716100	1.30847800	6.31025900
C	-0.78406900	1.23673000	6.31141500
C	5.87412200	-3.82619600	2.42828200
C	6.53447700	-2.53831000	2.42809500
C	5.94871400	-4.66534400	1.22202900
C	7.25915000	-2.10941700	1.22157300
C	-5.46472800	-4.38599800	2.43615400
C	-6.24869700	-3.16940000	2.43709700
C	-7.01366900	-2.81371000	1.23157300
C	-5.45823900	-5.22835900	1.22992300
C	0.38049400	6.99524500	2.43415800
C	-1.06506100	6.92383800	2.43519400
C	-1.79969000	7.33801800	1.22956200
C	1.06913200	7.47974600	1.22755700
C	-5.46823800	-4.38519100	-2.42996100
C	-6.25221300	-3.16859300	-2.42936700
C	-5.80984700	-4.61049800	0.00330700
C	-6.59710900	-3.38808200	0.00407900
C	6.23621000	-4.01601000	-0.00507900
C	6.89958200	-2.72223300	-0.00532800
C	-1.09028200	7.33370100	0.00204900
C	0.36191200	7.40533400	0.00100800
C	-1.80147700	7.33844400	-1.22443000
C	1.06734500	7.48017600	-1.22654200
C	-1.06859800	6.92469500	-2.43127800
C	0.37695800	6.99610900	-2.43231300
C	5.94691200	-4.66487300	-1.23200100
C	5.87051700	-3.82528900	-2.43781800
C	6.53088400	-2.53740000	-2.43814500
C	7.25730800	-2.10894400	-1.23252100
C	-5.46000300	-5.22795300	-1.22402000
C	-7.01544200	-2.81330600	-1.22262000

C	-3.18135400	7.58023400	-1.20528900
C	-3.85386100	7.74412900	0.00413100
C	-3.17959500	7.57979000	1.21251200
C	2.41832100	7.85679700	1.20855200
C	2.41656200	7.85721000	-1.20936600
C	3.07122900	8.08693500	-0.00084300
C	-8.01574300	-1.83254600	-1.20361600
C	-8.54037600	-1.38099500	0.00581600
C	-8.01399000	-1.83293900	1.21433900
C	-4.98094200	-6.54439900	-1.20654200
C	-4.97923200	-6.54480600	1.21132800
C	5.59921500	-6.02193500	-1.21392400
C	5.47252500	-6.70339900	-0.00503100
C	5.60101800	-6.02239600	1.20394400
C	8.15635100	-1.03456200	-1.21489000
C	8.63606300	-0.53376000	-0.00620700
C	8.15815000	-1.03502900	1.20300900
C	-4.78642300	-7.21007400	0.00214400
H	6.71562100	-0.65423800	3.42276200
H	4.44929200	-5.07234400	3.42248400
H	4.44422000	-5.07107900	-3.43035900
H	6.71058100	-0.65298200	-3.43243600
H	5.16319500	0.16157700	5.13820000
H	2.88073500	-4.28746400	5.13713600
H	2.87321900	-4.28561400	-5.14250000
H	5.15576400	0.16337900	-5.14544200
H	-2.78677700	6.13861700	3.43052600
H	2.17265900	6.38381400	3.42710300
H	2.16768800	6.38506300	-3.42806600
H	-2.79174100	6.13980800	-3.42440900
H	-2.71639100	4.38563800	5.14513900
H	2.27784800	4.63244300	5.14171200
H	2.27042000	4.63428000	-5.14343800
H	-2.72381700	4.38742800	-5.13973900
H	-6.61769000	-1.31117500	-3.42324900

H	-6.61273800	-1.31231800	3.43214800
H	-3.92744100	-5.48470100	-3.42417700
H	-3.92251300	-5.48585400	3.42777600
H	-2.43636600	-4.55022600	5.14079800
H	-5.14671400	-0.34810600	5.14600400
H	-5.15411300	-0.34633900	-5.13881100
H	-2.44377200	-4.54846900	-5.13905200
H	-3.72990700	7.65061800	-2.13896400
H	-4.91693800	7.96459600	0.00494500
H	-3.72678800	7.64982100	2.14701300
H	2.95724900	7.98083600	2.14223000
H	2.95413100	7.98156900	-2.14378600
H	4.10730100	8.41143200	-0.00154200
H	-8.39271300	-1.42778800	-2.13725100
H	-9.33870400	-0.64518400	0.00651600
H	-8.38961100	-1.42849100	2.14865000
H	-4.76886600	-7.05403700	-2.14083700
H	-4.76581700	-7.05474800	2.14515200
H	5.43690800	-6.54994600	-2.14798600
H	5.23573000	-7.76296000	-0.00505000
H	5.44009100	-6.55078400	2.13802900
H	8.49033400	-0.59472400	-2.14902400
H	9.35844400	0.27674100	-0.00658300
H	8.49352200	-0.59552500	2.13680300
H	-4.44701300	-8.24135700	0.00173100

Molecule **3** was calculated at B3LYP/6-31G(d,p) level

	X	Y	Z
C	-3.73488100	2.98606600	-2.74625900
C	-5.01066100	3.22651100	-2.08781500
C	-5.01069700	3.76797700	-0.75836600
C	-3.73488400	4.05598000	-0.11886700
C	3.73476100	4.05601700	-0.11878400
C	5.01065200	3.76779700	-0.75834400
C	5.01060000	3.22633900	-2.08766300

C	3.73476200	2.98600900	-2.74629500
C	-6.21430400	2.60039800	-2.59315400
C	-6.21404400	3.67105000	0.04085200
C	6.21410200	3.67108000	0.04089600
C	7.37575800	2.98994800	-0.46637500
C	7.37634200	2.46692600	-1.75446700
C	6.21435700	2.60036700	-2.59318400
C	9.09947000	0.85532100	-1.09147800
C	9.09935300	1.37422600	0.18412900
C	9.09950500	0.51748700	1.28644600
C	9.09977100	-0.84670700	1.09814300
C	9.09954800	-1.37282100	-0.19504100
C	9.09946100	-0.52774600	-1.28241000
C	-7.37570800	2.98992600	-0.46636400
N	-8.39215900	1.47523900	-2.14450400
C	-7.37629300	2.46692500	-1.75449400
C	-3.73502700	-3.87243000	-1.21278900
C	-5.01078800	-3.42169000	-1.75014000
C	-5.01061700	-2.54093100	-2.88360000
C	-3.73472000	-2.13024900	-3.45156400
C	3.73461200	-2.13015200	-3.45156800
C	5.01060400	-2.54095200	-2.88358400
C	5.01075600	-3.42156000	-1.75010000
C	3.73491000	-3.87254300	-1.21274500
C	-6.21448700	-3.54591400	-0.95517100
C	-7.37642500	-2.75303100	-1.25907200
C	-7.37576500	-1.89913900	-2.35624700
C	-6.21398400	-1.80048700	-3.19968900
C	6.21405200	-1.80046300	-3.19974900
C	7.37584300	-1.89918400	-2.35626500
C	7.37647300	-2.75300500	-1.25909600
C	6.21453700	-3.54592900	-0.95512400
C	3.73475600	-1.92467900	3.57090700
C	-3.73487400	-1.92458200	3.57089800
C	3.73490200	0.88560900	3.95863500

C	-3.73502000	0.88553300	3.95872100
C	-5.01097900	0.19488700	3.83860900
C	-5.01091200	-1.22726700	3.64277100
C	5.01087800	-1.22720400	3.64267700
C	5.01092300	0.19488800	3.83852500
C	-6.21460800	0.94560100	3.54856100
C	-7.37671000	0.28599600	3.01379900
C	-7.37613700	-1.09122700	2.82276100
C	-6.21428300	-1.87101700	3.15908400
C	6.21433000	-1.87104600	3.15904700
C	7.37617100	-1.09119200	2.82275700
C	7.37674500	0.28597300	3.01379900
C	6.21463500	0.94568700	3.54859200
N	8.39201100	1.47518500	-2.14436200
N	8.39189300	2.55305300	0.50490300
N	8.39180100	-0.83947000	-2.46364300
N	8.39220000	-2.59463300	-0.20538000
N	-8.39192800	-0.83949200	-2.46377200
N	-8.39232800	-2.59476900	-0.20535500
N	8.39229700	-1.71400100	1.95875000
N	8.39252800	1.11938500	2.34983300
N	-8.39268000	1.11946800	2.34992700
N	-8.39246600	-1.71411200	1.95884000
N	-8.39204100	2.55318400	0.50493700
C	-9.09963800	-0.84666700	1.09813900
C	-9.09937300	0.51744900	1.28642500
C	-9.09921900	1.37420700	0.18408200
C	-9.09933700	0.85532900	-1.09145400
C	-9.09931600	-0.52776500	-1.28237900
C	-9.09940600	-1.37279500	-0.19507200
C	-2.49739200	3.98972000	-0.85019800
C	-2.49739800	3.44951000	-2.17666200
C	-1.24695200	4.11271100	-0.15821600
C	-1.24695800	3.05421000	-2.75769200
C	-2.49739300	0.16064700	4.07500000

C	-2.49732000	-1.25817500	3.87885700
C	-1.24695100	-1.91900400	3.63940800
C	-1.24698400	0.86158700	4.02326200
C	-2.49729400	-2.73054500	-3.02874600
C	-2.49744300	-3.61053500	-1.89878200
C	-1.24696300	-3.91620900	-1.26597500
C	-1.24694400	-2.19275300	-3.48126900
C	2.49745200	0.16066400	4.07499200
C	2.49737400	-1.25821000	3.87888900
C	0.00000000	0.15198500	4.10695300
C	-0.00000300	-1.25847700	3.91187700
C	-0.00001000	4.01855200	-0.86653300
C	-0.00000800	3.48163600	-2.18513400
C	-0.00000600	-3.63375700	-1.92234300
C	-0.00000300	-2.75917800	-3.04578400
C	1.24700600	-3.91614700	-1.26594500
C	1.24699800	-2.19268800	-3.48118700
C	2.49749300	-3.61059800	-1.89879900
C	2.49735000	-2.73053800	-3.02875700
C	1.24699000	4.11263700	-0.15820300
C	2.49743800	3.98975500	-0.85018600
C	2.49744300	3.44951600	-2.17666800
C	1.24700400	3.05412800	-2.75762400
C	1.24704000	0.86158100	4.02315200
C	1.24700000	-1.91898400	3.63933800
C	1.22546400	-4.12201900	0.15356800
C	-0.00002200	-4.01121500	0.86435000
C	-1.22546700	-4.12197400	0.15356100
C	-1.22542900	-0.86788400	-4.03088700
C	1.22543500	-0.86788400	-4.03092500
C	-0.00001800	-0.15175000	-4.09922300
C	1.22549000	-3.05717300	2.76657500
C	-0.00002100	-3.47461500	2.18078600
C	-1.22549100	-3.05713300	2.76654800
C	1.22548100	2.19366000	3.49147600

C	-1.22547900	2.19363200	3.49145500
C	1.22548100	3.92599100	1.26407000
C	-0.00002400	3.62700800	1.91836400
C	-1.22548800	3.92593800	1.26404900
C	1.22539100	1.92779700	-3.64553200
C	-0.00002000	1.25672600	-3.90477800
C	-1.22539000	1.92778300	-3.64549600
C	-0.00002200	2.75389200	3.04028700
C	7.95946400	2.34191300	1.82062500
C	7.95944100	-2.74758800	1.11813800
C	7.95858000	0.40541300	-2.93780800
C	-7.95950900	-2.74760900	1.11815600
C	-7.95865300	0.40541200	-2.93786100
C	-7.95953700	2.34193500	1.82062900
C	-6.08995600	2.34687000	3.31402900
C	-6.93087100	3.01800400	2.34590600
C	-6.09010700	3.79033300	1.45625000
C	-4.82797900	2.93235700	3.19736700
C	-4.82815500	3.82251000	2.05246400
C	-3.65612100	2.25567000	3.56319100
C	-3.65616000	4.01041800	1.30654200
C	-2.42718700	2.81427900	3.10179400
C	-2.42723300	3.70130900	1.96169400
C	-6.93093200	-3.54078700	1.44079100
C	-6.09014200	-4.04354500	0.37539600
C	-6.08994200	-3.15649800	2.55433600
C	-4.82816700	-4.23590200	0.94062200
C	-4.82807000	-3.68856100	2.28358500
C	-3.65613300	-4.21514000	0.17156100
C	-3.65615100	-3.13617300	2.81867500
C	-2.42720700	-4.09453300	0.88591300
C	-2.42726100	-3.54931000	2.22360000
C	-6.93058600	0.52256100	-3.78643900
C	-6.08983000	1.69664500	-3.68935200
C	-4.82784800	1.30323200	-4.13832900

C	-4.82776900	-0.13355400	-4.33604300
C	-6.08968400	-0.63401000	-4.01045500
C	-3.65594100	1.95879900	-3.73549700
C	-2.42705000	1.27981700	-3.98807200
C	-2.42707300	-0.15134500	-4.18531300
C	-3.65598200	-0.87320400	-4.12512200
C	6.93067700	0.52257000	-3.78645100
C	6.08971300	-0.63404300	-4.01054800
C	6.08985400	1.69671900	-3.68943300
C	4.82782900	-0.13350000	-4.33578000
C	4.82789800	1.30311300	-4.13807100
C	3.65594000	-0.87319400	-4.12525300
C	3.65589200	1.95880600	-3.73557700
C	2.42704500	1.27988500	-3.98817500
C	2.42707200	-0.15138000	-4.18544300
C	6.93101000	-3.54080600	1.44078400
C	6.08996100	-3.15654800	2.55439600
C	6.09015200	-4.04365700	0.37537800
C	4.82812100	-3.68834600	2.28340300
C	4.82820900	-4.23562000	0.94059900
C	3.65610000	-3.13628900	2.81874500
C	3.65607500	-4.21525200	0.17159600
C	2.42725500	-3.54940400	2.22370000
C	2.42719800	-4.09466200	0.88590800
C	6.93095000	3.01803300	2.34591600
C	6.09013400	3.79048000	1.45626900
C	6.08996300	2.34693000	3.31411700
C	4.82820600	3.82227400	2.05236600
C	4.82802600	2.93222400	3.19712800
C	3.65610500	4.01053700	1.30660900
C	3.65607300	2.25576500	3.56324600
C	2.42722100	3.70146000	1.96172500
C	2.42717800	2.81435500	3.10190400

7. References

(1) Z. H. Wu, Z. T. Huang, R. X. Guo, C. L. Sun, L. C. Chen, B. Sun, Z. F. Shi, X. Shao, H. Li, H. L. Zhang, *Angew. Chem., Int. Ed.* **2017**, *56*, 13031−13035.

(2) X. Li, H. Wang, H. Chen, Q. Zheng, Q. Zhang, H. Mao, Y. Liu, S. Cai, B. Sun, C. Dun, M. P. Gordon, H. Zheng, J. A. Reimer, J. J. Urban, J. Ciston, T. Tan, E. M. Chan, J. Zhang, Y. Liu, *Chem.* **2020**, *6*, 933−944.

(3) T. Hamura, R. Nakayama, *Chem. Lett.* **2013**, *42*, 1013−1015.

(4) J. Wang, Q. Miao, *Org. Lett.* **2019**, *21*, 10120–10124.

(5) V. K. Patel, E. Kayahara, S. Yamago, *Chem. Eur. J.* **2015**, *21*, 5742–5749.

(6) Gaussian 09, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.