Supporting Information

Synthesis and Properties of Nanographene-Embedded Conjugated Macrocyclic Nanoring through Scholl Reaction

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1. General Information and Materials

All reagents including dry solvents and starting reactants for syntheses were purchased from commercial suppliers (Aldrich or Acros) and used directly. All glassware used in experiments was oven-dried and cooled under an inert atmosphere of argon. All air sensitive reactions were performed under argon atmosphere by standard Schlenk techniques. Flash column chromatography was carried out on silica gel (200～300 mesh). Nuclear magnetic resonance (NMR) spectra were recorded using a Bruker BioSpin (^{1}H 400 MHz, ^{13}C 100 MHz) spectrometer. Chemical shifts are quoted in ppm relative to $CHCl_3$ (δ 7.26 ppm), CH_2Cl_2 (δ 5.32 ppm), $C_2H_2Cl_4$ (δ 5.98 ppm) or tetramethylsilane (δ 0.00 ppm) for ^{1}H NMR and relative to $CDCl_3$ (δ 77.0 ppm) or $C_2D_2Cl_4$ (δ 73.8 ppm) for ^{13}C NMR. Data are reported as follows: chemical shift, multiplicity (s=singlet, d=doublet, m=multiplet), coupling constant (Hz), and integration. High-resolution mass spectrum (HR-MS) was acquired using MALDI-TOF-MS techniques. FTIR spectra were recorded on Infrared spectrometer (Thermo-Nicolet iS10) with DTGS Detector and EverGlo light source. UV-vis spectra were recorded on a UNIC-3802 spectrophotometer in quartz cuvettes.

2. Synthetic procedures of 10

Synthesis of compound 1. 4-bromo-4"-chloro-1',4'-dimethoxy-1',4'-dihydro-1,1':4',1"-terphenyl were prepared according to the published procedures. [S1]

Synthesis of compound 2. 4'-bromo-1-methoxy-[1,1'-biphenyl]-4(1*H*)-one were prepared according to the published procedures. [S2]

Synthesis of compound 3. (i). To a 250-mL round-bottom flask containing a magnetic stirring bar were added **1** (6.05 g, 14.34 mmol), and dry THF (100 mL). A solution of *n*-butyllithium in hexane (5.72 mL, 2.5 M, 14.34 mmol) was added at -78 °C. After stirring the mixture at -78 °C for 1.5 h, **2** (4.08 g, 14.61 mmol) was added, and the resultant mixture was further stirred at -78 °C for 3 h. After warmed up to room temperature, the mixture was quenched with H_2O, extracted with EtOAc, dried over Na_2SO_4, and concentrated under reduced pressure. (ii). NaH (1.03 g, 60% mineral oil, 25.74 mmol) was suspended in 20 mL anhydrous THF and cooled to 0 °C. The above crude product was put into the cooled suspension portionwise. After 30 min stirring, neat MeI (2.50 mL, 40.04 mmol) was added dropwise. The mixture was warmed to room temperature and stirred for 10 h. The excess sodium hydride was quenched by the addition of water (10 mL). After layer separation, the aqueous layer was extracted with diethyl ether three times. The combined organic layers were washed with brine, dried over Na_2SO_4 and the organic solvents were removed under reduced pressure. The residue was purified by silica gel column chromatography (EtOAc/petroleum ether = 1/6) to give **3** as a white solid (5.34 g, 8.61 mmol, 60%).^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 - 7.24 (m, 12H), 6.14 - 6.03 (m, 8H), 3.42 - 3.25 (m, 12H). ^{13}C NMR (101 MHz,

$CDCl_3$) δ 142.62, 142.49, 141.94, 134.14, 134.11, 133.60, 133.52, 133.44, 133.36, 133.04, 132.98, 131.43, 131.39, 128.44, 127.78, 127.76, 127.42, 127.40, 126.10, 126.01, 121.56, 74.53, 74.46, 74.41, 74.21, 51.99, 51.94.

Synthesis of compound 4. 2-(4"-chloro-1',4'-dimethoxy-1',4'-dihydro-[1,1':4',1"-terphenyl]-4-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane were prepared according to the published procedures. [S1]

Synthesis of compound 5. To a degassed suspension of **3** (3.89 g, 6.28 mmol), **4** (3.09 g, 6.59 mmol), potassium carbonate (8.68 g, 62.8 mmol) in THF (120 mL), H_2O (30 mL) was added $Pd(PPh_3)_4$ (362.5 mg, 0.31 mmol), then the mixture was degassed for 15 min. The mixture was then heated at 80 °C for 48 h under nitrogen atmosphere. After cooling down to room temperature, water was added and the mixture was extracted with CH_2Cl_2, dried over $MgSO_4$ and concentrated under vacuum. The crude product was purified by column chromatography (EtOAc/petroleum ether = 1/4) to afford compound **5** as a white solid (4.59 g, 83%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 - 7.52 (m, 6H), 7.46 - 7.32 (m, 14H), 6.18 - 6.02 (m, 12H), 3.46 - 3.30 (m, 18H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.88, 142.50, 142.21, 141.96, 140.06, 139.88, 133.87, 133.67, 133.61, 133.34, 133.07, 133.01, 128.47, 128.42, 127.45, 127.40, 127.13, 127.05, 126.40, 126.37, 126.33, 126.12, 126.08, 125.97, 74.61, 74.54, 74.47, 74.43, 74.34, 52.00. HR-MS (MALDI-TOF) *m/z* calcd. for: $C_{54}H_{50}Cl_2O_6$ $[M]^+$: 864.2985, found: 864.3044.

Synthesis of compound 6. A 250-mL flask containing **5** (5.60 g, 6.35 mmol), B_2pin_2 (3.87 g, 15.24 mmol), K_3PO_4 (6.70 g, 31.75 mmol), palladium(II) acetate (342 mg,

0.152 mmol), and SPhos (144 mg, 0.35 mmol) was evacuated and filled with argon three times, dry 1,4-dioxane (80 mL) was transferred to the flask via syringe under nitrogen at room temperature. The mixture was then stirred at 80 °C for 24 h. After cooling down to room temperature, the reaction was quenched with methanol (40 mL). Then the crude product was washed with cold methanol (40.0 mL) to give the product **6** as a white solid (6.08 g, 90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 - 7.74 (m, 4H), 7.66 - 7.37 (m, 16H), 6.16 - 6.08 (m, 12H), 3.46 - 3.30 (m, 18H). 1.37 - 1.31 (m, 24H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.39, 146.37, 142.75, 142.73, 142.65, 142.44, 142.42, 142.36, 140.02, 139.99, 139.95, 134.89, 134.88, 133.93, 133.84, 133.36, 133.33, 133.29, 133.22, 127.10, 127.08, 126.39, 126.35, 126.07, 126.05, 126.03, 125.30, 125.25, 91.49, 83.76, 83.74, 74.93, 74.91, 74.69, 74.65, 74.64, 74.62, 74.40, 51.98, 51.95, 24.83.

Synthesis of compound 7. 1,4-bis(4-bromophenyl)-2,3-bis(4-(*tert*-butyl)phenyl)-6,11-diiodotriphenylene were prepared according to the published procedures. [S3]

Synthesis of compound 8. To a round-bottom flask (500 mL) was added compound **6** (194.96 mg, 0.186 mmol), **7** (195.52 mg, 0.186 mmol), THF (250 mL) and H_2O (10 mL), then potassium carbonate (770 mg, 5.57 mmol) and $Pd(PPh_3)_4$ (30.06 mg, 0.026 mmol) was added after argon bubbling for 25 minutes. Then, the mixture was reacted at 80 °C for 48 hours. After cooling to room temperature, the solvent was removed under vacuum and the residue was extracted with CH_2Cl_2. The organic layer was dried by anhydrous $MgSO_4$, filtered and concentrated under reduced pressure to afford macrocycle intermediate **8** as a yellow solid for the next step without further

purification.

Synthesis of compound 9. To a 50-mL round-bottom flask (vessel A) containing a magnetic stirring bar were added $SnCl_2 \cdot 2H_2O$ (274 mg, 1.21 mmol), THF (25 mL) and concentrated HCl/H_2O (0.21mL, 12 mol/L) were added, and the resultant mixture was further stirred at room temperature for 30 min. To another 200-mL round-bottom flask (vessel B) containing a magnetic stirring bar were added the above crude product **8** and dry THF (10 mL). A solution of H_2SnCl_4/THF (18 mL, 0.72 mmol, 0.04 M in THF) in vessel A was added. After stirring the mixture at room temperature for 10 h, the mixture was added aqueous saturated sodium thiosulfate, extracted with CH_2Cl_2, dried over anhydrous $MgSO_4$, and concentrated under reduced pressure. Purification by column chromatography with petroleum ether/CH_2Cl_2 as the eluent (v/v, 4:1) afforded pure **9** (57.59 mg, 22%) as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, J = 9.0 Hz, 2H), 7.70 (d, J = 8.8 Hz, 2H), 7.60 - 7.52 (m, 20H), 7.47 (d, J = 8.6 Hz, 4H), 7.38 (t, J = 9.2 Hz, 6H), 7.31 (dd, J = 12.8, 4.6 Hz, 6H), 7.23 (d, J = 7.2 Hz, 2H), 7.14 (d, J = 7.8 Hz, 2H), 7.02 (d, J = 7.8 Hz, 4H), 6.87 (d, J = 8.2 Hz, 2H), 6.72 (d, J = 7.6 Hz, 2H), 6.25 (d, J = 8.0 Hz, 2H), 1.12 (s, 18H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.21, 146.03, 142.68, 142.25, 141.33, 139.99, 138.42, 138.38, 138.31, 138.18, 138.11, 138.02, 137.90, 137.83, 137.13, 136.91, 136.21, 134.56, 134.18, 132.50, 131.53, 131.47, 131.31, 130.51, 130.42, 130.06, 129.90, 129.66, 128.56, 127.33, 127.19, 127.08, 126.37, 124.26, 124.10, 123.70, 123.36, 122.78, 121.16, 120.31, 119.44, 34.12, 31.15. HR-MS (MALDI-TOF) *m/z* calcd. for: $C_{98}H_{72}Br_2$ $[M]^+$: 1408.3980, found: 1408.3987. IR (KBr) cm^{-1}: 3075.94, 3025.89, 2957.25, 2924.36, 2862.87, 1899.05, 1651.66,

1593.03, 1484.35, 1391.39, 1367.08, 1265.55, 1116.83, 1071.07, 1006.72, 812.24, 736.45, 682.11, 602.03, 566.28, 516.23.

Synthesis of compound 10. A solution of **9** (19.71 mg, 0.014 mmol) and DDQ (33.37 mg, 0.147 mmol) in 20 mL of anhydrous CH_2Cl_2 was degassed by argon bubbling for 20 minutes. The mixture was cooled with an ice bath and then was added TfOH (0.15 mL). After stirring at 0 °C for another 30 minutes, the reaction was quenched with saturated $NaHCO_3$ solution. The organic phase was separated, washed with saturated $NaHCO_3$ solution and brine, dried over anhydrous magnesium sulfate and evaporated. Purification by column chromatography with CS_2 as the eluent afforded pure **10** (8.78 mg, 45%) as an orange solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.38 (s, 2H), 9.14 (s, 2H), 9.06 (s, 2H), 8.88 (s, 2H), 8.63 - 8.49 (m, 4H), 8.32 (d, J = 10.5 Hz, 2H), 8.03 (d, J = 9.5 Hz, 2H), 7.52 (d, J = 9.0 Hz, 4H), 7.25 - 6.95 (m, 20H), 1.92 (s, 18H). ^{13}C NMR (101 MHz, CS_2/ $CDCl_3$ (1:1)) δ 148.79, 138.12, 137.96, 137.60, 137.52, 137.14, 132.47, 130.36, 129.73, 129.66, 128.63, 127.72, 127.38, 127.17, 127.00, 126.89, 126.78, 126.38, 125.84, 125.30, 125.03, 124.42, 122.18, 121.70, 120.86, 119.81, 119.34, 118.87, 118.25, 117.74, 35.76, 32.17. HR-MS (MALDI-TOF) *m/z* calcd. for: $C_{98}H_{58}Br_2$ $[M]^+$: 1394.2885, found: 1394.2878. IR (KBr) cm^{-1}: 2957.25, 2921.50, 2871.45, 2841.42, 1631.64, 1603.04, 1460.04, 1377.09, 1256.97, 813.67.

4. Computational details

Following the strategy of density functional theory (DFT) calculation, geometrical optimization were performed by the theoretical level of B3LYP/Def2-TZVP. Frontier molecular orbitals were plotted. Moreover, time-dependent DFT calculation in the theoretical level of B3LYP/DEF2-SVP were carried out. The strain energy (SE) was calculated using the computational methods reported by K. Itami[S4] (see Table S1), where the detailed energy information is displayed in Table S2. All of calculations were conducted in the ORCA 4.2.1[1]. [S5] As shown in Figure S15, the strain energy was estimated following the formula: Strain energy = E(**9**) + 9*E(biphenyl) – 8*E(Triphenyl) – E(**9**-Fragment) for **9**; Strain energy = E(**10**) + 7*E(biphenyl) – 6*E(Triphenyl) – E(**10**-Fragment) for **10**.

5. SCLC measurements.

Electron-only devices (ITO/ZnO/Active layer/Ca/Al) were fabricated as follows: 0.1 M zinc acetate in a solution mixture of 2-methoxy ethanol and ethanolamine was spin-coated onto the ITO substrates at 3000 rpm for 30 s, followed by heating at 200 °C for 30 min in air to form a ZnO film. The o-dichlorobenzene solution of **9** (5 mg/mL) and **10** (5 mg/mL), was spin-coated onto the ZnO layer at 1000 rpm for 40s, respectively. Then the devices were annealed at 125 °C for 10 min. Finally, 10 nm Ca/80 nm Al was deposited sequentially atop the active layer in a vacuum chamber (~10^{-5} Pa) with a defined active area of 2 × 5 mm^2.

The μ_e value is calculated from Mott-Gurney equation (1):

$$J_{SCLC} = \frac{9}{8}\varepsilon_0\varepsilon_r\mu_{e/h}\left(\frac{V^2}{L^3}\right) \quad (1)$$

where J_{SCLC} stands for current density, V is the applied potential, L is the thickness of the **9** (40 nm), **10** (40 nm), ε_r is the relative dielectric constant of the blend (3), ε_0 is the permittivity of free space (8.85 × 10^{-12} C V^{-1} s^{-1}).

6. Physical characterizations and photophysical properties

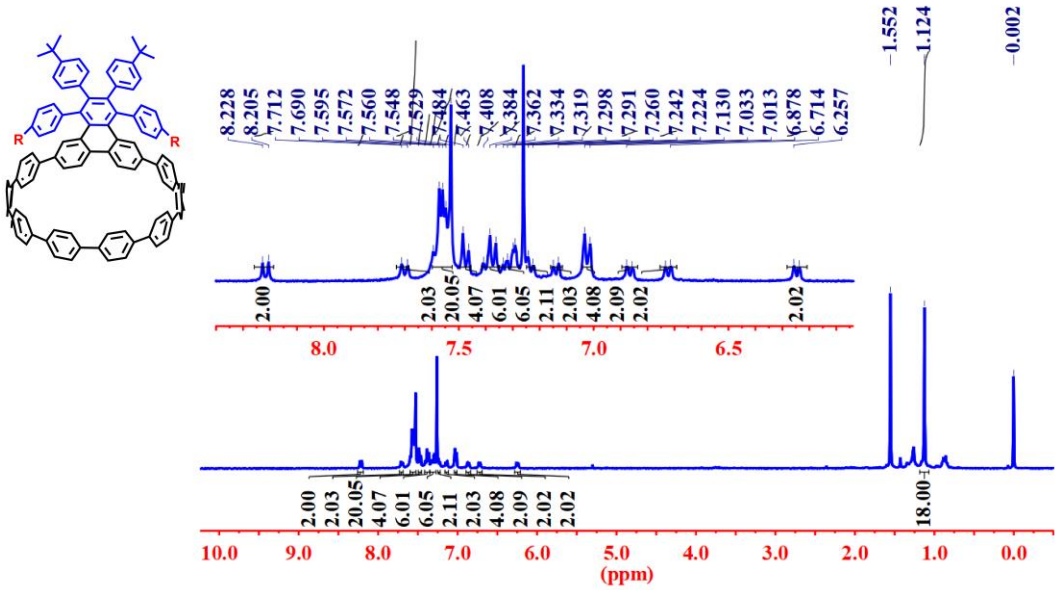

Figure S1. ^{1}H NMR spectrum of **9** in $CDCl_3$.

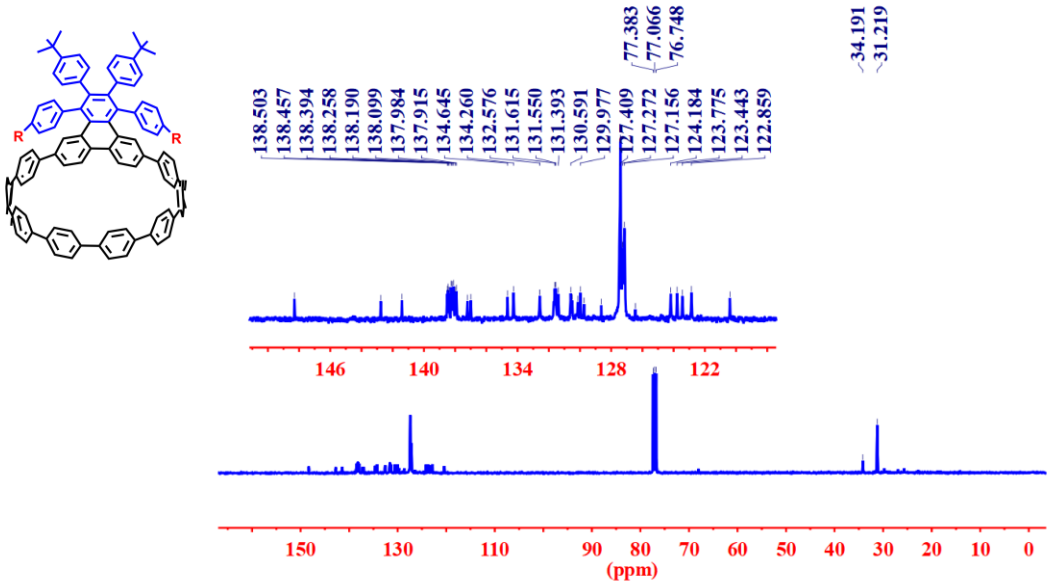

Figure S2. ^{13}C NMR spectrum of **9** in $CDCl_3$.

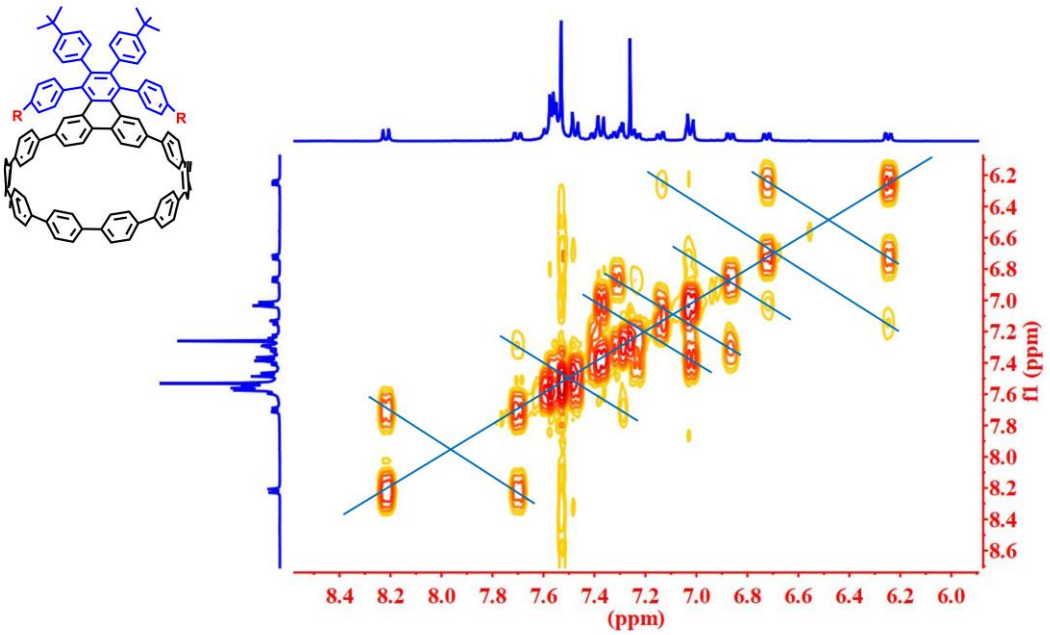

Figure S3. Expanded 2D ^{1}H-^{1}H COSY NMR spectrum (400 MHz, $CDCl_3$) of **9**.

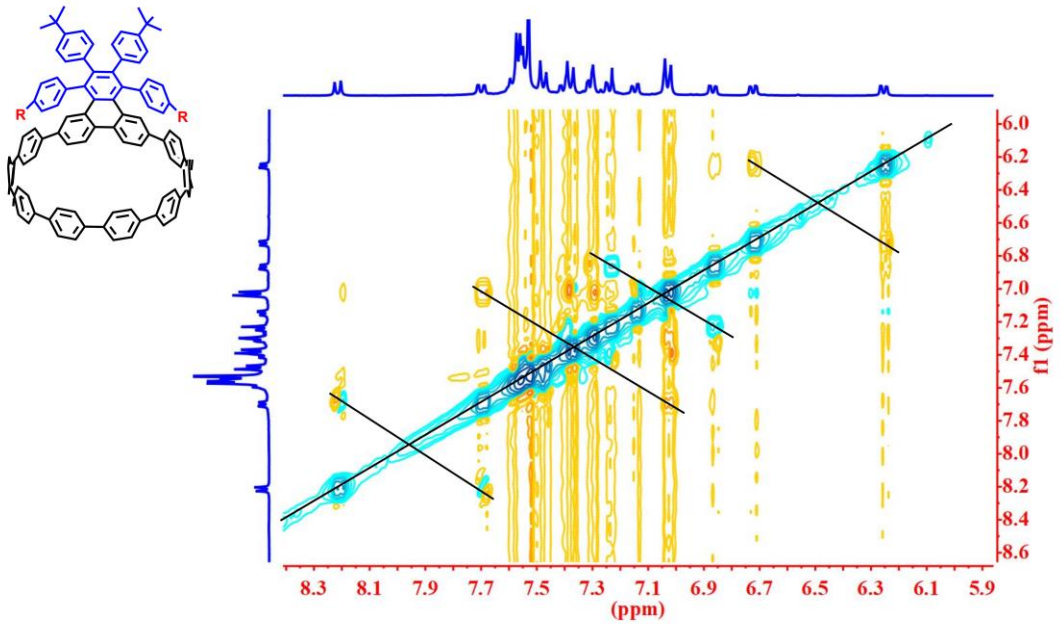

Figure S4. Expanded 2D ^{1}H-^{1}H NOESY NMR spectrum (400 MHz, $CDCl_3$) of **9**.

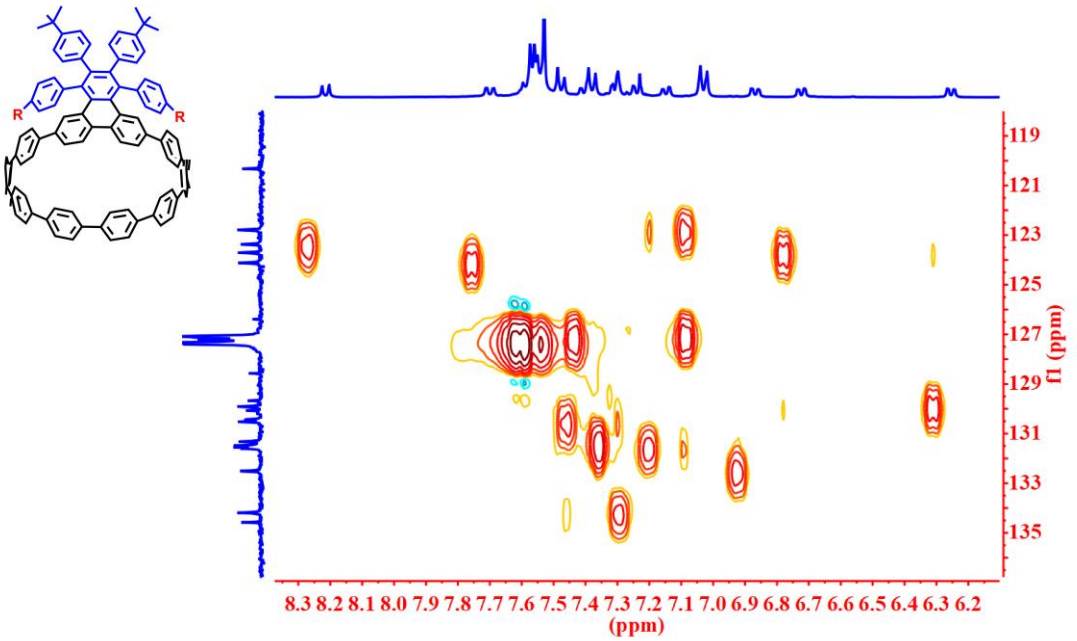

Figure S5. Expanded 2D (H, C)-HSQC NMR spectrum (400 MHz, $CDCl_3$) of **9**.

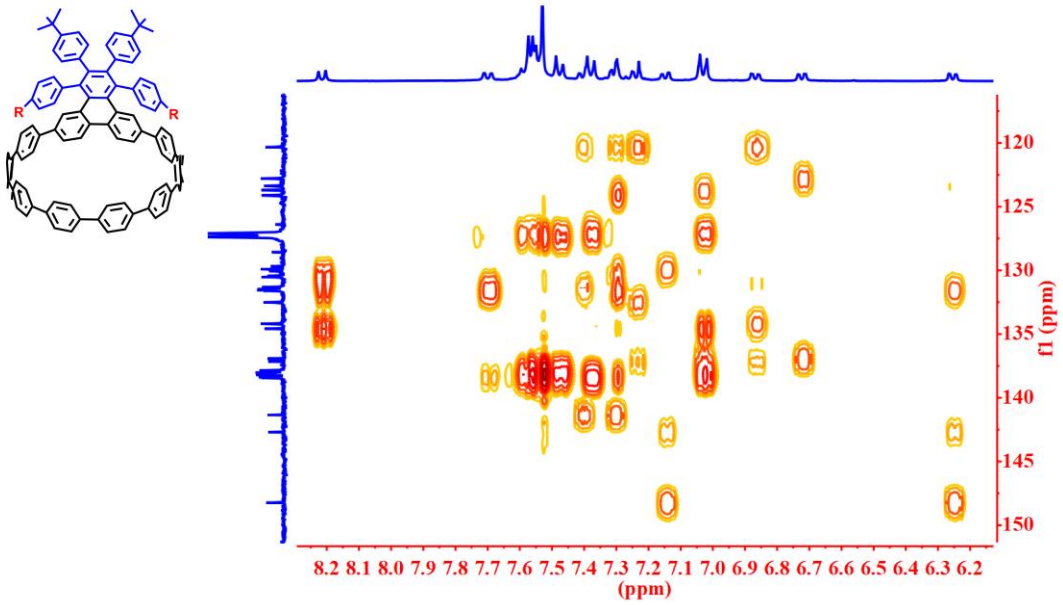

Figure S6. Expanded 2D (H, C)-HMBC NMR spectrum (400 MHz, $CDCl_3$) of **9**.

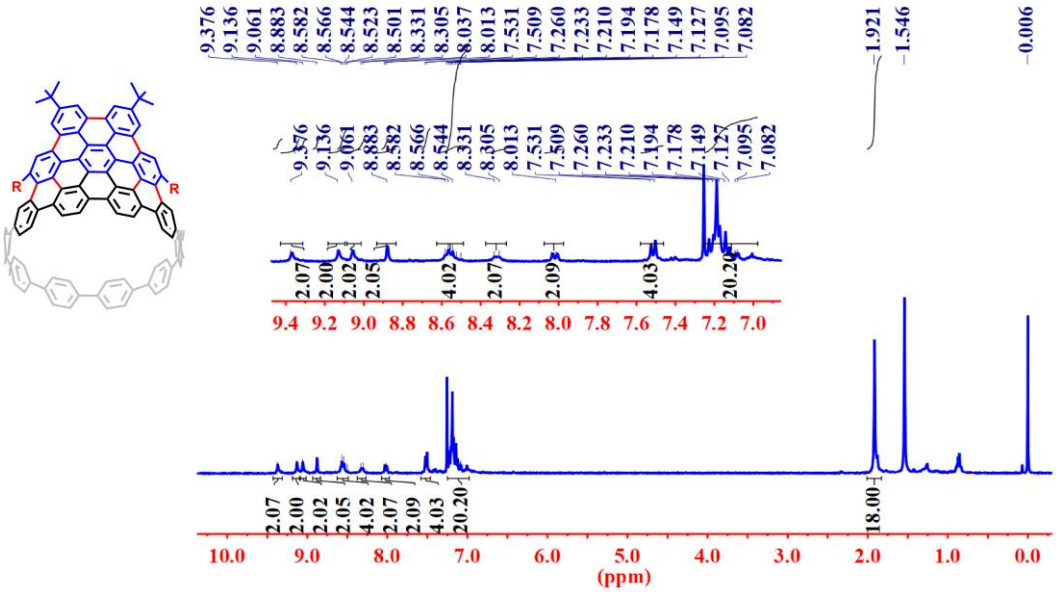

Figure S7. ^{1}H NMR spectrum of **10** in $CDCl_3$. (number of scans = 1024)

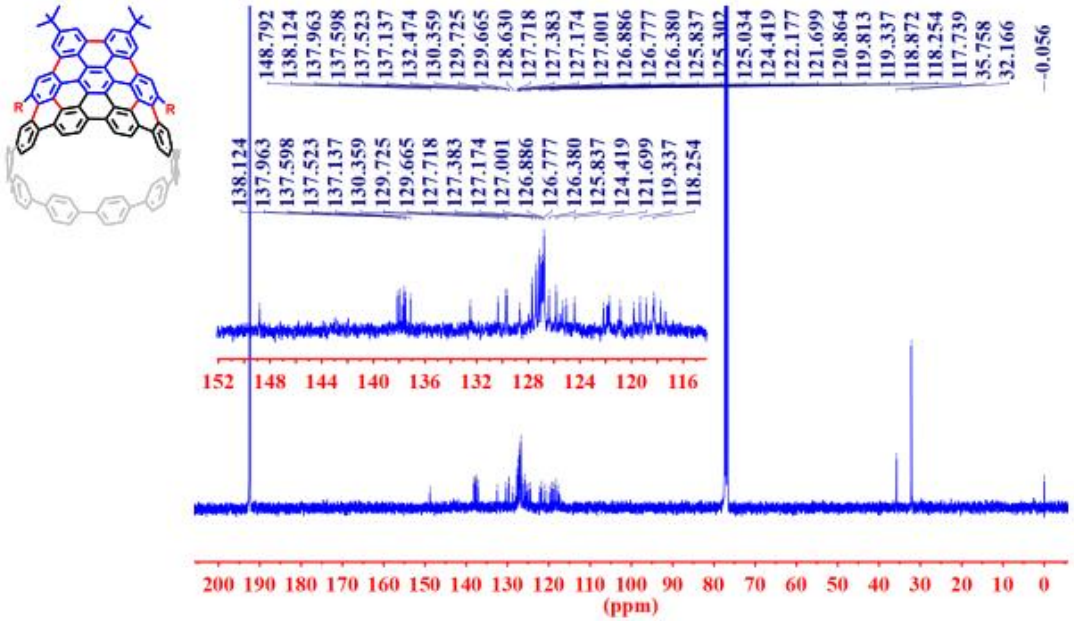

Figure S8. ^{13}C NMR spectrum of **10** in $CS_2/CDCl_3$ (1:1) (number of scans = 10240)

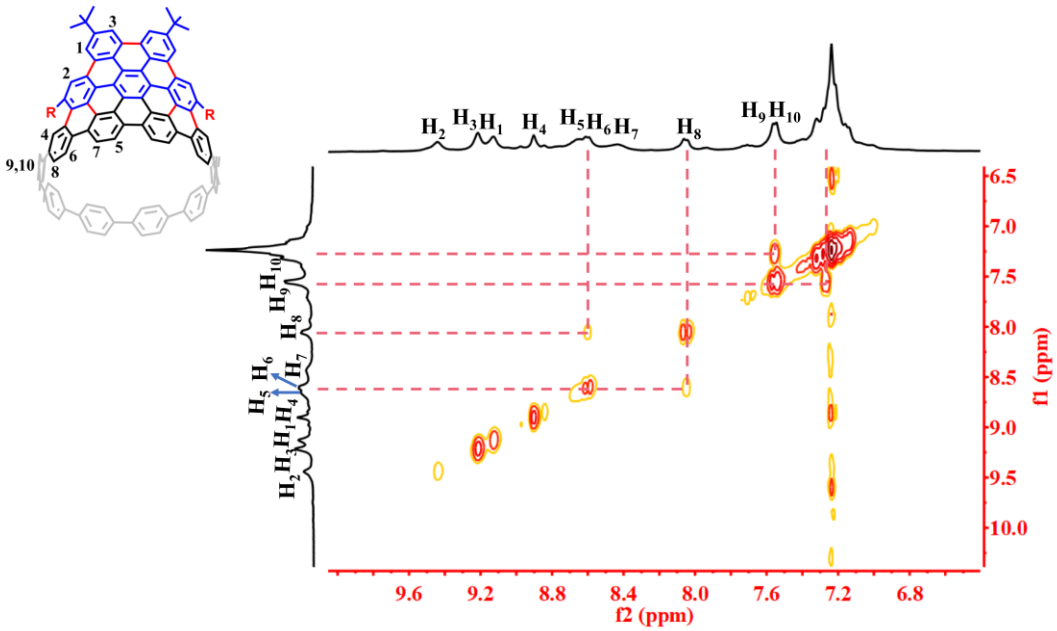

Figure S9. Expanded 2D ^{1}H-^{1}H COSY NMR spectrum (400 MHz, $CS_2/C_2D_2Cl_4$ (1:2)) of **10**.

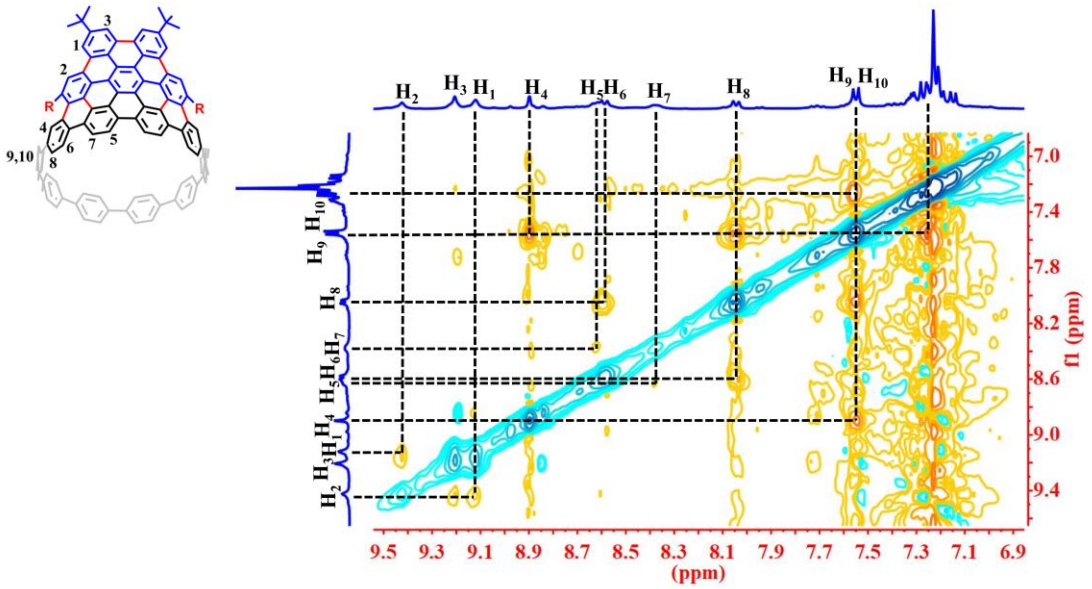

Figure S10. Expanded 2D ^{1}H-^{1}H ROESY NMR spectrum (400 MHz, $CS_2/C_2D_2Cl_4$ (1:2)) of **10**.

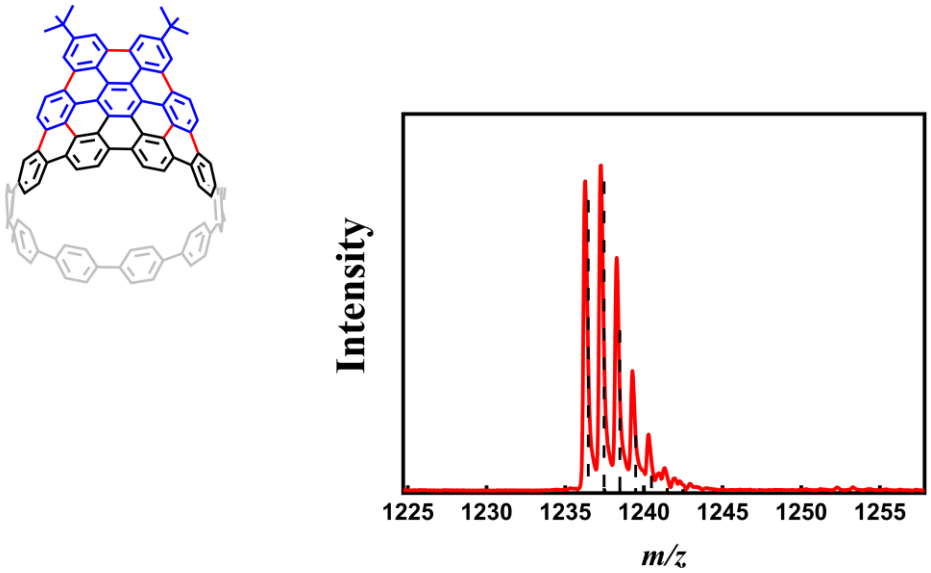

Figure S11. MALDI-TOF-MS spectrum (black) and simulated data (red) for **11**.

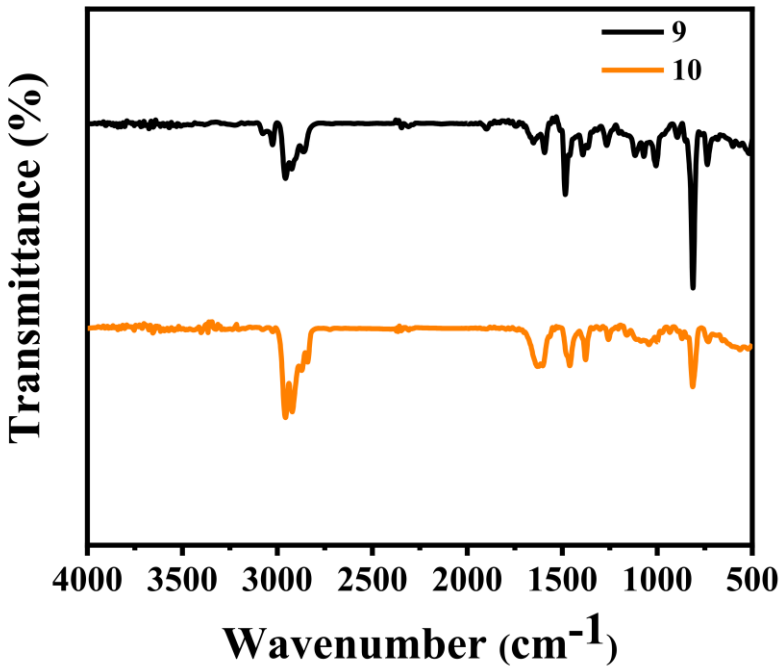

Figure S12. FTIR spectra of **9** and **10**.

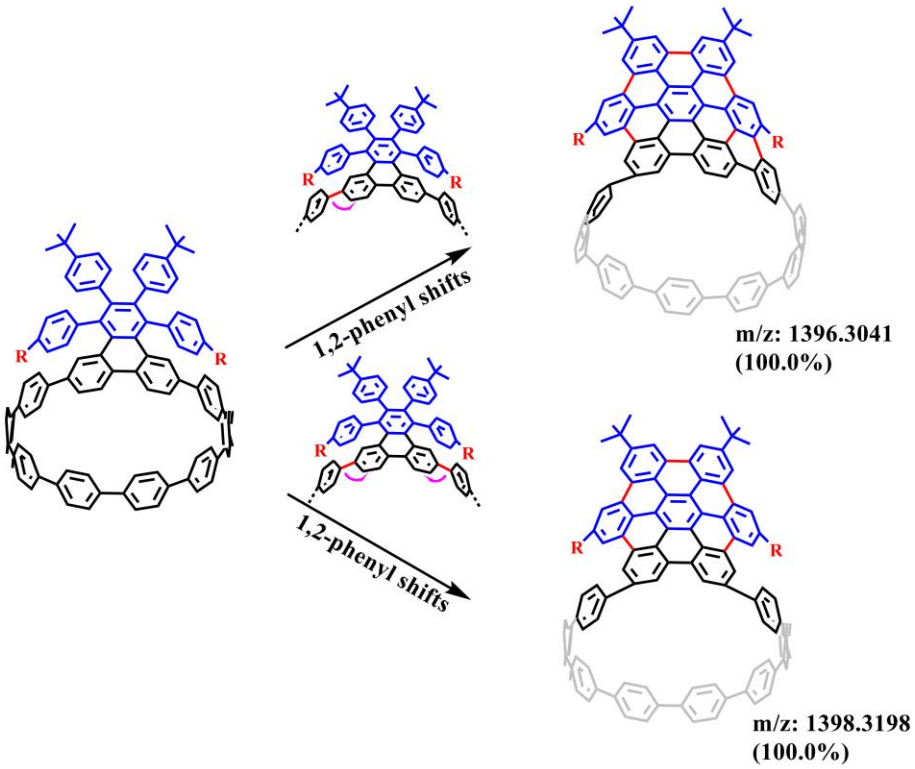

Figure S13. Possible molecular structures and their calculated molecular weights if 1,2-phenyl shifts occur during the Scholl reaction for synthesis of **10**.

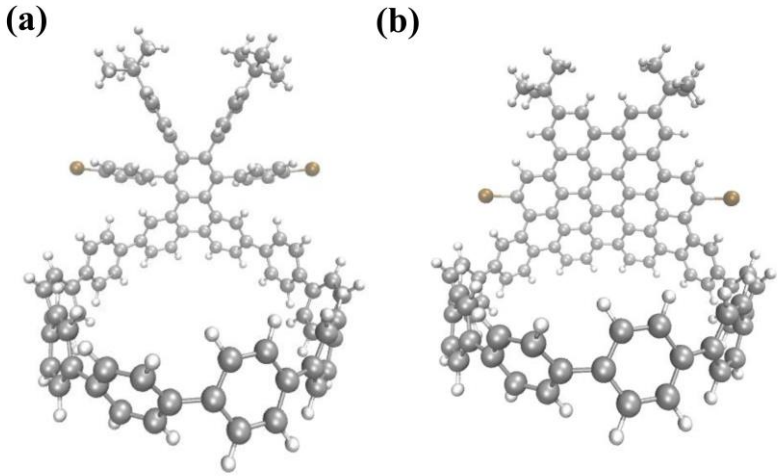

Figure S14. Relaxed configuration of **9** (a) and **10** (b).

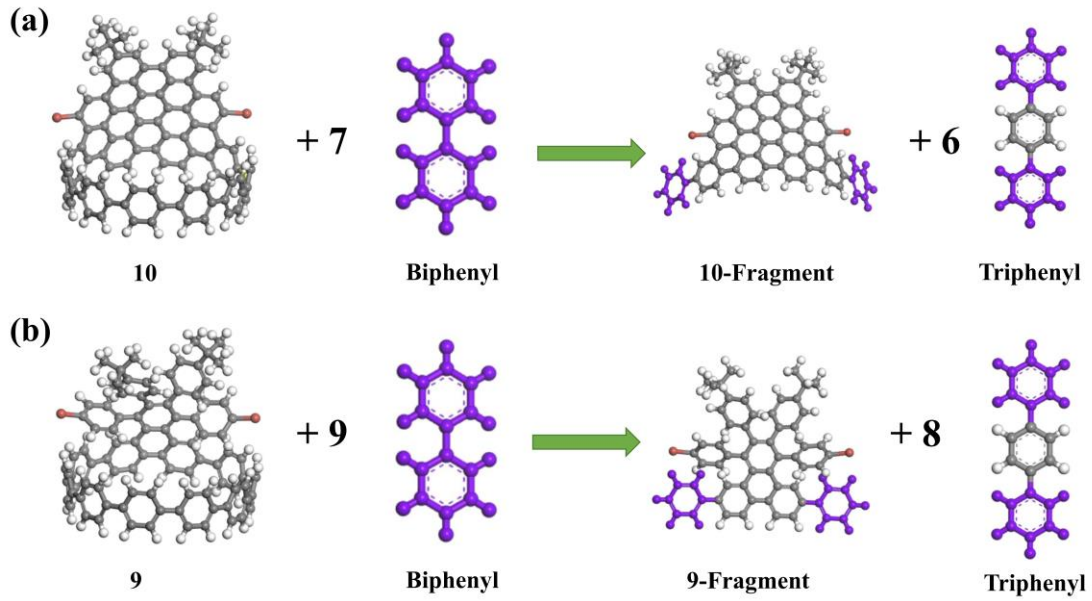

Figure S15. Homodesmotic equation for the calculation of strain energy： **10** (a) and **9** (b).

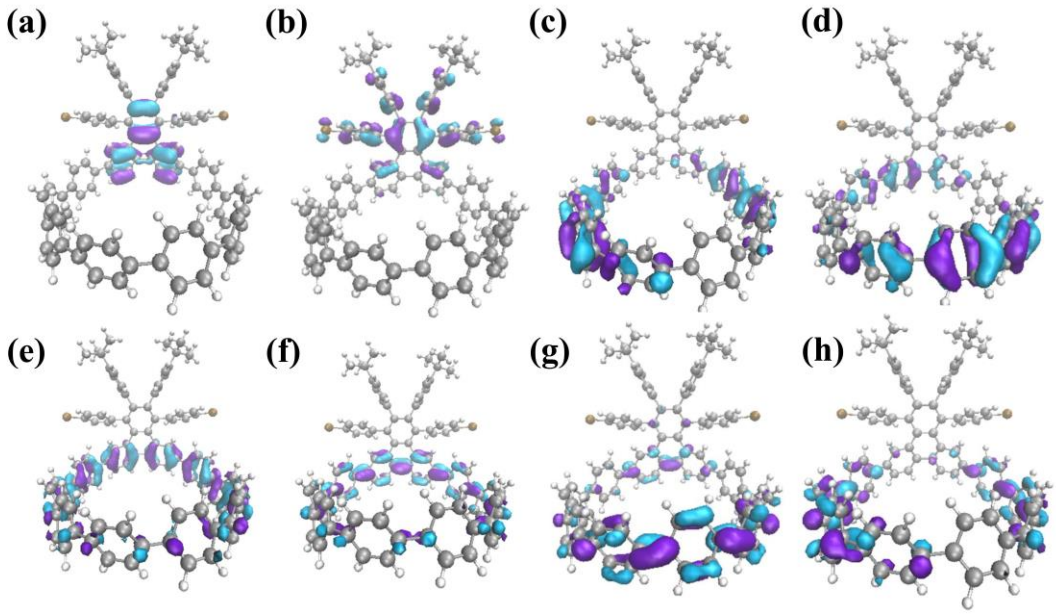

Figure S16. HOMO-3 (a), HOMO-2 (b), HOMO-1 (c), HOMO (d), LUMO (e), LUMO+1 (f), LUMO+2 (g) and LUMO +3 (h) of **9**.

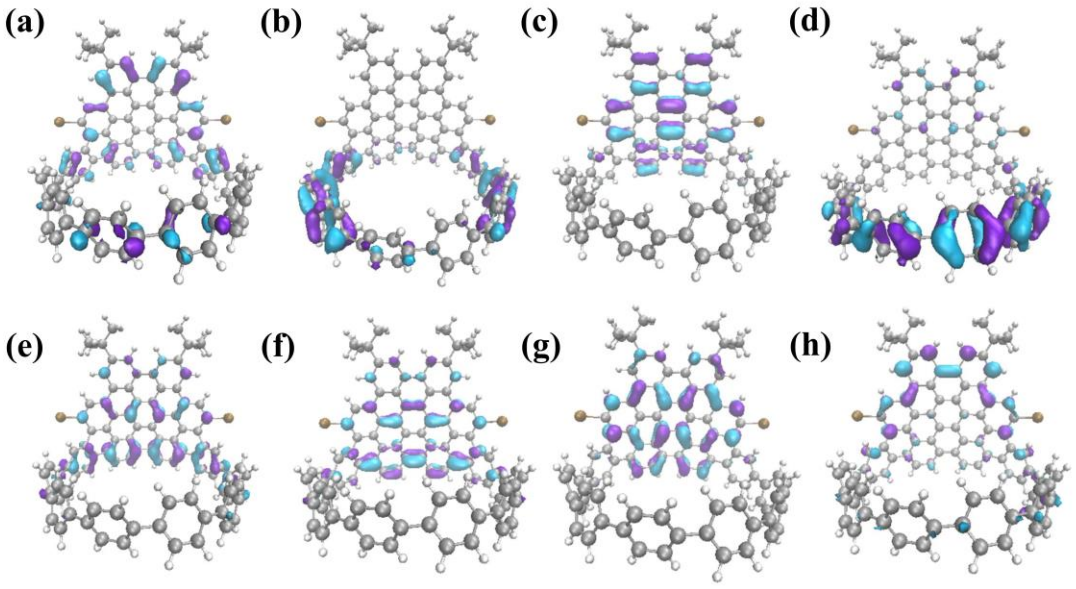

Figure S17. HOMO-3 (a), HOMO-2 (b), HOMO-1 (c), HOMO (d), LUMO (e), LUMO+1 (f), LUMO+2 (g) and LUMO +3 (h) of **10**.

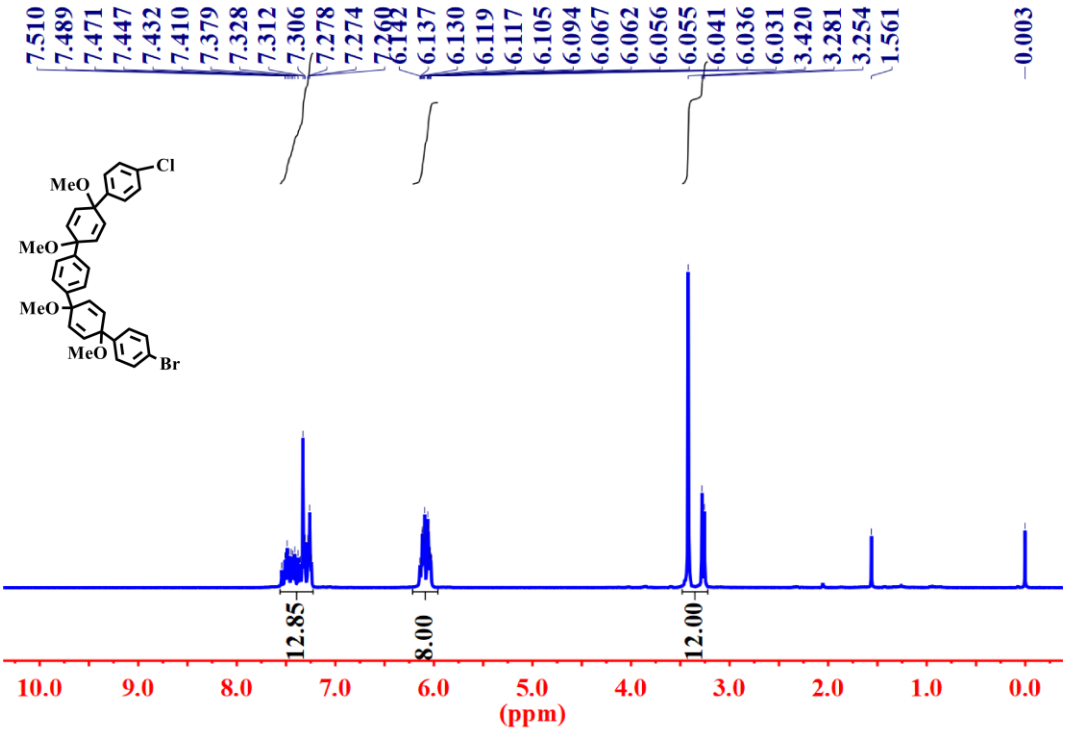

Figure S18. ^{1}H NMR spectrum of **3** in $CDCl_3$.

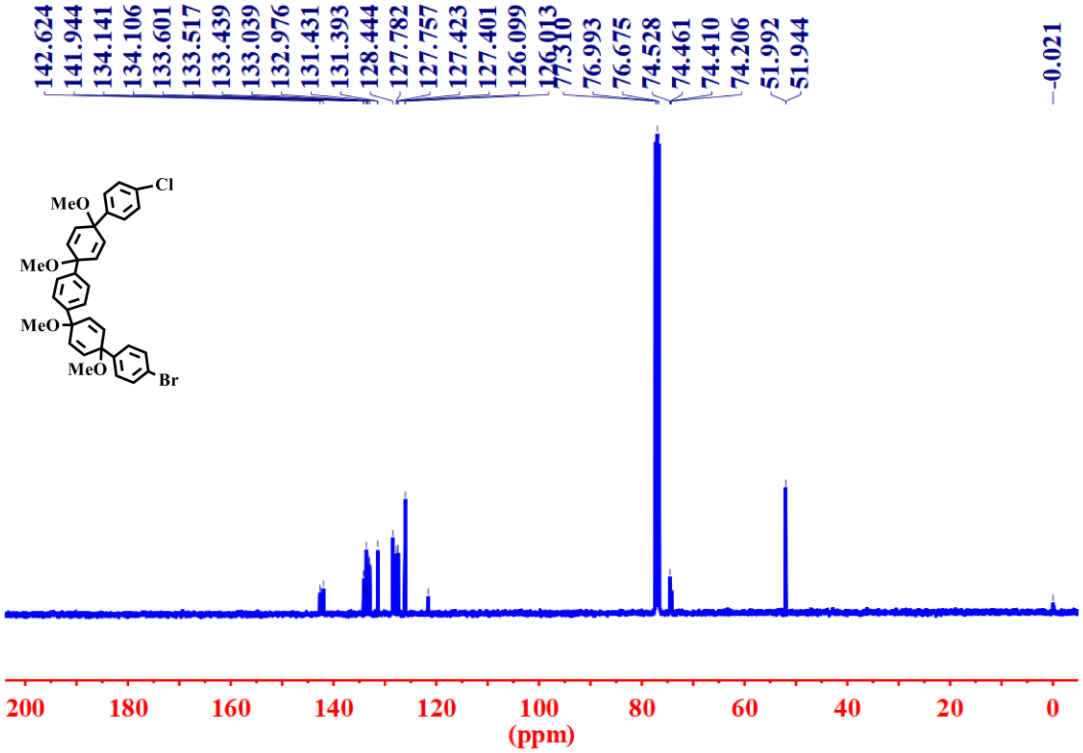

Figure S19. ^{13}C NMR spectrum of **3** in $CDCl_3$.

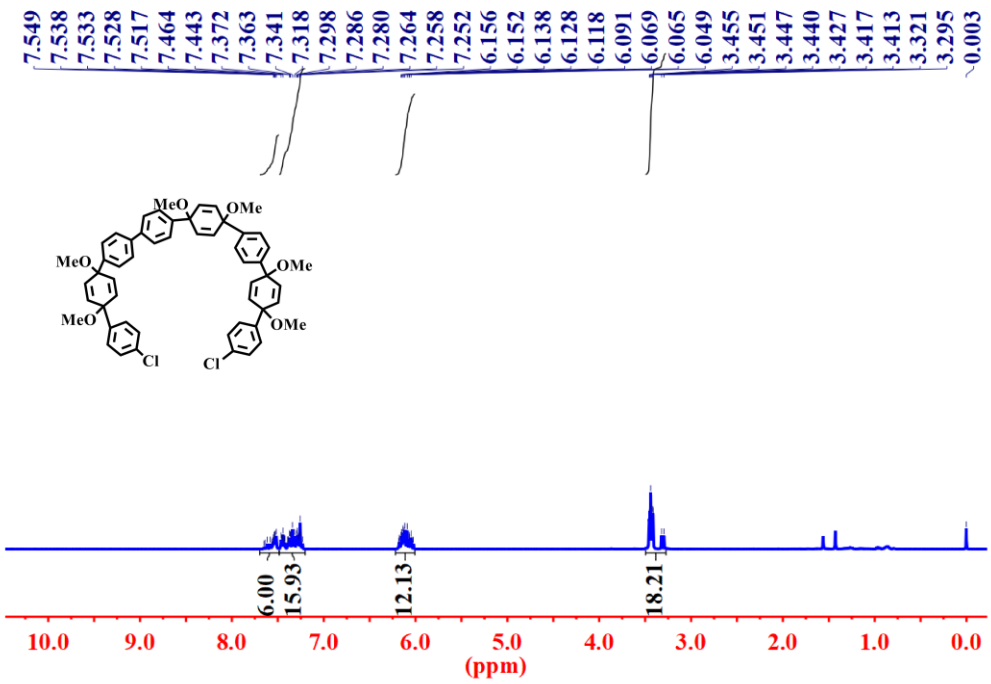

Figure S20. ^{1}H NMR spectrum of **5** in $CDCl_3$.

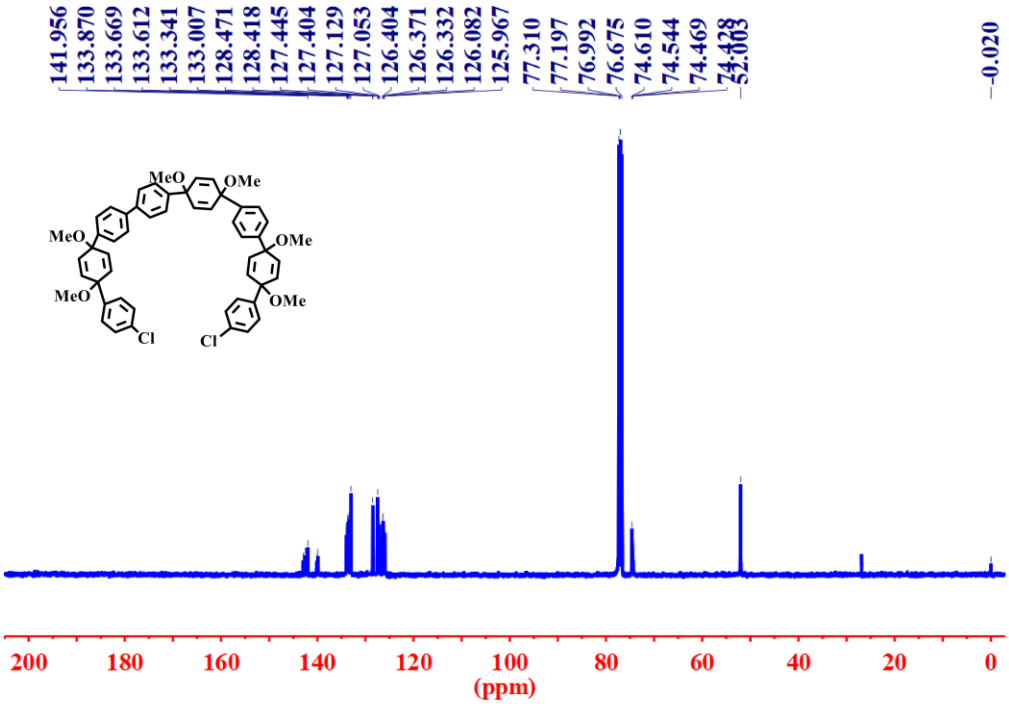

Figure S21. ^{13}C NMR spectrum of **5** in $CDCl_3$.

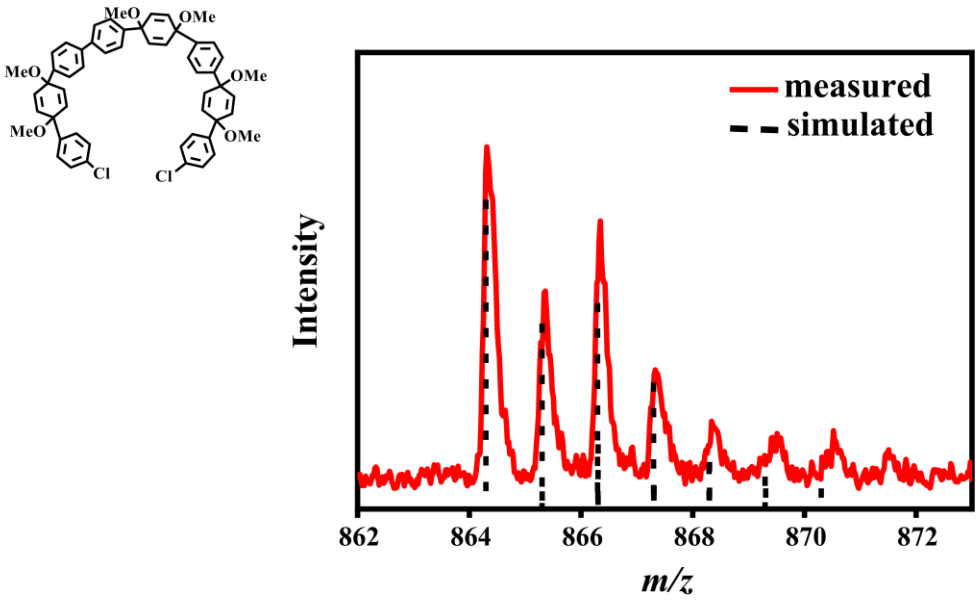

Figure S22. HR-MS (MALDI-TOF) data for **5**.

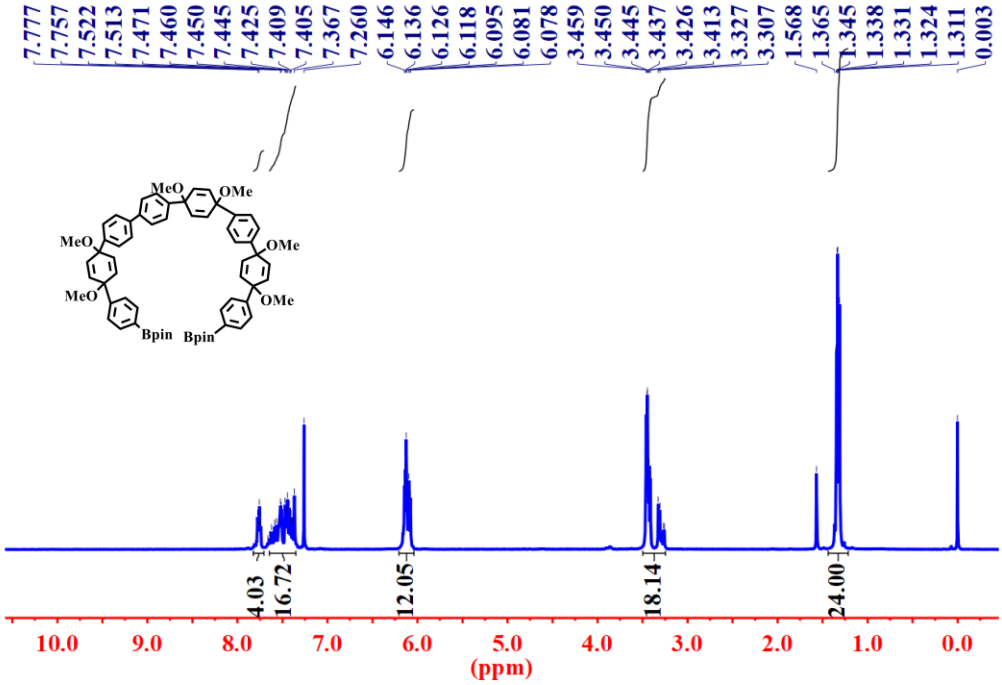

Figure S23. ^{1}H NMR spectrum of **6** in $CDCl_3$.

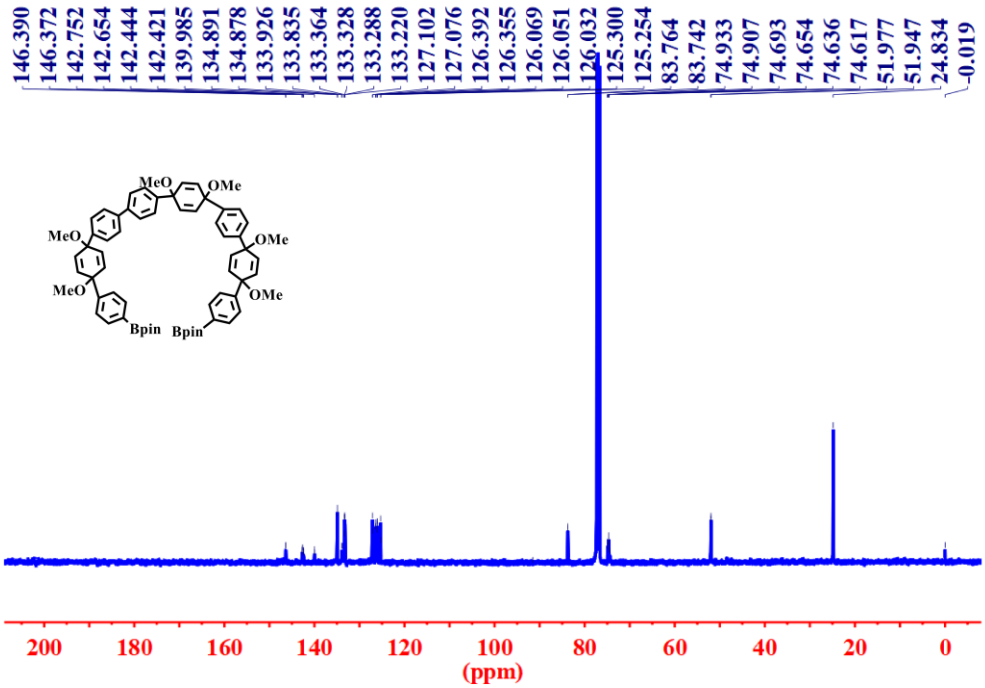

Figure S24. ^{13}C NMR spectrum of **6** in $CDCl_3$.

Table S1. Energy level by B3LYP/Def2-TZVP.

Orbital	10	9
LUMO+3	-1.7685	-1.3504
LUMO+2	-1.9831	-1.5974
LUMO+1	-2.0018	-1.7090
LUMO	-2.3699	-2.0924
HOMO	-5.1573	-5.2610
HOMO-1	-5.5183	-5.6441
HOMO-2	-5.5642	-5.7182
HOMO-3	-5.7306	-6.0272
Gap(HOMO-LUMO)	2.7874	3.1686

Table S2. Corresponding energy of strain energy by the level of B3LYP/Def2-TZVP.

	Energy(a.u.)		Energy(a.u.)
10	-8916.596944	**9**	-8924.807263
10-Fragment	-7993.913073	**9-Fragment**	-7540.146354
Biphenyl	-463.1732438	**Biphenyl**	-463.1732438
Triphenyl	-694.1616537	**Triphenyl**	-694.1616537
strain energy (kcal/mol)	46.02		45.69

Table S3. Oscillator strengths and transitions of the peaks from experiment and DFT calculations with the f_{osc} **> 0.10**.

λ_{Exp} **/nm**	λ_{DFT}**/nm**	f_{osc}	**Transitions**
		10	
490.5	506.7	0.2755	HOMO→LUMO (94%)
460.5	413.0	0.7374	HOMO-2→LUMO (31%) HOMO-3 →LUMO (32%) HOMO →LUMO+1 (28%)
400	399.1	0.1115	HOMO-3 →LUMO (48%) HOMO →LUMO+1 (11%)
370.5	380.8	0.4852	HOMO→LUMO+4 (37%) HOMO-2→LUMO+2 (11%) HOMO-2→LUMO+1 (18%)
	378.2	0.3906	HOMO-2→LUMO+2 (26%) HOMO→LUMO+4 (31%) HOMO-1→LUMO+2 (10%)
	361.3	0.2760	HOMO-1→LUMO+3 (38%) HOMO→LUMO+5 (41%)
		9	
343.5	375.9	1.053	HOMO→LUMO+1(61%) HOMO-1→LUMO(33%)
	368.5	0.8130	HOMO-2→LUMO(94%)
	342.9	0.1764	HOMO→LUMO+3(45%) HOMO-3→LUMO(38%)
	327.2	0.1584	HOMO-3→LUMO(48%) HOMO→LUMO+4(30%)

Table S4. Relaxed geometrical structure of **10**.

10							
C	6.773749	-4.563594	-2.107923	C	-3.880234	-5.774969	-5.661644
C	7.376928	-3.308548	-1.937487	C	-1.764069	-4.884523	-6.462759
C	6.615540	-4.718647	0.308944	C	-3.054161	-4.693936	-5.998388
C	6.490465	-5.291034	-0.946008	C	-2.101605	-7.246810	-6.433783
C	7.034752	-3.391128	0.467911	C	0.248240	-6.319179	-6.664644
C	7.509204	-2.738236	-0.680468	C	-1.223934	-6.167860	-6.606504
C	3.791635	7.771099	0.051548	C	1.079222	-5.391699	-7.308813
C	4.622118	7.311458	-1.165526	C	2.218253	-7.168275	-5.528759
C	2.880282	8.921318	-0.402147	C	0.870805	-7.263036	-5.839261
C	6.444563	-3.358380	2.927640	C	3.012298	-6.130539	-6.033413
C	6.696281	-2.672912	1.719634	C	2.429084	-5.302670	-7.004267
C	5.546265	-0.727702	2.664046	C	5.056650	-6.740698	-4.669863
C	6.330371	-1.334318	1.668230	C	4.286733	-5.791097	-5.357604
C	5.037010	0.630585	2.513435	C	5.552644	-4.063266	-4.211177
C	5.702066	1.701109	1.883840	C	4.625998	-4.445499	-5.167376
C	3.730777	3.110133	1.941103	C	5.980111	-6.358405	-3.708326
C	5.080797	2.902638	1.626675	C	6.183424	-5.007486	-3.391982
C	3.020502	4.329574	1.569582	C	-4.439251	8.330926	1.577802
C	3.676207	5.431306	1.020600	C	4.741609	8.311534	1.141647
C	1.615642	6.596310	0.754355	Br	-7.241345	1.783336	2.419675
C	3.000076	6.581192	0.618497	Br	7.575055	1.640368	1.445823
C	5.628745	-2.806576	3.886361	H	7.693394	-2.743419	-2.805990
C	3.814518	-1.149487	4.378499	H	6.253556	-5.274448	1.163188
C	5.046068	-1.533820	3.712074	H	6.038714	-6.271121	-1.025867
C	3.091916	-0.047275	3.873353	H	7.927196	-1.742544	-0.600678
C	3.734191	0.897435	2.998727	H	5.181345	8.153882	-1.579555
C	1.647611	2.207636	2.898852	H	3.977670	6.912971	-1.951985
C	3.050885	2.088206	2.632592	H	5.341751	6.536123	-0.898931
C	0.921258	3.302592	2.381121	H	2.188974	8.609346	-1.188369
C	1.611844	4.386108	1.745679	H	3.490378	9.732203	-0.804790
C	-0.565013	5.533600	1.380674	H	2.298014	9.330716	0.425832
C	0.898033	5.524319	1.295791	H	6.816233	-4.364989	3.069423
C	-1.326607	6.609455	0.911929	H	6.515708	-0.779882	0.762130
C	-2.681836	8.958716	-0.074103	H	5.656591	3.678907	1.148341
C	1.875757	-1.768919	5.700761	H	4.750044	5.398497	0.910261
C	3.196713	-1.942083	5.365078	H	1.075748	7.469838	0.429762
C	1.076835	-0.794171	5.071090	H	5.356007	-3.410879	4.740635
C	1.722229	0.123083	4.210613	H	-0.817349	7.468775	0.508990
C	-0.427556	1.209352	3.713406	H	-3.321232	9.772807	-0.420675
C	0.979662	1.194031	3.618695	H	-2.049723	8.659983	-0.913526
C	-1.164253	2.236246	3.085029	H	-2.039914	9.358342	0.714083

C	-0.490359	3.316127	2.472890	H	1.437754	-2.442356	6.424227
C	-2.656679	4.375499	1.920906	H	3.747945	-2.744528	5.835509
C	-1.236321	4.409882	1.923386	H	-4.436658	5.461711	1.450202
C	-3.356988	5.479684	1.435211	H	-3.851775	6.945071	-1.559512
C	-2.717462	6.613054	0.937672	H	-5.045509	8.170770	-1.111462
C	-4.452512	7.333902	-0.734549	H	-5.145126	6.548214	-0.428018
C	-3.553921	7.799630	0.431042	H	-0.581676	-2.403969	6.580511
C	-1.098269	-1.723456	5.918184	H	-5.337080	3.777731	1.855559
C	-0.370254	-0.774372	5.174037	H	-2.957777	-2.646726	6.323123
C	-2.513175	0.018972	4.261340	H	-6.392471	-4.225161	4.001362
C	-1.106414	0.156765	4.406094	H	-4.712395	-3.282541	5.464773
C	-3.246545	0.972286	3.471814	H	-6.332690	-0.666468	1.637620
C	-2.592645	2.144787	3.005819	H	-5.940125	-5.110225	2.007735
C	-4.719807	2.993163	2.262933	H	-8.123996	-2.692918	-1.681313
C	-3.336262	3.174535	2.396355	H	-8.030602	-1.675149	0.522007
C	-2.457273	-1.862511	5.772167	H	-6.019413	-6.112517	-0.177641
C	-4.504113	-1.422287	4.381450	H	-6.722664	-2.945007	-3.391589
C	-3.185755	-1.061214	4.872016	H	-5.086232	-7.547216	-3.966490
C	-5.121225	-0.615290	3.398087	H	-6.479204	-7.013848	-2.067399
C	-4.607493	0.729702	3.165379	H	-5.430430	-3.505360	-5.353936
C	-5.326770	1.808318	2.614189	H	-4.025156	-7.922487	-5.819102
C	-6.023475	-3.226585	3.805336	H	-1.126265	-4.019634	-6.593311
C	-5.082717	-2.681624	4.645709	H	-3.374218	-3.683634	-5.783116
C	-6.415281	-2.546426	2.632228	H	-1.750051	-8.256599	-6.608574
C	-6.039477	-1.214941	2.518824	H	0.652380	-4.693366	-8.018971
C	-6.458678	-4.580761	1.219554	H	2.624717	-7.839513	-4.782930
C	-6.912172	-3.274245	1.441494	H	0.269150	-8.004675	-5.329221
C	-7.639154	-3.234755	-0.878751	H	3.025455	-4.538790	-7.487855
C	-7.588374	-2.653752	0.380167	H	4.890600	-7.796566	-4.845985
C	-6.505062	-5.156760	-0.037237	H	5.687704	-3.008019	-4.011040
C	-6.638972	-4.908175	-2.506377	H	4.067632	-3.674510	-5.681769
C	-7.013009	-4.463172	-1.143301	H	6.510329	-7.124145	-3.155041
C	-6.401040	-3.970140	-3.520885	H	-5.114248	7.563645	1.959435
C	-5.466052	-6.538166	-3.875574	H	-5.051280	9.166666	1.229291
C	-6.245359	-6.227171	-2.773171	H	-3.829088	8.682951	2.412353
C	-5.055374	-5.552466	-4.785080	H	5.321205	9.154536	0.756933
C	-5.640035	-4.286705	-4.635032	H	5.445609	7.549120	1.478084
C	-3.398709	-7.054279	-5.980688	H	4.180568	8.655564	2.013147

Table S5. Relaxed geometrical structure of **9**.

				9			
C	6.129111	-5.639472	-2.331568	C	1.878413	-8.746867	-5.671812
C	6.768006	-4.394062	-2.266985	C	0.538179	-8.895088	-5.989400
C	5.798406	-5.498324	0.068939	C	2.660559	-7.743027	-6.257603
C	5.724563	-6.207219	-1.117525	C	2.082022	-7.032096	-7.320167
C	6.292094	-4.187108	0.112306	C	4.639717	-8.138504	-4.732734
C	6.855318	-3.690665	-1.073929	C	3.895937	-7.295390	-5.572144
C	3.761659	8.440637	-0.029063	C	5.052042	-5.413024	-4.559204
C	4.962317	7.932489	-0.854907	C	4.198465	-5.928332	-5.521982
C	2.773082	9.168302	-0.964349	C	5.484583	-7.622614	-3.761951
C	5.621666	-3.865532	2.523073	C	5.637459	-6.239352	-3.593033
C	6.003847	-3.328020	1.285966	C	-4.733013	8.609207	1.300330
C	5.256780	-1.164685	2.115740	C	4.285053	9.455278	0.998478
C	5.878427	-1.938070	1.149624	Br	-7.074605	3.743076	4.405234
C	5.228550	3.304558	4.389645	Br	7.895389	3.554053	3.374020
C	6.004845	3.299680	3.239663	H	7.162103	-3.946569	-3.171747
C	4.049338	2.942138	1.901684	H	5.357601	-5.938335	0.952659
C	5.425156	3.118089	1.992027	H	5.232263	-7.171112	-1.118492
C	2.219610	6.051299	2.580256	H	7.325034	-2.715620	-1.082556
C	2.873567	7.141297	2.012940	H	5.468323	8.770501	-1.340875
C	2.537836	6.212129	-0.151813	H	4.653144	7.233003	-1.633358
C	3.051640	7.250644	0.633613	H	5.687210	7.422819	-0.216574
C	4.974694	-3.098017	3.477630	H	2.401403	8.510529	-1.751720
C	3.683630	-1.033405	4.085709	H	3.260853	10.020872	-1.443680
C	4.695315	-1.740273	3.265143	H	1.910838	9.540140	-0.407002
C	2.989887	0.053214	3.560142	H	5.766102	-4.919084	2.723599
C	3.855671	3.122455	4.280556	H	5.152048	-0.103599	1.933672
C	1.751349	2.795779	2.965713	H	6.193286	-1.455786	0.233623
C	3.241031	2.937516	3.039971	H	5.685876	3.449643	5.358659
C	1.013218	3.848433	2.407291	H	3.602427	2.805366	0.925834
C	1.713728	5.022260	1.792040	H	6.035606	3.118267	1.099450
C	-1.538959	6.080214	2.858167	H	2.107019	6.005215	3.656968
C	1.883045	5.126566	0.410524	H	3.246440	7.910615	2.674260
C	-2.244850	7.176989	2.387135	H	2.645584	6.245309	-1.229195
C	-2.565603	9.809506	0.855801	H	4.606784	-3.593134	4.366181
C	2.017383	-1.131569	5.838978	H	3.320375	0.478506	2.628085
C	3.229475	-1.534254	5.322509	H	3.252080	3.125477	5.179841
C	1.215869	-0.178746	5.180816	H	-1.285550	6.024059	3.909858
C	1.801438	0.543090	4.116316	H	1.500820	4.344999	-0.235345
C	-0.333168	1.716041	3.675325	H	-2.522583	7.949138	3.093727
C	1.079726	1.697608	3.557959	H	-3.108387	10.695448	0.516350
C	-1.061212	2.828385	3.183982	H	-1.602700	9.784020	0.342225

C	-0.392934	3.862414	2.513024	H	-2.372419	9.927518	1.922981
C	-1.499890	5.166164	0.658308	H	1.643503	-1.630680	6.722517
C	-1.153336	5.048191	2.000796	H	3.787406	-2.303267	5.840195
C	-2.209793	6.267909	0.188599	H	-1.217572	4.385271	-0.037949
C	-2.600920	7.302295	1.039120	H	-2.453552	6.306314	-0.863870
C	-3.667200	8.490959	-0.951159	H	-2.747091	8.461335	-1.537787
C	-3.382389	8.534054	0.557697	H	-4.217458	9.386909	-1.246036
C	-0.937072	-1.049480	6.139963	H	-4.276209	7.626880	-1.225645
C	-0.234811	-0.145437	5.320052	H	-0.425065	-1.547408	6.952374
C	-2.268797	0.139586	4.052683	H	-2.749706	0.561231	3.186620
C	-0.980462	0.589949	4.369370	H	-2.241563	3.229603	5.581941
C	-2.960160	3.227290	4.771506	H	-5.547492	3.220392	1.911896
C	-2.522460	3.004940	3.463963	H	-3.167578	2.838744	1.421214
C	-4.822615	3.220415	2.714379	H	-2.723936	-2.137479	6.501122
C	-3.476123	3.007225	2.444554	H	-4.723994	0.039781	2.874867
C	-2.239509	-1.405399	5.868633	H	-4.620916	3.620866	6.077737
C	-4.061576	-1.593402	4.120711	H	-5.279588	-4.753873	3.835381
C	-2.893450	-0.908760	4.723323	H	-3.806034	-3.434401	5.216303
C	-4.817858	-1.015956	3.090181	H	-6.104637	-1.309620	1.422768
C	-4.301581	3.446453	5.059476	H	-5.028214	-5.706541	1.931518
C	-5.225197	3.440883	4.024088	H	-7.945092	-3.883304	-1.591048
C	-5.153453	-3.704777	3.600128	H	-7.643300	-2.637543	0.474961
C	-4.324230	-2.941517	4.404840	H	-5.334995	-6.943723	-0.111322
C	-5.751027	-3.169598	2.450942	H	-6.684976	-4.258548	-3.483017
C	-5.629857	-1.784630	2.271637	H	-5.097884	-8.908826	-3.735544
C	-5.706293	-5.309107	1.188261	H	-6.205524	-8.136943	-1.727532
C	-6.263532	-4.036188	1.364890	H	-5.672872	-5.059328	-5.532741
C	-7.303499	-4.295481	-0.821571	H	-4.310548	-9.507073	-5.682036
C	-7.129334	-3.583558	0.357741	H	-1.458289	-5.742937	-7.071744
C	-5.882241	-6.019857	0.015707	H	-3.644308	-5.297377	-6.151687
C	-6.448971	-6.102294	-2.394955	H	-2.096976	-9.950366	-6.586434
C	-6.623710	-5.500015	-1.053379	H	0.311864	-6.555261	-8.413334
C	-6.372954	-5.293742	-3.537377	H	2.282545	-9.333668	-4.857294
C	-5.472699	-7.894225	-3.711336	H	-0.058110	-9.591854	-5.414164
C	-6.086941	-7.446986	-2.553443	H	2.672734	-6.308555	-7.868682
C	-5.204692	-7.026088	-4.780052	H	4.508202	-9.211919	-4.795076
C	-5.775547	-5.747390	-4.703422	H	5.157232	-4.338456	-4.475914
C	-3.692954	-8.669175	-5.979850	H	3.660695	-5.237324	-6.158028
C	-4.138457	-7.356941	-5.755803	H	5.989127	-8.303032	-3.086345
C	-2.088695	-6.582006	-6.806944	H	-5.337553	7.721692	1.101782
C	-3.342871	-6.328400	-6.278507	H	-5.298644	9.485225	0.971420
C	-2.432071	-8.923606	-6.499100	H	-4.597885	8.686107	2.380173
C	-0.089186	-8.040644	-6.904138	H	4.789830	10.273715	0.480880
C	-1.559612	-7.877969	-6.833048	H	5.005972	9.004153	1.683984

C	0.738319	-7.174013	-7.632764	H	3.476427	9.889481	1.589544

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