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Supporting Information

Multifunctionalized Octamethoxy-[8]Cycloparaphenylene: Facile Synthesis, Analysis of Novel Photophysical and Photoinduced Electron Transfer Properties

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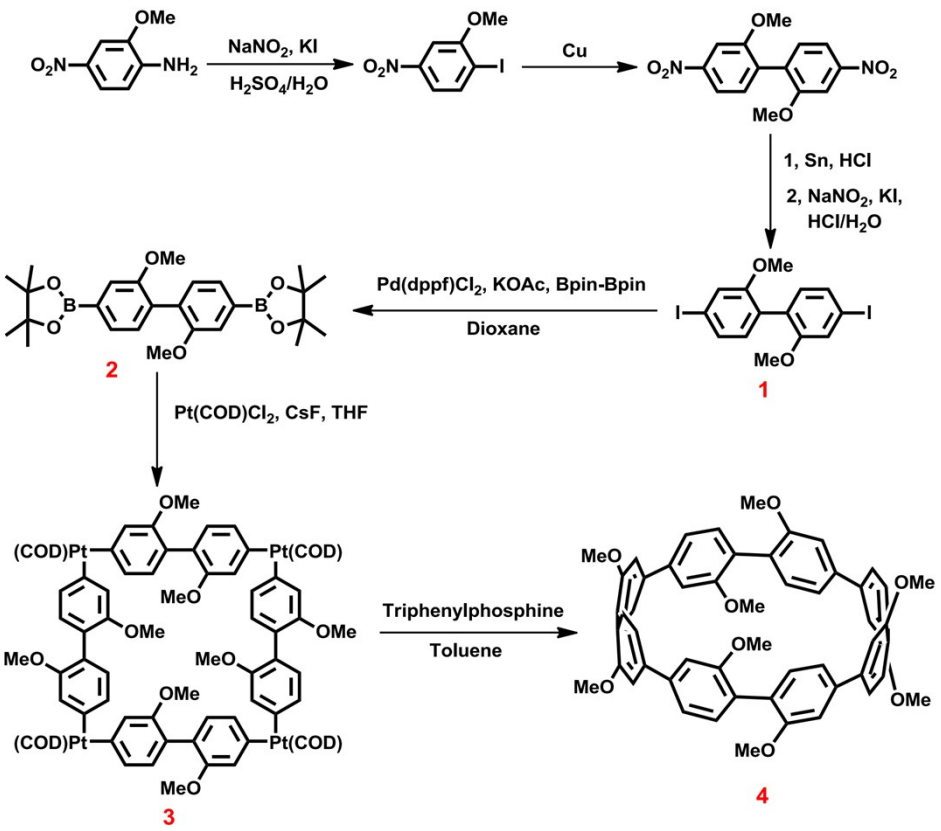
Materials and General Information

NMR spectra were recorded on Bruker BioSpin (^{1}H 400 MHz, ^{13}C 100 MHz) spectrometer, and chemical shifts were reported as the delta scale in ppm relative to CDC_{l3} (δ = 7.26 ppm) for ^{1}H NMR and $CDCl_3$ (δ = 77.0 ppm) for ^{13}C NMR. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet, br = broad signal), coupling constant (Hz), and integration. High resolution mass spectrometry (HR-MS) analyses were carried out using MALDI-TOF-MS techniques and *trans*-2-[3-(4-tert-Butylphenyl)-2-methyl-2-propenylidene]malononitrile as the matrix. Flash chromatography was performed on silica gel (200~300 mesh). Preparative thin-layer chromatography (PTLC) experiments were performed using silica gel GF 254 coated plates. UV-vis absorption spectra were performed on a UNIC-3802 spectrophotometer. All solvents for syntheses were dried by distillation under nitrogen prior to use. Tetrahydrofuran (THF), dioxane, and toluene were distilled after reflux with sodium under nitrogen. Other chemicals were obtained from commercial suppliers (Innochem or Acros) and used without further purification. Air-sensitive reactions were all carried out under nitrogen or argon atmosphere.

Synthetic procedures



Synthesis of 2-iodo-5-nitroanisole[S1]

2-methoxy-4-nitroaniline (15 g, 89.2 mmol) was dissolved in aqueous sulfuric acid (H_2SO_4/H_2O, 20 mL/75 mL) by heating, before cooling to 0-5 °C in an ice-water bath. To this suspension, a solution of sodium nitrite (6.46 g, 93.66 mmol) in water (20 mL) was added dropwise while maintaining the temperature below 10 °C before allowing to stir for another 30 minutes. The cold solution was then slowly added into a solution of potassium iodide (25.2 g, 152 mmol) in water (60 mL) with vigorous stirring, and left to warm to room temperature for another 5 hours. The crude solid was collected by filtration, washed with water several times, dried in air, and finally recrystallization from ethanol to afford of 2-iodo-5-nitroanisole as brown solid (20 g, 80 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97 (d, J = 8.3 Hz, 1H), 7.66-7.56 (m, 2H), 4.00 (s, 3H).

Synthesis of 2,2'-dimethoxy-4,4'-dinitro-1,1'-biphenyl [S1]

Copper (8 g, 157.5 mmol) and 2-iodo-5-nitroanisole (10 g, 35.9 mmol) were stirred at 200-205 °C under nitrogen atmosphere. The reaction is immediate with white smoke. The mixture was kept stirring overnight at 200 °C before cooling to room temperature. The resulting solid is extracted with plenty of hot chloroform. The resulting solution was concentrated with rotary evaporator. The crude product was purified by column chromatography (silica gel, PE/CH_2Cl_2 = 3/1) to afford 2,2'-dimethoxy-4,4'-dinitro-1,1'-biphenyl (2.0 g, 37%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.93 (d, J = 8.5 Hz, 2H), 7.84 (s, 2H), 7.38 (d, J = 8.2 Hz, 2H), 3.88 (s, 6H).

Synthesis of 4,4'-diiodo-2,2'-dimethoxy-1,1'-biphenyl (1) [S1]

Hydrochloric acid (25 mL, 37%), ethanol (12 mL) and 2,2'-dimethoxy-4,4'-dinitro-1,1'-biphenyl (2.0 g, 6.6 mmol) were stirred and heated to 90 °C. Tin powder (3.9 g, 33 mmol) was added to the mixture in three portions over 2 hours and then allowed to stir for a further 2 h at the same temperature before cooling. A solution of sodium hydroxide (15.0 g, 375 mmol) in water (30 mL) was then slowly added; initial clearing was soon followed by precipitation. This crude solid was collected by filtration, washed with water and dried in air for the next step without further purification.

To a 50-mL flask containing a magnetic stirring bar was added the above crude product, hydrochloric acid (10 mL, 37%) and water (20 mL). The mixture was heated into solution for 20 mins before cooling to 0-5 °C in an ice-water bath. A solution of sodium nitrite (1.05 g, 15 mmol) in water (5 mL) was then added dropwise while maintaining a temperature below 10 °C. After stirring for an additional 20 mins, the cold solution

was slowly added into a rapidly stirring solution of potassium iodide (4.5 g, 27.1 mmol) in water (20 mL) and then allowed to warm to room temperature overnight. The crude solid was collected by filtration, washed with water and dried in air. Purification by column chromatography (silica gel, PE/CH_2Cl_2 = 6/1) afford 4,4'-diiodo-2,2'-dimethoxy-1,1'-biphenyl as white solid (1.08 g, ~35 % over two steps). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.33 (d, *J* = 7.9 Hz, 2H), 7.25 (s, 2H), 6.90 (d, *J* = 7.9 Hz, 2H), 3.74 (s, 6H).

Synthesis of 4,4'-diboryl-2,2'-dimethoxy-1,1'-biphenyl (2)

A 50-mL flask containing 4,4'-diiodo-2,2'-dimethoxy-1,1'-biphenyl **1** (1.0 g, 2.1 mmol), bis(pinacolato)diboron (1.42 g, 5.6 mmol), KOAc (2.06 g, 21 mmol) and Pd(dppf)Cl_2 (73.2 mg, 0.1 mmol) was evacuated and refilled with argon for 3 cycles, and then anhydrous dioxane (30 mL) was transferred to the flask *via* syringe under argon at room temperature. The mixture was then stirred at 85 °C for 24 h. The crude product was purified by column chromatography (silica gel, PE/CH_2Cl_2 = 4/1) and recrystallization from CH_2Cl_2/MeOH to afford **2** as white solid (0.8 g, 80 %). Mp: 229-231 °C. IR (KBr): 2976, 2933, 1605, 1495, 1464, 1448, 1392, 1354, 1317, 1233, 1143, 1098, 1036, 1002, 966, 892, 852, 828, 771 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.47 (d, *J* = 7.3 Hz, 2H), 7.39 (s, 2H), 7.24 (d, *J* = 7.3 Hz, 2H), 3.80 (s, 6H), 1.35 (s, 24H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 24.90, 55.82, 83.80, 116.71, 127.08, 130.83, 131.02, 156.52. HR-MS (ESI) *m/z* calcd. for $C_{26}H_{37}B_2O_6$ $[M+H]^+$: 467.2771, Found 467.2756.

Synthesis of Octamethoxy-[8]CPP

To a degassed suspension of 4,4'-diboryl-2,2'-dimethoxy-1,1'-biphenyl **2** (100 mg,

0.215 mmol) and CsF (196.0 mg, 1.29 mmol) in anhydrous THF (30 mL) was added $Pt(COD)Cl_2$ (80.4 mg, 0.215 mmol), then the mixture was degassed for 10 min. The mixture was then heated at 50 °C for 48 h under argon atmosphere. After the reaction mixture was cooled to room temperature, removed the solvents under reduced pressure. The residue was recrystallization from MeOH to afford crude product **6** as a gray solid for the next step without further purification.

To a 50-mL flask containing a magnetic stirring bar was added the above crude product **6,** triphenylphosphine (564.0 mg, 2.15 mmol) and dry toluene (10 mL), then the mixture was degassed for 20 min. The mixture was then heated at 100 °C for 48 h under argon atmosphere. After the reaction mixture was cooled to room temperature, it was passed through a short silica gel column with CH_2Cl_2 as the eluent. The solvents were removed under reduced pressure. The residue was purified initially by silica gel column chromatography and then by preparative thin-layer chromatography (hexane/CH_2Cl_2 = 1/2) to afford the final product **4** as a pale yellow solid (~9 mg, ~10 % over two steps). Mp: 228-230 °C dec. IR (KBr): 2972, 2924, 2853, 1658, 1633, 1384, 1262, 1090, 1049, 880, 804 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ 7.34 (d, J = 8.1 Hz, 8H), 7.21 (s, 8H), 6.81 (d, J = 8.4 Hz, 8H), 3.96 (s, 24H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 56.44, 110.38, 122.45, 126.41, 131.93, 141.49, 157.23. HR-MS (MALDI-TOF-MS) *m/z* calcd. for $C_{56}H_{48}O_8$ $[M]^+$: 848.3349, Found 848.3373. UV-vis: λ_{max}: 341 nm.

Electrochemistry Details

Cyclic voltammetry (CV) and differential pulse voltammetry (DPV) were recorded using an electrochemical work station (CHI760E, Shanghai Chen Hua Instrument Co.,

Ltd.) through a standard three-electrode system using a glassy carbon working electrode, an $Ag/AgNO_3$ reference electrode, and a platinum wire counter electrode. The measurements were carried out in tetrabutylammonium hexafluorophosphate (Bu_4NPF_6, 0.1 mol L^{-1}) as a supporting electrolyte. And all the potentials in this study were referenced to the ferrocene/ferrocenium couple (Fc/Fc^+).

Computational Details

All density functional theory calculations were performed in the theoretical level of B3LYP/6-31G(d, p) using the ab-intio computational program of Gaussian 09.[S2] The initial structures were fully relaxed and validated by using frequency analysis. Polarizable continuum model (PCM) method was used to treat solvent effect.[S3] Time-dependent DFT calculation were used to identify the first excited state structures.

Reference.

S1. Reid, L. M.; Wu, G.; Crudden, C. M. *New J. Chem.* **2016**, *40*, 6487-6497.
S2. Gaussian 09, Revision A.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.
S3. Mennucci, B.; Tomasi, J.; Cammi, R.; Cheeseman, J. R.; Frisch,M. J.; Devlin, F. J.; Gabriel, S.; Stephens, P. J. *J. Phys. Chem. A*, **2002**, *106*, 6102-6113.

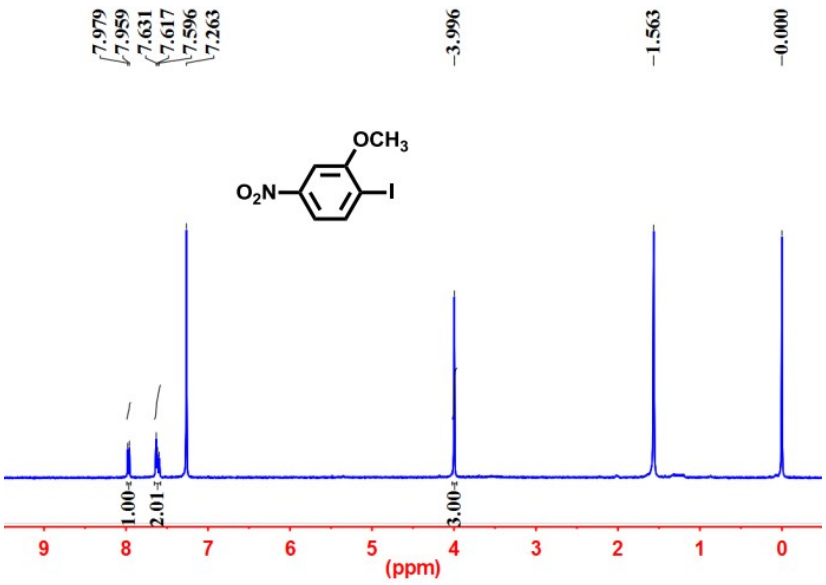


Figure S1. ^{1}H NMR spectrum of 2-iodo-5-nitroanisole in $CDCl_3$

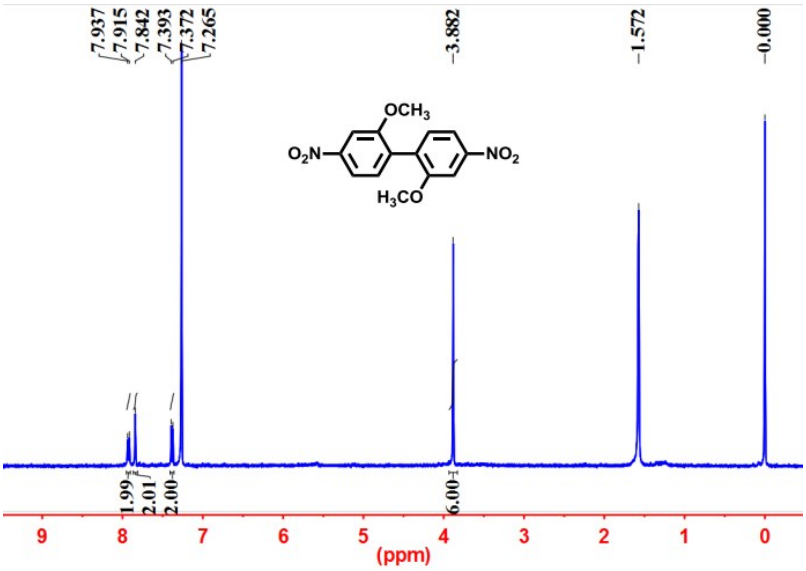


Figure S2. ^{1}H NMR spectrum of 2,2'-dimethoxy-4,4'-dinitro-1,1'-biphenyl in $CDCl_3$

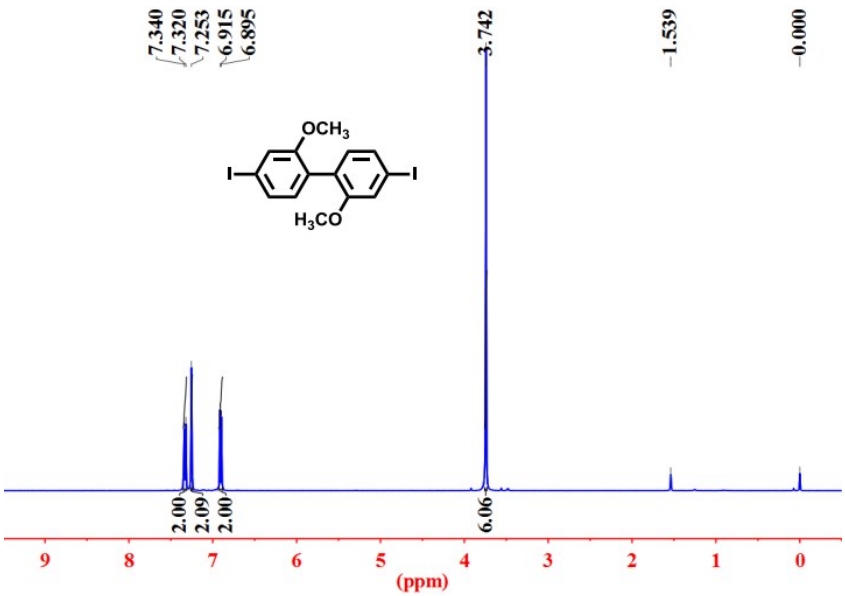


Figure S3. ^{1}H NMR spectrum of compound **1** in $CDCl_3$

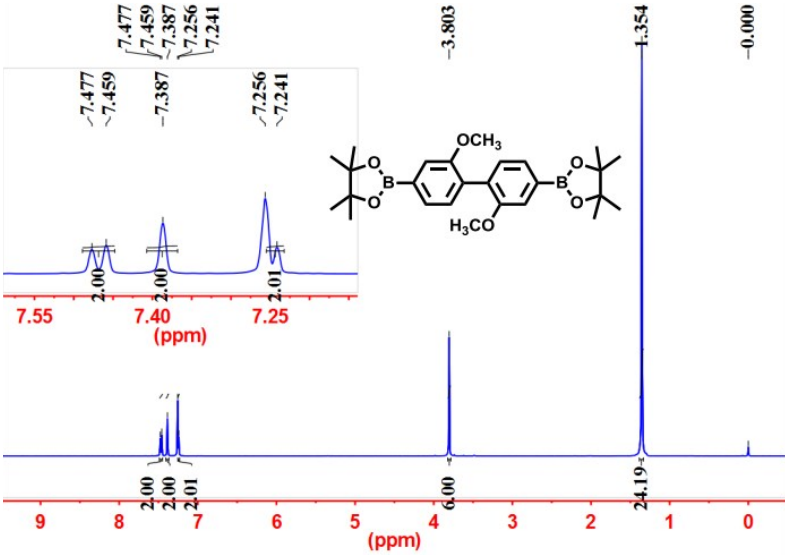


Figure S4. ^{1}H NMR spectrum of compound **2** in $CDCl_3$

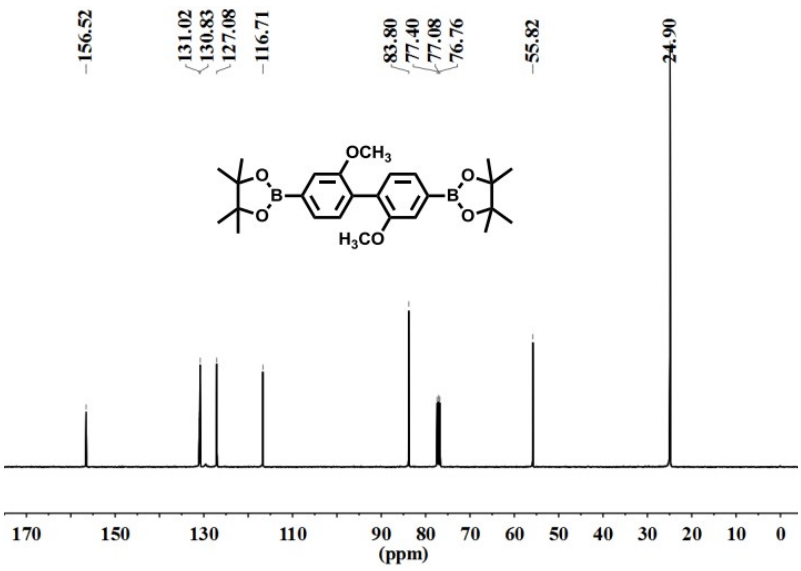


Figure S5. ^{13}C NMR spectrum of compound **2** in $CDCl_3$

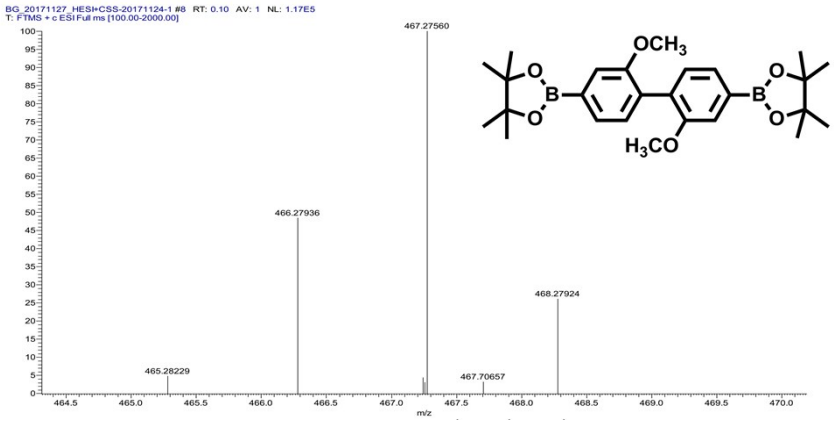


Figure S6. ESI-MS spectrum for compound **2.**

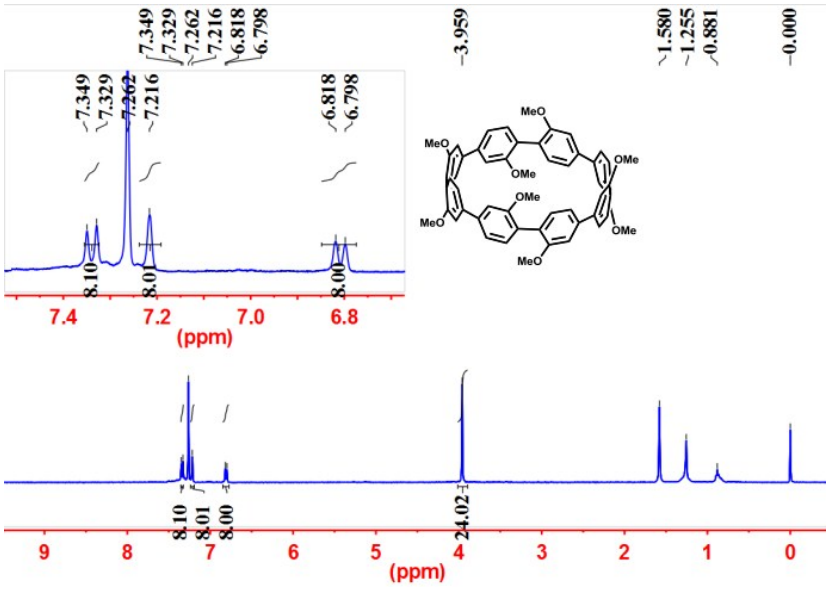


Figure S7. ^{1}H NMR spectrum of compound **4** in $CDCl_3$.

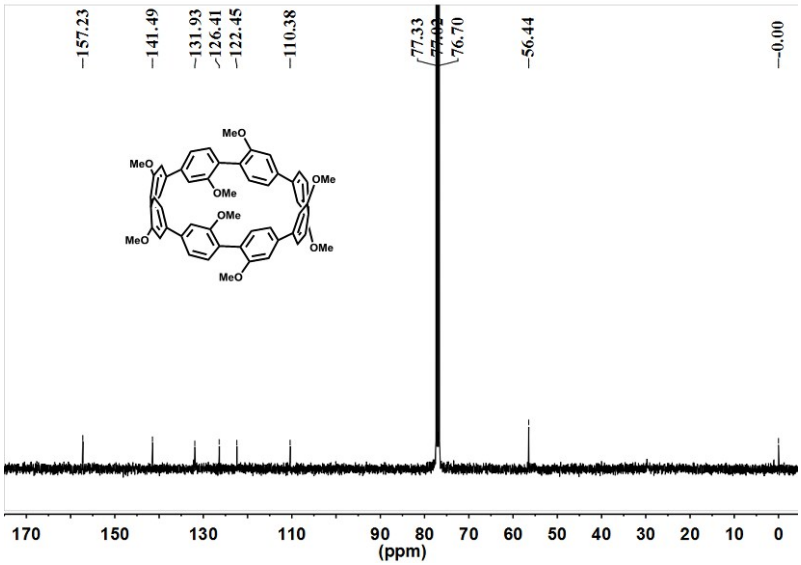


Figure S8. ^{13}C NMR spectrum of compound **4** in $CDCl_3$.

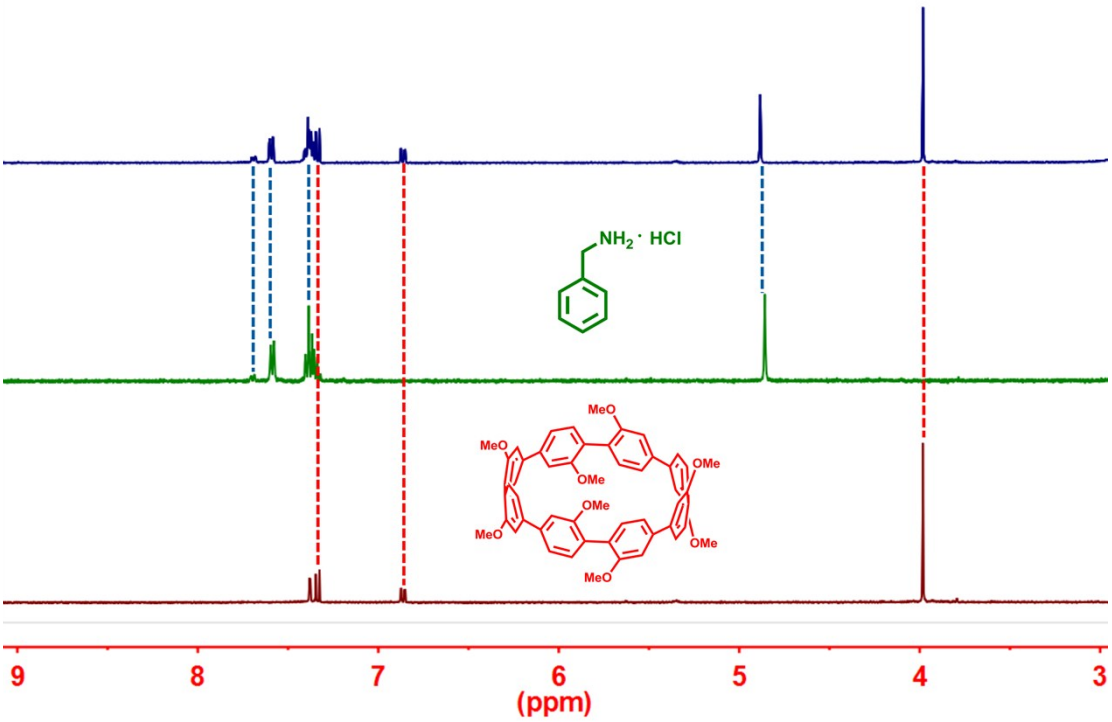


Figure S9. The ^{1}H NMR spectrum of (bottom) octamethoxy-[8]CPP **4**, (middle) benzylamine hydrochloride, (top) the mixture of **4** and benzylamine hydrochloride in acetone-d_6.

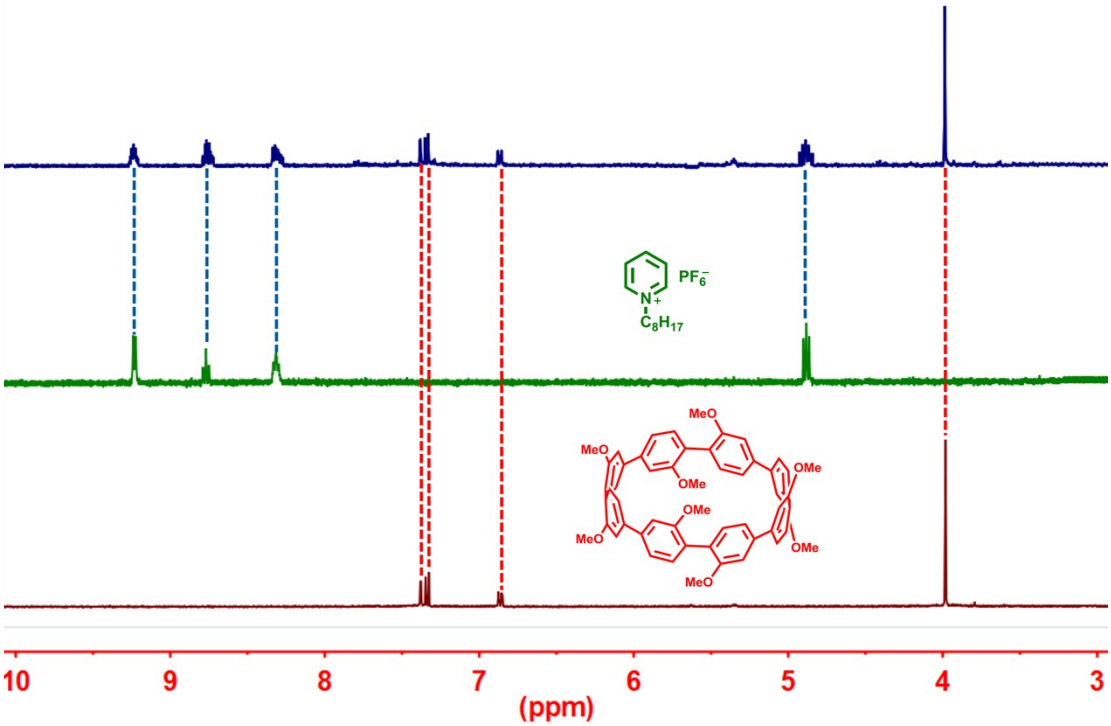


Figure S10. The ^{1}H NMR spectrum of (bottom) octamethoxy-[8]CPP **4**, (middle) 1-N-octylpyridinium hexafluorophosphate, (top) the mixture of **4** and 1-N-octylpyridinium hexafluorophosphate in acetone-d_6.

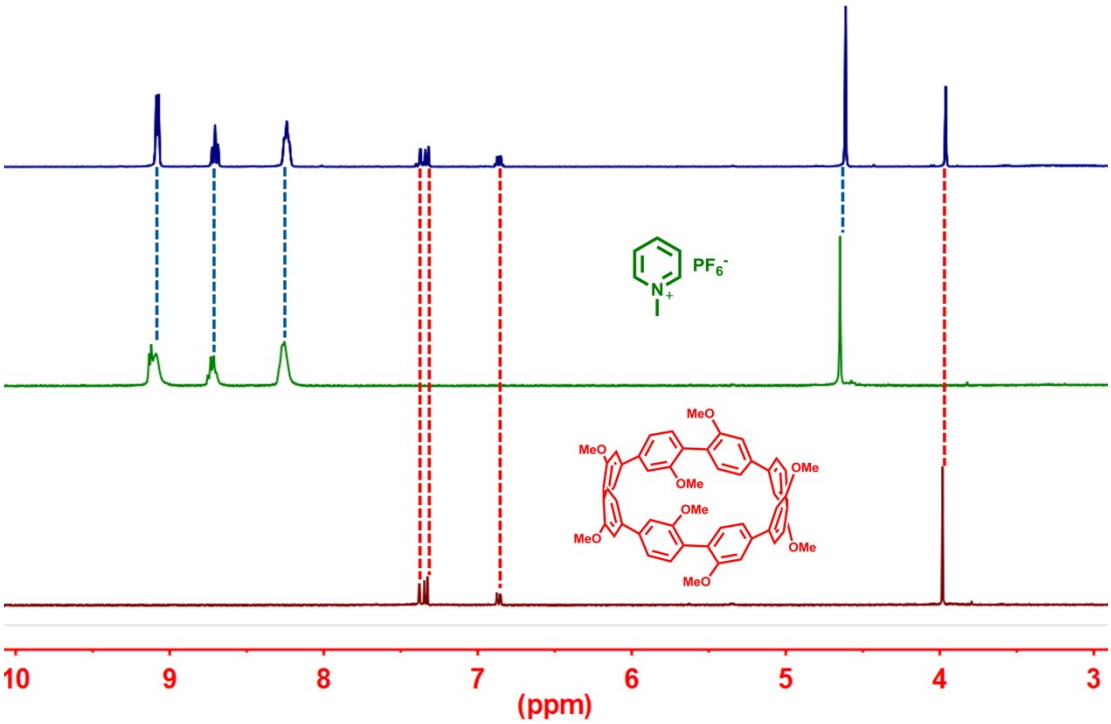


Figure S11. The ^{1}H NMR spectrum of (bottom) octamethoxy-[8]CPP **4**, (middle) 1-methylpyridinium hexafluorophosphate, (top) the mixture of **4** and 1-methylpyridinium hexafluorophosphate in acetone-d_6.

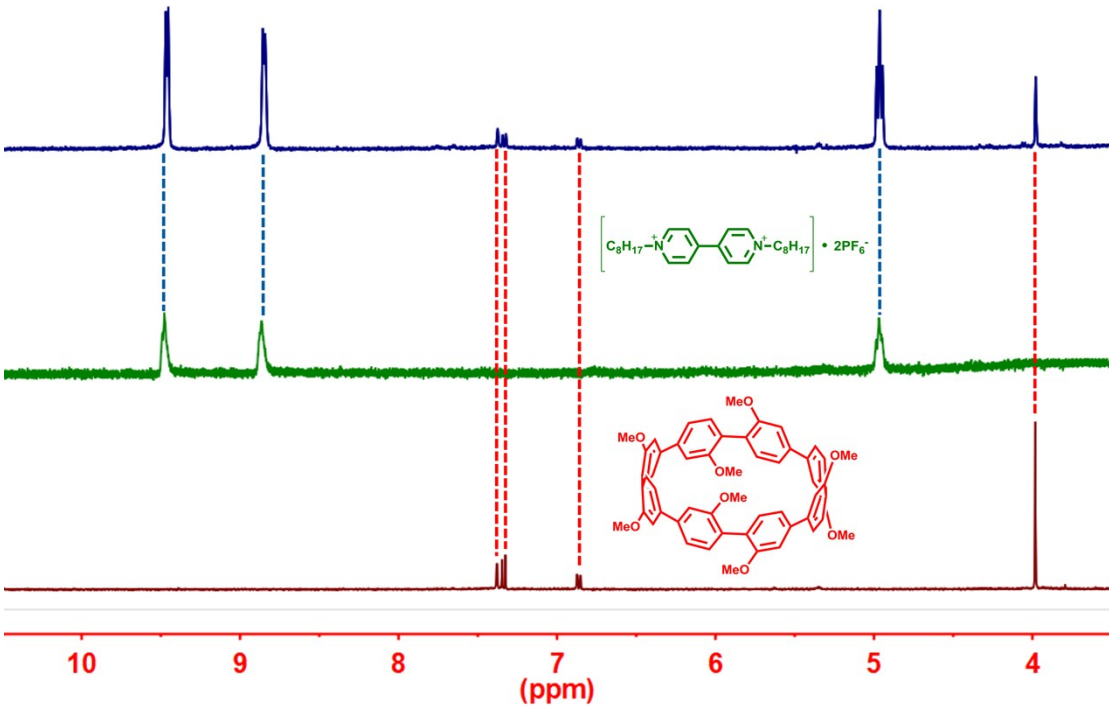


Figure S12. The ^{1}H NMR spectrum of (bottom) octamethoxy-[8]CPP **4**, (middle) *N,N′*-dioctyl-4,4'-bipyridinium bishexafluorophosphate salt, (top) the mixture of **4** and *N,N′*-dioctyl-4,4'-bipyridinium bishexafluorophosphate salt in acetone-d_6.

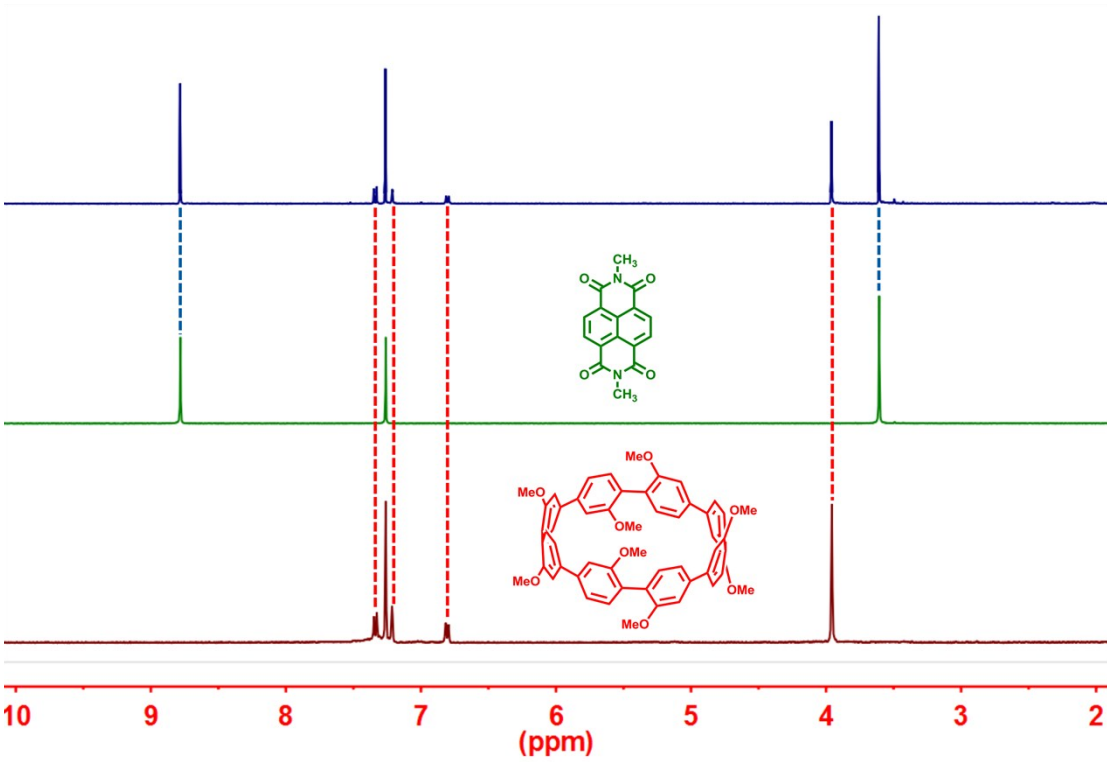


Figure S13. The ^{1}H NMR spectrum of (bottom) octamethoxy-[8]CPP **4**, (middle) *N*, *N*'-dimethyl-1,4,5,8-naphthalenetetracarboxylic diimide, (top) the mixture of **4** and *N*, *N*'-dimethyl-1,4,5,8-naphthalenetetracarboxylic diimide in $CDCl_3$.

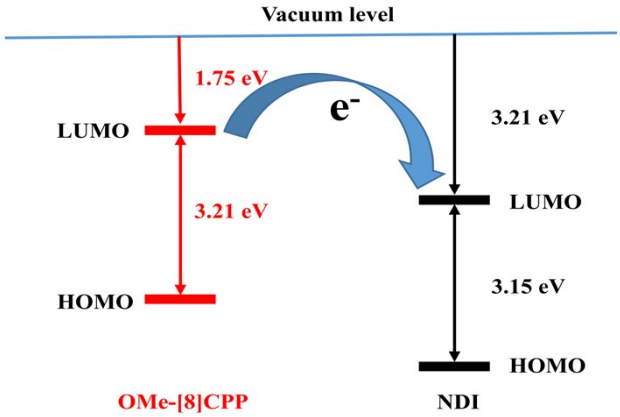


Figure S14. HOMO and LUMO levels of OMe-[8]CPP and NDI.

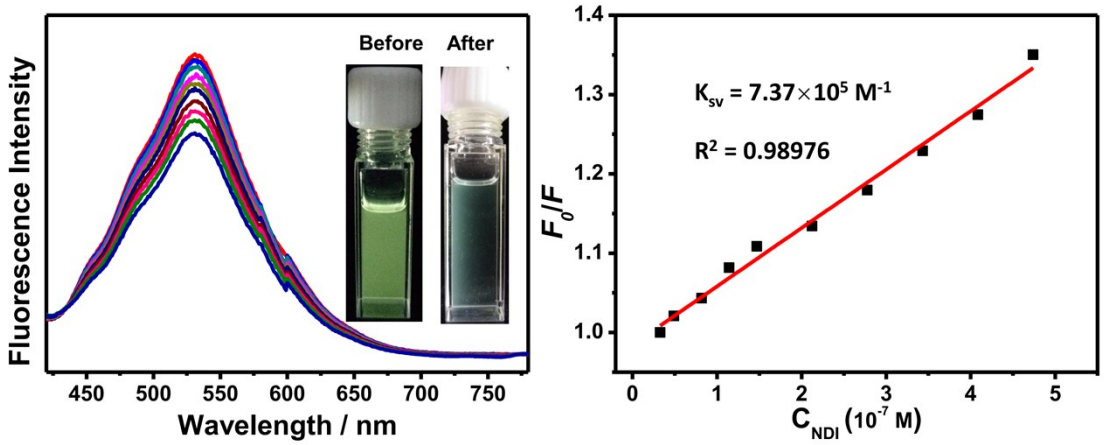


Figure S15. (a) Fluorescence spectra of [8]CPP titrated with NDI in CH_2Cl_2 at room temperature. Inset: Photographs of the fluorescence of [8]CPP before and after addition of NDI in CH_2Cl_2 under a UV lamp (365 nm). (b) Correlation of C_{NDI} on the fluorescent intensity of [8]CPP in CH_2Cl_2 for obtaining the K_{SV}. R^2 is the standard deviation.

Table S1. Energy level (unit: eV) of frontier molecular orbitals

Molecular Orbitals	OMe-[8]CPP	[8]CPP
HOMO-3	-5.90	-6.70
HOMO-2	-5.46	-5.70
HOMO-1	-5.42	-5.67
HOMO	-4.96	-5.10
LUMO	-1.75	-1.92
LUMO+1	-1.27	-1.32
LUMO+2	-1.16	-1.29
LUMO+3	-0.36	-0.59
HOMO-LUMO Gap	3.18	3.22

Table S2. Relaxed structure of OMe-[8]CPP and [8]CPP

Ground state of OMe-[8]CPP							
C	2.053807	-5.731689	-0.707193	O	-6.603403	0.898397	-2.154242
C	-2.162764	-4.499675	-1.509022	C	-7.913136	0.353090	-1.948818
C	-5.226696	-1.673768	-1.422299	O	0.928932	6.147917	-2.317212
C	-5.332194	2.514024	-1.014501	C	0.332252	7.447383	-2.222537
C	-1.522063	4.723592	-1.267038	O	6.268785	-1.121261	-2.118744
C	2.654520	5.059081	-1.150868	C	6.294597	-2.017969	-3.226690
C	4.968963	1.330208	-1.244855	O	0.071513	-4.821389	-2.360120
C	5.167354	-2.813767	-0.772021	C	-0.275654	-4.109969	-3.544247
C	3.317355	-5.158284	-0.563883	H	1.840842	-6.297195	-1.605821
C	-0.864190	-4.991353	-1.383257	H	-2.397431	-3.890527	-2.369545
C	-4.604868	-2.907485	-1.575950	H	-5.336428	-1.034477	-2.290390
C	-5.899915	1.237065	-1.016323	H	-5.481534	3.127503	-1.897682
C	-2.772919	4.114972	-1.268297	H	-0.901230	4.643321	-2.151674
C	1.360107	5.584141	-1.134312	H	3.211879	5.134903	-2.079347
C	4.321782	2.557257	-1.287535	H	4.855838	0.657642	-2.084885
C	5.747647	-1.551801	-0.931460	H	5.023274	-3.434238	-1.646589
C	-0.432598	-5.583031	-0.161078	H	4.054876	-5.320725	-1.343138
C	-4.256723	-3.673088	-0.450103	H	-4.292108	-3.207497	-2.569819
C	-5.636523	0.317363	0.030725	H	-3.090230	3.562426	-2.146309
C	-3.522399	4.040868	-0.084991	H	3.715350	2.798207	-2.154472
C	0.514887	5.405298	-0.011594	H	-3.482711	-5.668852	1.389274
C	4.285650	3.390911	-0.156017	H	-3.907187	2.456468	2.056538
C	5.722280	-0.608498	0.131536	H	2.820134	3.943734	2.043364
C	3.580748	-4.285432	0.504933	H	4.612746	-2.723063	2.572800
C	1.009628	-5.508585	0.207795	H	2.796515	-3.592280	2.384521
C	-3.111264	-4.624609	-0.477142	H	-1.183049	-6.417653	1.666828
C	-5.590669	-1.162231	-0.162885	H	-4.627073	-3.877600	1.662608
C	-4.530359	2.957539	0.048860	H	-4.844328	0.219102	2.028140
C	-0.971613	5.308944	-0.113923	H	-3.685361	4.815449	1.916590
C	3.182808	4.378942	-0.042399	H	0.549248	4.817106	2.056458
C	5.631511	0.865233	-0.089141	H	5.216047	3.684722	1.786072
C	4.629137	-3.228241	0.461722	H	5.448658	-0.466548	2.255547
C	1.379982	-4.856434	1.419223	H	-2.364780	5.339878	3.695276
C	-2.764190	-5.448744	0.606390	H	-3.139846	6.785490	2.984114
C	-5.525740	-2.084482	0.916740	H	-1.617730	6.946236	3.900573
C	-4.489662	2.145284	1.195601	H	-4.990405	-2.718312	3.556100
C	-1.843183	5.446249	1.000137	H	-6.483508	-3.527732	2.996931
C	2.439741	4.429188	1.150420	H	-6.584715	-2.064628	4.013700
C	5.806610	1.824258	0.940717	H	7.946169	0.159448	1.424078
C	4.899110	-2.412897	1.574094	H	8.339345	1.101848	2.884359
C	2.623496	-4.236476	1.535050	H	8.438077	1.871591	1.276185
C	-1.450364	-5.892169	0.758501	H	1.570087	-4.393764	4.110603
C	-4.830287	-3.289387	0.777648	H	-0.184384	-4.085033	4.188634
C	-5.020070	0.862811	1.176459	H	0.878853	-2.943157	3.325565

C	-3.081972	4.796529	1.017477	H	-7.875295	-0.630744	-1.471863
C	1.140996	4.921830	1.155638	H	-8.358820	0.255486	-2.940152
C	5.124090	3.043417	0.914848	H	-8.522170	1.030276	-1.339657
C	5.402369	-1.128986	1.399132	H	-0.623107	7.420256	-1.690445
O	-1.369298	6.175753	2.053673	H	0.162981	7.777506	-3.248885
C	-2.180873	6.309336	3.218022	H	1.009364	8.148050	-1.721127
O	-6.082268	-1.683636	2.098523	H	6.841617	-2.935777	-2.983341
C	-6.022100	-2.559551	3.221732	H	6.813288	-1.487130	-4.025335
O	6.535848	1.572316	2.085147	H	5.283439	-2.276448	-3.561679
C	7.891127	1.147551	1.890400	H	-1.097535	-4.597880	-4.080611
O	0.431740	-4.763403	2.394647	H	0.618640	-4.121412	-4.168069
C	0.705691	-3.998732	3.564625	H	-0.550616	-3.071706	-3.325675
			Ground state of [8]CPP				
C	-3.163639	4.082606	-1.288802	C	-4.597916	3.691114	1.051780
C	0.713064	5.744636	-1.214425	C	-0.679942	5.212882	1.122427
C	4.172398	3.084128	-1.232325	C	3.635230	4.648100	0.993396
C	5.889647	-0.750829	-0.849514	C	5.112654	0.732975	1.354368
C	3.546987	-4.370187	-1.214088	C	4.274202	-3.472427	1.298866
C	-0.708247	-4.978611	-1.406288	C	0.679717	-5.906303	0.802031
C	-4.541063	-3.361587	-1.077431	C	-3.302723	-4.413693	1.160461
C	-5.886086	0.674850	-0.908363	C	-5.108010	-0.625984	1.408929
C	-4.154520	3.108115	-1.232103	H	-2.577582	4.170068	-2.197847
C	-0.679863	5.748596	-1.214375	H	1.236966	5.965492	-2.139875
C	3.187180	4.064344	-1.288999	H	4.319307	2.446891	-2.098509
C	5.889838	0.640842	-0.908518	H	6.214815	-1.301450	-1.726432
C	4.521585	-3.387787	-1.077112	H	3.298503	-4.713434	-2.213267
C	0.679481	-4.982580	-1.406205	H	-1.213719	-4.555040	-2.266774
C	-3.572133	-4.349577	-1.214437	H	-4.981098	-2.953268	-1.980876
C	-5.893961	-0.716805	-0.849510	H	-6.201434	1.161476	-1.826921
C	-1.409570	5.366976	-0.070971	H	-4.305218	2.471809	-2.098320
C	2.812601	4.788906	-0.142199	H	2.601539	4.155123	-2.197987
C	5.388822	1.415431	0.155462	H	4.964122	-2.982198	-1.980564
C	4.821368	-2.817997	0.176839	H	-3.325466	-4.694060	-2.213641
C	1.414251	-5.338857	-0.259199	H	1.224987	4.934164	2.037183
C	-2.825183	-4.798375	-0.107433	H	4.741368	-1.120702	2.317933
C	-5.383812	-1.407574	0.269858	H	-1.233309	-6.280381	1.677557
C	-4.811883	2.807742	-0.024769	H	-4.744642	1.312026	2.216575
C	-2.784768	4.804918	-0.141992	H	-5.152934	3.560110	1.976261
C	1.440666	5.358862	-0.071073	H	-1.196173	4.941046	2.037261
C	4.828121	2.780033	-0.025031	H	3.449943	5.256050	1.874159
C	5.375546	-1.438501	0.269955	H	4.752418	1.284963	2.216468
C	2.797287	-4.814468	-0.107123	H	4.540930	-3.155910	2.301587
C	-1.445172	-5.330693	-0.259377	H	1.196711	-6.287351	1.677702
C	-4.837706	-2.790277	0.176577	H	-2.810322	-4.774597	2.057682
C	-5.380495	1.446407	0.155655	H	-4.747568	-1.093682	2.317791
C	-3.608088	4.668797	0.993674	H	-1.202570	5.972449	-2.139783
C	0.710253	5.208935	1.122380	H	6.207949	1.125535	-1.827145
C	4.619380	3.664699	1.051478	H	1.187455	-4.561916	-2.266644
C	5.104413	-0.655207	1.408977	H	-6.222394	-1.265433	-1.726459

C	3.276856	-4.432324	1.160777	H	-3.419211	5.275614	1.874456
C	-0.714025	-5.902329	0.801941	H	5.173705	3.530526	1.975919
C	-4.294520	-3.448071	1.298569	H	2.782245	-4.790204	2.057991
C	-5.108182	0.762229	1.354463	H	-4.559561	-3.130183	2.301305
C	-1.816024	-3.275519	-3.991790	O	5.647731	-1.389513	2.268125

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C	2.392018	-3.332029	-3.807248	C	7.017570	-1.625720	1.915796
C	4.658139	-1.702419	-0.498874	O	-1.758637	1.525355	6.300149
C	4.540815	0.526674	3.038312	C	-1.329644	2.241791	7.465960
C	0.851038	1.769123	4.934246	O	-6.855826	-1.772534	-0.235614
C	-3.318600	2.053569	4.633789	C	-7.023401	-3.185692	-0.325822
C	-5.663783	0.223720	1.478800	O	0.581036	-4.807266	-4.433097
C	-5.484660	-1.800000	-2.228680	C	1.293536	-5.918496	-3.893603
C	-3.076396	-2.926089	-3.551586	H	-1.308933	-4.099050	-3.508854
C	1.150825	-3.568892	-4.377788	H	2.919054	-4.144453	-3.324185
C	4.095803	-2.319237	-1.598563	H	4.586301	-2.191306	0.464281
C	5.159282	-0.128863	1.988895	H	4.487855	0.000653	3.985814
C	2.111432	1.407444	4.501404	H	0.209399	1.008075	5.359579
C	-2.079468	2.295418	5.199888	H	-3.929803	1.285472	5.095935
C	-5.091713	0.825356	2.580953	H	-5.750439	-0.854030	1.464607
C	-6.102133	-1.136689	-1.179105	H	-5.544430	-2.879077	-2.284235
C	0.365993	-2.490728	-4.923380	H	-3.504904	-3.480932	-2.724593
C	3.986365	-1.638973	-2.836986	H	3.593754	-3.269453	-1.455837
C	5.187837	0.434804	0.669400	H	2.412720	0.370302	4.597507
C	2.913303	2.312089	3.762829	H	-4.742404	0.190986	3.388284
C	-1.153073	3.215294	4.604894	H	2.763131	-0.065866	-4.698165
C	-4.785701	2.211358	2.588092	H	3.911660	3.493486	1.506014
C	-5.945314	0.283472	-1.006885	H	-3.284591	4.468113	2.243741
C	-3.710035	-1.746260	-4.017210	H	-4.343117	0.901857	-3.961181
C	-1.091724	-2.491886	-4.932065	H	-3.651176	-0.307479	-5.632208
C	2.970758	-2.034624	-3.801697	H	0.578392	-0.465985	-5.638655
C	5.167920	-0.376439	-0.545122	H	4.789999	0.045242	-3.932360
C	3.956765	1.809522	2.880198	H	4.949062	2.334750	-0.333773
C	0.297376	3.053819	4.685051	H	3.134535	4.416446	3.311682
C	-3.758412	2.739626	3.473091	H	-1.109076	4.859931	3.203042
C	-5.981152	0.948302	0.293027	H	-5.311465	4.057416	1.542305
C	-4.736471	-1.099818	-3.213065	H	-5.358397	2.050525	-2.094256
C	-1.875764	-1.497852	-5.620287	H	1.902047	6.220491	2.694285
C	2.339350	-1.060396	-4.615591	H	2.603218	6.389861	4.330204
C	5.330393	0.165966	-1.867937	H	1.127852	7.293371	3.891727
C	4.270337	2.483288	1.671005	H	5.303832	2.242581	-3.663211
C	1.234945	4.038484	4.216287	H	6.748786	1.224771	-3.933702
C	-2.974501	3.856810	3.084262	H	6.897894	2.776965	-3.065564
C	-5.959318	2.375143	0.445140	H	-7.948104	2.085965	-1.431341
C	-4.851058	0.312819	-3.205859	H	-8.031150	3.857393	-1.610050
C	-3.123794	-1.119945	-5.149489	H	-8.464120	3.099611	-0.052419
C	1.085447	-1.284260	-5.146830	H	-2.971341	-0.340644	-7.820407
C	4.726635	-0.432596	-2.963493	H	-1.380930	0.312731	-8.299920

C	4.858860	1.820239	0.613142	H	-2.197634	0.941377	-6.843302
C	2.484081	3.665726	3.741260	H	7.168540	-1.612862	0.832352
C	-1.725952	4.080193	3.628139	H	7.262402	-2.616347	2.302491
C	-5.359381	2.973514	1.538511	H	7.669726	-0.879752	2.383656
C	-5.426576	0.971116	-2.137492	H	-0.366332	2.736290	7.309957
O	0.802699	5.333389	4.238396	H	-1.229062	1.497700	8.257840
C	1.669991	6.357271	3.756664	H	-2.078629	2.986462	7.757852
O	6.075399	1.306309	-1.957409	H	-7.504468	-3.469028	-1.268768
C	6.257115	1.911546	-3.235524	H	-7.668524	-3.461814	0.508385
O	-6.434288	3.232809	-0.526772	H	-6.065359	-3.710116	-0.235237
C	-7.799760	3.042672	-0.921943	H	2.258357	-6.052391	-4.395467
O	-1.298134	-0.945406	-6.725858	H	0.664929	-6.790271	-4.075736
C	-2.015377	0.049427	-7.453479	H	1.457319	-5.805781	-2.815880

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C	-1.945661	-3.315771	-4.161817	C	-3.128671	-1.024886	-5.184563
C	2.272952	-3.400216	-3.822511	C	1.082037	-1.413651	-5.348390
C	4.750179	-1.811625	-0.697282	C	4.614675	-0.454216	-3.111850
C	4.509574	0.441078	2.878116	C	4.949170	1.760914	0.478564
C	1.007890	1.872397	4.910545	C	2.551362	3.677793	3.478624
C	-3.200354	2.078287	4.498170	C	-1.650315	4.183351	3.572709
C	-5.687437	0.387773	1.438619	C	-5.189110	3.115726	1.394632
C	-5.430673	-1.745184	-2.209222	C	-5.522612	1.026085	-2.271406
C	-3.210541	-2.952825	-3.747109	H	-1.507061	-4.208726	-3.730740
C	0.997017	-3.583783	-4.312586	H	2.732099	-4.211956	-3.268297
C	4.210137	-2.433200	-1.804495	H	4.773667	-2.365807	0.234259
C	5.023169	-0.248563	1.799928	H	4.391892	-0.088187	3.817870
C	2.273466	1.513973	4.493660	H	0.426419	1.137054	5.455180
C	-1.924502	2.258263	4.989436	H	-3.801324	1.275446	4.911943
C	-5.148436	1.004720	2.548747	H	-5.855872	-0.682243	1.484617
C	-5.943668	-1.051740	-1.133292	H	-5.450286	-2.829481	-2.178136
C	0.291987	-2.535400	-4.971226	H	-3.702099	-3.578671	-3.010890
C	3.983696	-1.728401	-3.019621	H	3.837507	-3.444498	-1.686687
C	5.125157	0.349348	0.510764	H	2.622351	0.515220	4.730985
C	3.039485	2.348178	3.632413	H	-4.921621	0.388321	3.411340
C	-1.041870	3.230900	4.437247	H	2.855928	-0.292407	-5.079087
C	-4.738549	2.367163	2.520129	H	4.202003	3.501111	1.423101
C	-5.873226	0.369379	-1.058658	H	-3.281526	4.696424	2.326563
C	-3.794348	-1.712715	-4.129286	H	-4.640726	0.905165	-4.191285
C	-1.160992	-2.468089	-4.992859	H	-3.586126	-0.150580	-5.635369
C	2.949862	-2.153106	-3.950935	H	0.641186	-0.610735	-5.928371
C	5.107897	-0.434531	-0.714696	H	4.616917	0.082552	-4.054549
C	4.056338	1.786278	2.756788	H	5.092946	2.303811	-0.448783
C	0.405028	3.094270	4.500354	H	3.151598	4.419209	2.961826
C	-3.699852	2.855754	3.413576	H	-1.067096	5.007868	3.178487
C	-5.861256	1.082641	0.209040	H	-5.047475	4.190880	1.366826
C	-4.805268	-1.075097	-3.300116	H	-5.530047	2.108971	-2.322829
C	-1.864593	-1.387755	-5.599336	H	0.505369	-4.532250	-4.123882
C	2.358608	-1.230149	-4.858376	H	5.288097	-1.291745	1.936401

C	5.154383	0.167032	-2.005332	H	-1.575197	1.589585	5.769014
C	4.435901	2.451075	1.557466	H	-6.345444	-1.619261	-0.300569
C	1.286503	4.035995	3.895174	H	-1.380338	-0.783845	-6.359419
C	-2.926902	4.003353	3.081154	H	5.559273	1.166603	-2.123483
C	-5.728014	2.499172	0.285189	H	0.943822	5.044319	3.688145
C	-5.009949	0.332310	-3.348128	H	-5.988610	3.115050	-0.569034