Electronic Supporting Information

Highly Emissive Phenylene-Expanded [5]Radialene

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Contents

General experiments

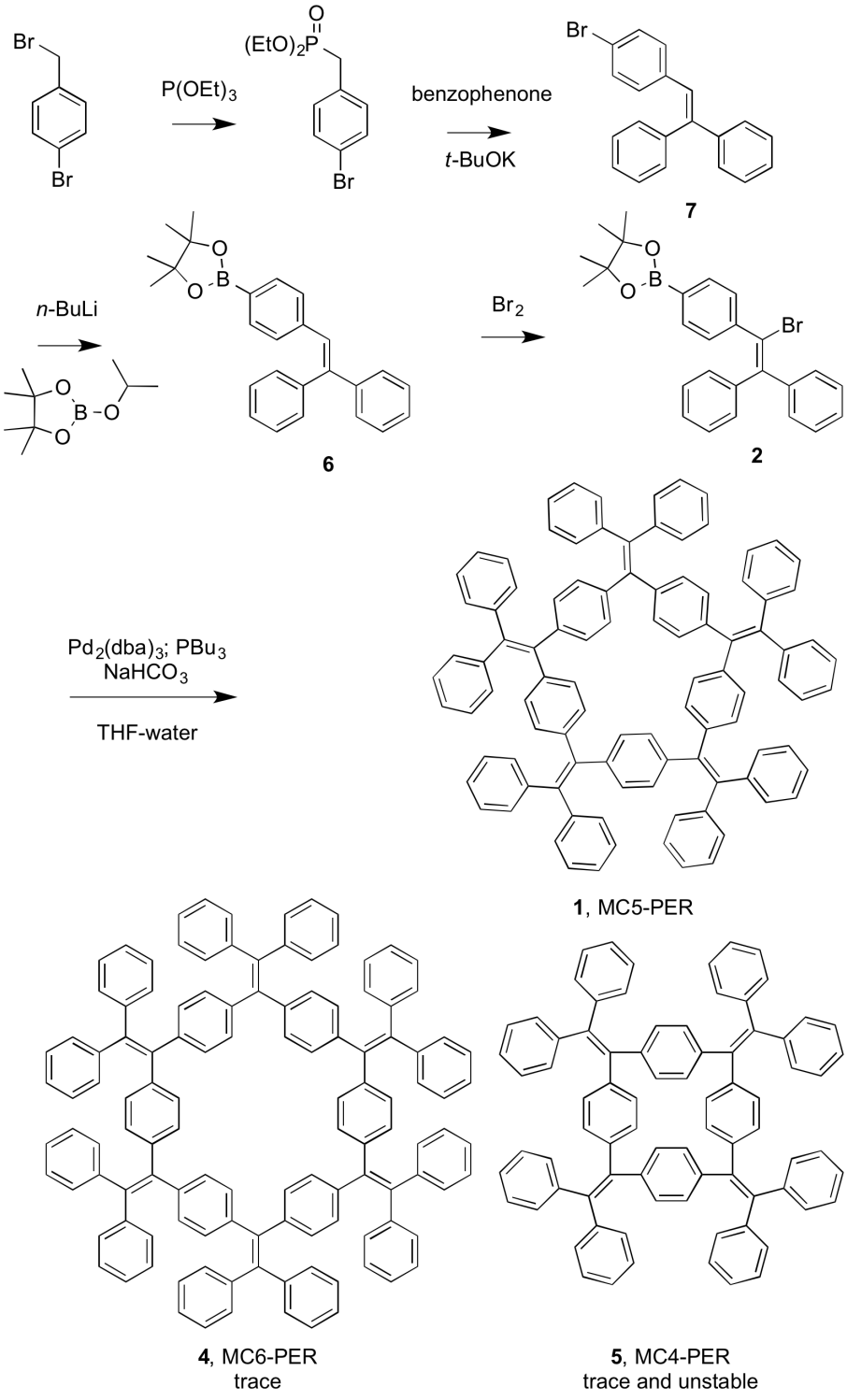
Materials

Tetrahydrofuran (THF) was distilled from sodium benzophenone ketyl immediately prior to use. Other solvents were directly used without further purification. The reagents, such as 4-bromobenzyl bromide, triethyl phosphite ($P(OEt)_3$), benzophonone, potassium *tert*-butoxide (*t*-BuOK), *n*-butyl lithium (*n*-BuLi, 2.0 M in cyclohexane), bromine (Br_2), tris(dibenzylideneacetone)dipalladium (Pd_2dba_3), tributylphosphine tetrafluoroborate (PBu_3•HBF_4) and sodium hydrogen carbonate ($NaHCO_3$) were purchased from commercial companies and directly used without purification. Picric acid is unstable and it may explode if it is struck, ground or heated. Keep it wet. Wear protective cloth and goggles while using picric acid.

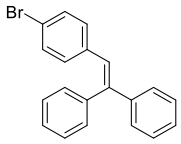
Instrumentation

^{1}H and ^{13}C-NMR spectra were measured on a Bruker ARX 400 (300) spectrometer using $CDCl_3$ or CD_2Cl_2 as solvent and tetramethylsilane (TMS) as internal standard. High-resolution mass spectra (HRMS) were recorded on a GCT premier CAB048 mass spectrometer performed in a MALDI-TOF mode. The UV-vis absorption spectra were taken on a Milton Roy Spectronic 3000 Array spectrometer and the emission spectra were measured on a Perkin-Elmer LS 55 spectrofluorometer.

1. Synthesis



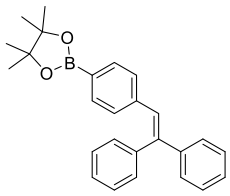
Scheme S1 Synthetic route to compound **1**.



(2-(4-bromophenyl)ethane-1,1-diyl)dibenzene[1] **(7)**

A solution of benzophenone (2.73 g, 15 mmol) and diethyl 4-bromobenzyl phosphonate (5.5 g, 18 mmol) in anhydrous THF (50 mL) was stirred under nitrogen atmosphere at 0 °C. Potassium *tert*-butoxide (2.0 g, 18 mmol) was added quickly and the mixture was stirred for over night at room temperature. The reaction mixture was quenched with 2 mol/L HCl and extracted with DCM (3×100 ml). The combined organic solvent was dried over anhydrous magnesium sulfate and removed under reduced pressure. The residue was purified with silica gel chromatographic using pure hexane as eluent. Colorless oil product was obtained and became solid after one night.

^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.19-7.36 (m, 12H), 6.91 (d, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) = 143.64, 143.26, 140.14, 136.53, 131.29, 131.25, 130.46, 128.97, 128.46, 127.94, 127.85, 127.79, 126.99, 120.77. HRMS (MALDI-TOF) Calcd. for $C_{20}H_{15}Br$ 334.0357, Found 334.0367.

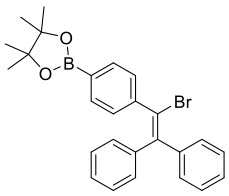


2-(4-(2,2-diphenylvinyl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane **(6)**

Into an oven-dried two-necked round-bottom flask were added (2-(4-bromophenyl)ethene-1,1-diyl)dibenzene (**7**, 1.34 g, 4.0 mmol) and 20 mL of THF under nitrogen atmosphere, which was then cooled to −78 °C. Then *n*-BuLi (2 M, 2.0 mL) was added dropwisely into the reaction mixtures and the temperature was kept at −78 °C for 0.5 h. 2-Isopropoxy-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (9.8 mmol, 2.0 ml) was injected and the mixture was allowed to recover to room temperature and further reacted for 2 h. After quenched with aqueous ammonium chloride, the mixture was extracted with dichloromethane (60 ml×3) and dried over anhydrous magnesium sulfate. The organic solvent was removed under reduced pressure. The residue was purified with silica gel chromatographic using hexane/CH_2Cl_2 (1:3 to 1:2) as eluent. Colorless oil product was got in a yield of 95% (1.445 g).

^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) = 7.60 (d, J = 8.0 Hz, 2H), 7.34 (m, 8H), 7.22 (t, J = 4.0 Hz, 2H), 7.04 (d, J = 8.0 Hz, 2H), 6.99 (s, 1H), 1.33 (s, 12H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) = 143.73, 143.49, 140.41, 134.58, 130.55, 129.03, 128.84, 128.41, 128.34, 127.87, 127.83, 127.66, 83.89, 25.07. HRMS (MALDI-TOF) Calcd. for $C_{26}H_{27}BO_2$ 382.2104, Found 382.2095.

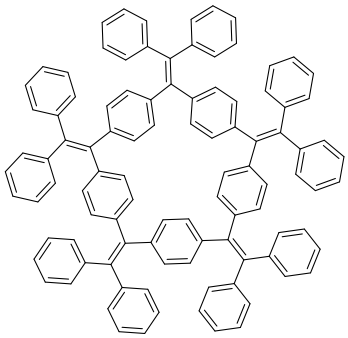
[1] Debabrata Jana, Shatabdi Boxi, Binay K. Ghorai. *Dyes and Pigments* **2013**, *99*, 740-747.



2-(4-(1-bromo-2,2-diphenylvinyl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane **(2)**

Into an two-necked round-bottom flask were added 2-(4-(2,2-diphenylvinyl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane **6** (1.53 g, 4.0 mmol) and 40 mL of $CHCl_3$. The flash was cooled to 0 °C and Br_2 (4.4 mmol, 704 mg in 6 ml $CHCl_3$) was then added dropwise into the reaction mixtures. After stirring at 0 °C for 0.5 h, the mixture was allowed to warm to room temperature and further stirred for 2 h. The reaction was quenched by addition of an aqueous $NaHCO_3$. The mixture was extracted with dichloromethane (60 mL×3) and dried over anhydrous magnesium sulfate. The organic solvent was removed under reduced pressure. The residue was purified with silica gel chromatography using hexane/CH_2Cl_2 (1:3 to 1:2) as eluent. Crystalline product was obtained after recrystallization from ethanol in 86% yield (1.59 g).

^{1}HNMR (400 MHz, $CDCl_3$), δ (ppm) = 7.64 (d, J = 7.6 Hz, 2H), 7.39 (s, 4H), 7.33 (d, J = 7.6 Hz, 3H), 7.08 (t, 3H), 6.97 (d, J = 5.2 Hz, 2H), 1.33 (s, 12H). ^{13}C NMR (100 MHz, $CDCl_3$), δ (ppm) = 144.08, 144.00, 143.96, 141.12, 134.57, 130.52, 129.78, 129.70, 128.38, 128.14, 127.79, 127.28, 122.15, 84.08, 25.09. HRMS (MALDI-TOF): Calcd. for $C_{26}H_{26}BBrO_2$ 460.1209, Found 460.1214.



MC5-PER **(1)**

Into a round-bottom flask were added compound **2** (231 mg, 0.5 mmol), $Pd_2(dba)_3$ (23 mg, 0.025 mmol), PBu_3•HBF_4 (15 mg, 0.05 mmol), $NaHCO_3$ (2.1 g, 12.5 mmol) under nitrogen atmosphere. Degassed water (30 ml) and THF (300 ml) was purged with nitrogen for one hour and injected to the reaction system. The reaction was stirred for 120 h under gently reflux. After cooling to room temperature, solvent was removed under vacuum. The residue was then extracted with DCM (3×50 ml), and dried over anhydrous magnesium sulfate. The organic solvent was removed under reduced pressure. The residue was then sonicated with hexane (50 ml) for 10 minutes, a cotton-like precipitate was formed and filtered, washed by hexane for several times. The precipitate was then purified with silica gel chromatography using DCM/hexane

(1:4) as the eluent. A white solid was obtained in 31% yield (39 mg). High resolution MALDI-TOF spectra of crude product give trace amount of MC4-PER and MC6-PER peaks. After purification by column chromatography and recrystallization from DCM/hexane system, high resolution MS peaks of MC4-PER and MC6-PER can not be found.

^{1}H NMR (400 MHz, CD_2Cl_2), δ (ppm) = 7.08 (t, 30H), 6.98 (d, 20H), 6.70 (s, 20H). ^{13}C NMR (100 MHz, $CDCl_3$), δ (ppm) = 143.51, 142.29, 141.13, 140.70, 131.48, 130.48, 128.18, 126.90. HRMS (MALDI-TOF): Calcd. For $C_{100}H_{70}$ 1271.5511, Found 1271.5516. Elemental analysis calcd for C100H70: C, 94.45; H, 5.55. Found: C, 94.28; H, 5.58.

MC4-PER: HRMS (MALDI-TOF), Calcd. For $C_{80}H_{56}$ 1016.4382, Found 1016.4731.

MC6-PER: HRMS (MALDI-TOF), Calcd. For $C_{120}H_{84}$ 1525.6607, Found 1525.6620.

Characterization

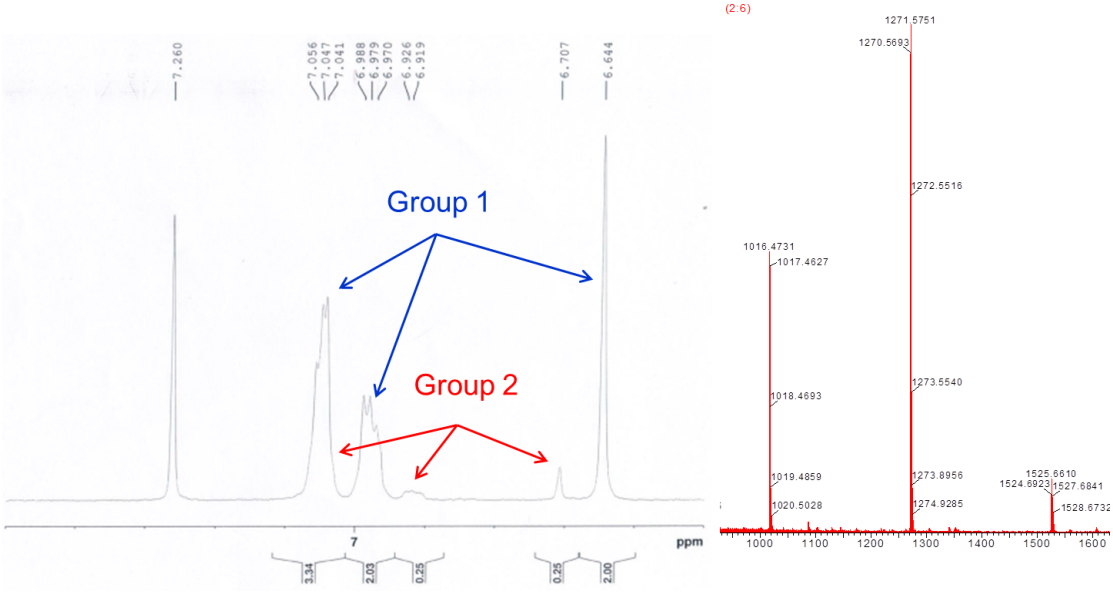


Fig. S1 ^{1}H NMR ($CDCl_3$) and MALDI-TOF mass spectra of crude products.

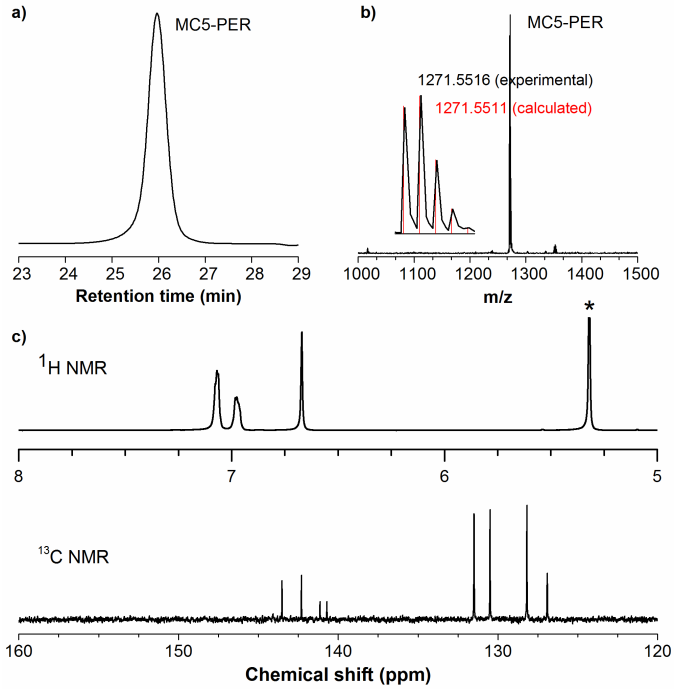


Fig. S2 a) GPC trace of MC5-PER in THF. b) MALDI-TOF MS data of MC5-PER. Insets: Comparison of experimental (dark) and calculated (red) peak patterns. c) ^{1}H and ^{13}C NMR spectra of MC5-PER in CD_2Cl_2 (star).

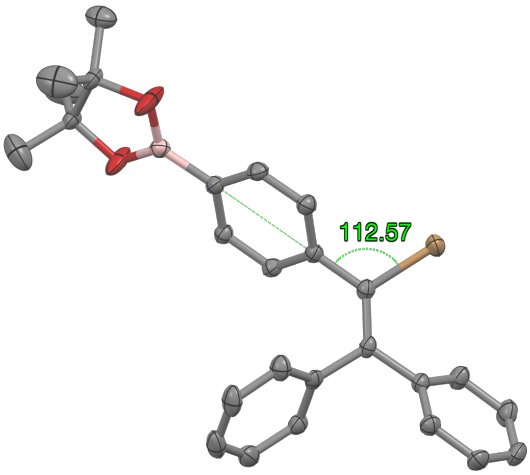


Fig. S3 Single crystal structure of **2** and its linking angle.

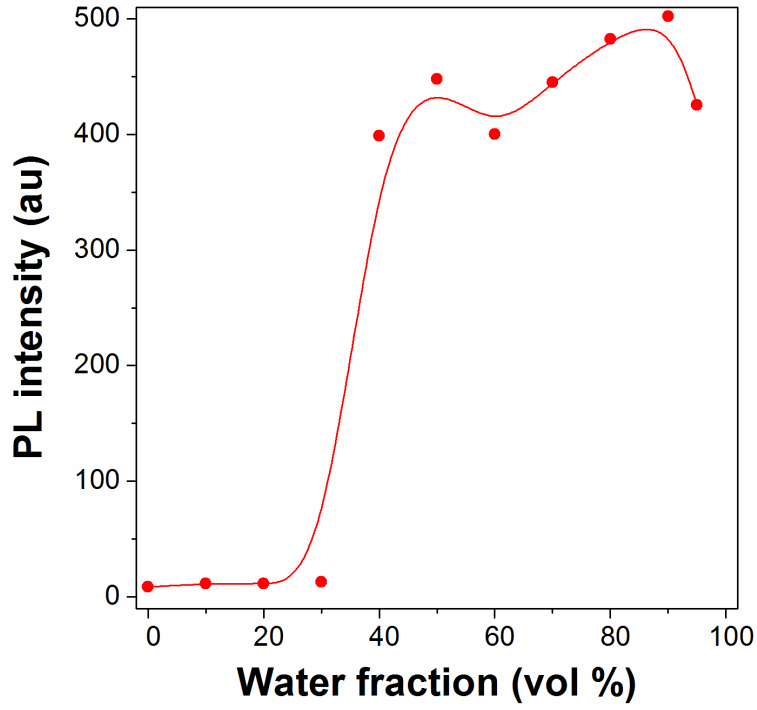


Fig. S4 Plot fluorescence intensity of MC5-PER versus the compositions of the aqueous mixtures. Solution concentration: 10 μM; excitation wavelength: 340 nm.

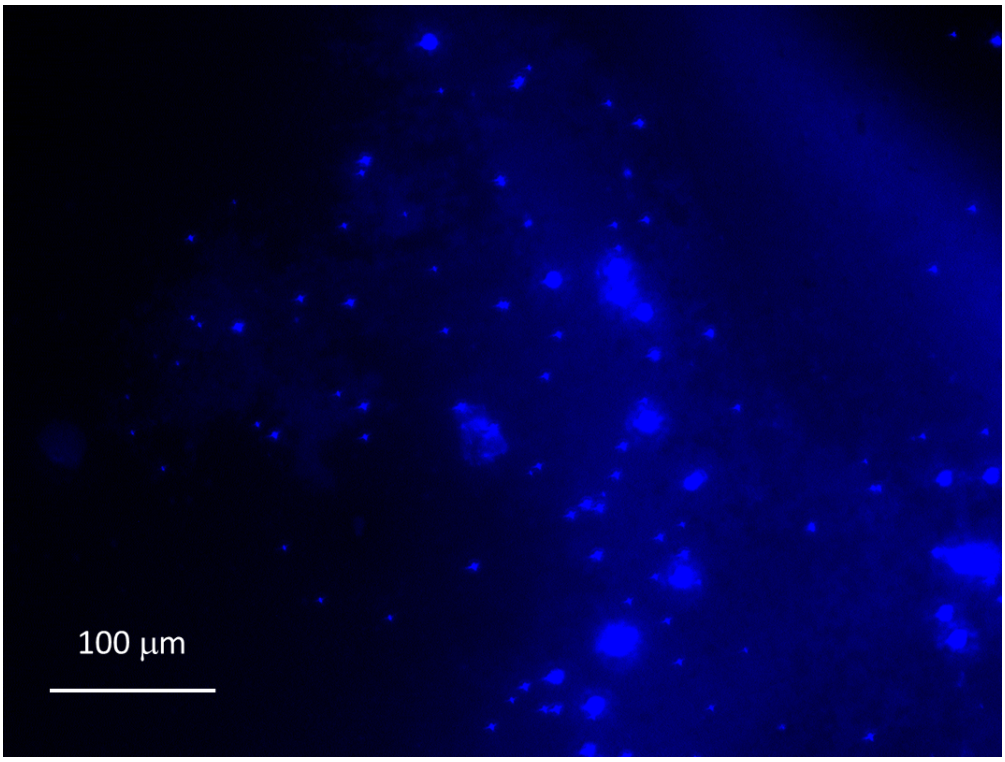


Fig. S5 Fluorescence microscopy photograph of irregular particles obtained from THF-water mixtures with water fractions of 60-95%.

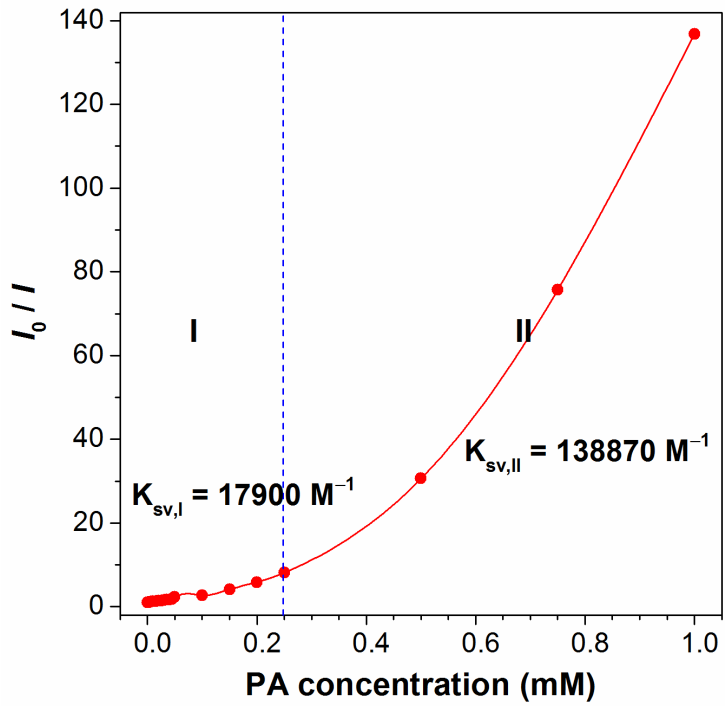
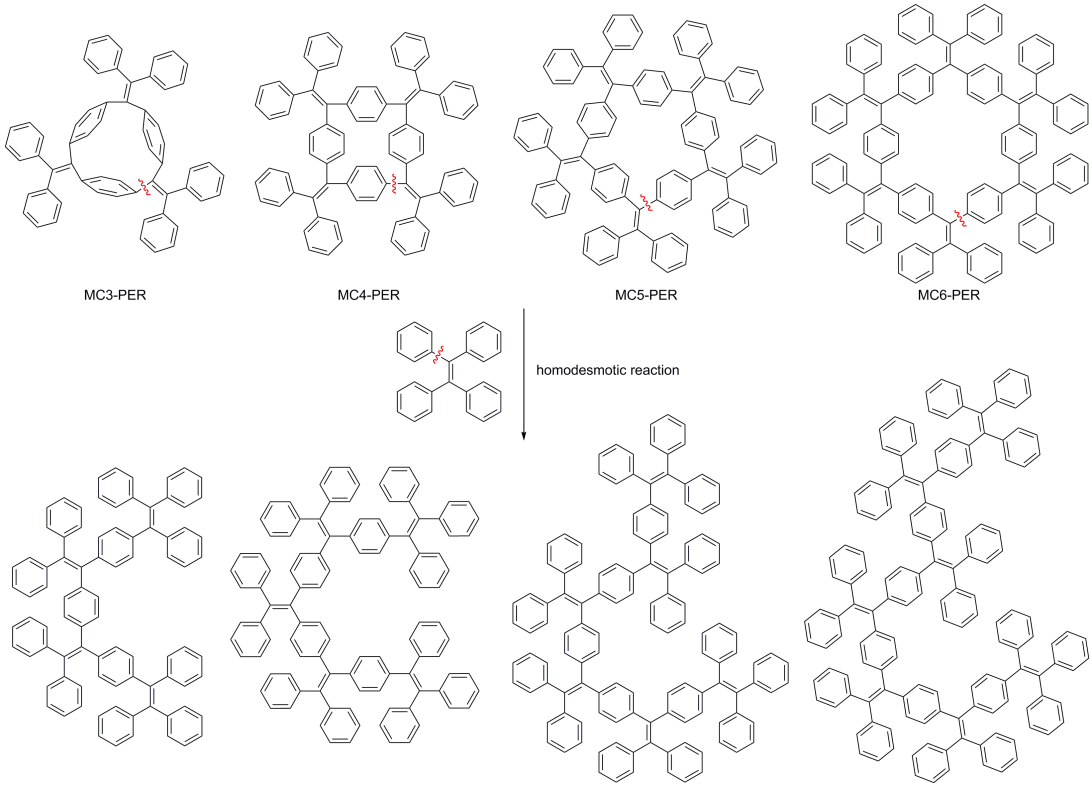


Fig. S6 Stern–Volmer plots of (I_0/I) value versus [PA] in s. Stern–Volmer plots of relative PL intensity (I_0/I) versus PA concentration in the nanoaggregates suspended in the THF–water mixture with 80% water content.

2. Density functional theory calculations

The geometry of MC5-PER and c-MC5-PER was first optimized at the B3LYP level of DFT coupled with 6-31G(d, p) basis set. To characterize the energy levels, a single point calculation was carried out at the B3LYP/6-31G(d, p) level. All of the calculations were performed using Gaussian 09 program package.[2]

The strain energies of MC3-PER, MC4-PER, MC5-PER, and MC6-PER were estimated by a hypothetical homodesmotic reaction in the following ways (as shown in Scheme S3). Molecules structures were optimized by DFT calculation at the B3LYP/6-31G(d, p) basis set and the molecules energies was calculated at the B3LYP/6-311++G(d, p) basis set.



Sheme S2. Homodesmotic reactions for estimation the ring strain.

[2] Gaussian 09, Revision A.1, 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.

Table S1 Computed Cartesian coordinates of MC5-PER

	X	Y	Z
C	7.79256200	-4.23569000	2.49943500
C	8.53782000	-3.70249200	1.44506800
C	7.90676300	-3.41701500	0.23346400
C	6.54053800	-3.65358800	0.07924100
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C	6.43002700	-4.48009100	2.34082300
C	4.31226700	-4.45741800	0.99058800
C	3.88721900	-5.82439500	1.42789000
C	3.43275600	-3.52826100	0.53293300
C	3.81200200	-2.10199800	0.25835900
C	1.98079900	-3.80231500	0.29293800
C	2.86094500	-6.01013300	2.36796400
C	2.51172300	-7.28881700	2.80212200
C	3.17679100	-8.40876500	2.30058900
C	4.20253900	-8.23903200	1.36820200
C	4.56139600	-6.95994800	0.94667700
C	1.00778200	-3.03856500	0.95846700
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C	3.90222300	-1.62170100	-1.05602300
C	4.17729700	-0.28009800	-1.31404600
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C	6.87873300	1.89810800	-1.12854300
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C	-3.00988700	-3.03359300	-0.45363900
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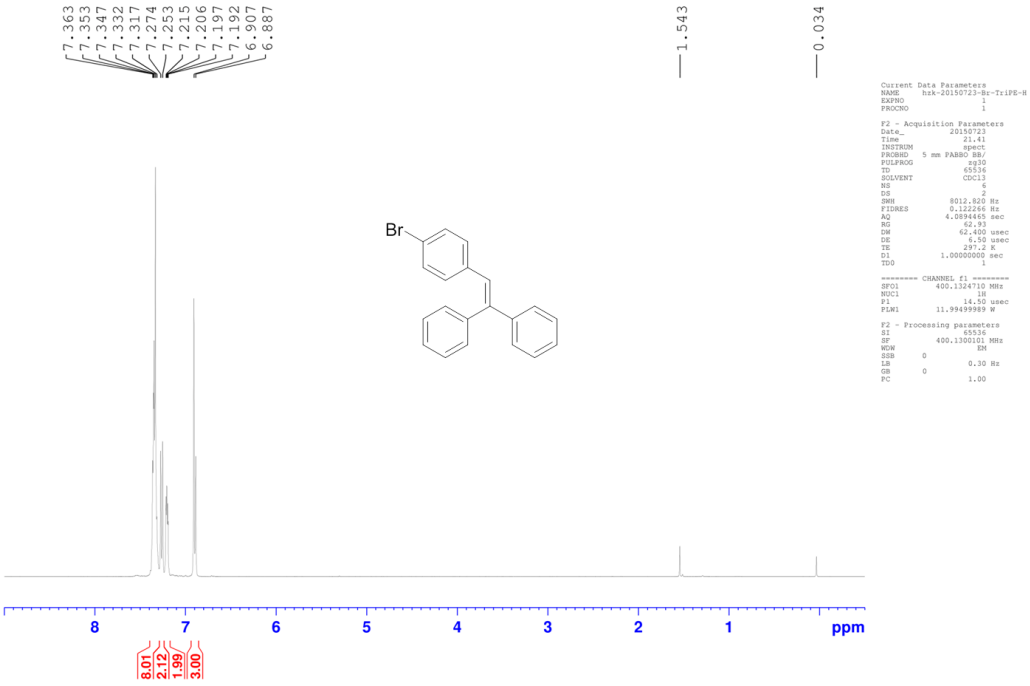
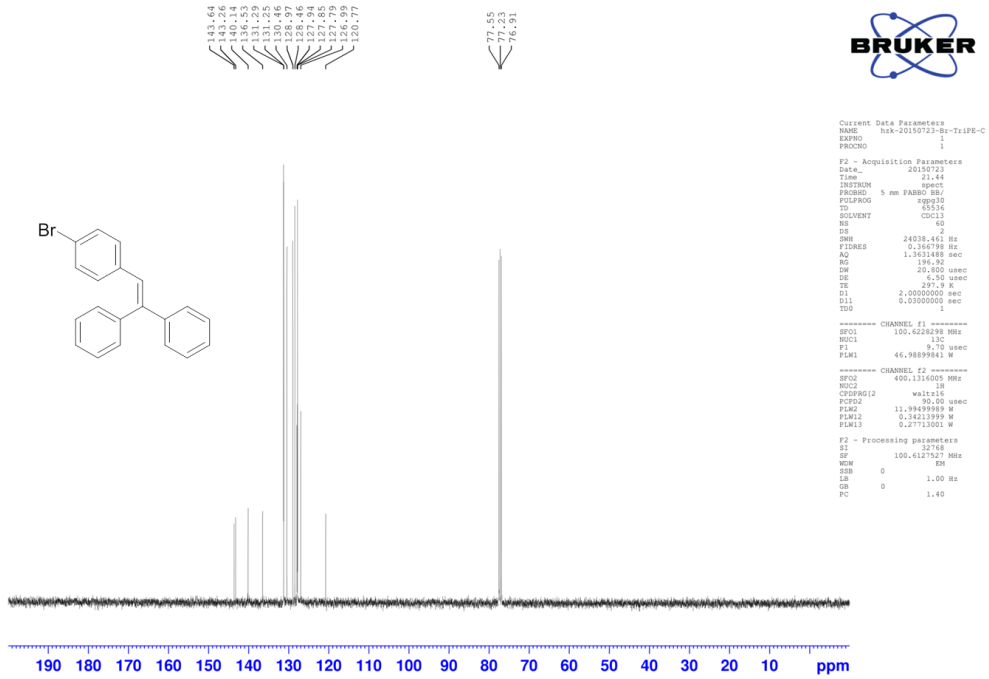
H	7.43310900	4.52269700	-0.23612000
H	2.03972200	1.67928600	-1.68416000
H	-0.07538700	2.85085000	-1.28631800
H	1.85673500	5.34863200	1.62863400
H	3.99253100	4.22102400	1.17523700
H	-4.92469200	-7.04197800	0.28801800
H	-7.23459200	-7.23116400	-0.56938700
H	-7.92889800	-5.94569300	-2.58515400
H	-6.28358700	-4.46298400	-3.72219000
H	-3.98581800	-4.24993300	-2.83830100
H	-2.81267100	-7.69899900	-2.31589500
H	-1.78088700	-9.90265700	-1.87694900
H	-0.64548600	-10.33980000	0.29492700
H	-0.55170300	-8.54379000	2.01495400
H	-1.56601600	-6.33483700	1.56131400
H	-4.46799600	-3.67936000	0.99520300
H	-5.55595800	-1.48342800	1.21051500
H	-2.79702500	0.15845900	-1.64355500
H	-1.70408100	-2.03354700	-1.84981300
H	-4.68459700	3.32678400	-1.22401600
H	-2.89793600	5.00441600	-1.00789600
H	-0.88294500	2.49518700	1.83550000
H	-2.67336100	0.82300700	1.62855500
H	-8.48670600	0.36819800	1.24914200
H	-10.17578200	-1.26978100	0.49174000
H	-9.88697100	-2.44797700	-1.68221000
H	-7.88455400	-1.96996900	-3.08106900
H	-6.18481100	-0.35234000	-2.30520400
H	-5.66773600	2.48316700	2.30493700
H	-6.68621100	4.59540600	3.08573800
H	-8.38865700	5.75477800	1.68827700
H	-9.07367700	4.76061900	-0.48880800
H	-8.07223600	2.63347600	-1.25124800
H	0.03742200	8.19356100	2.31896200
H	1.77343100	9.90171000	1.89385600
H	3.00592700	9.91868300	-0.26914000
H	2.48230900	8.20303400	-1.99416500
H	0.76143200	6.48339100	-1.55405300
H	-2.16185800	8.31594200	-0.27916300
H	-4.25993000	9.29244800	0.58827700
H	-5.35074600	8.32119600	2.60421400
H	-4.31908400	6.35560800	3.73127100
H	-2.24148300	5.36044400	2.83673300

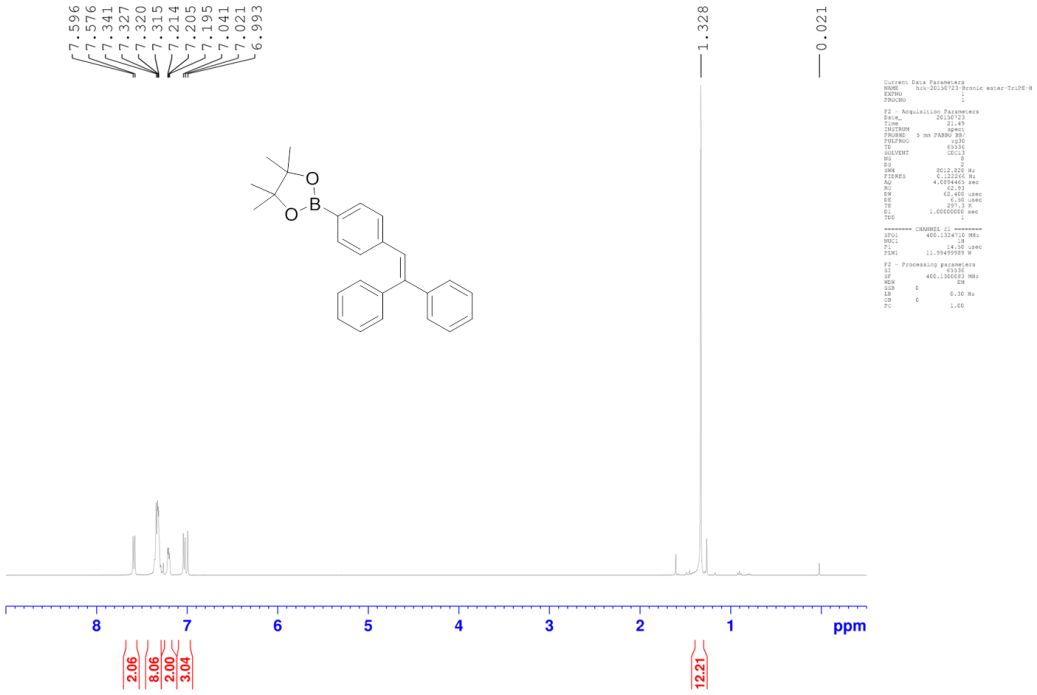
3. ^{1}H NMR and ^{13}C NMR spectra



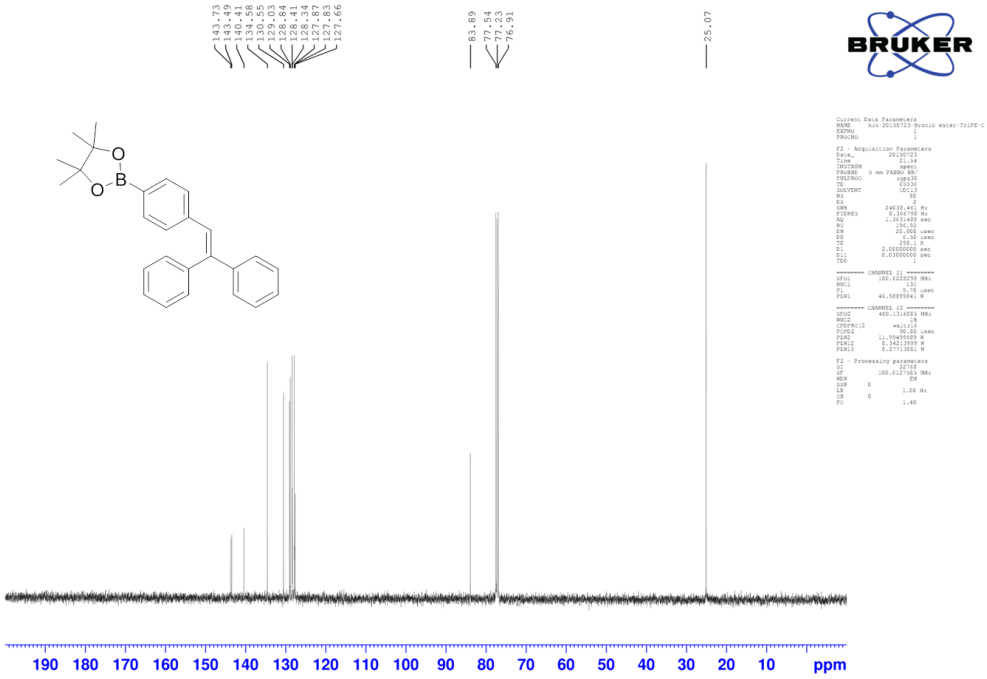
^{1}H NMR spectra of **7** in $CDCl_3$.



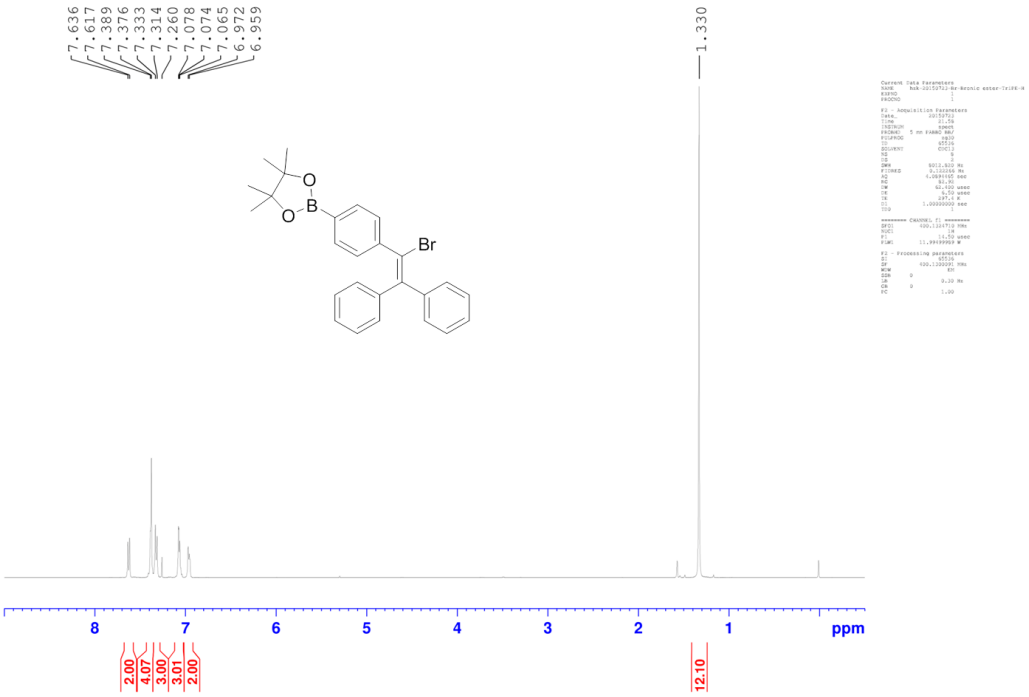
^{13}C NMR spectra of **7** in $CDCl_3$.



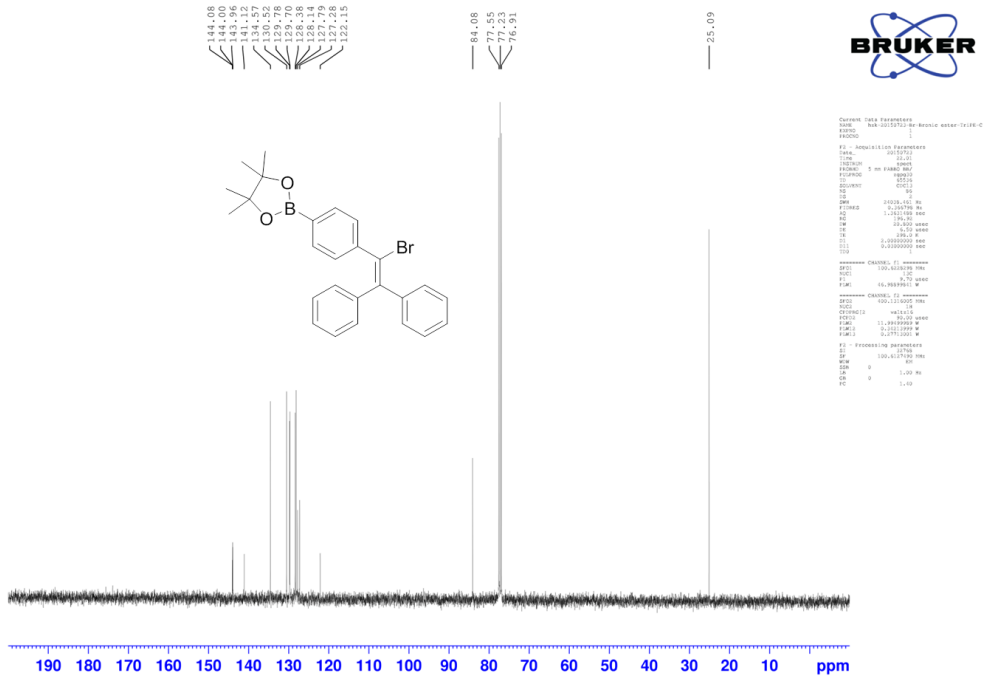
^{1}H NMR spectra of **6** in $CDCl_3$.



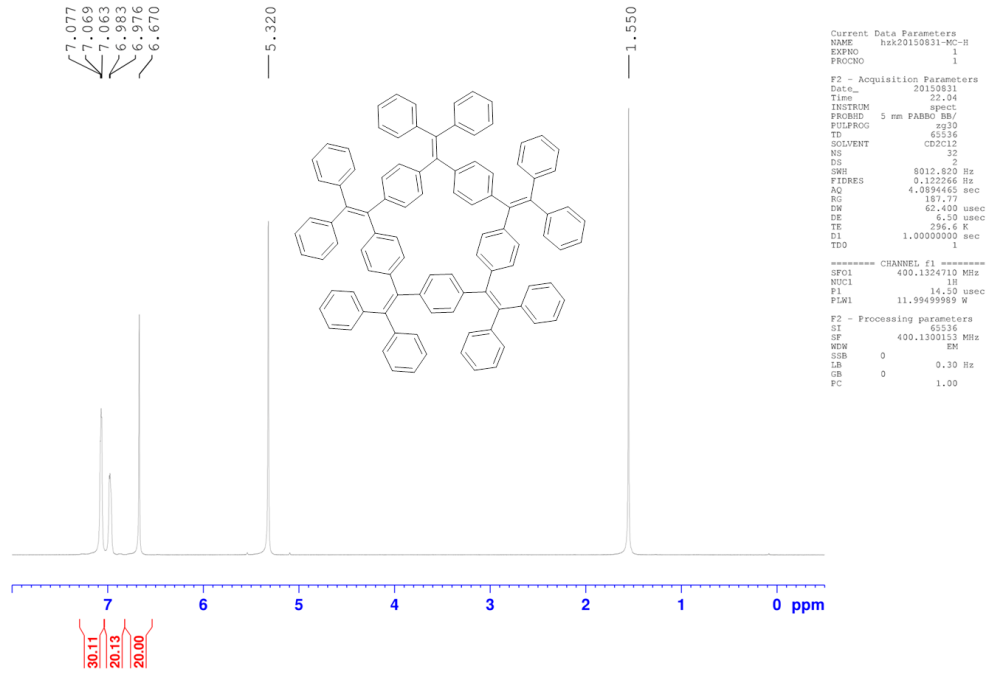
^{13}C NMR spectra of **6** in $CDCl_3$.



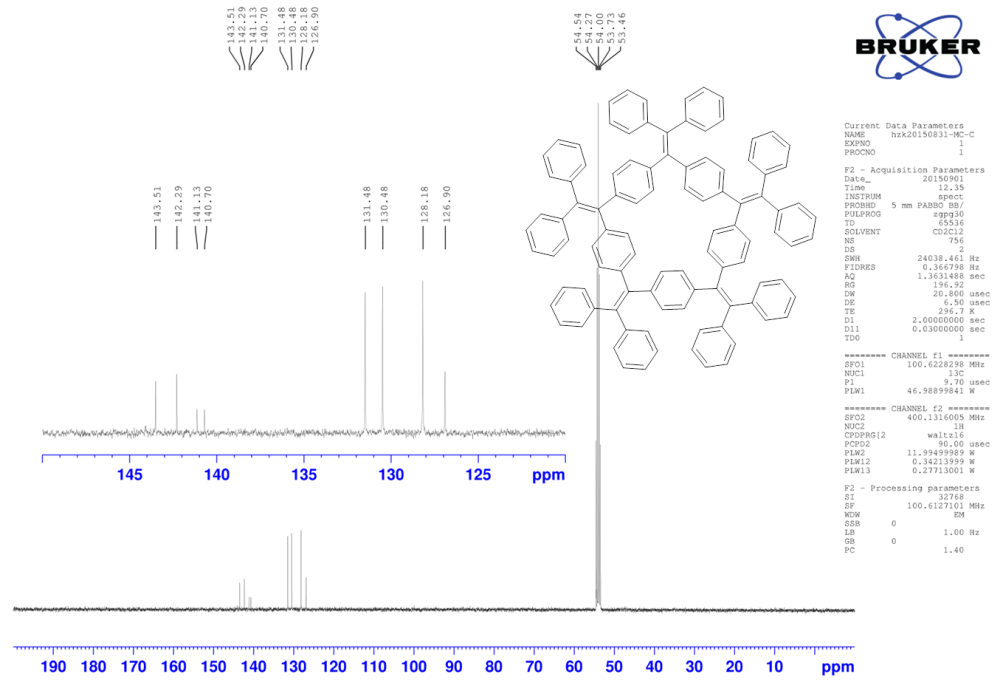
^{1}H NMR spectra of **2** in $CDCl_3$.



^{13}C NMR spectra of **2** in $CDCl_3$.



^{1}H NMR spectra of MC5-PER in CD_2Cl_2.



^{13}C NMR spectra of MC5-PER in CD_2Cl_2.

Table S2 Crystal Data and Structure Refinement for **2**.

Empirical formula	C26 H26 B Br O2
Formula weight	412.19
Temperature	150 (2) K
Wavelength	1.54184 Å
Crystal system	triclinic
Space group	P $\bar{1}$ (2)
Unit cell dimensions	a = 10.1232(4) Å alpha = 68.2965(19) deg.
	b = 10.2530(4) Å beta = 86.379(2) deg.
	c = 12.6447(5) Å gamma = 67.7741(18) deg.
Volume	1124.29(8) $Å^3$
Z	2
Density (calculated)	1.362 Mg/m^3
Absorption coefficient	2.633 mm^{-1}
F(000)	476
Crystal size	0.10 x 0.06 x 0.05 mm^3
Theta range for data collection	3.778 to 70.074
Index ranges	-12<=h<=12, -12<=k<=12, -15<=l<=15
Reflections collected	34775
Independent reflections	4275 [R(int) = 0.0509]
Absorption correction	Multi-scan
Max. and min. transmission	0.7538 and 0.5062
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	4275 / 0 /275
Goodness-of-fit on F2	1.008
Final R indices [I>2sigma(I)]	R1 = 0.0334, wR2 = 0.0822
R indices (all data)	R1 = 0.0364, wR2 = 0.0797
Largest diff. peak and hole	0.364 and -0.537 $e.Å^{-3}$

Table S3 Crystal Data and Structure Refinement for MC5-PER.

Empirical formula	C112 H80 Cl2
Formula weight	1496.66
Temperature	153 (2) K
Wavelength	1.54184 Å
Crystal system	monoclinic
Space group	$P12_1/c1$
Unit cell dimensions	a = 25.9806(9) Å alpha = 90 deg. b = 24.2530(8) Å beta = 97.253(2) deg. c = 26.5964(8) Å gamma = 90 deg.
Volume	16624.5(9) $Å^3$
Z	8
Density (calculated)	1.196 Mg/m^3
Absorption coefficient	1.088 mm^{-1}
F(000)	6288
Crystal size	0.12 x 0.05 x 0.05 mm^3
Theta range for data collection	2.475 to 67.079
Index ranges	-31<=h<=31, -28<=k<=28, -30<=l<=31
Reflections collected	29528
Independent reflections	29528 [R(int) = 0.1790]
Absorption correction	Multi-scan
Max. and min. transmission	0.7538 and 0.4413
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	29528 / 198 /2120
Goodness-of-fit on F2	1.038
Final R indices [I>2sigma(I)]	R1 = 0.0945, wR2 = 0.2318
R indices (all data)	R1 = 0.1439, wR2 = 0.2680
Largest diff. peak and hole	0.899 and -1.085 $e.Å^{-3}$