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Supporting Information for:

Transannularly Conjugated Tetrameric Perylene Diimide Acceptors Containing [2.2]Paracyclophane for Non-fullerene Organic Solar Cells

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General Information.

^{1}H and ^{13}C NMR spectra were recorded on a Bruker AV-400 MHz NMR spectrometer. Chemical shifts are reported in parts per million (ppm, δ). ^{1}H NMR and ^{13}C NMR spectra were referenced to tetramethylsilane (0 ppm) for $CDCl_3$. Mass spectra were collected on a MALDI Micro MX mass spectrometer, or an API QSTAR XL System.

Materials. P3TEA,[1] ***o*CP-Br4 and *p*CP-Br4** was synthesized according to a previous report.[2] [2.2]paracyclophane was purchased from J&K Scientific. Tetrahydrofuran were freshly distilled before use from sodium using benzophenone as the indicator. All other reagents and chemicals were purchased from commercial sources and used without further purification.

Optical characterizations. Film UV-Vis absorption spectra were acquired on a Perkin Elmer Lambda 20 UV/VIS Spectrophotometer. All film samples were spin-cast on ITO/ZnO substrates. UV-Vis absorption spectra were collected from the solution of two small molecules with the concentration of 1.0×10^{-5} M in dichloromethane. A cuvette with a stopper (Sigma Z600628) was used to avoid volatilization during the measurement.

Electrochemical characterizations. Cyclic voltammetry was carried out on a CHI610E electrochemical workstation with three electrodes configuration, using Ag/AgCl as the reference electrode, a Pt plate as the counter electrode, and a glassy carbon as the working electrode. 0.1 mol L^{-1} tetrabutylammonium hexafluorophosphate in anhydrous acetonitrile was used as the supporting electrolyte. The polymer and small molecules were drop-cast onto the glassy carbon electrode from chloroform solutions (5 mg/mL) to form thin films. Potentials were referenced to the ferrocenium/ferrocene couple by using ferrocene as external standards in acetonitrile solutions. The scan rate is 100 mV s^{-1}.

AFM analysis. AFM measurements were performed by using a Scanning Probe MicroscopeDimension 3100 in tapping mode. All film samples were spin-cast on ITO/ZnO substrates.

Solar cell fabrication and testing. Diethylzinc (15 % wt in toluene) and molybdenum trioxide (MoO_3) were purchased from Sigma-Aldrich and used as received without further treatment. Prepatterned ITO-coated glass substrates were cleaned by sequential sonication in soap deionized water, deionized water, acetone, and isopropanol for 30 min of each step. Active layer solutions (D:A ratio 1:1.5 w/w) were prepared in 1,2,4-trimethylbenzene with 2% 1,8-octanedithiol (polymer concentration: 8.5 mg mL^{-1}). To completely dissolve the polymer, the active layer solution should be stirred on a hotplate at 100 °C for at least 1 hour. Active layers were spin-coated onto the glass/ITO/ZnO substrates at 100 °C in a N_2 glovebox at 1500-2500 rpm. The optimized active layer thickness was ~110 nm. The active layers were then treated with vacuum to remove the solvent. Subsequently, the blend films were thermally annealed at 100 °C for 5 min before being transferred to the vacuum chamber of a thermal evaporator inside the same glovebox, and a thin layer (7 nm) of MoO_3 was deposited as the anode interlayer, followed by the deposition of 100 nm of Al as the top electrode at a vacuum level of ~1.0×10^{-4} Pa. All devices were encapsulated using epoxy and thin glass slides inside the glovebox. Device *J-V* characteristics were measured under AM 1.5G (100 mW cm^{-2}) using a Newport solar simulator in ambient atmosphere. The light intensity was calibrated using a standard Si diode (with KG5 filter, purchased from PV Measurement) to bring spectral mismatch to unity. *J-V* characteristics were recorded using a Keithley 2400 source meter unit. Typical cells have devices area of 5.9 mm2, defined by a metal mask with an aperture aligned with the device area. EQEs were measured using an Enlitech QE-S EQE system equipped with a standard Si diode. Monochromatic light was generated from a Newport 300W lamp source.

EQE measurements. EQEs were measured using an Enlitech QE-S EQE system equipped with a standard Si diode. Monochromatic light was generated from a Newport 300W lamp source.

Hole-mobility measurements. The hole-mobilities were measured using the space charge limited current (SCLC) method, employing a device architecture of ITO/PEDOT:PSS/blend film/MoO_3/Al. The mobilities were obtained by taking current-voltage curves and fitting the results to a space charge limited form, where the SCLC is described by:

$$J = \frac{9\varepsilon_0\varepsilon_r\mu(V_{appl} - V_{bi} - V_s)^2}{8L^3}$$

Where ε_0 is the permittivity of free space, ε_r is the relative permittivity of the material (assumed to be 3), μ is the hole mobility and L is the thickness of the film. From the plots of $J^{1/2}$ vs $V_{appl} - V_{bi} - V_s$, hole mobilities can be deduced.

Electron mobility measurements. The electron mobilities were measured using the SCLC method, employing a device architecture of ITO/ZnO/blend film/Ca/Al. The mobilities were obtained by taking current-voltage curves and fitting the results to a space charge limited form, where the SCLC is described by:

$$J = \frac{9\varepsilon_0\varepsilon_r\mu(V_{appl} - V_{bi} - V_s)^2}{8L^3}$$

Where ε_0 is the permittivity of free space, ε_r is the relative permittivity of the material (assumed to be 3), μ is the hole mobility and L is the thickness of the film. From the plots of $J^{1/2}$ vs $V_{appl} - V_{bi} - V_s$, electron mobilities can be deduced.

GIWAXS characterization. GIWAXS measurements were performed at beamline 7.3.3 at the Advanced Light Source.[3] Samples were prepared on Si substrates using identical blend solutions as those used in devices. The 10 keV X-ray beam was incident at a grazing angle of 0.11° - 0.15°, which maximized the scattering intensity from the samples. The scattered X-rays were detected using a Dectris Pilatus 2M photon counting detector. In-plane and out-of-plane sector averages were calculated using the

Nika software package.[4] The uncertainty for the peak fitting of the GIWAXS data is 0.3 A. The coherence length was calculated using the Scherrer equation:

$$L_c = \frac{2\pi K}{\Delta q}$$

R-SoXS characterization. R-SoXS transmission measurements were performed at beamline 11.0.1.2 at the Advanced Light Source.[5] Samples for R-SoXS measurement were prepared on a PSS modified Si substrate under the same conditions as those used for device fabrication, and then transferred by floating in water to a 1.5 mm × 1.5 mm, 100 nm thick Si_3N_4 membrane supported by a 5 mm × 5 mm, 200 µm thick Si frame (Norcada Inc.). 2D scattering patterns were collected on an in-vacuum CCD camera (Princeton Instrument PI-MTE). The sample detector distance was calibrated from diffraction peaks of a triblock copolymer poly(isoprene-b-styrene-b-2-vinyl pyridine), which has a known spacing of 391 Å. The beam size at the sample is approximately 100 µm by 200 µm.

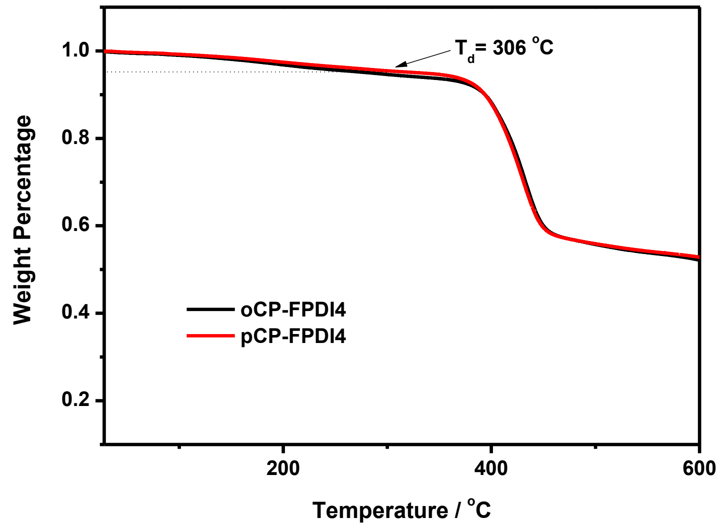


Figure S1. Thermogravimetric curves of *o*CP-FPDI4 and *p*CP-FPDI4. The thermal degradation temperature (T_d at 5% weight loss) of two SMAs are 306 ºC.

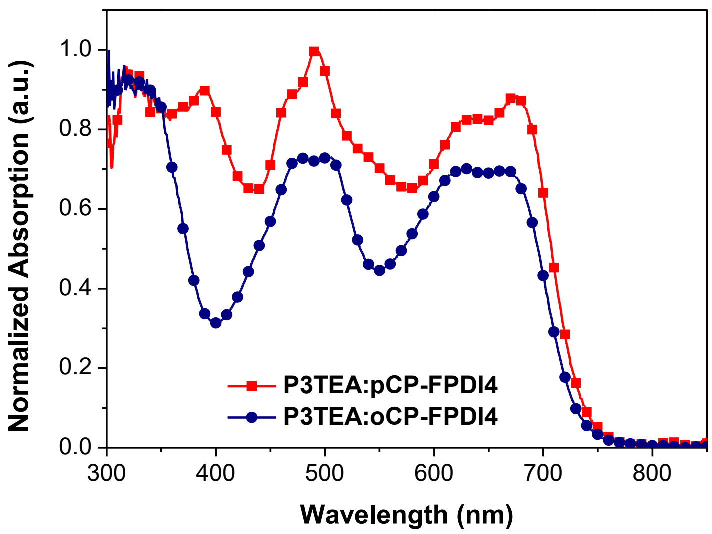


Figure S2. Blend film absorption of P3TEA:*o*CP-FPDI4 and P3TEA:*p*CP-FPDI4.

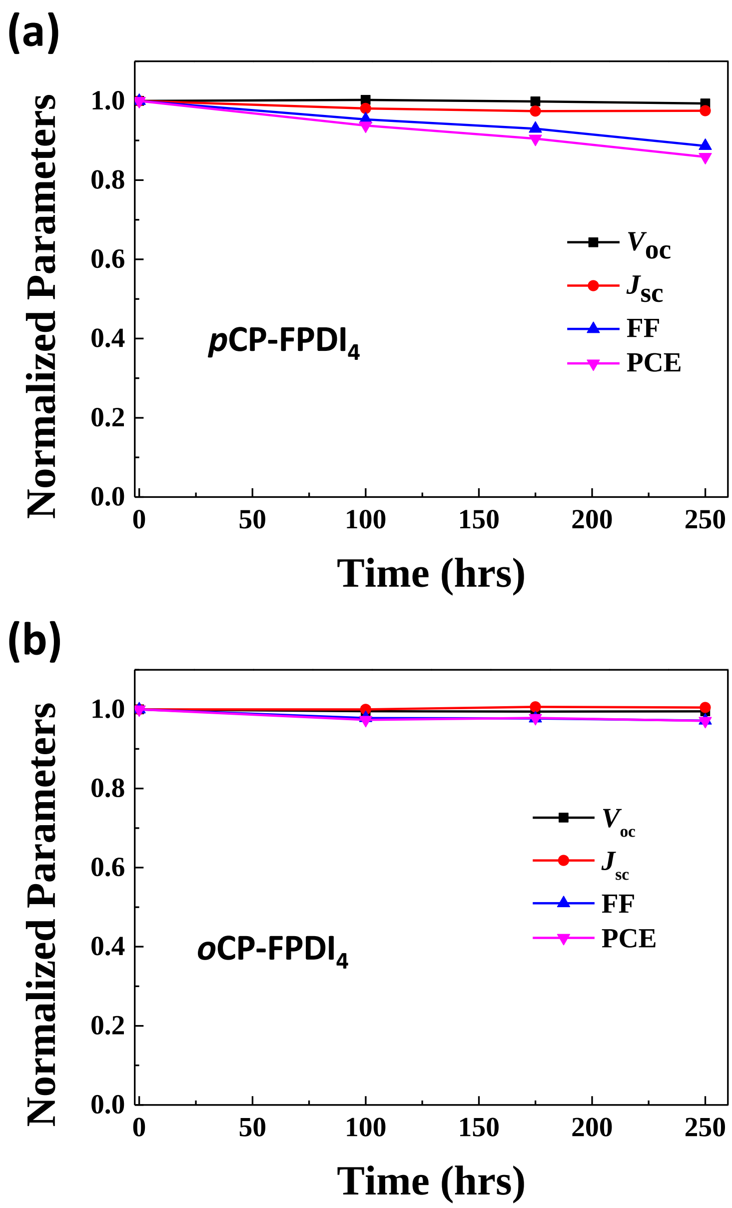


Figure S3. Shelf life stability plots of encapsulated devices based on (a) P3TEA: *p*CP-FPDI4 and (b) P3TEA: *o*CP-FPDI4 PDI for 250 hours.

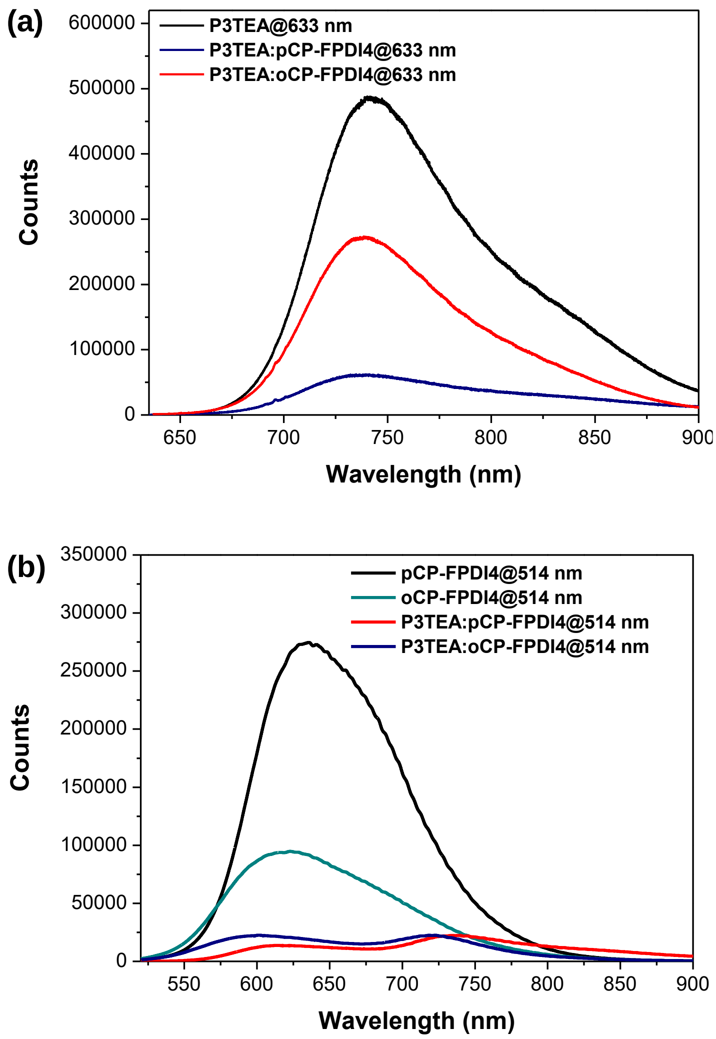
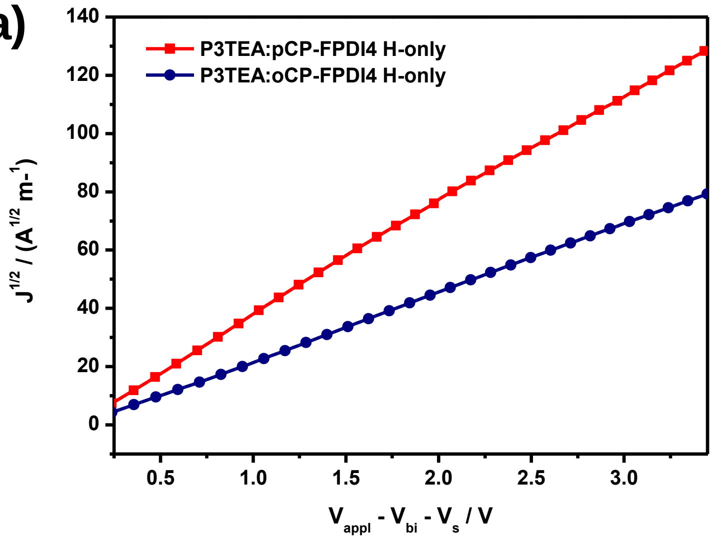


Figure S4. Photoluminescence quenching experiment of (a) the pristine P3TEA film, the P3TEA:*p*CP-FPDI4 and P3TEA: *o*CP-FPDI4 blend films excited at 633 nm; (b) the pristine *p*CP-FPDI4 film and P3TEA: *p*CP-FPDI4 blend films excited at 514 nm; the pristine *o*CP-FPDI4 film and P3TEA: *o*CP-FPDI4 blend films excited at 514 nm.

(a)



(b)

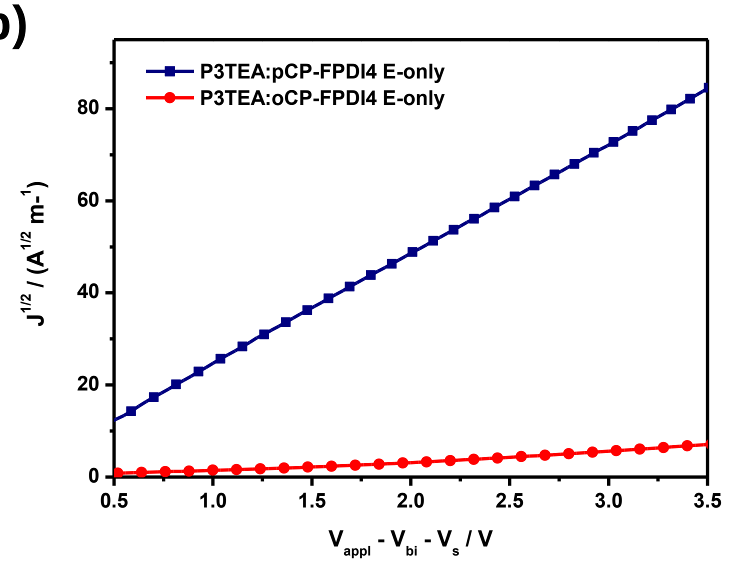


Figure S5. $J^{1/2}$~V characteristics of (a) hole-only devices and (b) electron-only devices of the P3TEA: *p*CP-FPDI4 and P3TEA: *o*CP-FPDI4 films.

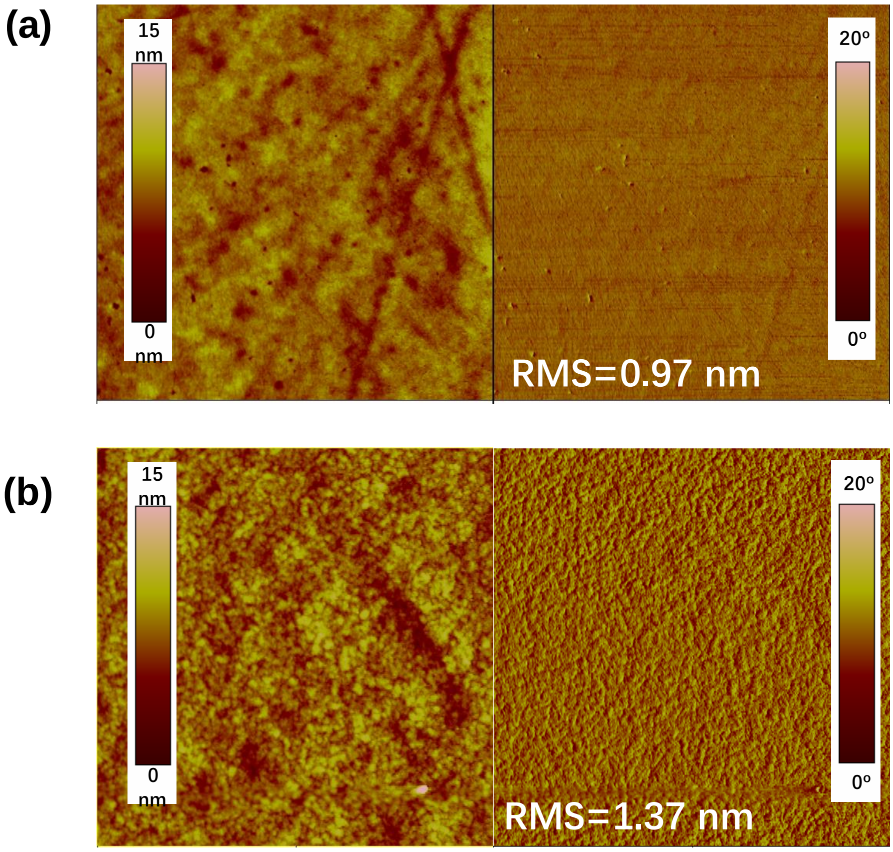


Figure S6. AFM images (5 μm × 5 μm) of (a) the P3TEA: *p*CP-FPDI4 blend, and (b) the P3TEA: *o*CP-FPDI4 blend.

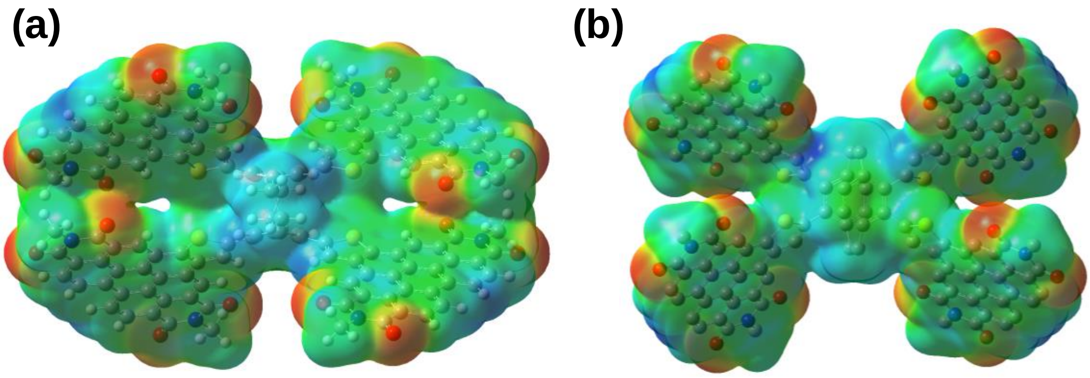
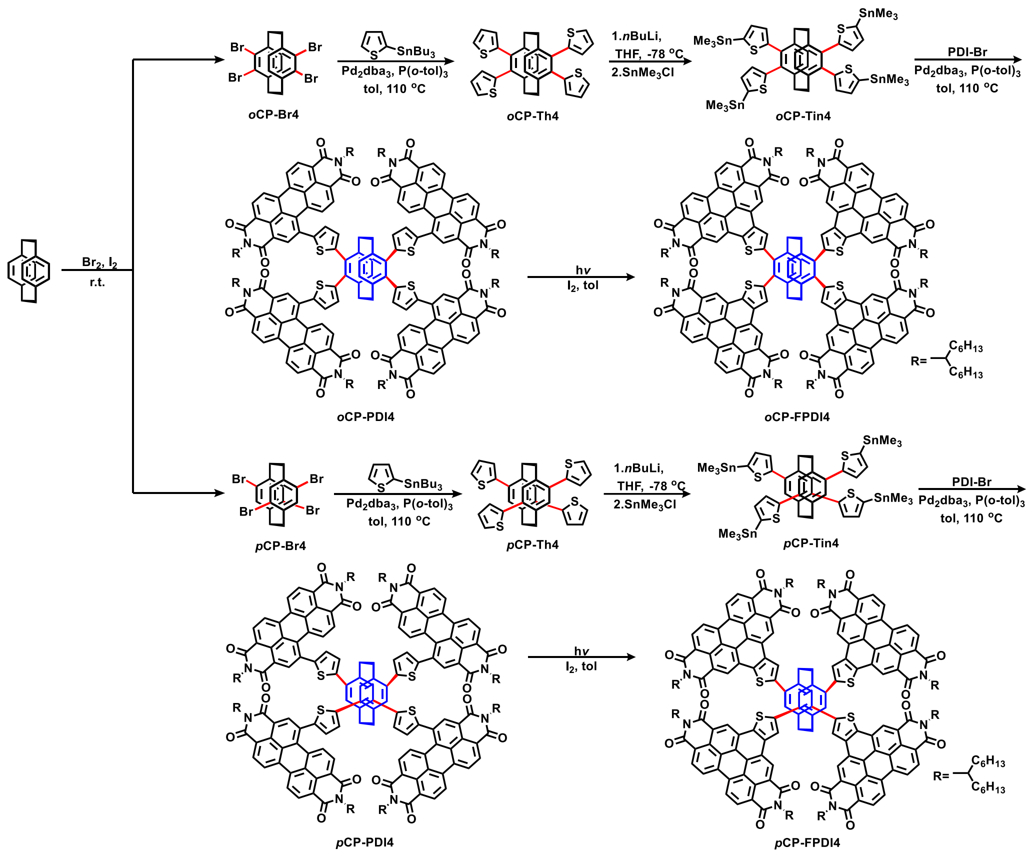


Figure S7. Electrostatic potential graphs of (a) *p*CP-FPDI4 and (b) *o*CP-FPDI4.

Synthesis of *o*CP-FPDI4 and *p*CP-FPDI4



Synthesis of *o*CP-Th4. To a solution of ***o*CP-Br4** (500 mg, 0.954 mmol), $Pd_2(dba)_3$ (73 mg, 0.127 mmol) and P(*o*-tol)$_3$ (155 mg, 0.508 mmol) in toluene (20 mL), 2-(tributylstannyl)thiophene (2.37 g, 6.35 mmol) was added under N_2. The reaction mixture was stirred for 12 h at 110 °C. Then, the reaction mixture was cooled and poured into an aqueous potassium fluoride. The mixture was extracted with chloroform. The combined organic phase was washed with water followed by brine. Then the solution was dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography (stationary phase: silica gel; eluent: n-hexane:DCM = 1:1) to get the product as light yellow solid (450 mg, 88%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.28 (dd, J = 5.1, 1.1 Hz, 4H), 6.95 (dd, J = 5.1, 3.5 Hz, 4H), 6.90 (s, 4H), 6.82 (dd, J = 3.5, 1.1 Hz, 4H), 3.04 (tq, J = 14.2, 10.5 Hz, 8H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.3, 140.3, 134.6, 131.8, 128.2, 126.5, 125.9, 33.9. HRMS (MALDI+) Calcd for $C_{32}H_{24}S_4$ (M+): 536.0761, Found: 536.0769.

Synthesis of *p*CP-Th4. To a solution of ***p*CP-Th4** (500 mg, 0.954 mmol), $Pd_2(dba)_3$ (73 mg, 0.127 mmol) and P(*o*-tol)$_3$ (155 mg, 0.508 mmol) in toluene (20 mL), 2-(tributylstannyl)thiophene (2.37 g, 6.35 mmol) was added under N_2. The reaction mixture was stirred for 12 h at 110 °C. Then, the reaction mixture was cooled and poured into an aqueous potassium fluoride. The mixture was extracted with chloroform. The combined organic phase was washed with water followed by brine. Then the solution was dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography (stationary phase: silica gel; eluent: n-hexane:DCM = 1:1) to get the product as light yellow solid (400 mg, 78%). m.p. 217 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37 (dd, J = 4.2, 2.1 Hz, 4H), 7.14-7.10 (m, 8H), 6.97 (s, 4H), 3.76-3.65 (m, 4H), 2.91-2.79 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 143.1, 137.0, 134.1, 132.8, 127.8, 125.7, 125.6. HRMS (MALDI+) Calcd for $C_{32}H_{24}S_4$ (M+): 536.0761, Found: 536.0747.

Synthesis of *o*CP-Tin4. To a solution of ***o*CP-Th4** (100 mg, 0.219 mmol) in anhydrous THF (50 mL) was added *n*-BuLi (0.55 mL, 1.09 mmol, 2 M in hexane) dropwise at -78 °C under N2. The mixture was kept at 0 °C for 1 h and then cooled to -78 °C again. Trimethyltin chloride (1.3 mL, 1.31 mmol, 1 M in hexane) was added dropwise and the mixture was allowed to react for 2 h. Then, the reaction mixture was poured into aqueous potassium fluoride and extracted with diethyl ether. The combined organic phase was washed with water followed by brine. Then the solution was dried over Na_2SO_4 and concentrated under reduced pressure. The crude product (light yellow solid, 218 mg, 90%) was directly used for the next step without further purification. ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.99 (d, J = 3.2 Hz, 4H), 6.89 (s, 4H), 6.86 (d, J = 3.2 Hz, 4H), 3.14-2.96 (m, 8H), 0.34 (m, 9H).

Synthesis of *p*CP-Tin4. To a solution of ***p*CP-Br4** (100 mg, 0.219 mmol) in anhydrous THF (50 mL) was added n-BuLi (0.55 mL,1.09 mmol, 2 M in hexane) dropwise at -78

^{o}C under N2. The mixture was kept at 0 ^{o}C for 1 h and then cooled to -78 ^{o}C again. Trimethyltin chloride (1.3 mL, 1.31 mmol, 1 M in hexane) was added dropwise and the mixture was allowed to react for 2 h. Then, the reaction mixture was poured into aqueous potassium fluoride and extracted with diethyl ether. The combined organic phase was washed with water followed by brine. Then the solution was dried over Na2SO4 and concentrated under reduced pressure. The crude product (light yellow solid, 201 mg, 83%) was directly used for the next step without further purification. ^{1}H NMR (400 MHz, $CDCl_3$): δ *J*7.22 (d, *J* = 3.3 Hz, 4H), 7.19 (d, *J* = 3.3 Hz, 4H), 6.97 (s, 4H), 3.77-3.66 (m, 4H), 2.94-2.82 (m, 4H), 0.42 (s, 9H).

Synthesis of *o*CP-PDI4. To a mixture of ***o*CP-Tin4** (100 mg, 0.0903 mmol), C6-PDI-Br (301 mg, 0.361 mmol), $Pd_2(dba)_3$ (8 mg, 0.00903 mmol) and P(*o*-tol)$_3$ (22 mg, 0.0722 mmol) in a microwave tube, toluene (5 mL) was added. The reaction was performed by using microwave reactor at 120 ^{o}C. After 2 h, the reaction was stopped and the mixture was extracted by chloroform. The combined organic phase was washed with water followed by brine. Then the solution was dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash column chromatography (stationary phase: silica gel; eluent: n-hexane: dichloromethane = 2:3) to get the product as dark violet solid (215 mg, 69%). The Stille coupling product is so active that it could be oxidized to cyclization under air condition during column chromatography process. We are not able to get the pure product so we used it directly without further purification. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.67-8.57 (m, 20H), 8.34 (s, 4H), 8.16 (m, 4H), 7.37 (s, 4H), 7.09 (s, 4H), 6.93 (s, 4H), 5.28-4.90 (m, 8H), 3.55-3.13 (m, 8H), 2.37-1.50 (m, 64H), 1.37-0.63 (m, 144H).

Synthesis of *p*CP-PDI4. To a mixture of ***p*CP-Tin4** (100 mg, 0.0903 mmol), C6-PDI-Br (301 mg, 0.361mmol), $Pd_2(dba)_3$ (8 mg, 0.00903 mmol) and P(*o*-tol)$_3$ (22 mg, 0.0722 mmol) in a microwave tube, toluene (5 mL) was added. The reaction was performed by using microwave reactor at 120 ^{o}C. After 2 h, the reaction was stopped and the mixture was extracted by chloroform. The combined organic phase was washed with water followed by brine. Then the solution was dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash column chromatography (stationary phase: silica gel; eluent: n-hexane: dichloromethane = 2:3) to get the product as dark red solid (234 mg, 75%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.80 (s, 4H), 8.46 (s, 8H), 8.28 (s, 4H), 8.11 (s, 4H), 7.80 (s, 4H), 7.47 (s, 4H), 7.33 (s, 4H), 6.92 (s, 4H), 5.28 (s, 4H), 4.94 (d, J = 34.5 Hz, 4H), 3.92 (s, 4H), 2.88 (dd, J = 6.8 Hz, 4H), 2.57-1.67 (m, 32H), 1.48-0.68 (m, 176H). ^{13}C NMR (100 MHz, CDCl3): δ 163.85, 145.60, 142.64, 136.73, 134.74, 133.56, 133.24, 132.78, 132.03, 129.57, 128.89, 128.60, 128.22, 127.63, 126.90, 123.02, 121.90, 54.36, 34.30, 32.41, 32.16, 31.83, 31.66, 29.13, 27.05, 26.92, 22.64, 14.07. MALDI-TOF MS: Calcd for $C_{232}H_{264}N_8O_{16}S_4$ (M+): 3548.88, Found: 3548.79.

Synthesis of *o*CP-FPDI4. To a standard photocyclization glassware was added 50 mg of ***o*CP-PDI4**, 50 ml of toluene and 1 mg of I_2 as catalyst. The mixture was illuminated by 500 W mercury lamp for 2 hours. The solvent was removed under reduced pressure. The crude product was purified by flash column chromatography (stationary phase: silica gel; eluent: Chloroform) to afford ***o*CP-FPDI4** as orange (yield: 85%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.90 (s, 4H), 9.52 (s, 4H), 9.11 (s, 8H), 8.89 (s, 8H), 8.65 (s, 4H), 7.69 (s, 4H), 5.22 (d, J = 29.4 Hz, 8H), 3.64 (s, 8H), 2.25 (d, J = 9.8 Hz, 16H), 1.84 (s, 16H), 1.43-0.58 (m, 176H). ^{13}C NMR (100 MHz, CDCl3): 165.11, 164.01, 144.16, 144.18, 140.41, 137.05, 134.09, 133.50, 132.97, 129.26, 128.48, 126.94, 126.43, 125.84, 124.44, 123.45, 123.06, 122.70, 122.02, 54.92, 35.44, 34.51, 33.04, 32.42, 31.71, 31.63, 30.51, 29.72, 29.54, 29.21, 29.11, 28.16, 26.92, 24.68, 22.54, 22.47, 13.99, 13.94. MALDI-TOF MS: Calcd for $C_{232}H_{256}N_8O_{16}S_4$ (M+): 3537.83, Found: 3537.47.

Synthesis of *p*CP-FPDI4. To a standard photocyclization glassware was added 50 mg of ***p*CP-PDI4**, 50 ml of toluene and 1 mg of I_2 as catalyst. The mixture was illuminated by 500 W mercury lamp for 2 hours. The solvent was removed under reduced pressure.

The crude product was purified by flash column chromatography (stationary phase: silica gel; eluent: n-hexane: dichloromethane = 1:2) to afford ***p*CP-FPDI4** as red solid (yield: 91%). ^{1}H NMR (400 MHz, $C_2D_2Cl_4$, 333 K): δ 9.79 (s, 4H), 9.50 (s, 4H), 9.35 (s, 8H), 9.04 (s, 8H), 8.80 (s, 4H), 7.95 (s, 4H), 4.99 (s, 8H), 4.47 (s, 4H), 3.73 (s, 4H), 2.61-2.01 (br, 32H), 1.51-1.31 (br, 128H), 0.98-0.72 (br, 48H). ^{13}C NMR (100 MHz, CDCl3): 163.85, 145.60, 142.64, 136.73, 134.74, 133.56, 133.24, 132.78, 132.03, 129.57, 128.89, 128.60, 128.22, 127.63, 126.90, 123.02, 121.90, 54.36, 34.30, 32.41, 32.16, 31.83, 31.66, 29.13, 27.05, 26.92, 22.64, 14.07. MALDI-TOF MS: Calcd for $C_{232}H_{256}N_8O_{16}S_4$ (M+): 3537.83, Found: 3537.74.

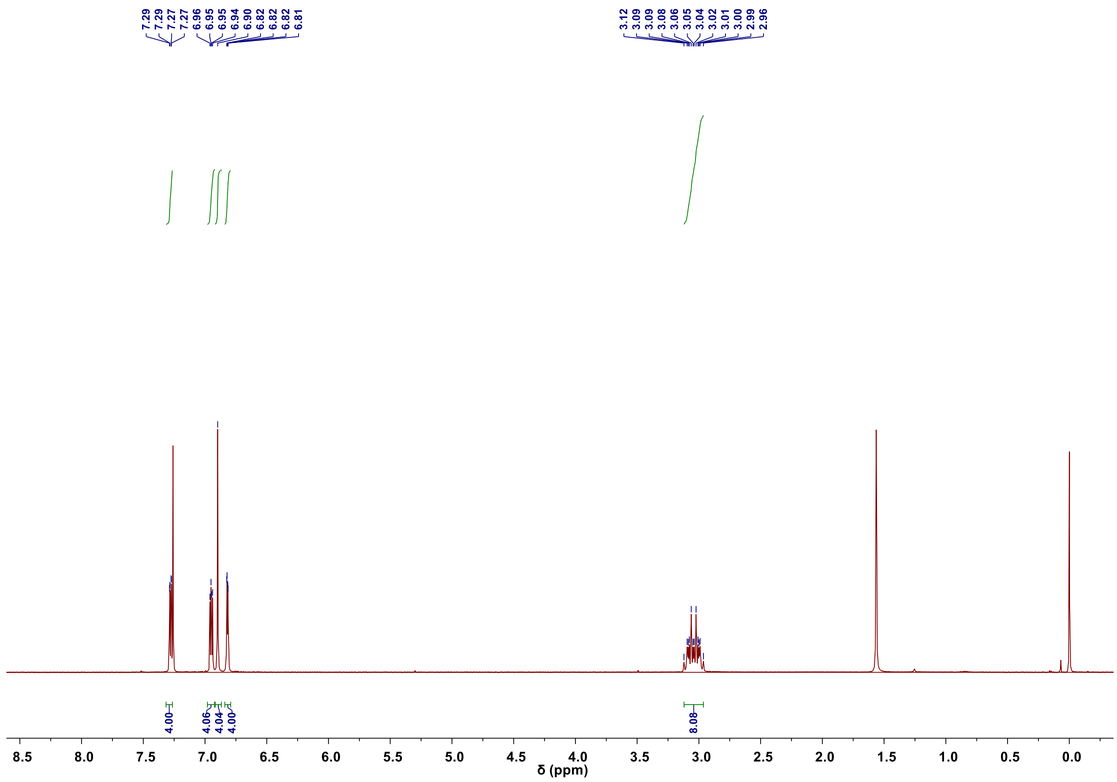


Figure S8. ^{1}H NMR spectrum of *o*CP-Th4.

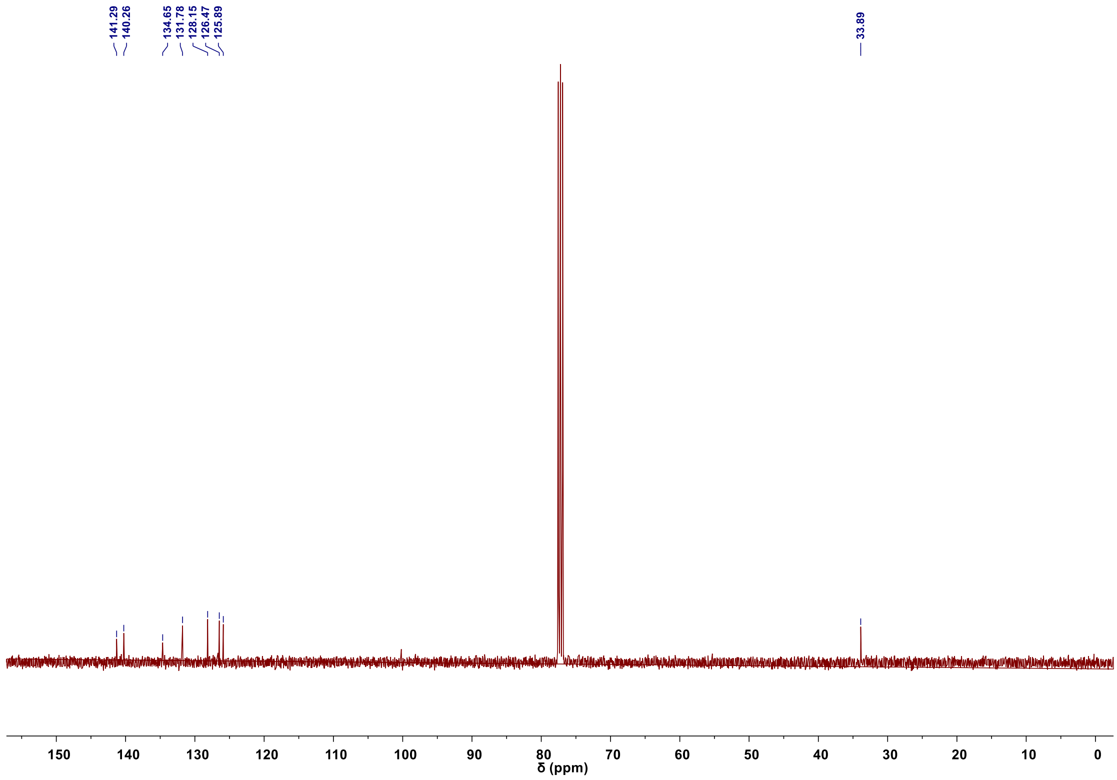


Figure S9. ^{13}C NMR spectrum of *o*CP-Th4.

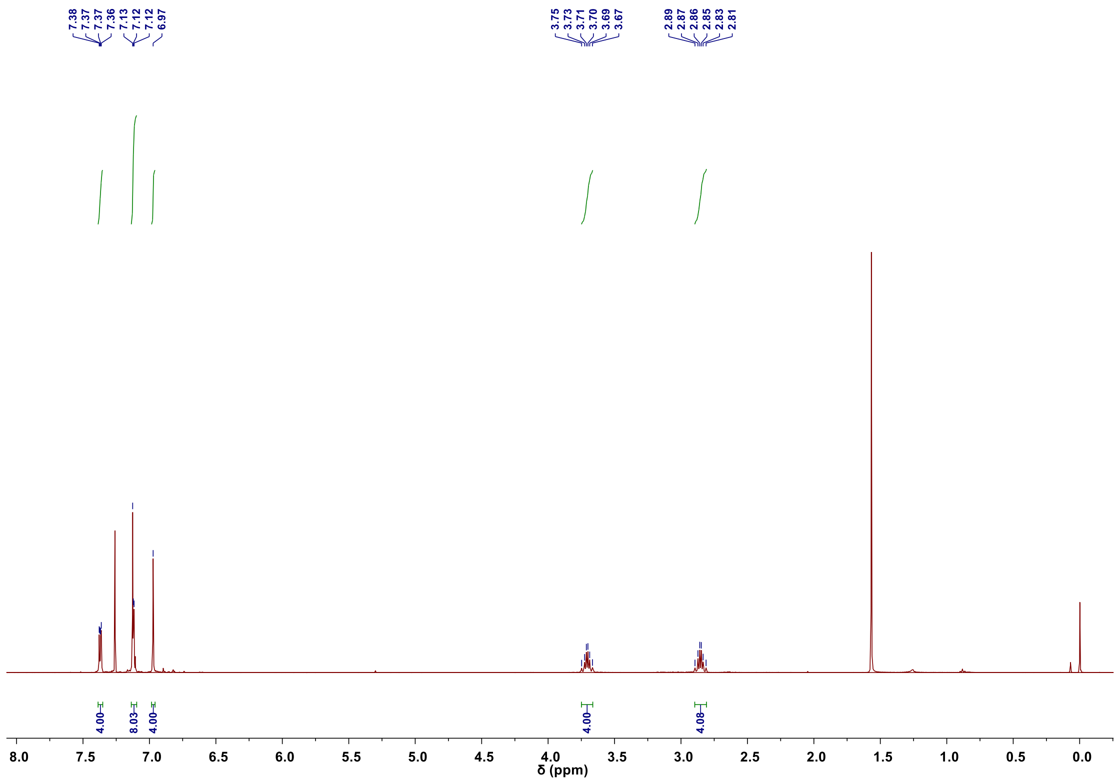


Figure S10. ^{1}H NMR spectrum of *p*CP-Th4.

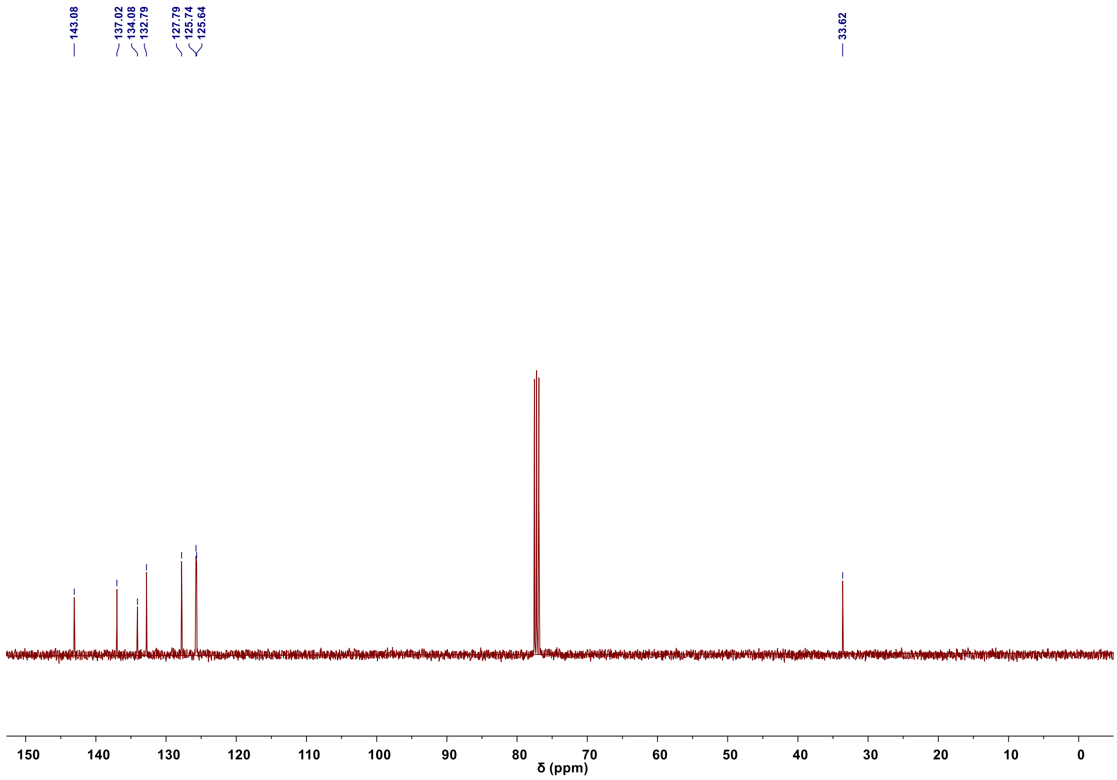


Figure S11. ^{13}C NMR spectrum of *p*CP-Th4.

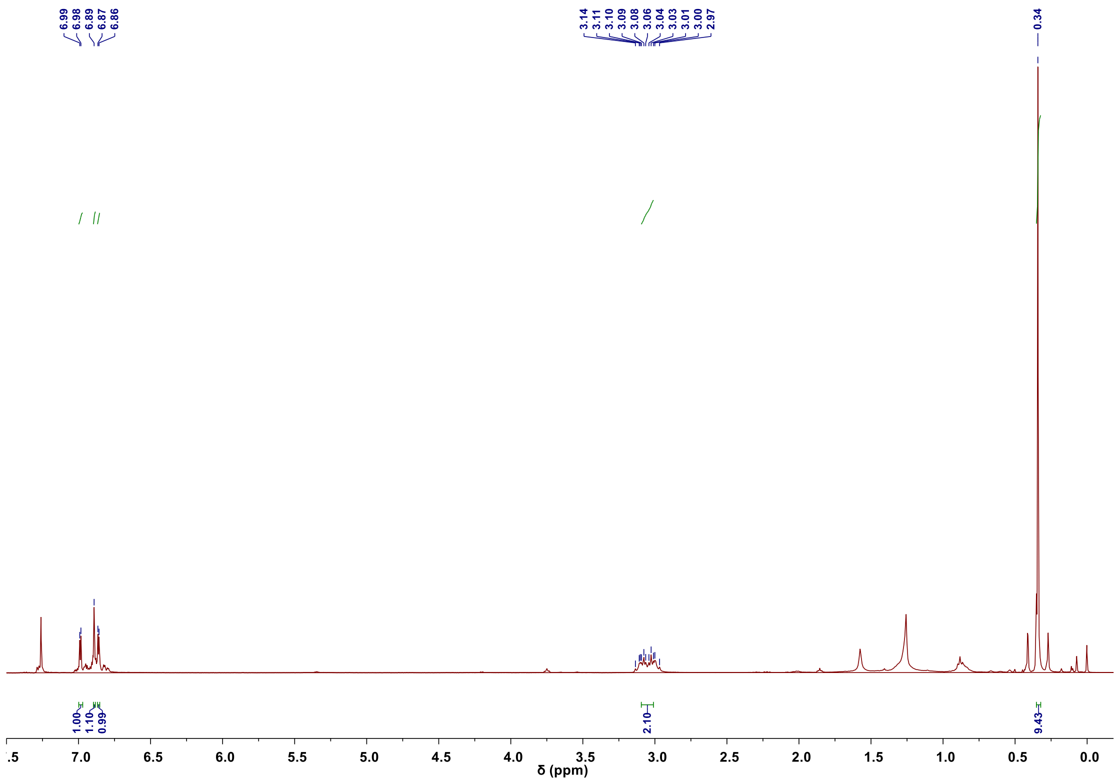


Figure S12. ^{1}H NMR spectrum of *o*CP-Tin4.

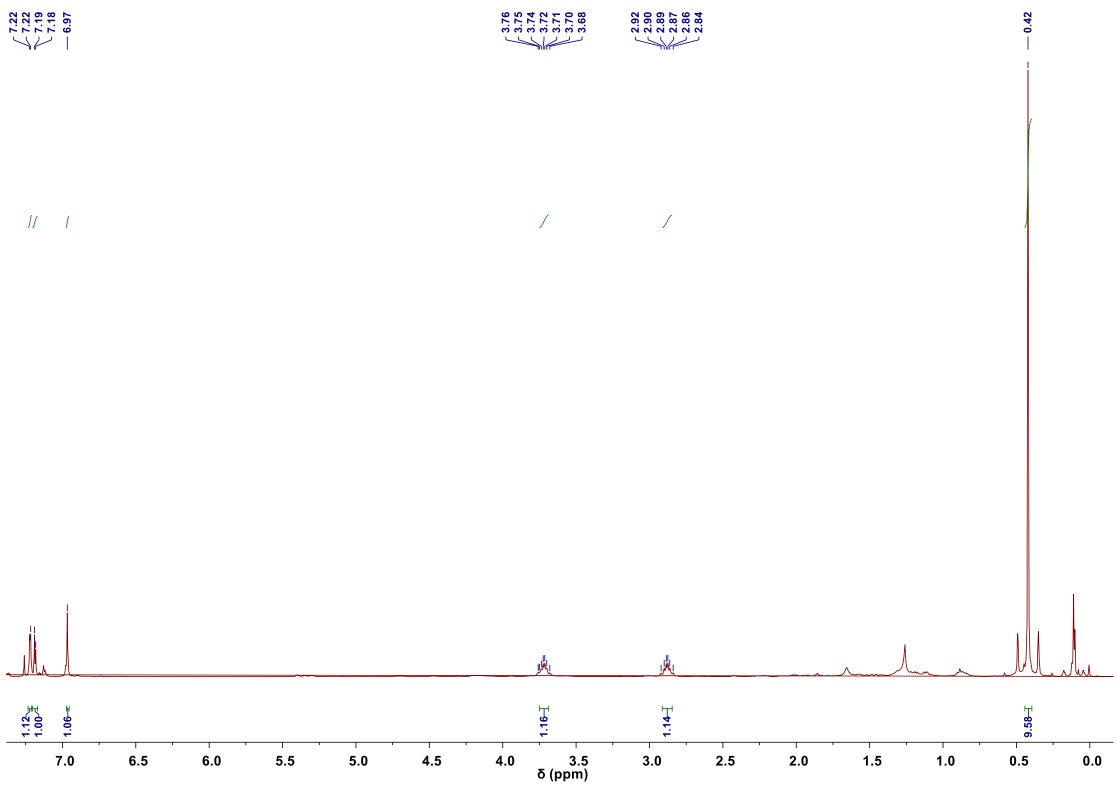


Figure S13. ^{1}H NMR spectrum of *p*CP-Tin4.

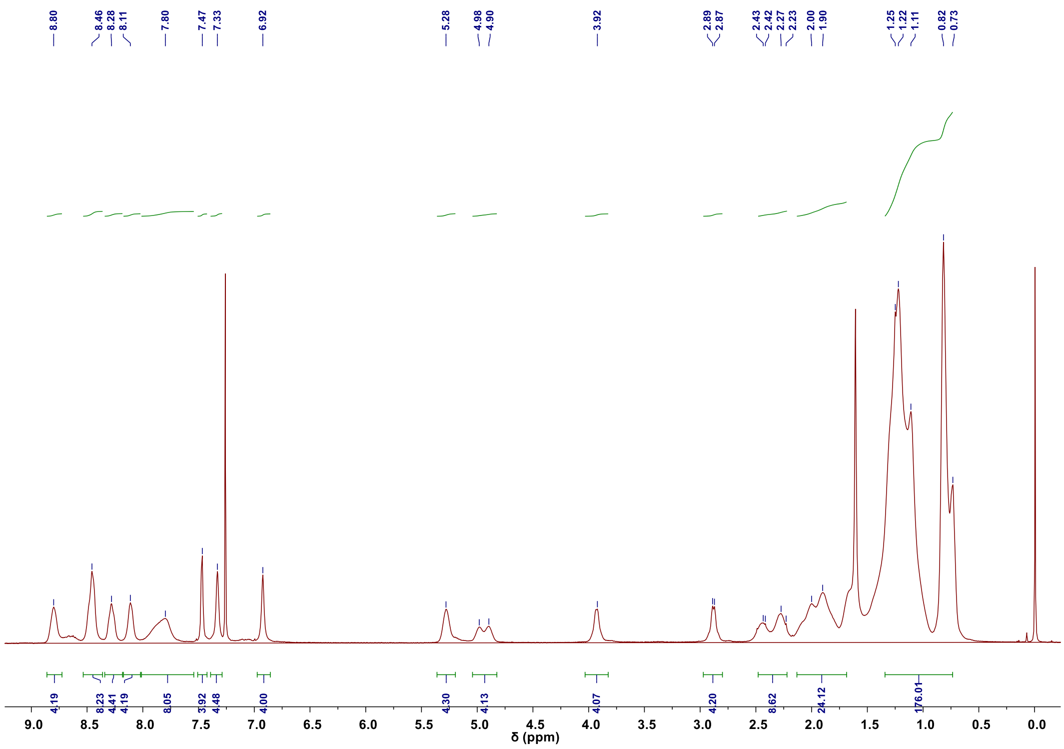


Figure S14. ^{1}H NMR spectrum of *p*CP-PDI4.

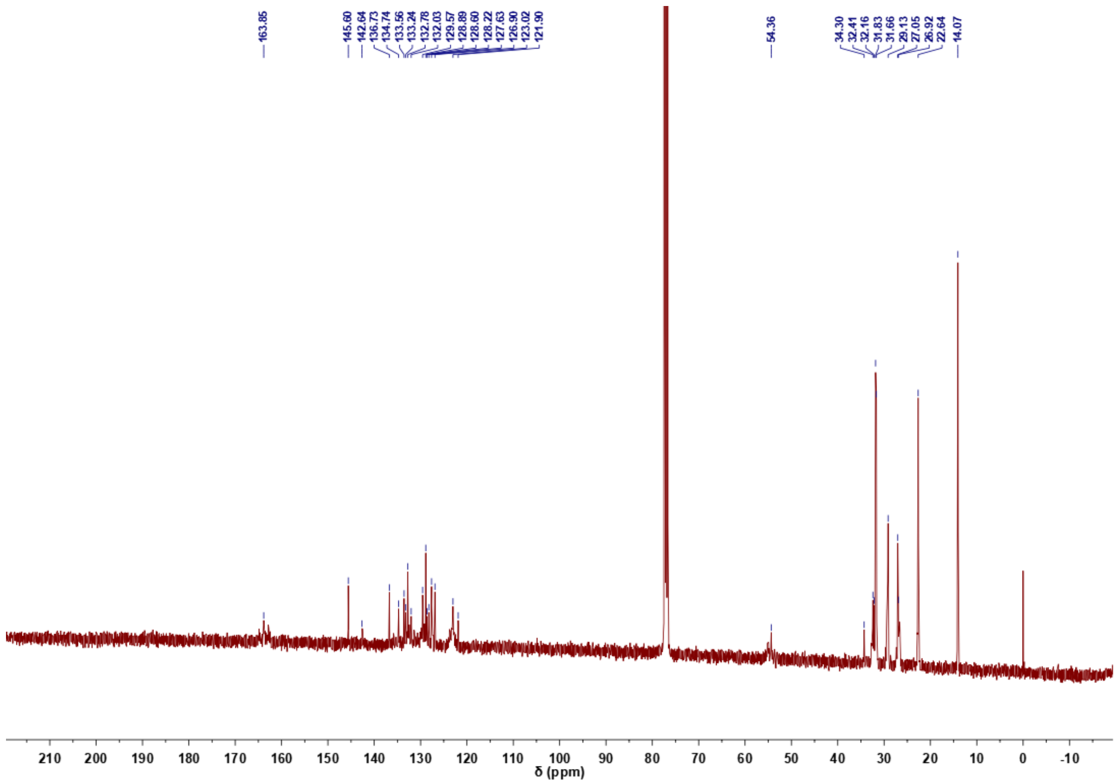


Figure S15. ^{13}C NMR spectrum of *p*CP-PDI4.

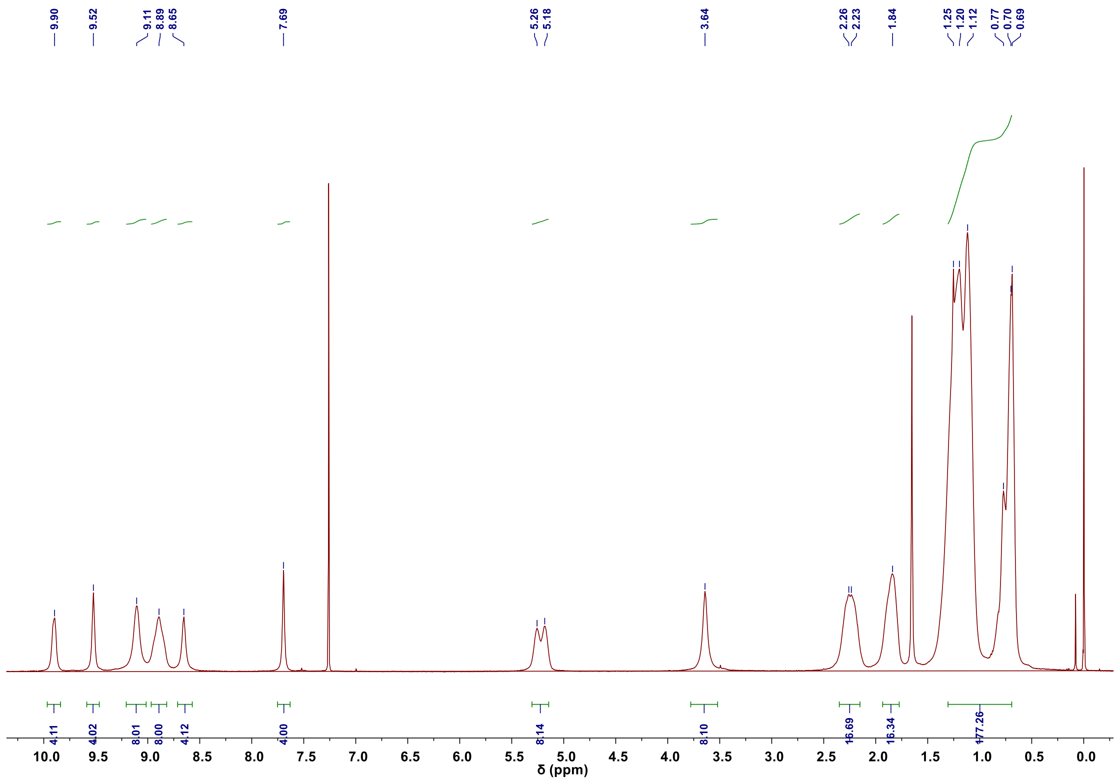


Figure S16. ^{1}H NMR spectrum of *o*CP-FPDI4.

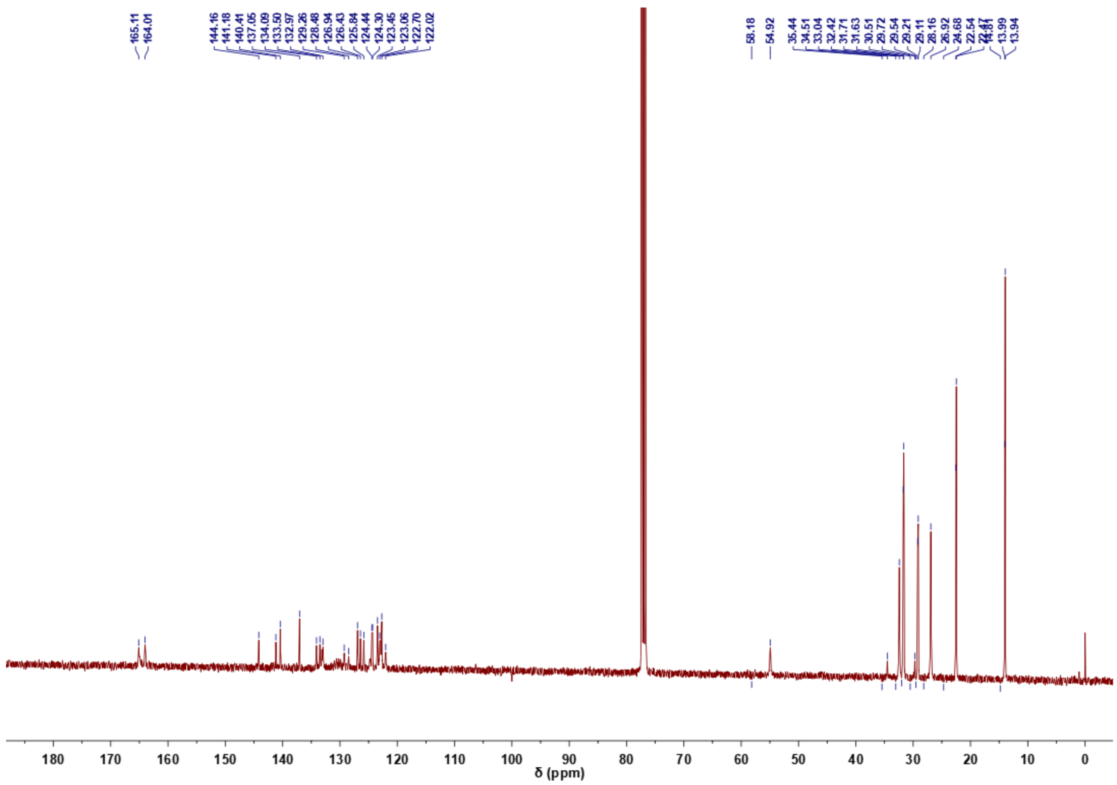


Figure S17. ^{13}C NMR spectrum of *o*CP-FPDI4.

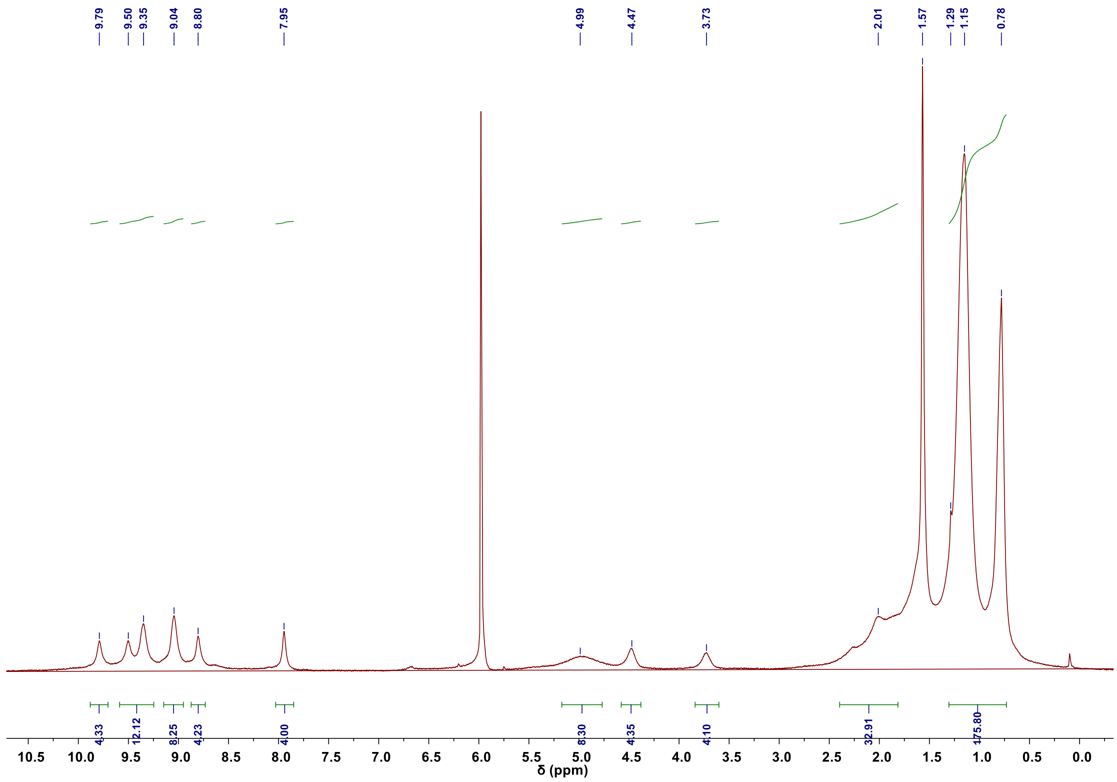


Figure S18. ^{1}H NMR spectrum of *p*CP-FPDI4 (CD_2Cl_4, 60 ºC).

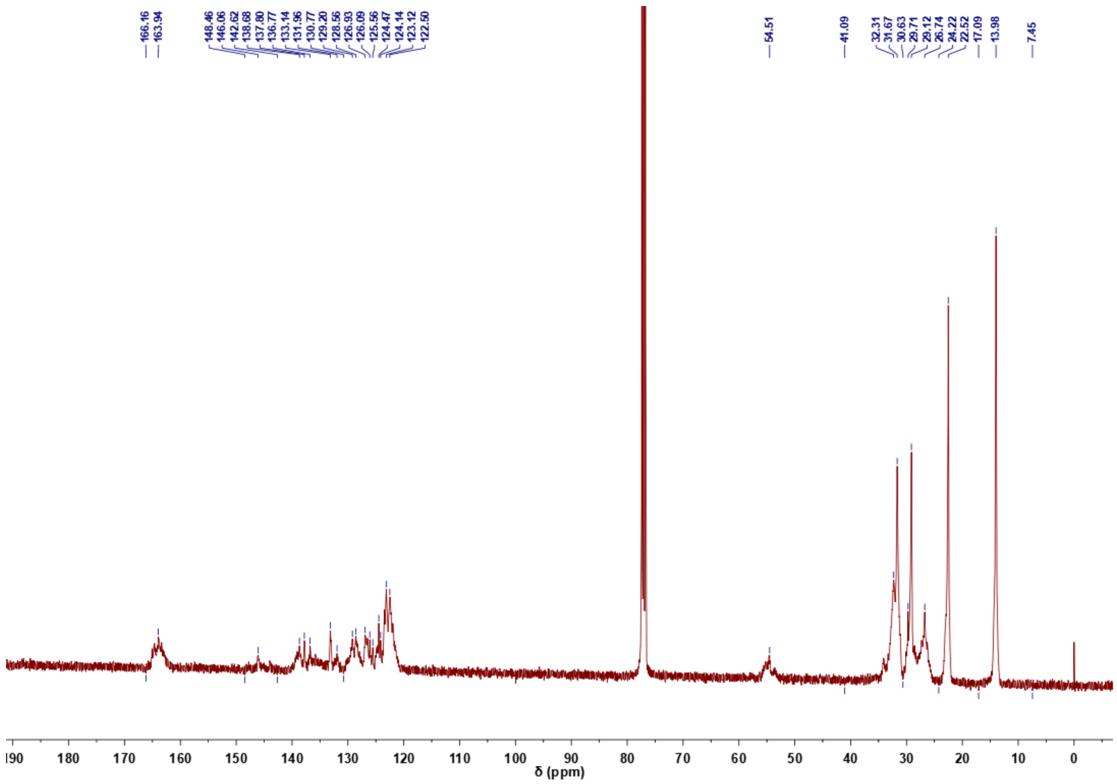


Figure S19. ^{13}C NMR spectrum of *p*CP-FPDI4.

Table S1. OSC performance metrics for the reported PDI-based devices.

Donor	**Acceptor**	***PCE*** (%)	V_{OC} (V)	***FF*** (%)	J_{SC} (mA·cm^{-2})	**Ref**
PTB7-Th	di-PBI	5.9	0.80	59	12.0	*Adv. Mater.*, 2014, **26**, 5708
P3TEA	SF-PDI$_2$	9.5	1.11	64	13.3	*Nat. Energy*, 2016, **1**, 16089
PDBT-T1	SdiPBI-S	7.2	0.90	66	11.7	*JACS*, 2015, **137**, 11156
PDBT-T1	SdiPBI-Se	8.4	0.95	70	12.5	*JACS*, 2016, **138**, 375
PTB7-Th	TPE-PDI$_4$	5.5	0.91	52	11.7	*Adv. Mater.*, 2015, **27**, 1015
PffBT-T3(1,2)-2	TPPz-PDI$_4$	7.1	0.99	56	12.5	*Adv. Mater.*, 2016, **28**, 8546
PTB7-Th	TPB	8.5	0.79	58	17.9	*JACS*, 2016, **138**, 7248
PTB7-Th	helical PDI	6.1	0.80	55	13.5	
PTB7-Th	hPDI3	7.9	0.80	67	14.3	*Nat. Commun*, 2015, **6**, 8242
PTB7-Th	hPDI4	8.3	0.80	68	15.0	
PTB7-Th	FPDI-T	3.0	0.91	39	8.5	
PTB7-Th	FPDI-T	6.7	0.93	58	12.0	*Adv. Mater.*, 2016, **28**, 951
PTB7-Th	FPDI-Se	5.8	0.92	55	11.2	
PDBT-T1	TPH	8.3	0.97	70	12.0	*JACS*, 2016, **138**, 10184
PDBT-T1	TPH-Se	9.3	1.00	72	12.5	
P3TEA	FTTB-PDI4	10.6	1.13	66	13.9	*JACS*, 2017, **139**, 16092
PTTEA	Aq$_3$-PDI	7.8	0.87	66	13.6	*Adv. Funct. Mater.*, 2019,
PTTEA	Aq$_3$-PDI2	9.5	0.85	71	15.7	**29**, 1902079
PTTEA	TPP-PDI	6.2	1.02	50	12.2	
PTTEA	TPO-PDI	11.0	0.99	75	14.9	*Adv. Funct. Mater.*, 2019,
PTTEA	TPD-PDI	9.7	0.97	70	14.2	**29**, 1906587
P3TEA	*p*CP-FPDI4	9.1	1.16	57	13.8	***This work***
P3TEA	*o*CP-FPDI4	2.4	1.16	34	6.1	***This work***

Cartesian coordinates of optimized molecular geometry of *p*CP-FPDI4

C	-1.08713	-0.80042	-1.61268	**C**	-9.4419	-0.44939	-1.71336
C	-1.25721	0.59317	-1.71002	**C**	-11.68613	-1.42097	-1.3845
C	-0.12417	1.40932	-1.43428	**C**	-3.40161	9.00955	-6.61601
C	1.12411	0.80946	-1.60244	**O**	-6.13963	9.03043	-6.89814
C	1.29512	-0.58441	-1.69685	**O**	-2.43606	6.88534	-5.29705
C	0.15908	-1.40011	-1.43119	**O**	-12.69958	0.76695	-2.56168
C	2.59598	-1.16104	-2.04946	**O**	-8.95096	-1.39461	-1.10857
C	-2.55633	1.16791	-2.07223	**C**	8.7537	-6.05582	-5.36131
C	-2.78805	2.33836	-2.75308	**C**	8.22785	-4.94538	-4.6825
C	-4.16739	2.58831	-3.03594	**C**	6.81277	-4.86492	-4.50852
C	-4.99636	1.56155	-2.56111	**C**	5.98572	-5.90875	-5.01317
S	-4.06886	0.30532	-1.78159	**C**	6.55594	-7.00569	-5.685
C	2.82934	-2.33793	-2.71872	**C**	7.93615	-7.06805	-5.8555
C	4.20865	-2.58846	-3.00065	**C**	6.20535	-3.75594	-3.83693
C	5.03659	-1.55572	-2.53712	**C**	4.79381	-3.71147	-3.67481
S	4.10793	-0.29325	-1.76891	**C**	4.00243	-4.77543	-4.18343
C	-6.41077	1.59193	-2.68929	**C**	4.57239	-5.84042	-4.83374
C	-6.99121	2.70551	-3.35675	**C**	9.07163	-3.87555	-4.14579
C	-8.41208	2.78069	-3.50273	**C**	8.45193	-2.774	-3.48191
C	-9.22285	1.74169	-2.96246	**C**	7.03153	-2.70187	-3.32962
C	-8.61251	0.63887	-2.29211	**C**	10.47153	-3.88856	-4.25166
C	-7.25013	0.57007	-2.16637	**C**	11.25519	-2.86484	-3.72796
C	-9.03168	3.8788	-4.17239	**C**	10.66113	-1.78386	-3.08179
C	-10.43215	3.89633	-4.26955	**C**	9.26214	-1.72781	-2.95476
C	-11.21644	2.88019	-3.73207	**C**	8.65181	-0.62286	-2.28792
C	-10.62235	1.80233	-3.08082	**C**	7.28987	-0.55726	-2.15563
C	-6.16417	3.75291	-3.87629	**C**	6.45081	-1.58444	-2.66868
C	-6.77137	4.85746	-4.55534	**C**	11.51586	-0.70785	-2.52876
C	-8.18703	4.94057	-4.7236	**N**	10.86499	0.37667	-1.92082
C	-4.75211	3.70615	-3.71911	**C**	9.4818	0.46991	-1.71878
C	-3.9599	4.76307	-4.24093	**C**	3.69709	-6.92345	-5.34794
C	-4.52961	5.82334	-4.89918	**N**	4.3242	-7.98469	-6.00937
C	-5.94348	5.894	-5.07341	**C**	5.70976	-8.10117	-6.2174
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C	-7.89416	7.05072	-5.91871	**C**	11.71908	1.45993	-1.41752
C	-8.71255	6.04584	-5.41105	**O**	8.99389	1.41303	-1.10817
C	-3.65341	6.89883	-5.42746	**O**	12.73813	-0.73703	-2.58794
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C	-5.66636	8.0738	-6.30004	**O**	6.18332	-9.06225	-6.80807
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N	-10.82696	-0.34756	-1.89988	**C**	1.25687	0.59288	1.70679

C	1.08717	-0.80071	1.6089	**O**	12.69896	0.7692	2.56335
C	-0.15891	-1.40064	1.42722	**O**	8.95162	-1.39108	1.10489
C	-1.29515	-0.58532	1.69319	**C**	-8.7497	-6.05828	5.36324
C	-1.12452	0.80861	1.59923	**C**	-8.2247	-4.94804	4.68342
C	-2.59574	-1.16248	2.04593	**C**	-6.80976	-4.86718	4.50845
C	2.55575	1.16786	2.0695	**C**	-5.98201	-5.91044	5.01313
C	2.78685	2.33779	2.75144	**C**	-6.55139	-7.00719	5.68597
C	4.16602	2.588	3.0349	**C**	-7.93147	-7.06994	5.85744
C	4.99552	1.56202	2.55931	**C**	-6.20319	-3.75833	3.83589
S	4.0687	0.30617	1.77836	**C**	-4.79176	-3.7134	3.67291
C	-2.82835	-2.33936	2.71548	**C**	-3.99966	-4.77681	4.18156
C	-4.20742	-2.59041	2.99801	**C**	-4.56882	-5.84168	4.83278
C	-5.03601	-1.55817	2.53452	**C**	-9.06921	-3.87882	4.14668
S	-4.10818	-0.29548	1.76562	**C**	-8.45035	-2.77742	3.48176
C	6.40988	1.59276	2.68802	**C**	-7.03007	-2.70483	3.32853
C	6.98967	2.70576	3.35701	**C**	-10.46902	-3.89224	4.25356
C	8.41045	2.78117	3.50378	**C**	-11.25341	-2.86907	3.72987
C	9.2218	1.74303	2.96272	**C**	-10.66016	-1.78825	3.08268
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C	6.16209	3.75231	3.87738	**C**	-9.48262	0.46508	1.71745
C	6.76863	4.85624	4.55801	**C**	-3.69279	-6.92408	5.34704
C	8.18418	4.93955	4.72708	**N**	-4.31908	-7.98518	6.00946
C	4.75011	3.7053	3.7195	**C**	-5.70447	-8.10208	6.21841
C	3.95735	4.7614	4.24214	**C**	-3.4406	-9.04644	6.51457
C	4.52643	5.82107	4.90189	**C**	-11.72035	1.45445	1.41761
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C	6.50948	6.98335	5.75845	**O**	-12.73788	-0.74237	2.58987
C	7.89012	7.04822	5.9245	**O**	-2.47604	-6.91234	5.21097
C	8.70904	6.04416	5.41609	**O**	-6.1773	-9.06302	6.8099
C	3.64966	6.89568	5.43101	**C**	0.23956	2.76816	0.75936
N	4.27588	7.95158	6.10177	**C**	-0.26586	-2.75798	0.74877
C	5.66184	8.07024	6.30591	**C**	0.26629	-2.75766	-0.75319
C	11.4763	0.73677	2.51273	**C**	-0.24036	2.76837	-0.76178
N	10.82702	-0.34444	1.89832	**H**	-1.97091	-1.4343	-1.60916
C	9.44208	-0.44647	1.71105	**H**	2.00762	1.44366	-1.59164
C	11.68687	-1.41698	1.38221	**H**	-1.98045	2.98231	-3.076
C	3.39666	9.00488	6.62201	**H**	2.02259	-2.98583	-3.03566
O	6.13456	9.02634	6.90528	**H**	-6.82708	-0.28336	-1.64651
O	2.43238	6.88199	5.3	**H**	-10.93175	4.71794	-4.76819

H	-12.29772	2.90728	-3.80813	**H**	2.87865	4.75406	4.13501
H	-2.88116	4.75592	-4.13434	**H**	8.30824	7.89646	6.45476
H	-8.31278	7.89945	-6.44778	**H**	9.77816	6.13283	5.56557
H	-9.78176	6.13439	-5.55989	**H**	11.04455	-2.24264	1.08688
H	-12.26225	-1.07596	-0.52206	**H**	12.38491	-1.72257	2.16227
H	-12.38759	-1.72245	-2.16304	**H**	12.26682	-1.06929	0.52345
H	-11.04378	-2.24859	-1.09477	**H**	4.02172	9.74197	7.11915
H	-2.68333	8.57932	-7.31677	**H**	2.67801	8.57352	7.32169
H	-2.84598	9.46596	-5.79421	**H**	2.84147	9.46231	5.80047
H	-4.02715	9.74718	-7.11174	**H**	-9.8184	-6.14555	5.51644
H	9.82254	-6.14283	-5.51371	**H**	-8.34969	-7.92249	6.38066
H	8.35503	-7.92075	-6.37795	**H**	-2.92144	-4.7713	4.06985
H	2.92413	-4.77028	-4.07238	**H**	-10.96803	-4.71586	4.74946
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H	12.33604	-2.88816	-3.81113	**H**	-6.86779	0.29379	1.63511
H	6.86704	0.29765	-1.638	**H**	-2.89	-9.49625	5.68579
H	2.89523	-9.49585	-5.68575	**H**	-4.0656	-9.78728	7.00618
H	2.72429	-8.62562	-7.21685	**H**	-2.71795	-8.62474	7.21603
H	4.07205	-9.78763	-7.0049	**H**	-12.22709	1.15601	0.49561
H	12.2263	1.16143	-0.49579	**H**	-11.08704	2.31673	1.22416
H	11.08517	2.32165	-1.22356	**H**	-12.47899	1.68087	2.16625
H	12.47738	1.68728	-2.16623	**H**	1.27734	3.09951	0.78906
H	1.97112	-1.43436	1.60515	**H**	-0.34998	3.53055	1.28171
H	-2.00819	1.44259	1.58868	**H**	0.29608	-3.52942	1.2883
H	1.97891	2.98113	3.07473	**H**	-1.30815	-3.07701	0.74212
H	-2.02116	-2.98678	3.03232	**H**	-0.29549	-3.52903	-1.293
H	6.82726	-0.28112	1.64315	**H**	1.30863	-3.0765	-0.74661
H	10.92893	4.71752	4.77301	**H**	-1.27821	3.09952	-0.79131
H	12.2959	2.90828	3.81169	**H**	0.349	3.53108	-1.28388

Cartesian coordinates of optimized molecular geometry of *o*CP-FPDI4

C	1.27363	-1.6729	-1.39929	**C**	7.45076	-1.81948	5.56584
C	0.30404	-1.31725	-2.3204	**C**	8.57208	-1.5753	7.74215
C	0.08529	0.02934	-2.60942	**C**	7.30891	-8.30439	-4.83569
C	0.86783	0.97933	-2.01722	**O**	9.255	-8.94054	-3.06092
C	2.13065	0.67782	-1.33648	**O**	5.59328	-6.36374	-4.02974
C	2.28502	-0.75281	-0.93789	**O**	10.15845	-3.64424	7.06971
C	3.17326	1.3401	-2.24372	**O**	6.71492	-0.8708	5.86986
C	3.27022	-1.53189	-0.15153	**C**	8.96321	7.04731	0.99471
C	3.86109	-2.69549	-0.72041	**C**	8.48143	6.08599	0.085
C	4.97917	-3.20027	-0.00983	**C**	7.1322	5.63739	0.26321
C	5.19825	-2.43581	1.18165	**C**	6.34423	6.13266	1.34491
S	4.11946	-1.15346	1.25419	**C**	6.87158	7.09574	2.2331
C	3.53121	2.40926	-1.27916	**C**	8.18154	7.5466	2.03938
C	4.66944	3.25309	-1.34184	**C**	6.56736	4.68683	-0.64466
C	5.41881	2.93263	-2.46055	**C**	5.23498	4.21017	-0.42405
S	4.28574	2.04675	-3.21176	**C**	4.49593	4.70645	0.6792
C	6.21769	-2.81885	2.12738	**C**	5.0176	5.65826	1.54159
C	7.06403	-3.92749	1.81481	**C**	9.29172	5.54117	-0.9961
C	8.08193	-4.31824	2.74331	**C**	8.71115	4.60993	-1.91473
C	8.20964	-3.62904	3.98594	**C**	7.35218	4.2056	-1.74888
C	7.34504	-2.53973	4.29202	**C**	10.64673	5.87302	-1.19218
C	6.38897	-2.1496	3.36604	**C**	11.40678	5.32814	-2.23056
C	8.96753	-5.39869	2.42514	**C**	10.84032	4.42563	-3.13963
C	9.93366	-5.74599	3.39008	**C**	9.48196	4.0682	-2.98763
C	10.04425	-5.08021	4.61195	**C**	8.89178	3.15612	-3.91014
C	9.18975	-4.01649	4.92644	**C**	7.5532	2.81459	-3.76954
C	6.91058	-4.63469	0.57225	**C**	6.77602	3.31877	-2.69686
C	7.80843	-5.69736	0.23395	**C**	11.65763	3.86956	-4.2225
C	8.84428	-6.08003	1.14551	**N**	11.02807	2.95427	-5.08622
C	5.8673	-4.28658	-0.33489	**C**	9.67749	2.57127	-5.00246
C	5.74975	-4.98927	-1.56031	**C**	4.18765	6.16331	2.64134
C	6.63306	-5.99441	-1.91918	**N**	4.75723	7.14797	3.46321
C	7.6738	-6.36296	-1.0212	**C**	6.07501	7.62665	3.34465
C	8.57357	-7.38691	-1.39185	**C**	3.92407	7.6784	4.53812
C	9.58553	-7.75295	-0.49605	**C**	11.82413	2.39696	-6.1763
C	9.70838	-7.1167	0.74109	**O**	9.21179	1.76624	-5.81849
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C	8.46787	-8.06167	-2.68998	**O**	6.50999	8.4605	4.14751
C	9.32499	-3.32734	6.21256	**C**	-2.01388	0.48553	-0.25679
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C	-0.76042	-1.49224	0.5573	**O**	-11.27853	-2.74686	6.25991
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C	-2.99328	1.40297	-0.89571	**C**	-7.40588	5.6525	-0.16646
C	-2.96737	-1.99495	0.4286	**C**	-6.92105	6.33483	0.99312
C	-3.56921	-3.09663	-0.22362	**C**	-7.67503	7.36801	1.58816
C	-4.75174	-3.59245	0.4287	**C**	-8.90431	7.71052	1.01546
C	-5.01436	-2.85768	1.62807	**C**	-6.62687	4.59431	-0.73067
S	-3.72997	-1.81411	1.92909	**C**	-5.37636	4.24784	-0.13986
C	-3.39103	2.59518	-0.22881	**C**	-4.92045	4.96707	0.99257
C	-4.6141	3.15632	-0.67995	**C**	-5.66429	5.98422	1.56257
C	-5.12776	2.41427	-1.78922	**C**	-9.16435	5.31773	-1.98234
S	-4.08336	1.15348	-2.16041	**C**	-8.35416	4.25723	-2.49995
C	-6.2406	-3.02609	2.36563	**C**	-7.11285	3.88347	-1.88386
C	-7.19934	-3.97444	1.88964	**C**	-10.41073	5.78584	-2.51149
C	-8.44169	-4.1259	2.58437	**C**	-10.70224	4.99067	-3.7114
C	-8.70913	-3.3329	3.73962	**C**	-9.98755	3.94906	-4.29371
C	-7.73977	-2.39791	4.20637	**C**	-8.78412	3.54361	-3.67207
C	-6.54007	-2.26403	3.52517	**C**	-8.02621	2.46637	-4.20025
C	-9.41664	-5.06458	2.11297	**C**	-6.8528	2.09954	-3.56558
C	-10.62543	-5.15176	2.83207	**C**	-6.36698	2.78584	-2.42315
C	-10.88327	-4.37368	3.96163	**C**	-10.45493	3.28362	-5.50901
C	-9.9325	-3.45961	4.43335	**N**	-9.67305	2.21397	-5.9859
C	-6.92346	-4.75518	0.71697	**C**	-8.48266	1.75146	-5.39485
C	-7.88634	-5.70542	0.2462	**C**	-5.14257	6.67495	2.74813
C	-9.13081	-5.86918	0.93441	**N**	-5.96659	7.66128	3.31553
C	-5.70593	-4.57692	-0.00601	**C**	-7.20083	8.07499	2.78237
C	-5.46124	-5.36684	-1.15837	**C**	-5.49039	8.34065	4.51639
C	-6.37076	-6.30624	-1.61245	**C**	-10.1228	1.56421	-7.21479
C	-7.60169	-6.48013	-0.91927	**O**	-7.87375	0.78939	-5.88137
C	-8.53547	-7.42574	-1.39911	**O**	-11.48193	3.60687	-6.11917
C	-9.74974	-7.58171	-0.71944	**O**	-4.04293	6.42045	3.25231
C	-10.03413	-6.81925	0.41563	**O**	-7.83077	8.98917	3.32681
C	-6.05349	-7.09398	-2.80841	**C**	0.98525	-2.99456	-0.65498
N	-7.04041	-7.99017	-3.2532	**C**	0.26212	2.3777	-1.83749
C	-8.25958	-8.22965	-2.59506	**C**	-0.325	-2.9328	0.26516
C	-10.22301	-2.65432	5.62304	**C**	-0.49162	2.57278	-0.44182
N	-9.23469	-1.73612	6.02532	**H**	-0.45131	-2.04375	-2.62509
C	-7.99295	-1.5672	5.38863	**H**	-0.83307	0.31258	-3.12644
C	-9.49834	-0.92919	7.21354	**H**	3.52597	-3.08489	-1.67735
C	-6.75547	-8.76367	-4.45754	**H**	2.97637	2.60156	-0.34505
O	-9.04828	-9.07339	-3.03986	**H**	5.74645	-1.30946	3.62734
O	-4.98375	-7.00063	-3.42023	**H**	10.64625	-6.55461	3.24547

H	10.81057	-5.40007	5.3161	**H**	-4.53059	-5.24402	-1.7073
H	4.96552	-4.72396	-2.26469	**H**	-10.49329	-8.2949	-1.07061
H	10.29439	-8.53804	-0.75363	**H**	-11.00574	-7.01445	0.86353
H	10.53063	-7.47259	1.35731	**H**	-9.09622	-1.42205	8.11073
H	8.07009	-2.15581	8.52982	**H**	-10.574	-0.77027	7.34512
H	9.62775	-1.45062	8.01133	**H**	-9.03733	0.06023	7.11857
H	8.12704	-0.5766	7.70665	**H**	-6.22463	-9.69297	-4.20442
H	6.26904	-8.32147	-5.17937	**H**	-6.14368	-8.17966	-5.15414
H	7.91887	-7.76633	-5.57621	**H**	-7.68357	-9.01711	-4.98172
H	7.64968	-9.34447	-4.78385	**H**	-10.33495	7.401	-0.47799
H	9.96828	7.45946	0.93824	**H**	-9.5167	8.49821	1.45016
H	8.6144	8.28951	2.70687	**H**	-3.96737	4.71403	1.44992
H	3.47565	4.3651	0.84091	**H**	-11.34951	6.27233	-2.75115
H	11.18687	6.55464	-0.53891	**H**	-11.61444	5.15866	-4.325
H	12.45286	5.61593	-2.31831	**H**	-6.29405	1.26416	-3.98718
H	7.10602	2.11391	-4.47292	**H**	-6.33075	8.5853	5.17648
H	4.31334	8.6357	4.8988	**H**	-4.96157	9.26805	4.25293
H	3.88189	6.97199	5.37953	**H**	-4.8145	7.69368	5.08583
H	2.90472	7.86061	4.17558	**H**	-11.21494	1.47615	-7.2298
H	11.76413	3.04266	-7.06466	**H**	-9.71705	0.55111	-7.29366
H	11.47209	1.39533	-6.44315	**H**	-9.80036	2.1425	-8.09316
H	12.87364	2.2996	-5.88011	**H**	0.90044	-3.82008	-1.37783
H	0.97869	-1.11488	1.76325	**H**	1.80651	-3.25988	0.01801
H	0.87758	1.29555	1.45103	**H**	-0.47143	2.55931	-2.63814
H	-3.24393	-3.39689	-1.21578	**H**	1.04046	3.14569	-1.96334
H	-2.88748	2.92681	0.67382	**H**	-0.16266	-3.48325	1.20422
H	-5.82734	-1.53216	3.90386	**H**	-1.13235	-3.44727	-0.27438
H	-11.43205	-5.82447	2.54954	**H**	0.17978	3.12302	0.23609
H	-11.83921	-4.48633	4.47011	**H**	-1.34426	3.23907	-0.6026

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