

Electronic Supplementary Information (ESI)

**Segregated co-assembly of fullerene-triphenylene hybrid dendrimers in
columnar mesophases showing ambipolar charge transport**

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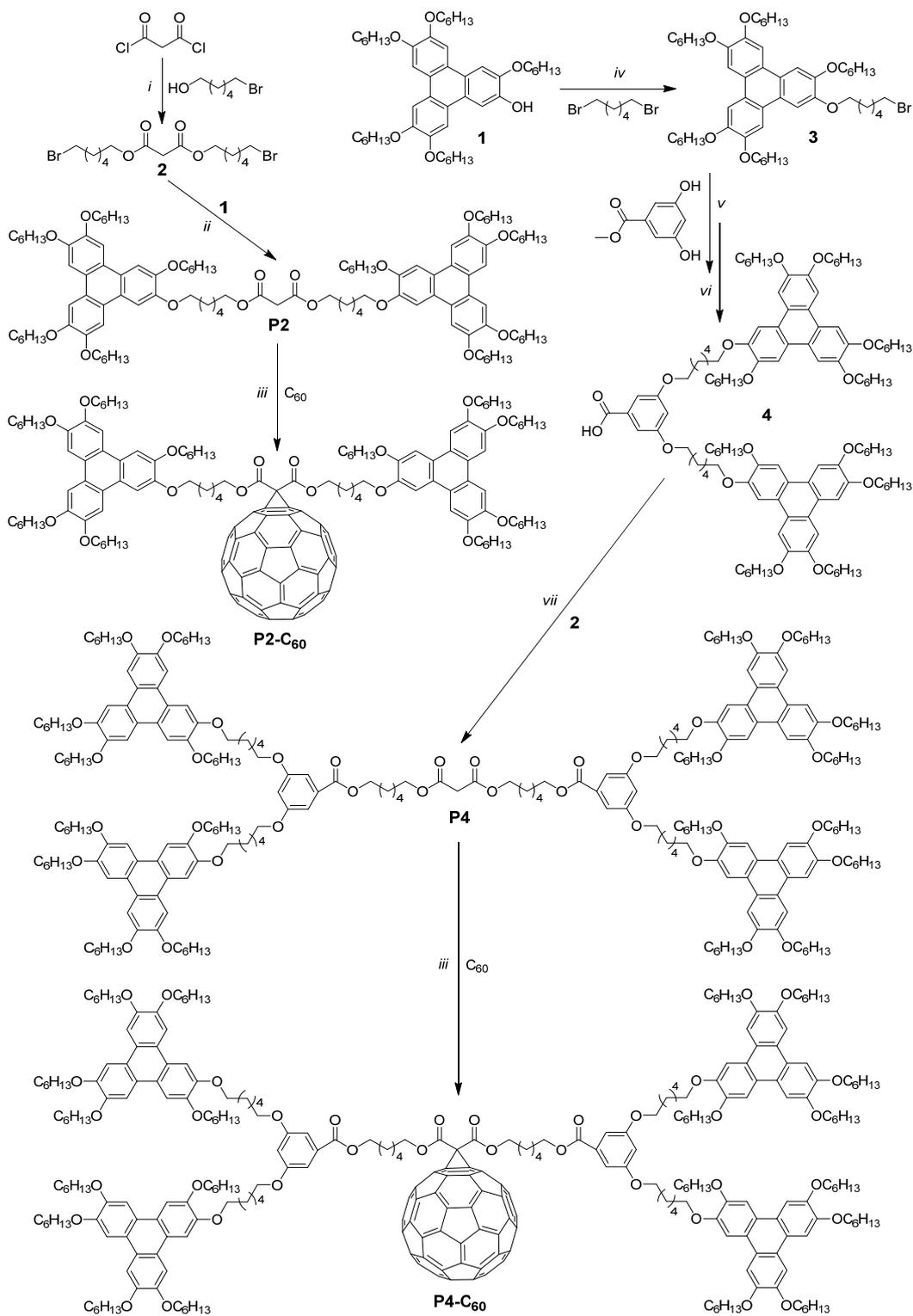
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1. Experimental Details

Materials. 6-Bromo-1-hexanol (>95.0%, TCI), 1,6-dibromohexane (>97.0%, TCI), malonyl chloride (>97.0%, TCI), 1,8-diazabicyclo[5.4.0]-7-undecene (DBU, >98.0%, TCI), fullerene (C₆₀, >99.0%, TCI), methyl 3,5-dihydroxybenzoate (>98.0%, TCI) were used as received. All other chemical reagents were commercially available and used as received.

Measurements. ¹H NMR and ¹³C NMR spectra in solution were obtained from 400 MHz Bruker Avance III 400 instruments. Multiplicities are denoted as follows: s = singlet, d = doublet, t = triplet, and m = multiplet. Matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF-MS) was performed on a Bruker Autoflex II instrument, with dithranol employed as the matrix substance. Elemental analyses were carried out with an Elementar Vario EL Cube. Polarized optical microscopy (POM) was adopted to characterize thermal transitions, observe and photograph textures with a Nikon E400POL microscope equipped with an Instec HCS302 hot and cold stage. Differential scanning calorimetry (DSC) thermograms were recorded on a Mettler Toledo DSC 1 system equipped with a cooling accessory and under nitrogen atmosphere at a flow rate of 20 mL min⁻¹. X-ray scattering experiments were performed with Anton Paar SAXSess mc² or SAXSpoint 2.0 small-angle X-ray scattering instruments. The scattering vector q is defined as $4\pi\sin\theta/\lambda$, where the wavelength λ is 0.1542 nm of Cu-K α radiation and 2θ is the scattering angle. Ultraviolet visible (UV-vis) absorption spectra were recorded on a Shimadzu UV-2550 spectrometer. The electrochemical properties were measured using a CHI-760E electrochemical workstation at a scan rate of 0.1 V s⁻¹ in dichloromethane with tetrabutylammonium hexafluorophosphate (TBAPF₆) as supporting electrolyte. A three-electrode system (a glassy carbon working electrode, Pt counter electrode, and Ag/AgCl reference electrode) was used in all cases. The time-of-flight (TOF) mobilities were measured using a TOF-401 device with the samples filled in LC cells (E.H.C. Company, Japan) with semi-transparent indium tin oxide electrodes. Current transients were generated in the samples upon exposure to a 337 nm laser pulse from a N₂ laser (USHO KEC 160), and recorded by a NF low-digital phosphor oscilloscope (Tektronix TDS 3032C). The mobility was calculated as $\mu = d^2/Vt_T$, where d is the thickness of the charge-transport layer (ca. 9 μ m), V is the applied bias voltage (40 V), and t_T is the transit time of the photogenerated charge carriers travelling the LC layer.



Scheme S1 Synthesis of the C₆₀-core discotic LC dendrimers. Reagents and conditions: (i) pyridine, dichloromethane, 25 °C, 24 h; (ii) K₂CO₃, KI, acetone, 75 °C, 48 h; (iii) iodine (I₂), 1,8-diazabicyclo[5.4.0]-7-undecene (DBU), toluene, 25 °C, 24 h; (iv) K₂CO₃, KI, acetone, 75 °C, 30 h; (v) K₂CO₃, KI, acetone, 75 °C, 72 h; (vi) NaOH, methanol/tetrahydrofuran, 60 °C, 6 h; (vii) K₂CO₃, dimethylformamide, 60 °C, 12 h.

2-Hydroxy-3,6,7,10,11-penta(hexyloxy)triphenylene (1). This was synthesized according to the same procedure as described in our previous report (Bin Mu, et al. *Macromolecules* 2015, 48, 2388-2398).

Bis(6-bromohexyl) malonate (2). To a solution of 6-bromo-1-hexanol (2.3 g, 12.7 mmol) and pyridine (1.0 mL, 13.0 mmol) in 75 mL dichloromethane, a solution of malonyl chloride (0.6 mL, 6.0 mmol) in 10 mL dichloromethane was added under ice-water bath and then allowed to stir at room temperature for 24 h. The reaction mixture was washed with water, and then was purified by silica-gel column chromatography using mixed solvents of petroleum ether/ethyl acetate (10:1, v/v) as the eluent to give a desired product (2.2 g) in colorless oil. Yield 85%. ¹H NMR (400 MHz, CDCl₃): δ (ppm) = 4.15 (t, 4H, *J* = 6.4 Hz), 3.41 (t, 4H, *J* = 6.8 Hz), 3.38 (s, 2H), 1.92-1.82 (m, 4H), 1.72-1.61 (m, 4H), 1.52-1.34 (m, 8H).

The discotic LC compound of TP dimer (P2). A mixture of monohydroxy triphenylene derivative **1** (1.6g, 2.15 mmol), **2** (0.4 g, 0.92 mmol), potassium carbonate (3.0 g, 21.7 mmol) and catalytic amount of potassium iodide in 50 mL acetone was stirred at 75 °C for 48 h. After removal of insoluble inorganic components and evaporation of the solvent, the crude product was purified by silica-gel column chromatography using mixed solvents of petroleum ether/ethyl acetate (15:1, v/v) as the eluent to give a desired product (1.3 g) in light yellow solid. Yield 82%. ¹H NMR (400 MHz, CDCl₃): δ (ppm) = 7.82 (s, 12H), 4.26-4.19 (m, 24H), 4.17 (t, 4H, *J* = 6.4 Hz), 3.38 (s, 2H), 1.99-1.86 (m, 24H), 1.76-1.30 (m, 72H), 0.97-0.89 (m, 30H). ¹³C NMR (100 MHz, CDCl₃): δ (ppm) = 166.73, 148.99, 123.57, 107.27, 69.68, 65.56, 41.63, 31.75, 29.48, 28.53, 25.91, 22.72, 14.12. MALDI-TOF-MS calcd for C₁₁₁H₁₆₈O₁₆, 1757.23; found, 1757.21. Elemental analysis: Calcd for C₁₁₁H₁₆₈O₁₆, C 75.81%, H 9.63%, O 14.56%; Found, C 75.96%, H 9.70%.

The C₆₀-TP hybrid discotic LC compound (P2-C₆₀). To a solution of **P2** (150 mg, 0.084 mmol) and C₆₀ (90 mg, 0.12 mmol) in 60 mL toluene, DBU (54 mg, 0.36 mmol) and iodine (I₂, 37 mg, 0.15 mmol) was added under ice-water bath and then allowed to stir at room temperature for 24 h. The reaction mixture was directly subjected to silica-gel column chromatography by firstly using toluene as the eluent to remove the residual C₆₀, and then a mixed solvent of petroleum ether/dichloromethane (1:2, v/v) was used to give a desired product (140 mg) in brown solid. Yield 76%. ¹H NMR (400 MHz, CDCl₃): δ (ppm) = 7.84-7.74 (m, 12H), 4.52 (t, 4H, *J* = 6.4 Hz), 4.26-4.15 (m, 24H), 1.99-1.84 (m, 24H), 1.66-1.31 (m, 72H), 0.97-0.88 (m, 30H). ¹³C NMR (100 MHz, CDCl₃): δ (ppm) = 163.74, 148.98,

145.15, 144.95, 144.82, 144.72, 144.47, 144.40, 144.27, 143.62, 142.84, 142.65, 141.92, 141.62, 140.77, 138.75, 123.65, 107.36, 71.51, 69.75, 67.34, 52.42, 31.74, 29.46, 28.71, 25.91, 22.72, 14.12. MALDI-TOF-MS calcd for C₁₇₁H₁₆₆O₁₆, 2475.21; found, 2475.31. Elemental analysis: Calcd for C₁₇₁H₁₆₆O₁₆, C 82.91%, H 6.75%, O 10.33%; Found, C 82.96%, H 6.82%.

2-((6-Bromohexyl)oxy)-3,6,7,10,11-pentakis(hexyloxy)triphenylene (3). A mixture of monohydroxy triphenylene derivative **1** (3.0 g, 4.0 mmol), 1,6-dibromohexane (5.0 g, 20.5 mmol), potassium carbonate (11.0 g, 79.7 mmol) and catalytic amount of potassium iodide in 100 mL acetone was stirred at 75 °C for 30 h. After removal of insoluble inorganic components and evaporation of the solvent, the crude product was purified by silica-gel column chromatography using mixed solvents of petroleum ether/ethyl acetate (50:1, v/v) as the eluent to give a desired product (3.1 g) in light yellow solid. Yield 82%. ¹H NMR (300 MHz, CDCl₃) δ (ppm): 7.83 (s, 6H), 4.23 (t, 12H, *J* = 6.4 Hz), 3.45 (t, 2H, *J* = 6.8 Hz), 2.00-1.88 (m, 14H), 1.66-1.51 (m, 14H), 1.46-1.32 (m, 20H), 0.93 (t, 15H, *J* = 7.2 Hz).

Methyl 3,5-bis((6-((3,6,7,10,11-pentakis(hexyloxy)triphenylen-2-yl)oxy)hexyl)oxy)benzoate. A mixture of **3** (1.9 g, 2.1 mmol), methyl 3,5-dihydroxybenzoate (0.17 g, 1.0 mmol), potassium carbonate (3.0 g, 21.7 mmol) and catalytic amount of potassium iodide in 45 mL acetone was stirred at 75 °C for 72 h. After removal of insoluble inorganic components and evaporation of the solvent, the crude product was purified by silica-gel column chromatography using mixed solvents of petroleum ether/ethyl acetate (30:1, v/v) as the eluent to give a desired product (1.4 g) in light yellow solid. Yield 77%. ¹H NMR (400 MHz, CDCl₃): δ (ppm) = 7.84 (s, 12H), 7.17 (d, 2H, *J* = 2.4 Hz), 6.65 (t, 1H, *J* = 2.4 Hz), 4.23 (t, 24H, *J* = 6.4 Hz), 4.00 (t, 4H, *J* = 6.4 Hz), 3.88 (s, 3H), 2.02-1.81 (m, 28H), 1.70-1.51 (m, 28H), 1.46-1.32 (m, 40H), 0.98-0.89 (m, 30H).

3,5-Bis((6-((3,6,7,10,11-pentakis(hexyloxy)triphenylen-2-yl)oxy)hexyl)oxy)benzoic acid (4). To a solution of the above obtained yellow solid (1.4 g, 0.77 mmol) in 50 mL tetrahydrofuran and 5 mL methanol, a solution of sodium hydroxide in water (20 mL, 4 mol/L) was added and then allowed to stir at 60 °C for 6 h. After cooling down to room temperature, the reaction mixture was acidified by 4 mol/L hydrochloric acid aqueous solution to neutral, and then extracted by dichloromethane to give a desired product (1.35 g) in light yellow solid. Yield 97%. ¹H NMR (400 MHz, CDCl₃): δ (ppm) = 7.83 (s, 12H), 7.22 (d, 2H, *J* = 2.4 Hz), 6.59 (t, 1H, *J* = 2.4 Hz), 4.23 (t, 24H, *J* = 6.4 Hz), 4.01 (t, 4H, *J* = 6.4 Hz), 2.02-1.81 (m, 28H), 1.70-1.50 (m, 28H), 1.46-1.31 (m, 40H), 0.98-0.89 (m, 30H).

The discotic LC dendrimer (P4). A mixture of **4** (140 mg, 0.078 mmol), **2** (14 mg, 0.033 mmol) and potassium carbonate (150 mg, 1.1 mmol) in 8 mL dimethylformamide was stirred at 65 °C for 12 h. The reaction mixture was cooled down to room temperature and was then poured into 45 mL water. After extraction with dichloromethane, the crude product was purified by silica-gel column chromatography using mixed solvents of petroleum ether/ethyl acetate (50:1-10:1, v/v) as the eluent to give a desired product (96 mg) in light yellow solid. Yield 75%. ¹H NMR (400 MHz, CDCl₃): δ (ppm) = 7.83 (s, 24H), 7.18 (d, 4H, *J* = 2.0 Hz), 6.64 (t, 2H, *J* = 2.0 Hz), 4.27 (t, 4H, *J* = 6.8 Hz), 4.22 (t, 48H, *J* = 6.4 Hz), 4.13 (t, 4H, *J* = 6.8 Hz), 3.99 (t, 8H, *J* = 6.0 Hz), 3.35 (s, 2H), 2.03-1.81 (m, 56H), 1.71-1.50 (m, 72H), 1.46-1.31 (m, 80H), 0.98-0.88 (m, 60H). ¹³C NMR (100 MHz, CDCl₃): δ (ppm) = 166.74, 166.59, 160.14, 148.96, 132.23, 123.61, 107.65, 107.29, 106.15, 69.69, 68.30, 65.68, 65.26, 41.66, 31.73, 29.46, 28.73, 28.48, 26.26, 26.11, 25.89, 22.71, 14.12. MALDI-TOF-MS calcd for C₂₄₅H₃₆₄O₃₆, 3882.67; found, 3882.79. Elemental analysis: Calcd for C₂₄₅H₃₆₄O₃₆, C 75.73%, H 9.44%, O 14.82%; Found, C 75.90%, H 9.51%.

The C₆₀-core discotic LC dendrimer (P4-C₆₀). To a solution of **P4** (78 mg, 0.020 mmol) and C₆₀ (25 mg, 0.035 mmol) in 35 mL toluene, DBU (18 mg, 0.12 mmol) and iodine (I₂, 12 mg, 0.05 mmol) was added under ice-water bath and then allowed to stir at room temperature for 24 h. The reaction mixture was directly subjected to silica-gel column chromatography by firstly using toluene as the eluent to remove the residual C₆₀, and then a mixed solvent of petroleum ether/ dichloromethane (1:2, v/v) was used to give a desired product (66 mg) in brown solid. Yield 75%. ¹H NMR (400 MHz, CDCl₃): δ (ppm) = 7.83 (s, 24H), 7.14 (d, 4H, *J* = 2.0 Hz), 6.63 (t, 2H, *J* = 2.0 Hz), 4.48 (t, 4H, *J* = 6.4 Hz), 4.27 (t, 4H, *J* = 6.8 Hz), 4.22 (t, 48H, *J* = 6.4 Hz), 3.98 (t, 8H, *J* = 6.4 Hz), 2.01-1.81 (m, 56H), 1.69-1.47 (m, 72H), 1.45-1.31 (m, 80H), 0.97-0.85 (m, 60H). ¹³C NMR (100 MHz, CDCl₃): δ (ppm) = 166.45, 166.67, 160.14, 148.98, 145.18, 145.02, 144.97, 144.91, 144.60, 144.47, 144.40, 143.64, 142.92, 142.78, 142.75, 141.93, 141.70, 140.84, 138.82, 132.14, 123.62, 107.74, 107.31, 106.15, 71.51, 69.71, 68.20, 67.22, 64.93, 52.33, 31.73, 29.45, 28.76, 28.83, 26.11, 26.04, 25.89, 22.71, 14.12. MALDI-TOF-MS calcd for C₃₀₅H₃₆₂O₃₆, 4600.65; found, 4600.89. Elemental analysis: Calcd for C₃₀₅H₃₆₂O₃₆, C 79.57%, H 7.93%, O 12.51%; Found, C 79.62%, H 7.99%.

Co-assembled mixture of P4-C₆₀/SymTP. Predesigned amount of discotic LC dendrimer P4-C₆₀ and SymTP compound were co-dissolved in dichloromethane, and then sonicated for 10 min before slow removal of the solvent and final dryness under vacuum to yield a homogeneous co-assembled

mixture in viscous solid. In all cases, the obtained mixture was heating to isotropic melt and then allowed to cool to room temperature to eliminate the influence from thermal history before subjecting to thermal analysis, X-ray scattering, and semiconducting property measurements.

2. Analysis of Experimental Data

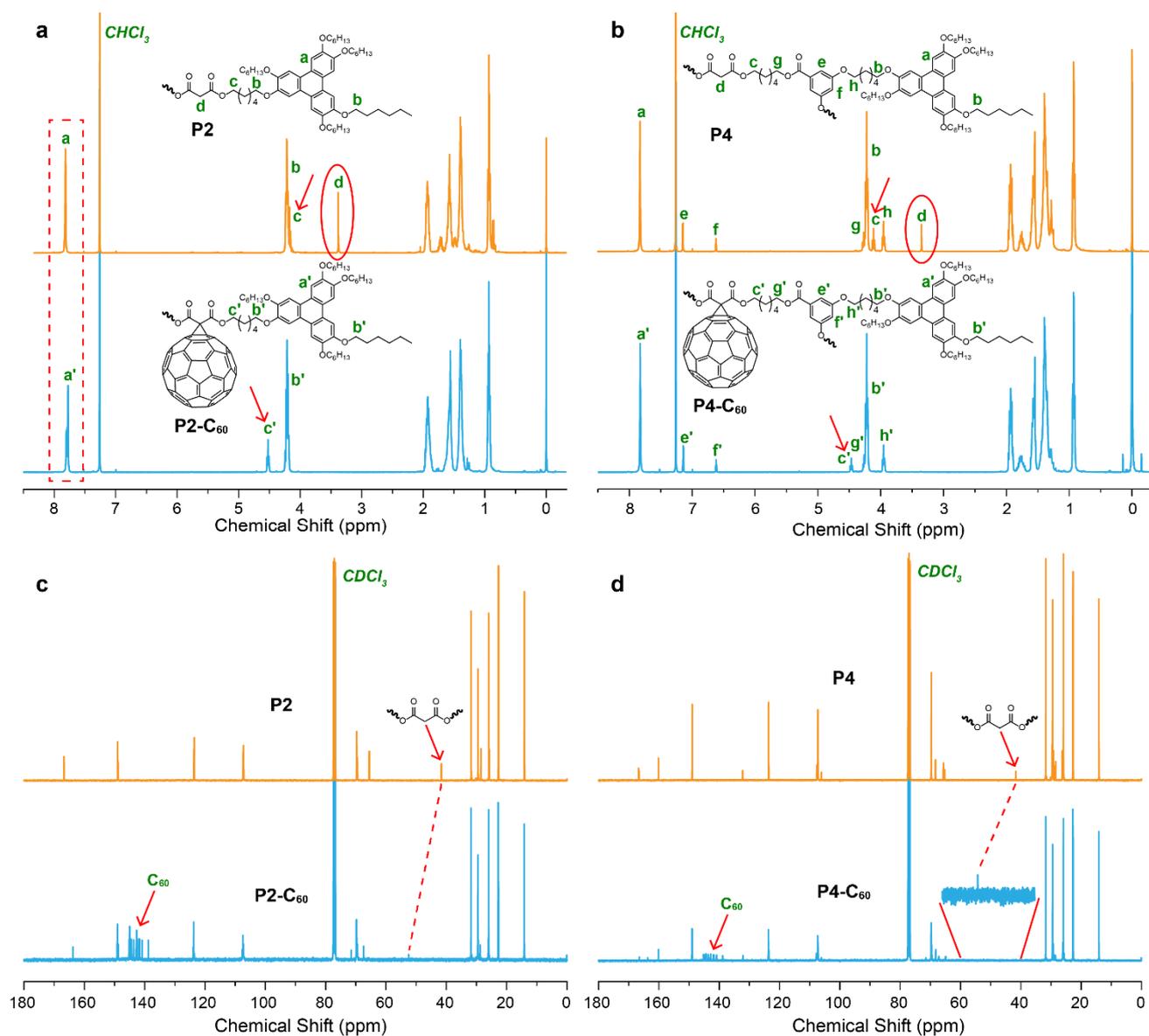


Fig. S1 (a,b) ^1H NMR and (c,d) ^{13}C NMR spectra comparison for the discotic LC compounds with and without the fullerene core of (a,c) P2 and P2- C_{60} , and (b,d) the dendrimer P4 and P4- C_{60} .

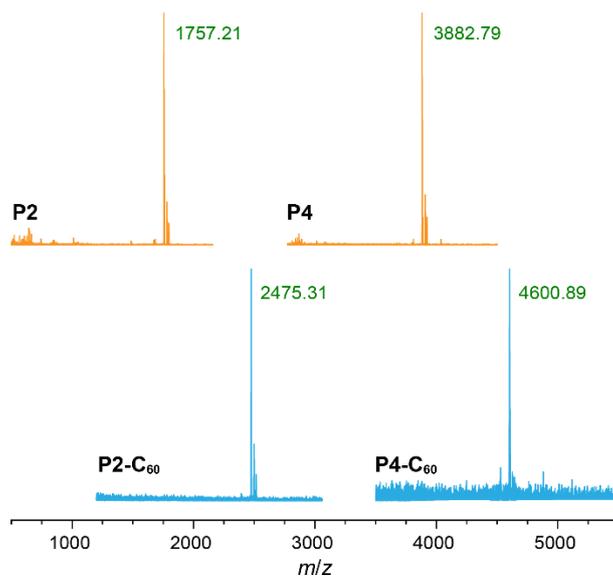


Fig. S2 MALDI-TOF mass spectra of the discotic LC compounds with and without the fullerene core indicated with the molecular ion peak.

Table S1 Summary of thermal transitions and thermotropic phase behavior assignments of all dendrimers and co-assembled mixtures.

Sample	Phase transitions ^a (°C; enthalpy changes/J g ⁻¹)
P2 ^b	Cr 53(47.8) Iso
P2-C ₆₀ ^b	Lam 41(30.9) Iso
P4 ^b	Col _r 47(13.0) Iso
P4-C ₆₀ ^b	Lam 34(14.5) Iso
SymTP ^d	Cr 91(32.0) Col _{hp} 142(21.6) Iso
P4-C ₆₀ /SymTP (2:1) ^c	Col-Lam 72(8.5) Iso
P4-C ₆₀ /SymTP (1:1) ^d	Col _{r-s} 114(1.9) Iso
P4-C ₆₀ /SymTP (1:2) ^d	Cr 91(13.2) Col _{ob} 133(9.4) Iso

^a Cr = crystalline phase; Iso = isotropic liquid; Lam = lamellar phase; Col_r = rectangular columnar lattice; Col_{hp} = hexagonal columnar plastic phase; Col-Lam = lamellar columnar phase; Col_{r-s} = rectangular columnar superlattice; Col_{ob} = oblique columnar lattice. ^b Heating at 10 °C min⁻¹ after annealing below the isotropization temperature. ^c Heating at 10 °C min⁻¹ after cooling from isotropic liquid at a slow rate of 1 °C min⁻¹. ^d Heating at 10 °C min⁻¹ after cooling from isotropic liquid at a rate of 10 °C min⁻¹.

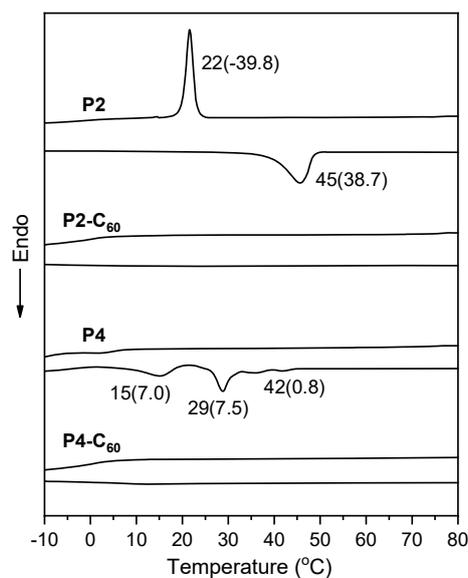


Fig. S3 DSC cooling and subsequent heating traces at a rate of $10\text{ }^{\circ}\text{C min}^{-1}$ for the series discotic LC compounds.

P2 exhibited a normal DSC cycle irrespective of the annealing process, due to its high assembly ability in ordered crystalline state. P4 exhibited multiple thermal transition peaks in the DSC heating trace, similar to what we have observed in assembled disordered discotic LC polymers. P2-C₆₀ and P4-C₆₀ both showed no thermal transition peak in both heating and cooling runs, implying very slow assembly kinetics in comparison with the results after annealing treatment (Fig. 2 in the main text).

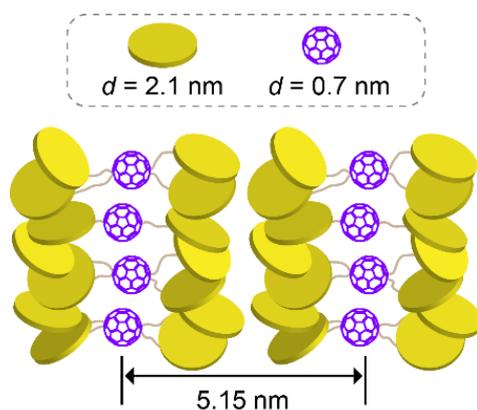


Fig. S4 Arrangement of the TP disc and C₆₀ core in the lamellar structure for P2-C₆₀ and P4-C₆₀.

According to the dimensions of TP disc (diameter $d_{\text{disc}} = 2.1\text{ nm}$) and C₆₀ core (diameter $d_{\text{C60}} = 0.7\text{ nm}$), the interlamellar distance of 5.15 nm in the lamellar structure should be corresponding to two TP discs and one C₆₀ core ($2d_{\text{disc}} + d_{\text{C60}} = 4.9\text{ nm}$), thus the most probable molecular packing mode was depicted in Fig. S4. The absence of scattering signal in middle and wide angle regions suggested that both the TP disc and C₆₀ core stacked in a relatively disordered manner.

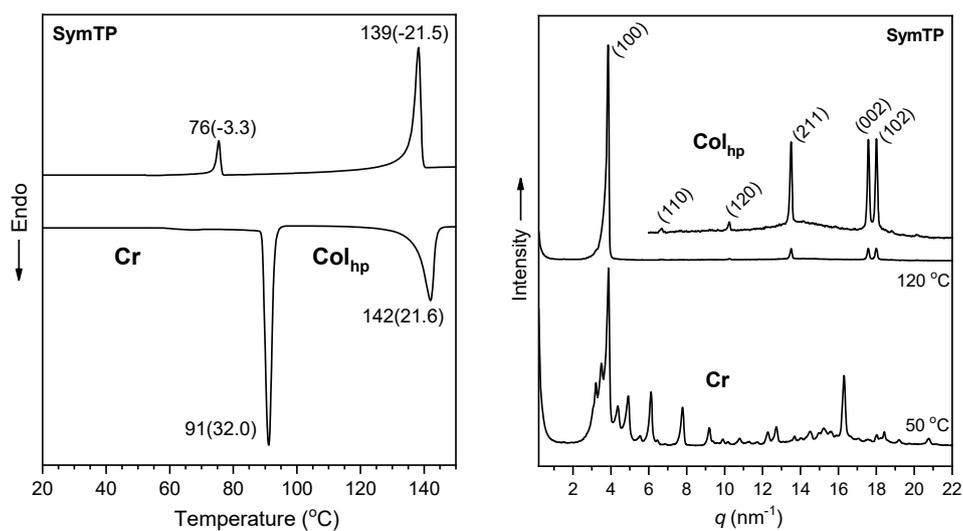


Fig. S5 DSC cooling and subsequent heating traces at a rate of $10\text{ }^{\circ}\text{C min}^{-1}$, and X-ray scattering patterns at indicated temperatures for the low-molar-mass symmetric TP derivative SymTP.

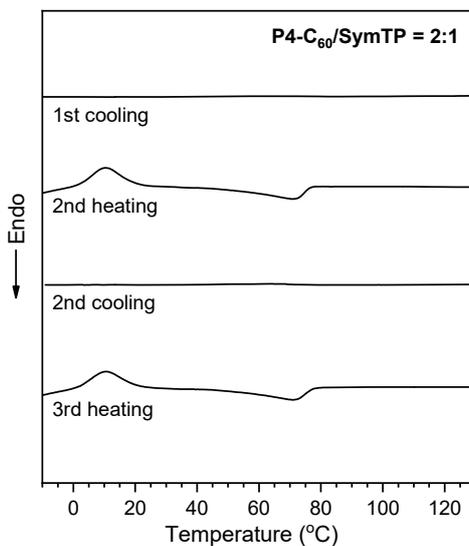
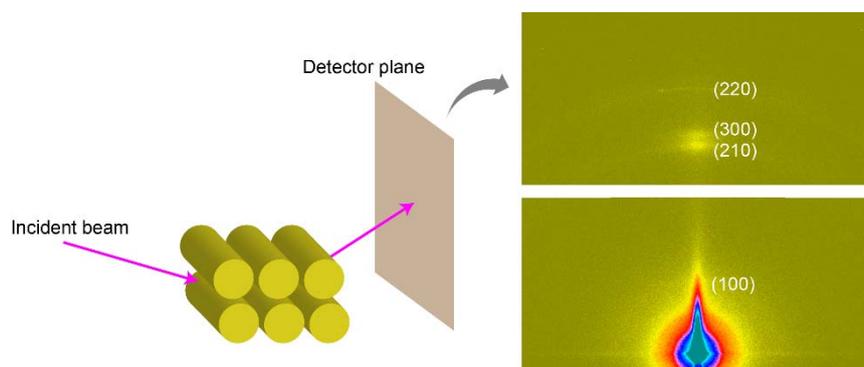


Fig. S6 DSC cooling and subsequent heating cycles at a rate of $10\text{ }^{\circ}\text{C min}^{-1}$ for the co-assembled mixture P4-C₆₀/SymTP in a TP ratio of 2:1.

Table S2 X-ray scattering data for the co-assembled mixture P4-C₆₀/SymTP (1:1).

<i>hkl</i>	<i>d</i> _{obs} (nm)	<i>d</i> _{calc} (nm)	lattice parameter	ρ_{calc}
100	4.85	4.85	$a = 4.85$ nm	1.05 g cm ⁻³
210	1.92	1.91	$b = 3.10$ nm	
300	1.61	1.62	$c = 0.38$ nm	
120	1.48	1.48		
220	1.27	1.30		
030/130	1.02	1.03/1.01		
230	0.96	0.95		
600	0.80	0.81		
440	0.68	0.65		
	0.43 (diffuse halo)			
001	0.38			

The calculated density ρ_{calc} based on measured lattice parameters was determined as $\rho = M \cdot Z / (N_A \cdot V_{\text{unit cell}})$, where $V_{\text{unit cell}}(\text{Col}_{\text{r-s}}) = a \cdot b \cdot c$, $Z = 4$, and M is the average molecular weight of the repeat unit about 906 g mol⁻¹.

**Fig. S7** Grazing incidence small-angle X-ray scattering pattern for the co-assembled film of P4-C₆₀/SymTP (1:1) formed by spin-coating on a silicon wafer and annealing at 60 °C for 24 hours.

The grazing incidence small-angle X-ray scattering pattern of annealed P4-C₆₀/SymTP (1:1) film confirmed the columnar structure with columnar orientation parallel to the substrate, and the X-ray incidence was perpendicular to the columnar direction (Fig. S7). The series scattering arcs indicated the existence of two-dimensional columnar structure, which was assigned to (100), (210), (300) and (220) scattering in a rectangular lattice according to the result obtained in the X-ray scattering experiment (Fig. 4 in the main text).

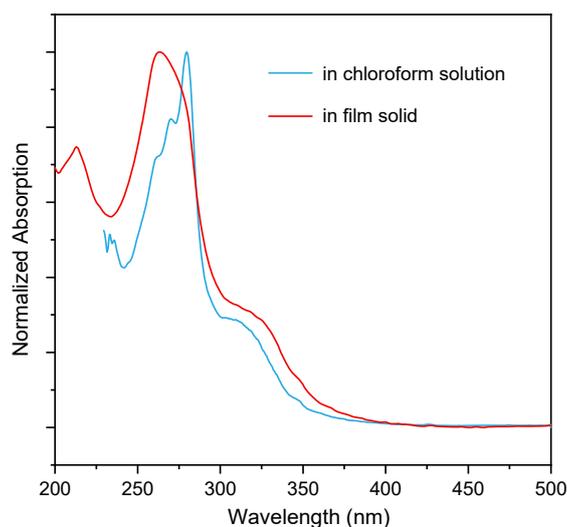


Fig. S8 Normalized UV-vis absorption spectra comparison for the co-assembled mixture P4-C₆₀/SymTP (1:1) in chloroform solution and film solid state.

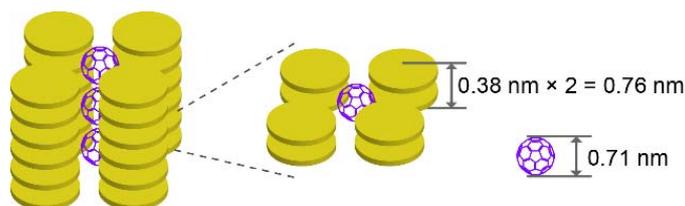


Fig. S9 Proposed intra-columnar arrangement of the TP disc and C₆₀ core for the co-assembled mixture P4-C₆₀/SymTP (1:1).

P4-C₆₀ has four TP discs and one C₆₀ core, and thus the mixture P4-C₆₀/SymTP (1:1) has eight TP discs and one C₆₀ core. According to the proposed structure with four TP columns surrounding one C₆₀ column, the stacking stratum can be depicted as in Fig. S9 by assuming a linear stacking mode of C₆₀. X-ray scattering revealed the intracolumnar interdisc spacing about 0.38 nm, thus the average distance between the neighboring C₆₀ cores may be calculated as 0.76 nm, which is slightly larger than the dimension of the C₆₀ around 0.71 nm, manifesting relatively close packing of the C₆₀ within the assembled columnar superstructure. Actually, the C₆₀ core may be arranged in a nonlinear mode, however within the small region between TP columns, neighboring C₆₀ units should still approach to enable the effective π - π interacting distance and possible charge transport along the columns.

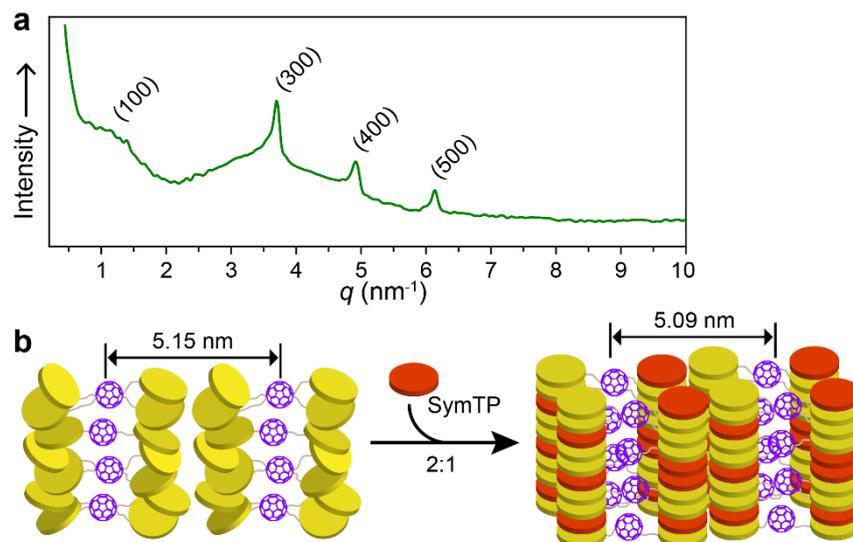


Fig. S10 (a) X-ray scattering pattern and (b) proposed packing structure for the co-assembled mixture P4-C₆₀/SymTP (2:1).

Table S3 X-ray scattering data for the co-assembled mixture P4-C₆₀/SymTP (2:1).

hkl	d_{obs} (nm)	d_{calc} (nm)	lattice parameter	ρ_{calc}
100	5.09	5.09	$L = 5.09$ nm	/
300	1.70	1.70	$c = 0.38$ nm	
400	1.27	1.27		
500	1.02	1.02		
	0.42 (diffuse halo)			
001	0.38			

The density ρ_{calc} cannot be calculated based on a lamellar phase.

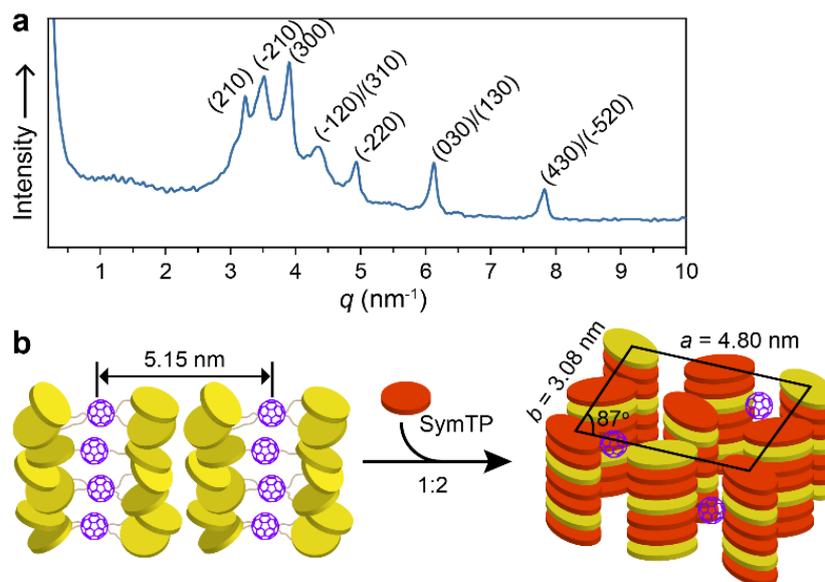


Fig. S11 (a) X-ray scattering pattern and (b) proposed packing structure for the co-assembled mixture P4-C₆₀/SymTP (1:2).

Table S4 X-ray scattering data for the co-assembled mixture P4-C₆₀/SymTP (1:2).

<i>hkl</i>	<i>d</i> _{obs} (nm)	<i>d</i> _{calc} (nm)	lattice parameter	ρ_{calc}
210	1.94	1.94	<i>a</i> = 4.80 nm	0.98 g cm ⁻³
-210	1.81	1.84	<i>b</i> = 3.08 nm	
300	1.61	1.60	γ = 87°	
-120/310	1.44	1.43/1.45	<i>c</i> = 0.38 nm	
-220	1.27	1.26		
030/130	1.02	1.03/1.01		
430/-520	0.80	0.80/0.79		
	0.43 (diffuse halo)			
001	0.38			

The calculated density ρ_{calc} based on measured lattice parameters was determined as $\rho = M \cdot Z / (N_A \cdot V_{\text{unit cell}})$, where $V_{\text{unit cell}} (\text{Col}_{\text{ob}}) = a \cdot b \cdot \sin \gamma \cdot c$, $Z = 4$, and M is the average molecular weight of the repeat unit about 824 g mol⁻¹.

Table S5 Electrochemical data for the C₆₀-core discotic LC dendrimer P4-C₆₀.

E^{red} vs Ag/AgCl	E^{red} vs FOC	E^{ox} vs Ag/AgCl	E^{ox} vs FOC	HOMO	LUMO
-1.32 V	-1.75 V	1.17 V	0.74 V	-5.54 eV	-3.05 eV
$E_{1/2} = 0.43$ V vs Ag/AgCl. $E_{\text{HOMO}} = -e(E^{\text{ox}}$ vs FOC + 4.8 V). $E_{\text{LUMO}} = -e(E^{\text{red}}$ vs FOC + 4.8 V).					