

Supporting Information

Hydrogen Bond-Assisted Supramolecular Assembly of Doubly Discotic Supramolecules Based on Porphyrin and Triphenylene

Jianjun Miao[†] and Lei Zhu^{†,‡,*}

[†] Polymer Program, Institute of Materials Science and Department of Chemical, Materials and Biomolecular Engineering, University of Connecticut, Storrs, Connecticut 06269-3136

[‡] Department of Macromolecular Science and Engineering, Case Western Reserve University, Cleveland, Ohio 44106-7202, Email: lxz121@case.edu, Tel. (216)368-6355

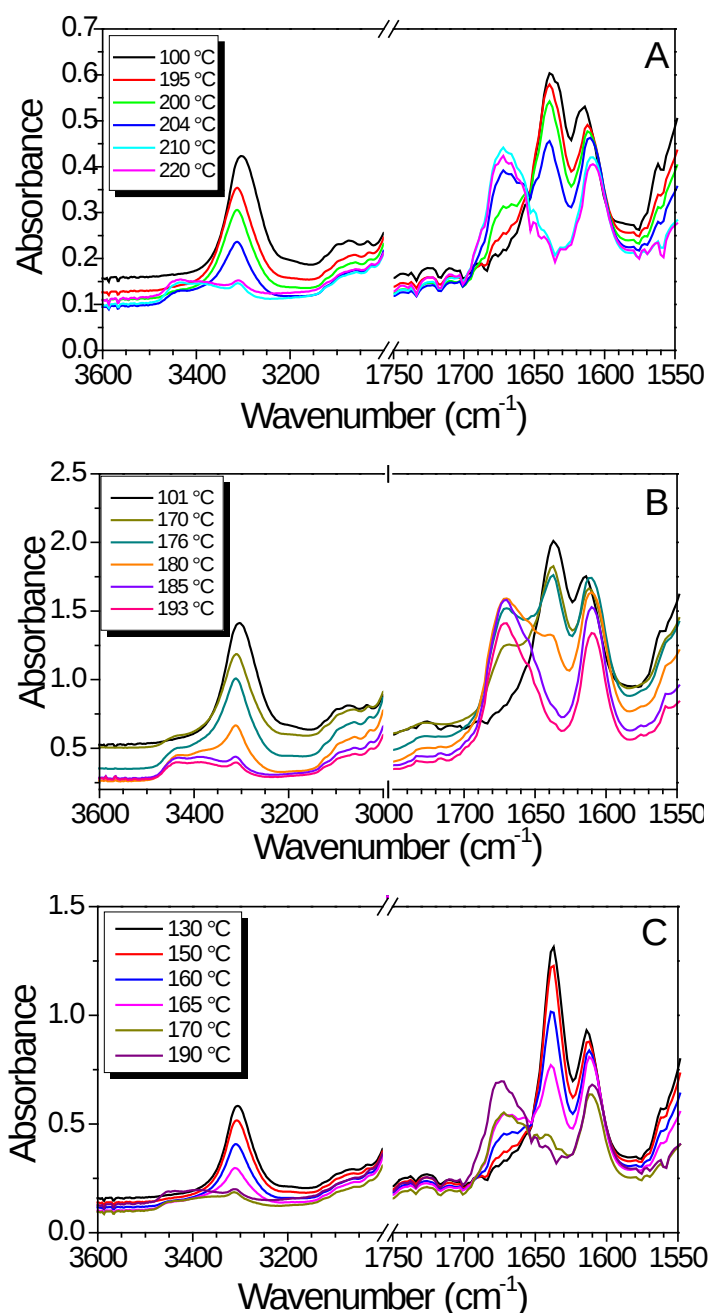


Figure S1. FTIR spectra for sample (A) 1, (B) 2 and (C) 4 at different temperatures.

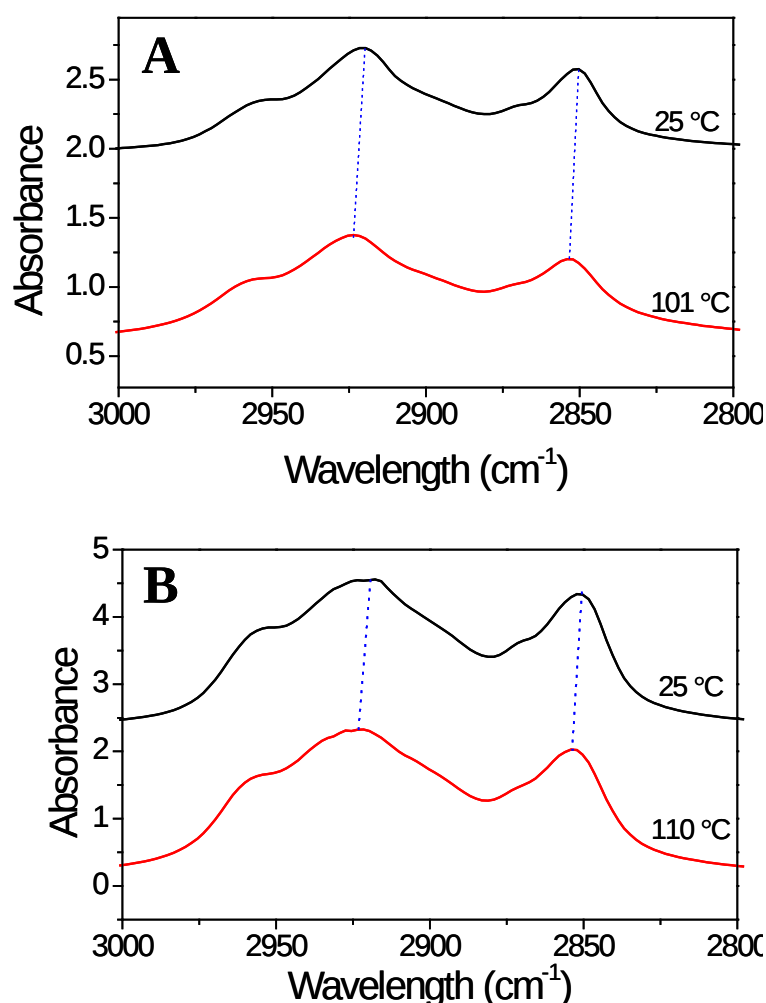


Figure S2. FTIR spectra for (A) the sample **3** at 25 and 101 °C and (B) the sample **4** at 25 and 110 °C, respectively.

Table S1. Observed and Calculated Spacings for Different Reflections for Sample **1**. The orthorhombic unit cell dimensions are $a = 4.82$ nm, $b = 3.50$ nm, and $c = 0.49$ nm.

$hk0$	(100)	(200)	(020)	(300)	(220)	(130)	(230)	(330)	(240)	(530)	(150)
Obs. (nm)	4.82	2.42	1.85	1.61	1.385	1.084	1.042	0.954	0.817	0.734	0.688
Calc. (nm)	4.82	2.41	1.75	1.607	1.416	1.134	1.05	0.944	0.822	0.743	0.693
$hk0$	(160)	(360)	(170)	(470)	(380)	(001)	(221)	(241)	Tp		
Obs. (nm)	0.590	0.536	0.494	0.466	0.422	0.490	0.461	0.426	0.350		
Calc. (nm)	0.579	0.548	0.497	0.462	0.422	0.490	0.461	0.421			

Note: Based on the unit cell dimensions, the theoretical density of sample **1** should be 1.17 g/cm^3 . The experimental density is 1.154 g/cm^3 .

Table S2. Observed and Calculated Spacings for Different Reflections for Sample **2**. The orthorhombic unit cell dimensions are $a = 4.89$ nm, $b = 3.50$ nm, and $c = 0.49$ nm.

$hk0$	(100)	(020)	(300)	(220)	(130)	(330)	(350)	(360)	(180)	(001)
Obs. (nm)	4.89	1.76	1.63	1.395	1.13	0.920	0.613	0.541	0.443	0.490
Calc. (nm)	4.89	1.745	1.63	1.42	1.132	0.947	0.642	0.548	0.435	0.490
$hk0$	(221)	(331)	(361)	Tp						
Obs. (nm)	0.471	0.433	0.374	0.350						
Calc. (nm)	0.463	0.435	0.365							

Note: Based on the unit cell dimensions, the theoretical density of sample **2** should be 1.22 g/cm^3 . The experimental density is 1.197 g/cm^3 .

Table S3. Observed and Calculated Spacings for Different Reflections for Sample 4. The orthorhombic unit cell dimensions are $a = 5.78$ nm, $b = 3.50$ nm, and $c = 0.49$ nm.

$hk0$	(100)	(200)	(300)	(030)	(340)	(160)	(180)	(001)	(031)	(341)
Obs. (nm)	5.78	2.78	1.926	1.159	0.799	0.579	0.431	0.490	0.463	0.432
Calc. (nm)	5.78	2.89	1.927	1.167	0.797	0.58	0.436	0.490	0.460	0.424

Note: Based on the unit cell dimensions, the theoretical density of sample 4 should be 1.12 g/cm^3 (assuming the average face-to-face distance between neighboring triphenylenes is 0.5 nm). The experimental density is 0.935 g/cm^3 . Therefore, the crystallinity/liquid crystallinity is 83.5%.

Table S4. Observed and Calculated Spacings for Different Reflections for Sample 3 at 175 °C. The oblique columnar unit cell dimensions are $a = 7.88$ nm, $b = 6.10$ nm and $\gamma = 95^\circ$.

$hk0$	(100)	(010)	($1\bar{1}0$)	(110)	(200)	(210)	(300)	(220)	($3\bar{2}0$)
Obs. (nm)	7.82	6.06	5.09	4.55	3.89	3.09	2.55	2.25	2.05
Calc. (nm)	7.85	6.07	5.02	4.61	3.92	3.17	2.61	2.30	2.07

Table S5. Observed and Calculated Spacings for Different Reflections for Sample 3 at 120 °C. The monoclinic unit cell dimensions are $a = 8.03$ nm, $b = 5.50$ nm, $c = 0.49$ nm, and $\gamma = 95^\circ$.

$hk0$	(100)	(010)	($1\bar{1}0$)	(200)	($2\bar{1}0$)	($3\bar{1}0$)	($2\bar{2}0$)	(220)	($3\bar{2}0$)	(320)
Obs. (nm)	8.0	5.48	4.71	3.95	3.37	2.47	2.31	2.13	1.99	1.90
Calc. (nm)	8.0	5.48	4.72	4.00	3.37	2.48	2.35	2.17	1.99	1.83
$hk0$	(130)	(001)	(581)							
Obs. (nm)	1.79	0.49	0.39							
Calc. (nm)	1.74	0.49	0.38							

Table S6. Observed and Calculated Spacings for Different Reflections for Sample 3 at 25 °C. The orthorhombic unit cell dimensions are $a = 7.82$ nm, $b = 5.37$ nm, and $c = 0.49$ nm.

$hk0$	(100)	(010)	(110)	(210)	(120)	(220)	(400)	(130)	(050)	(560)
Obs. (nm)	7.82	5.37	4.48	3.17	2.47	2.26	1.94	1.79	1.08	0.79
Calc. (nm)	7.82	5.37	4.43	3.16	2.54	2.21	1.96	1.74	1.07	0.77
$hk0$	(580)	(590)	(001)	($5\bar{1}10$)	(151)	(581)				
Obs. (nm)	0.61	0.55	0.49	0.45	0.45	0.4				
Calc. (nm)	0.61	0.55	0.49	0.46	0.44	0.38				