Supporting Information

Both Raising the Iso-to-Col Transition and Lowering the Solidifying Temperatures of the Triazine-based Dendrimer by Introducing CN Polar Groups in the Dendritic Core

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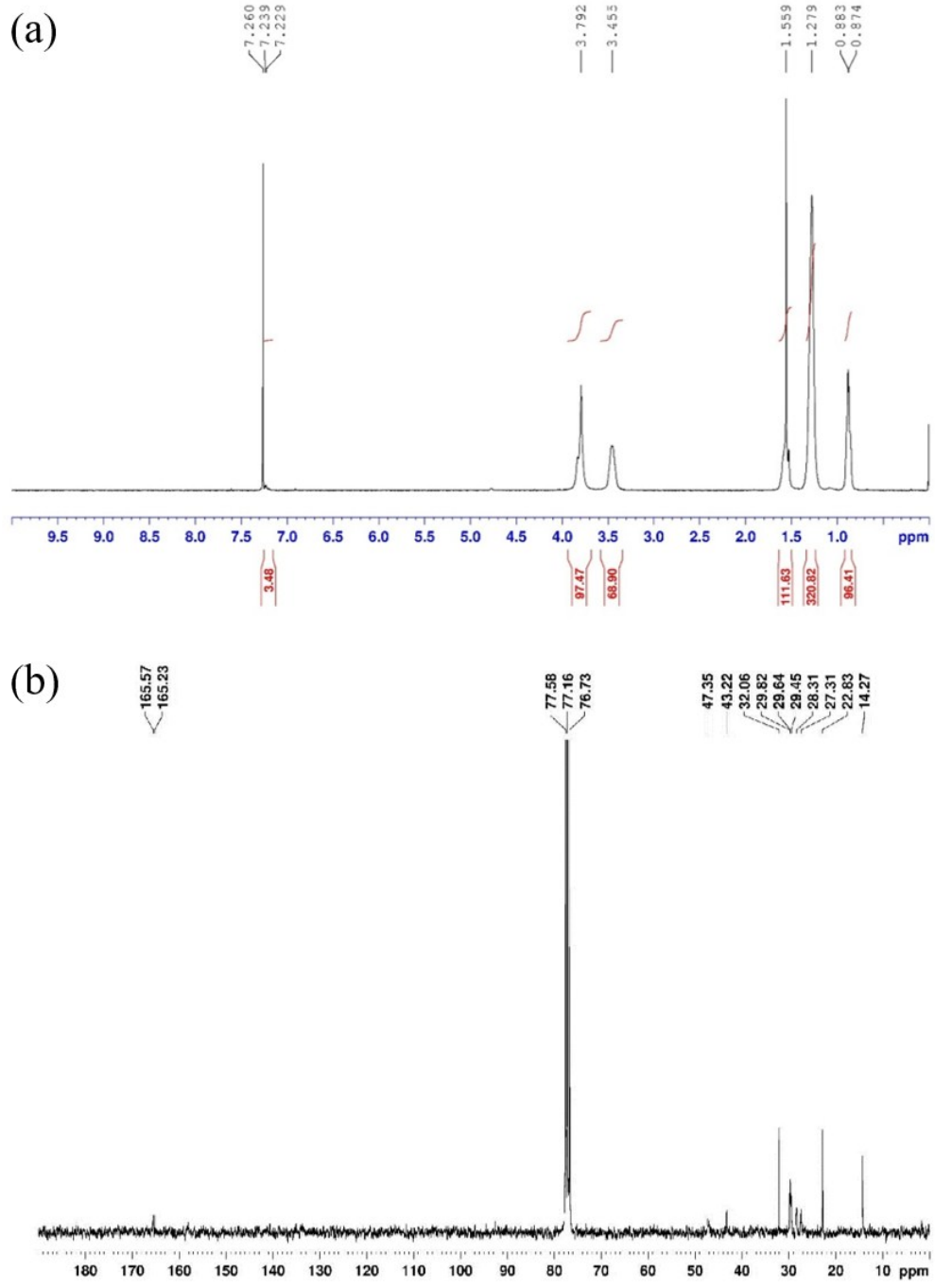

Figure S1. The (a) ^{1}H- NMR and (b) ^{13}C-NMR spectrum of **1a**.

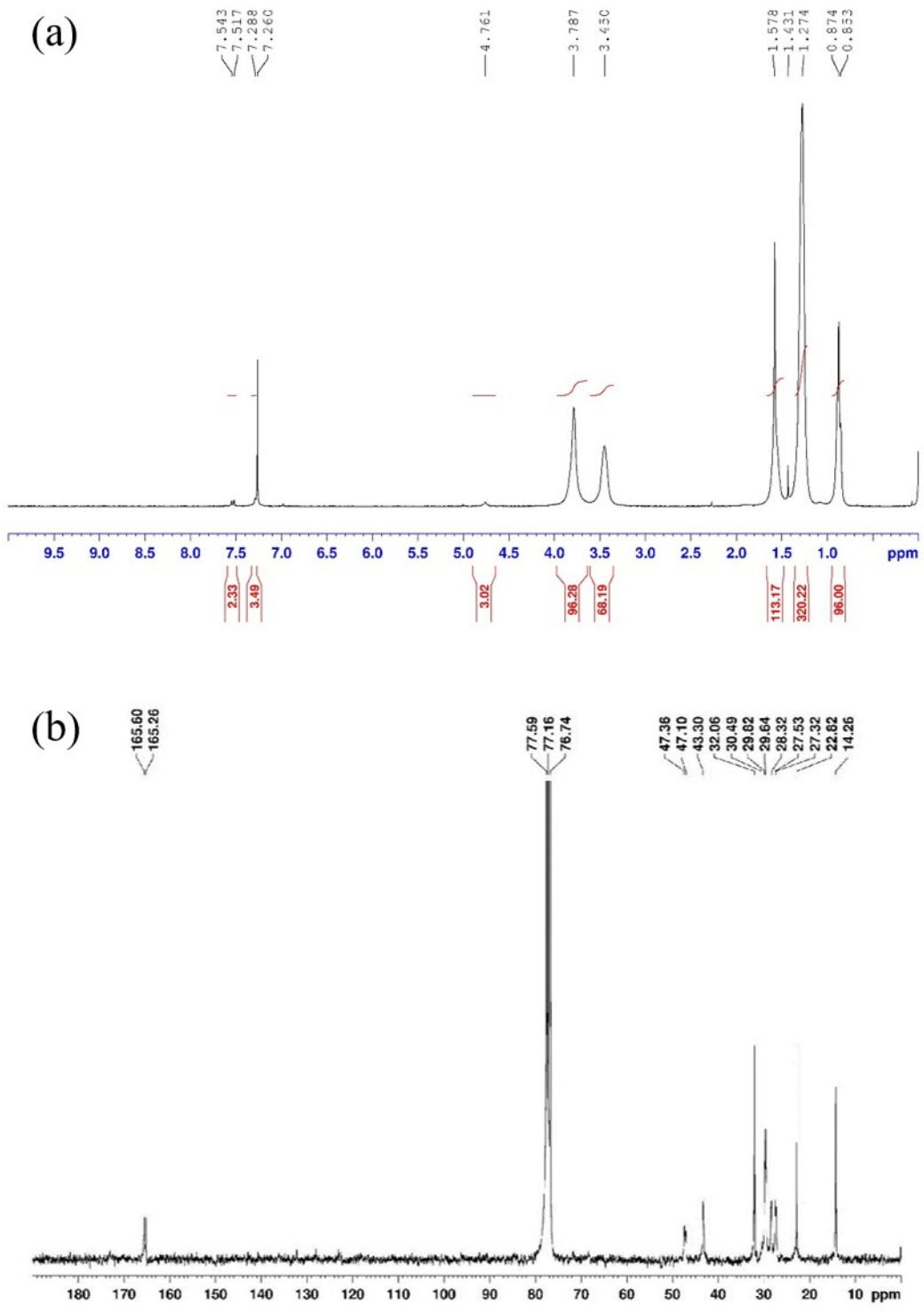

Figure S2. The (a) ^{1}H- NMR and (b) ^{13}C-NMR spectrum of **1b**.

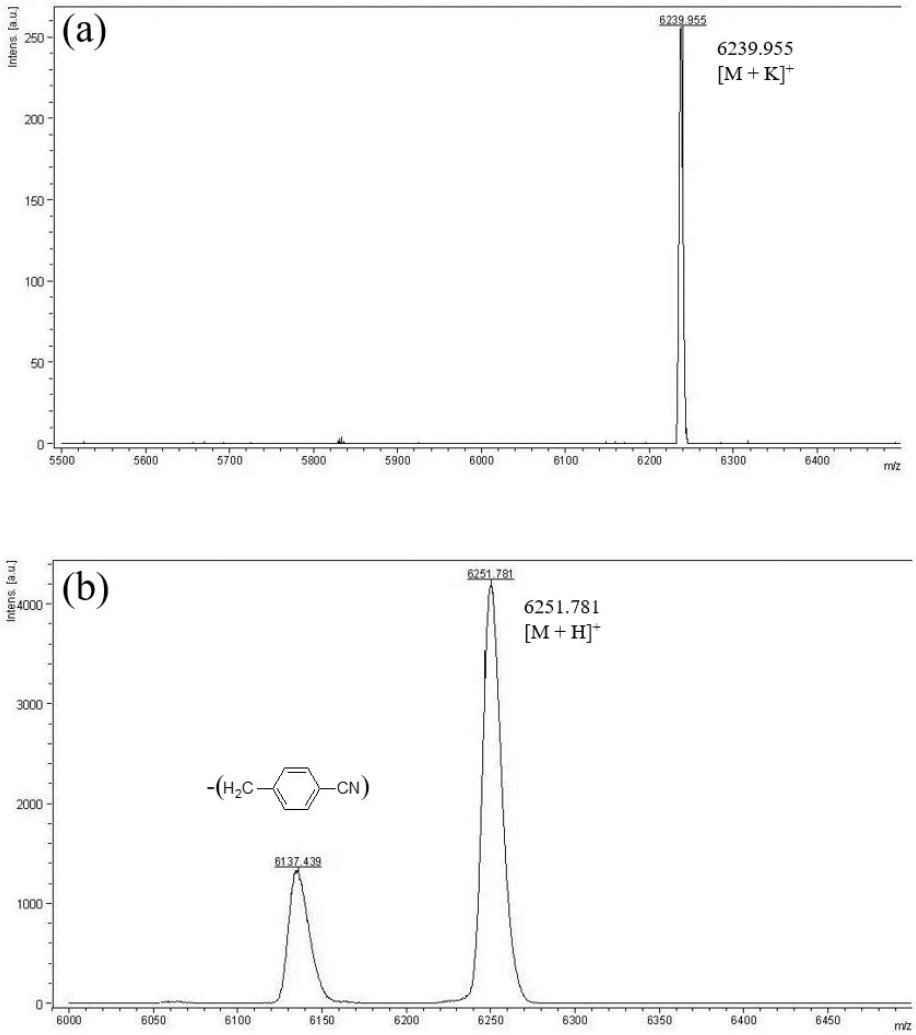

Figure S3. The MALDI-TOF mass spectrum of (a) **1a** and (b) **1b**.

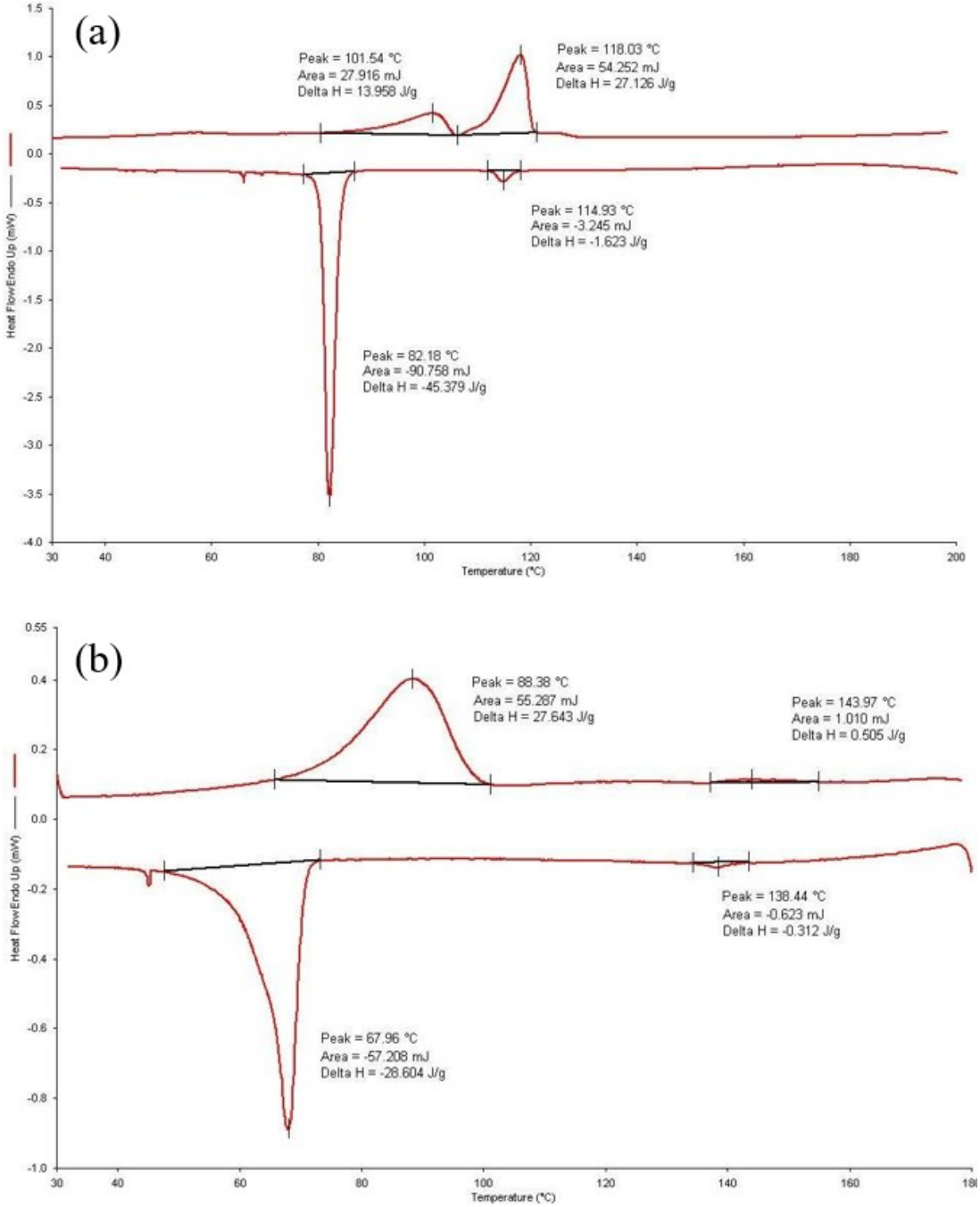

Figure S4. DSC data of compounds (a) **1a** and (b) **1b**.

Table S1. Calculated data of compounds **1a**, **1b** and **1c**.[a]

Cpd	phase (T (°C))	M_r	N_{ch}	N_C	T (°C)	V_{CH2} (Å^3)	ΔV_{CH3} (Å^3)	V_{CH} (Å^3)	V_m (Å^3)	d_{100} (Å)	a (Å)	S_{col} (Å^2)	h (Å)	V_{cell} (Å^3)	$N_{cell} = V_{cell}/V_m$	V_m/V_{cell}
1a	Col_h (110)	6202	32	8	110	28.8	34.1	8462.9	10981.1	36.29	41.9	1520.7	9	13686.3	1.25	0.80
1b	Col_h (130)	6252	32	8	130	29.2	36.4	8642.2	11225.9	32.85	38.4	1278.9	9	11510.1	1.03	0.98
1c	Col_h (C114)	6022	16	6	115	28.9	34.6	3328.6	10700.0	32.86	37.9	1246.8	9	11221.4	1.05	0.95
1c	Col_h (C110)	6022	16	6	110	28.8	34.1	3309.9	10662.4	32.87	38.0	1247.8	9	11230.3	1.05	0.95
1c	Col_h (C105)	6022	16	6	105	28.7	33.5	3291.6	10624.8	32.88	38.0	1248.3	9	11235.1	1.06	0.95
1c	Col_h (94)	6022	16	6	94	28.5	32.4	3252.5	10542.0	32.98	38.1	1255.9	9	11303.5	1.07	0.93

[a] M_r is the molecular weight. V_m and V_{cell} are the molecular and cell volumes respectively. S_{col} is the area of one columnar stratum. The equations and calculations corresponding to these values are detailed in the supporting information.

Synthesis of 2 (*N,N*-di(4-cyanobenzal)amino-propane):

1,3-Propandiamine (0.74 g, 10.0 mmol) and 4-cyanobenzaldehyde (2.62 g, 20.0 mmol) were added to dry EtOH (40 ml). The reaction was stirred at room temperature for 24 h. $NaBH_4$ (3.78 g, 100.0 mmol) was then added and the resulting solution was stirred at room temperature for 3 h. Ethanol was removed to give a sticky residue. 0.5M K_2CO_3 aqueous solution (30 ml) was added and then extracted with CH_2Cl_2 (30 mL) and. The organic extract was washed by water (20 mL), and then dried over $MgSO_4$. It was evaporated at reduced pressure, and the residue was purified by column (SiO_2: 2.1 cm × 20 cm; eluent: CH_2Cl_2:THF = 5:1) to give compound **2** in 93.2% (2.85g) yield as an oily solid. ^{1}H NMR (300MHz, $CDCl_3$, 25°C, TMS): 1.25 (s, 2H, 2×NH), 1.71−1.77 (m, 2H, 1×CH3), 2.70 (t, J = 6.6 Hz, 4H, 2×CH2), 3.84 (s, 4H, 2×CH2), 7.19 (d, J = 8.1 Hz, 4H, 4×CH), 7.60 (d, J = 8.1 Hz, 4H, 4×Ar-H) ppm. ^{13}C NMR (75MHz, $CDCl_3$, 25 °C, TMS): δ29.47, 29.66, 29.92, 30.34, 48.12, 53.73, 110.93, 119.06, 128.72, 132.36, 146.23. HR-MS cacld for $C_{19}H_{21}N_4$ $(M+H)^+$: 305.1766; found 305.1765(80%) + 306.1802(20%).

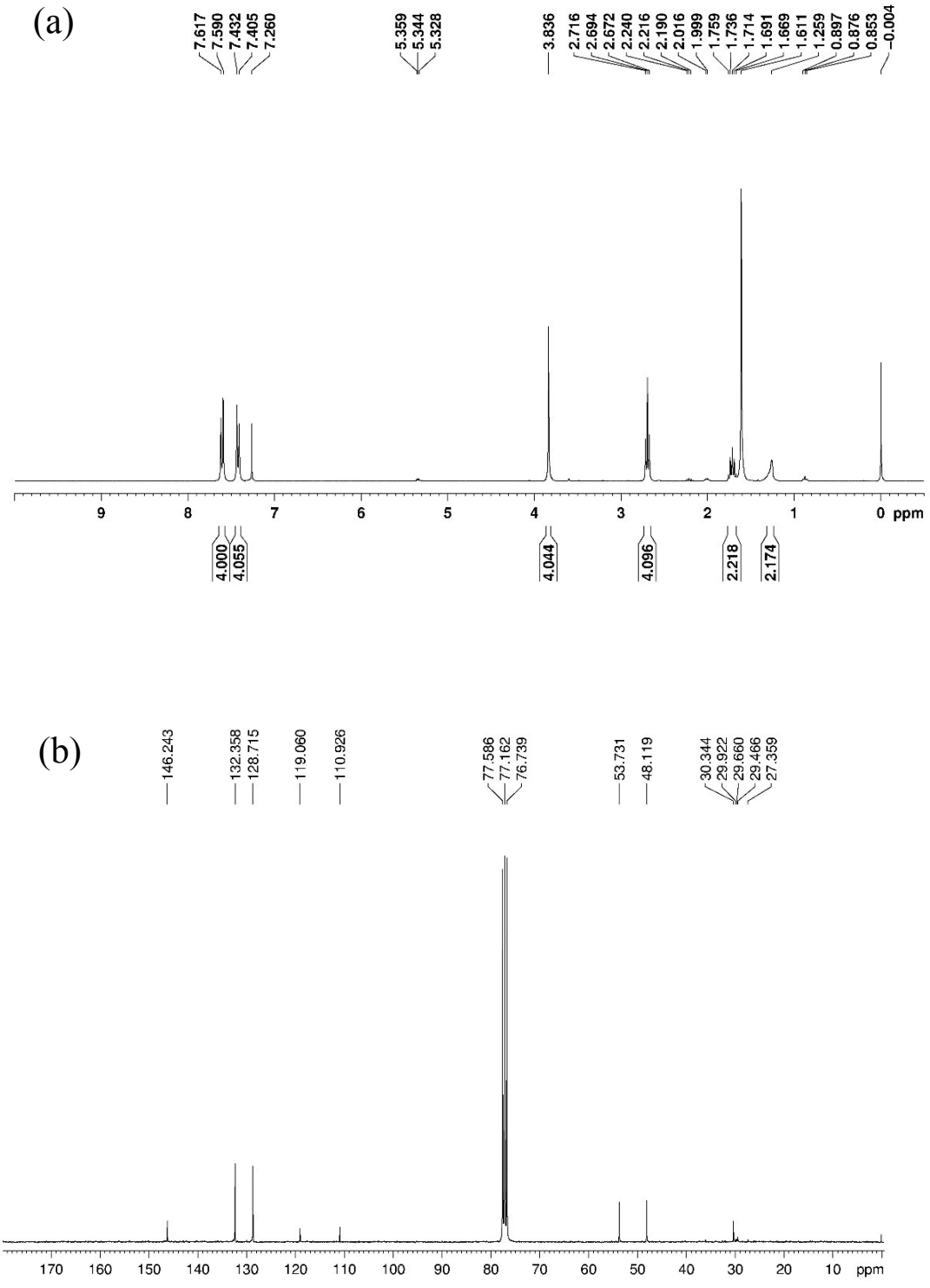

Figure S6. The (a) ^{1}H- NMR and (b) ^{13}C-NMR spectrum of **2**.

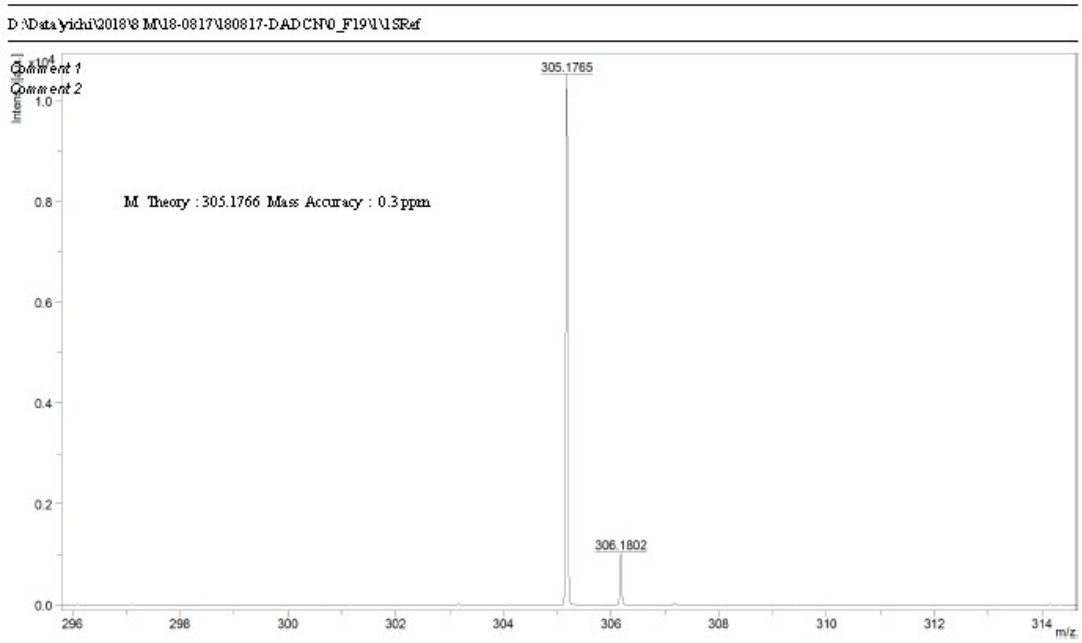

Figure S7. The HR mass spectrum of **2**.

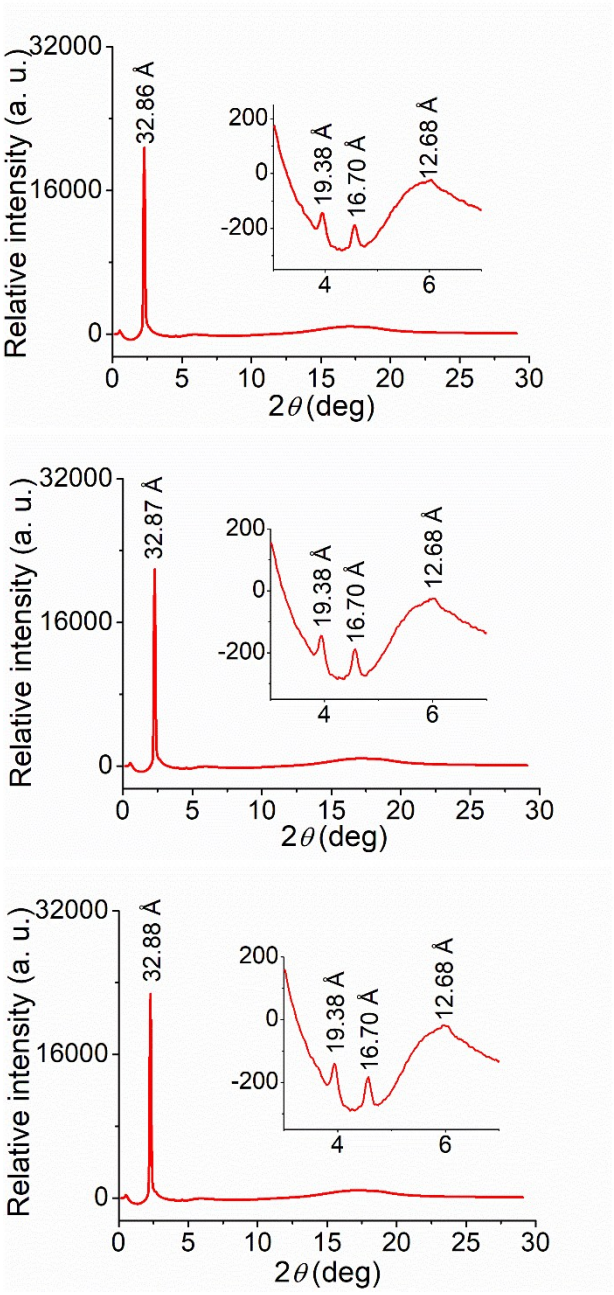

Figure S8. The powder-XRD patterns of **1c** upon cooling at 114 (top), 110 (middle), and 105 °C (bottom). For comparison, the d-spacings of **1c** at 94 °C are 32.98, 19.20, 16.58, 13.14, 4.52 Å for d10, d11, d20, columnar slice and chain-correlation respectively as reported previously.[16e]