

Supporting Information

Folded Discotic Dimers

Kevin J. A. Bozek and Vance E. Williams
Department of Chemistry
Simon Fraser University

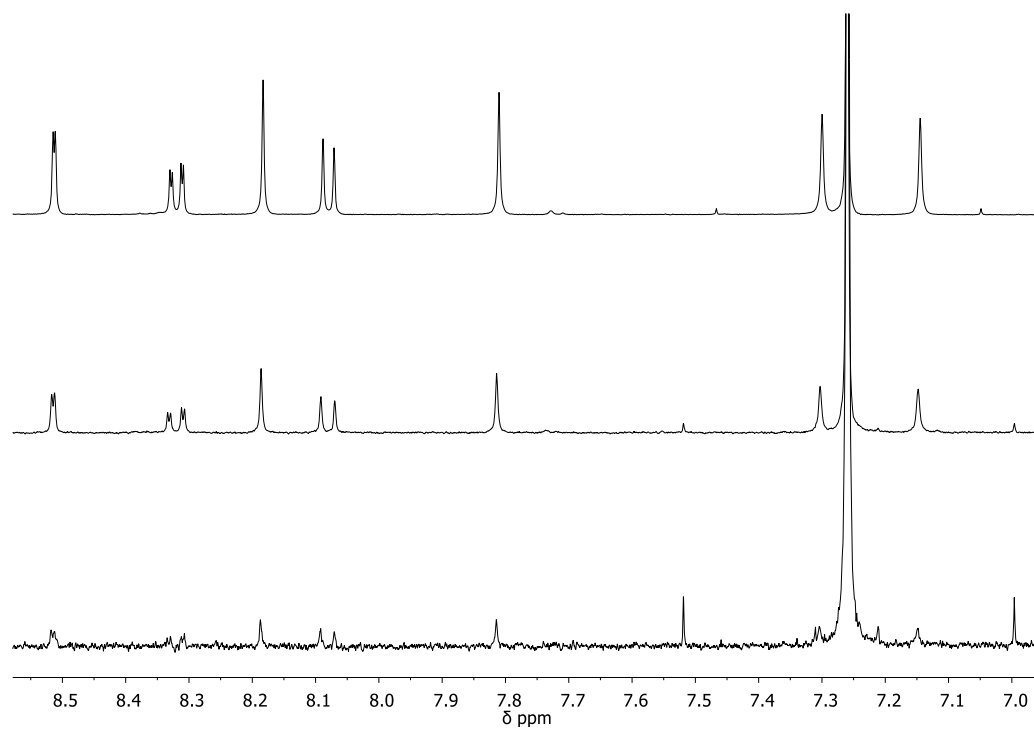


Figure S1: ^1H -NMR spectra (400 MHz) in CDCl_3 of **2** (a) 0.002 M (b) 0.00141 M (c) 0.000141 M

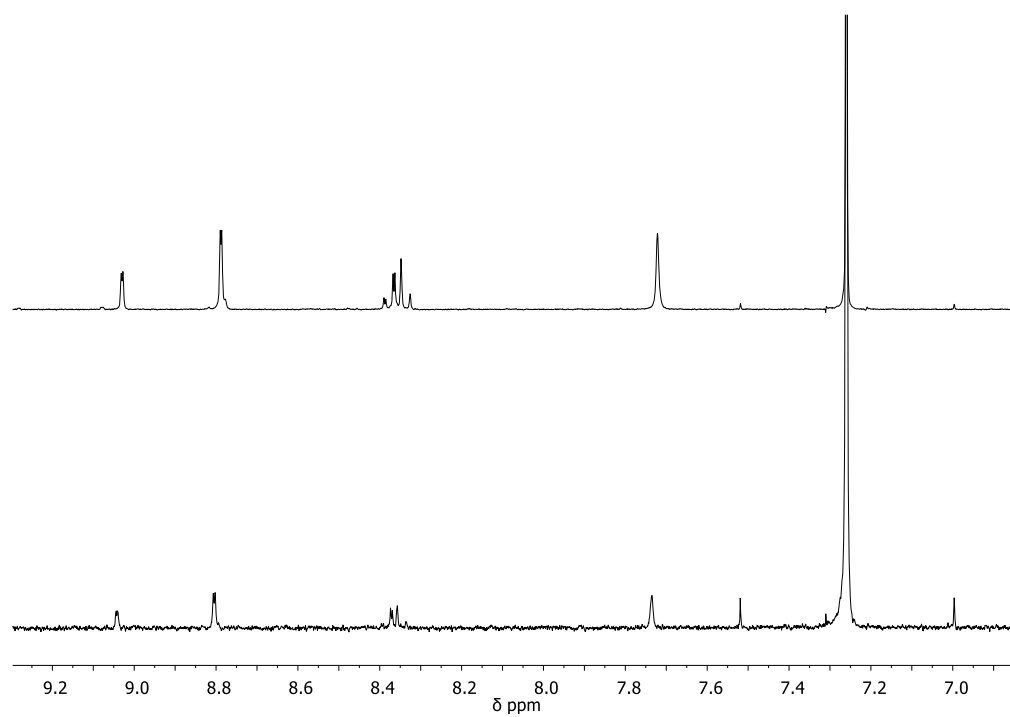


Figure S2: ^1H -NMR spectra (400 MHz) in CDCl_3 of **4** (a) 0.00268 M (b) 0.000268 M

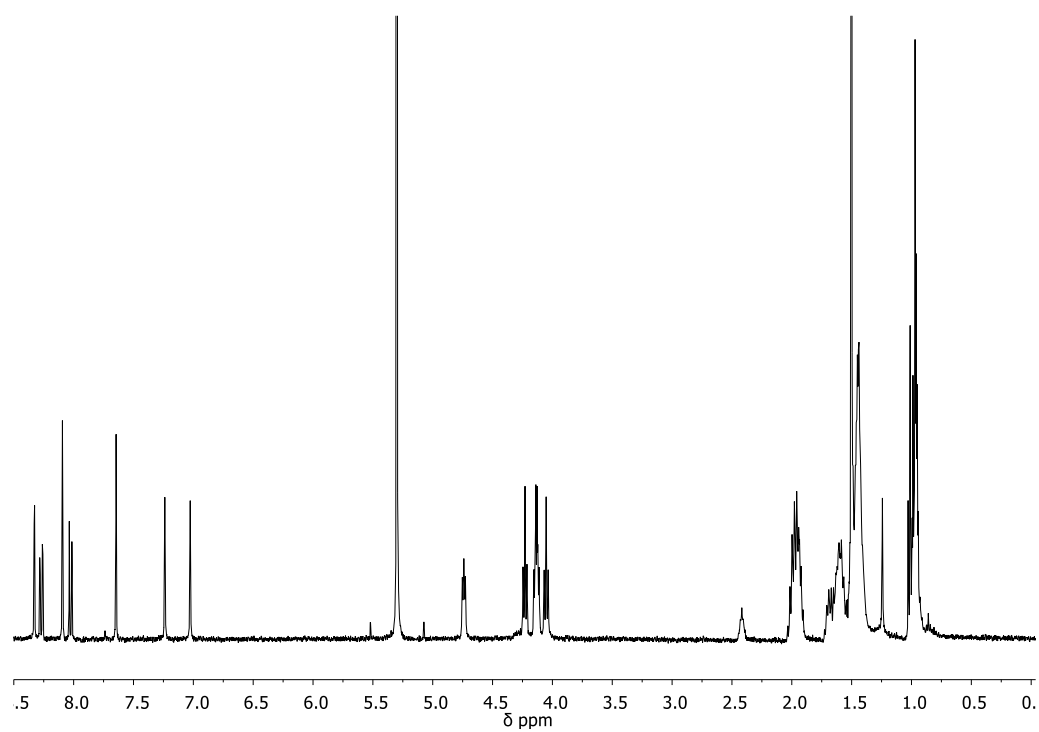


Figure S3: ^1H -NMR spectra (400 MHz) in CD_2Cl_2 of **2**

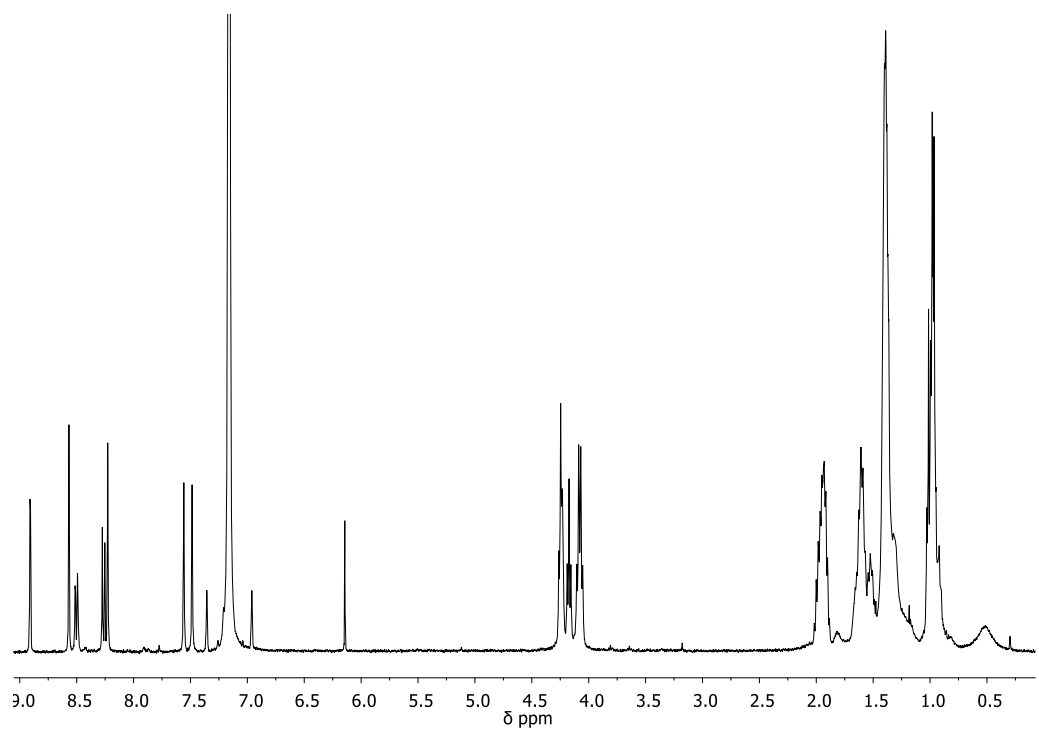


Figure S4: ^1H -NMR spectra (400 MHz) in benzene- d_6 of **2**

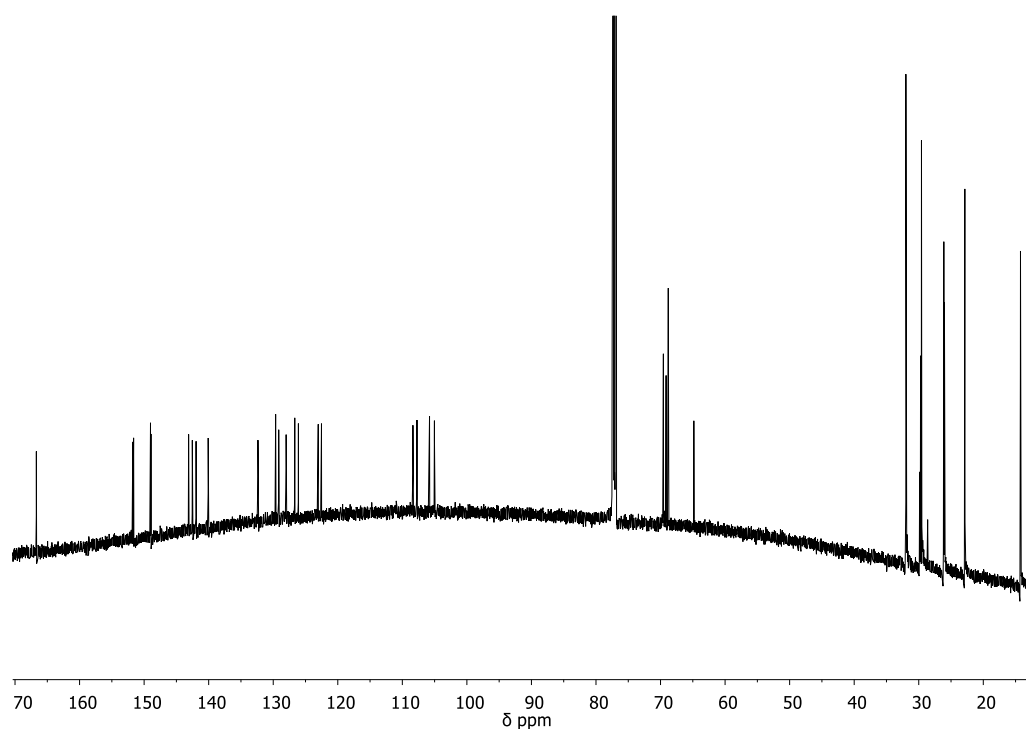


Figure S5: ^{13}C -NMR spectra (150 MHz) in CDCl_3 of **2**

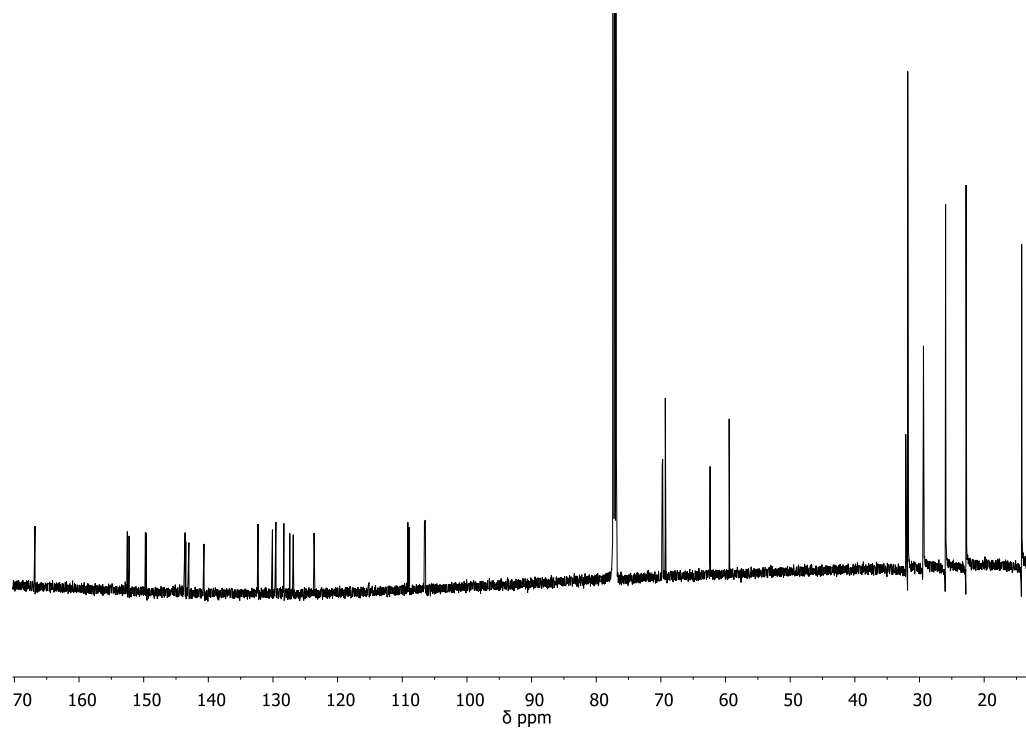


Figure S6: ^{13}C -NMR spectra (150 MHz) in CDCl_3 of **4**

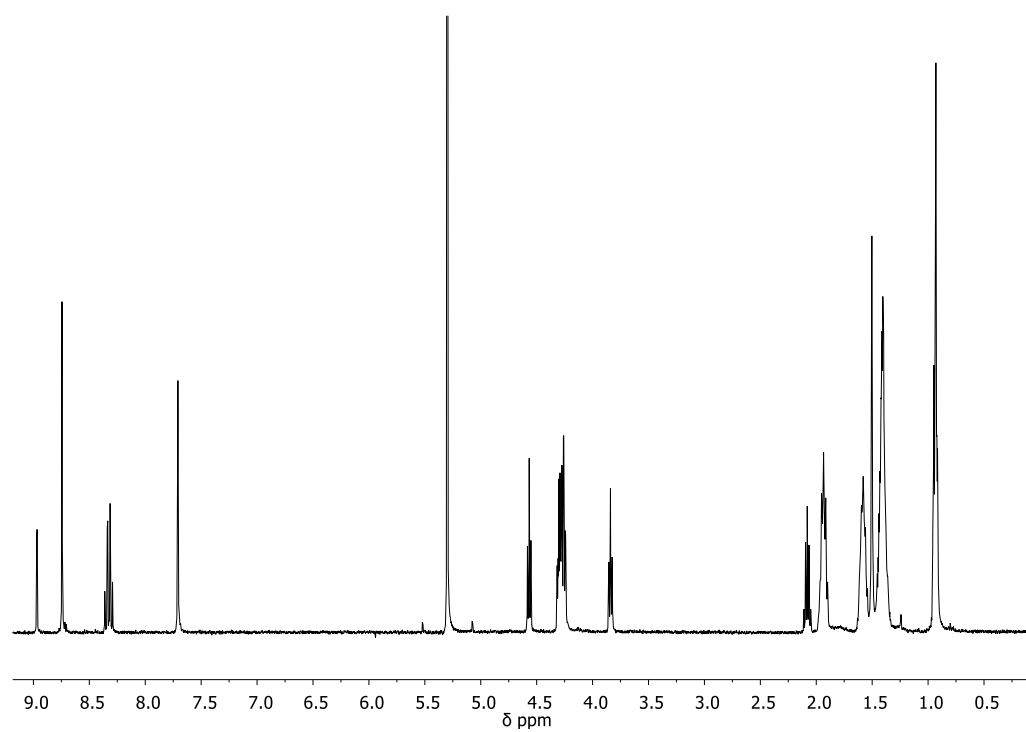


Figure S7: $^1\text{H-NMR}$ spectra (400 MHz) in CD_2Cl_2 of **4**

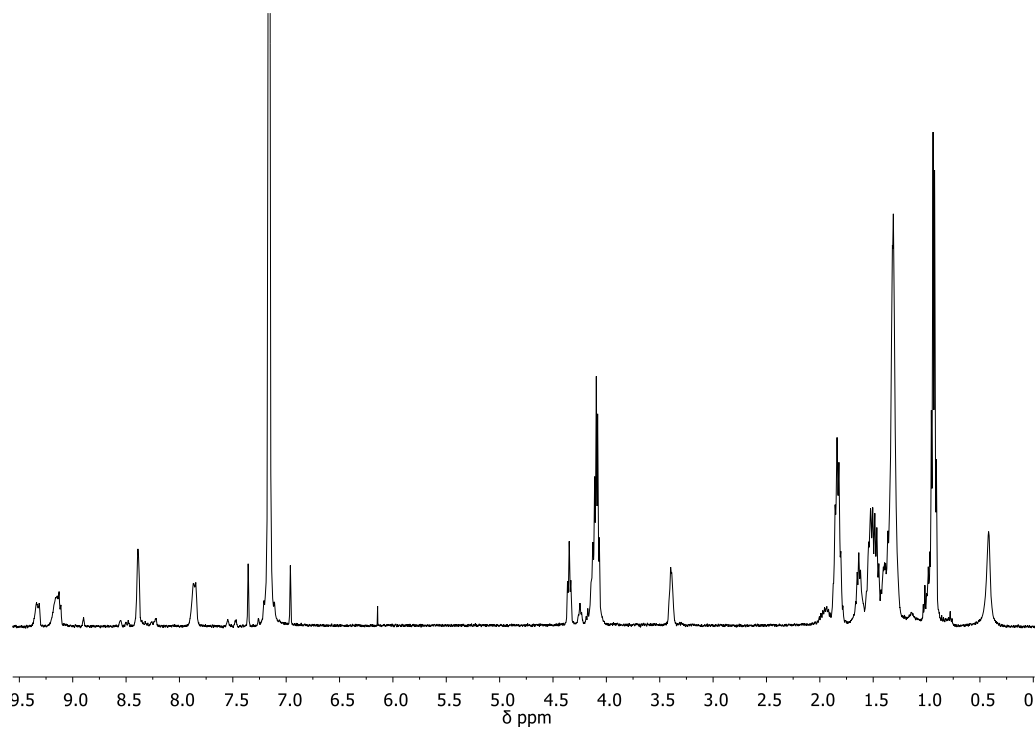


Figure S8: $^1\text{H-NMR}$ spectra (400 MHz) in benzene-d_6 of **4**

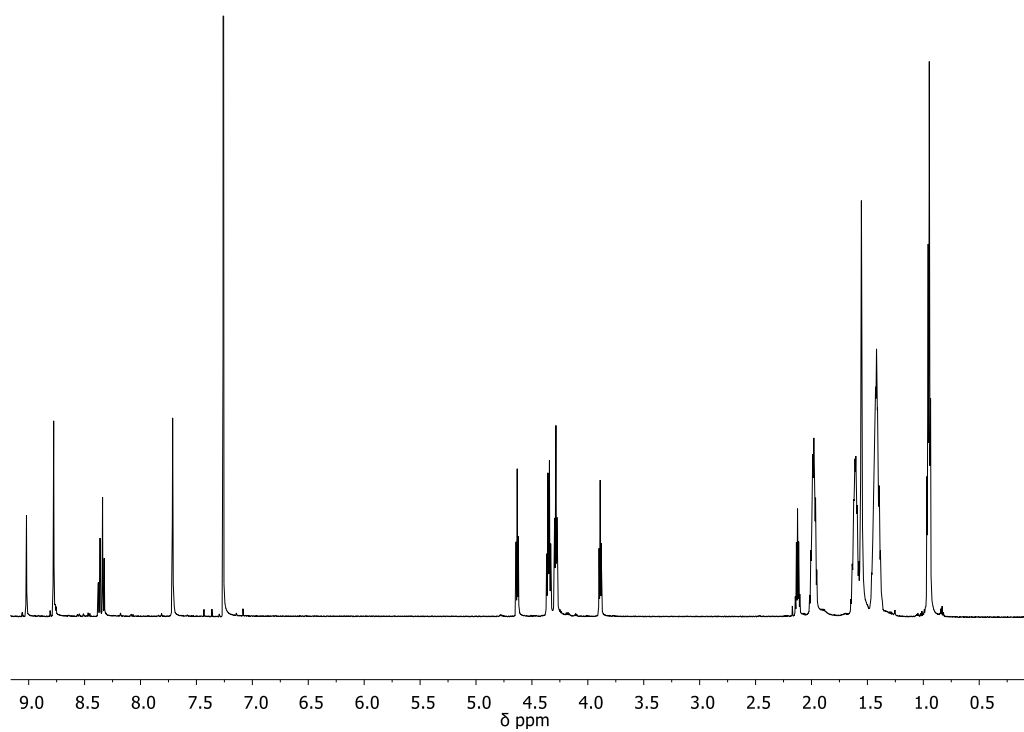


Figure S9: $^1\text{H-NMR}$ spectra (400 MHz) in CDCl_3 of **4**

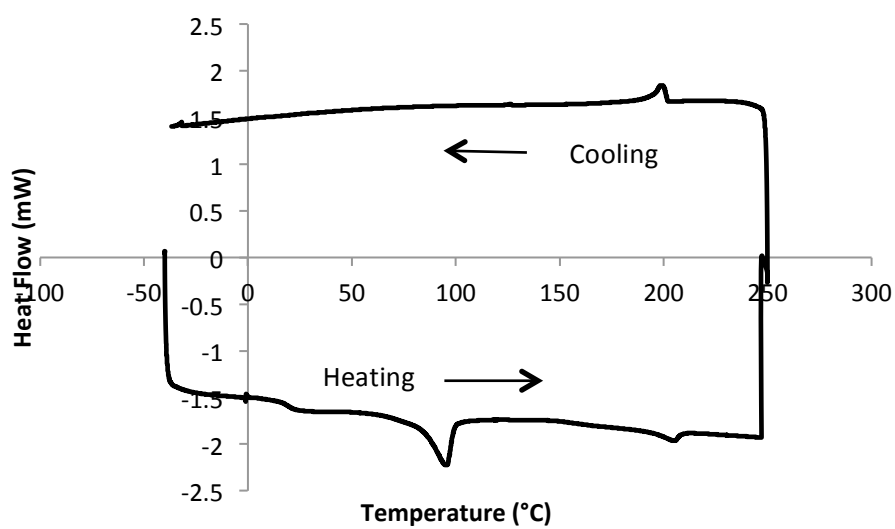


Figure S10: DSC Trace for **2** with a heating and cooling rate of $10\text{ }^\circ\text{C min}^{-1}$

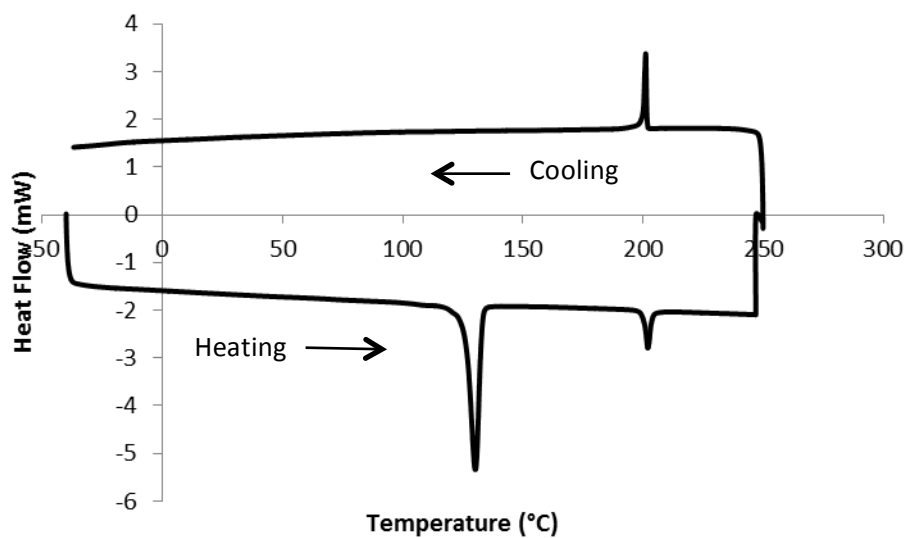


Figure S11: DSC Trace for **4** with a heating and cooling rate of $10\text{ }^{\circ}\text{C min}^{-1}$

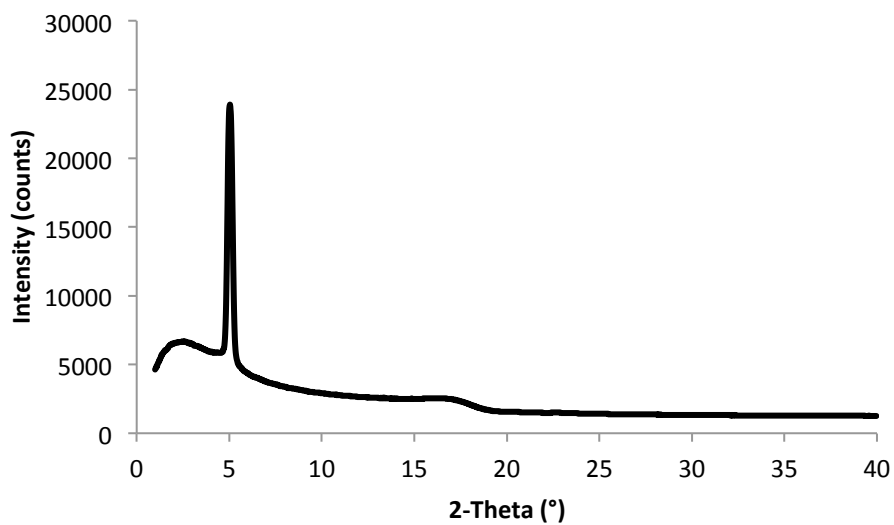


Figure S12: XRD trace of **4** at $178\text{ }^{\circ}\text{C}$

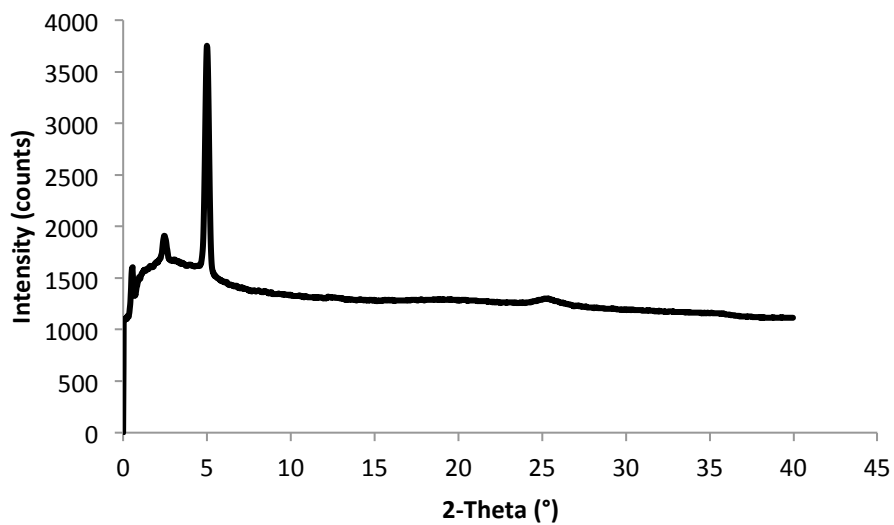


Figure S13: XRD trace of **4** at 170 °C

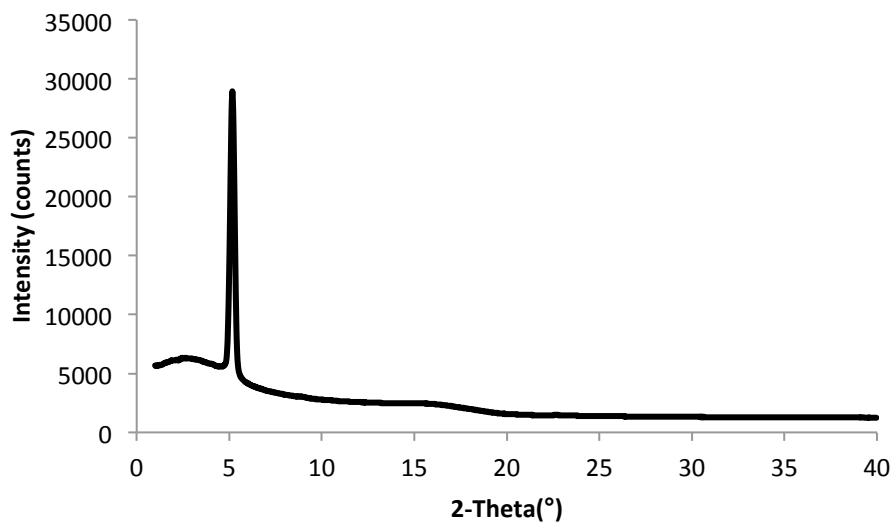


Figure S14: XRD trace of **2** at 166 °C

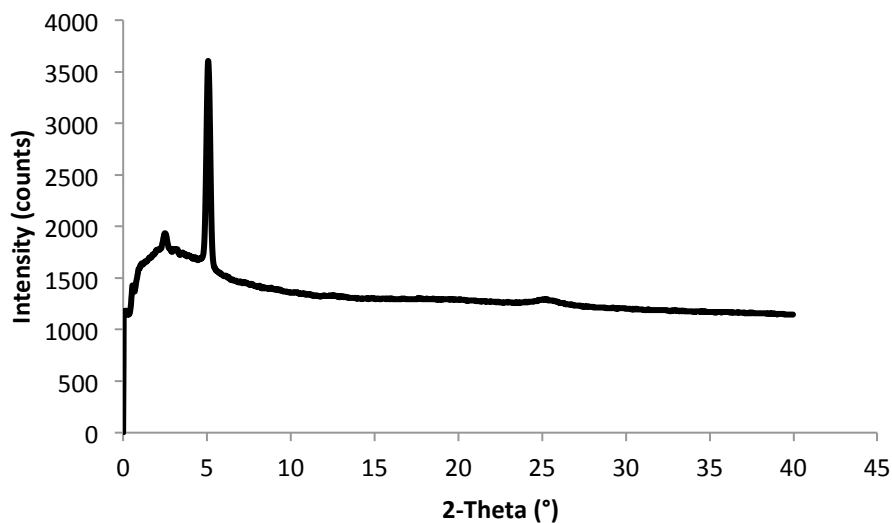


Figure S15: XRD trace of **2** at 190 °C

Cmpd	Phase ^a	T/ °C ($\Delta H/J g^{-1}$) ^b	Phase ^a		
2	Cr	96 (27)	→	Col _h	205 (5)
					⇌
4	Cr	130 (72)	→	Col _h	202 (9)
					⇌

Table S1: Phase behavior of **2** and **4**. ^a Cr = crystal, Col_h = hexagonal columnar, I = isotropic liquid. ^b Transition temperatures and enthalpies determined by DSC on first heating (scan rate = 10 °C min⁻¹).

Cmpd	Temp (°C)	d-spacings (Å)	Miller index (hkl)	Phase (lattice constants)
2	166	17.1	100	Col _h
		3.55	π - π stacking	(a = 19.7 Å)
4	178	17.5	100	Col _h
		3.55	π - π stacking	(a = 20.2 Å)

Table S2: X-ray diffraction data of **2** and **4**