

Supporting Information

Self-Assembly of Columnar Mesophases from Diaminotriazines

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Sample: KM-V-227
Size: 0.9610 mg
Method: ken

DSC

File: C:\...\DSC\Mars 2006\Ken\KM-V-227.001
Operator: ED
Run Date: 03-Mar-06 15:17
Instrument: DSC Q1000 V7.3 Build 249

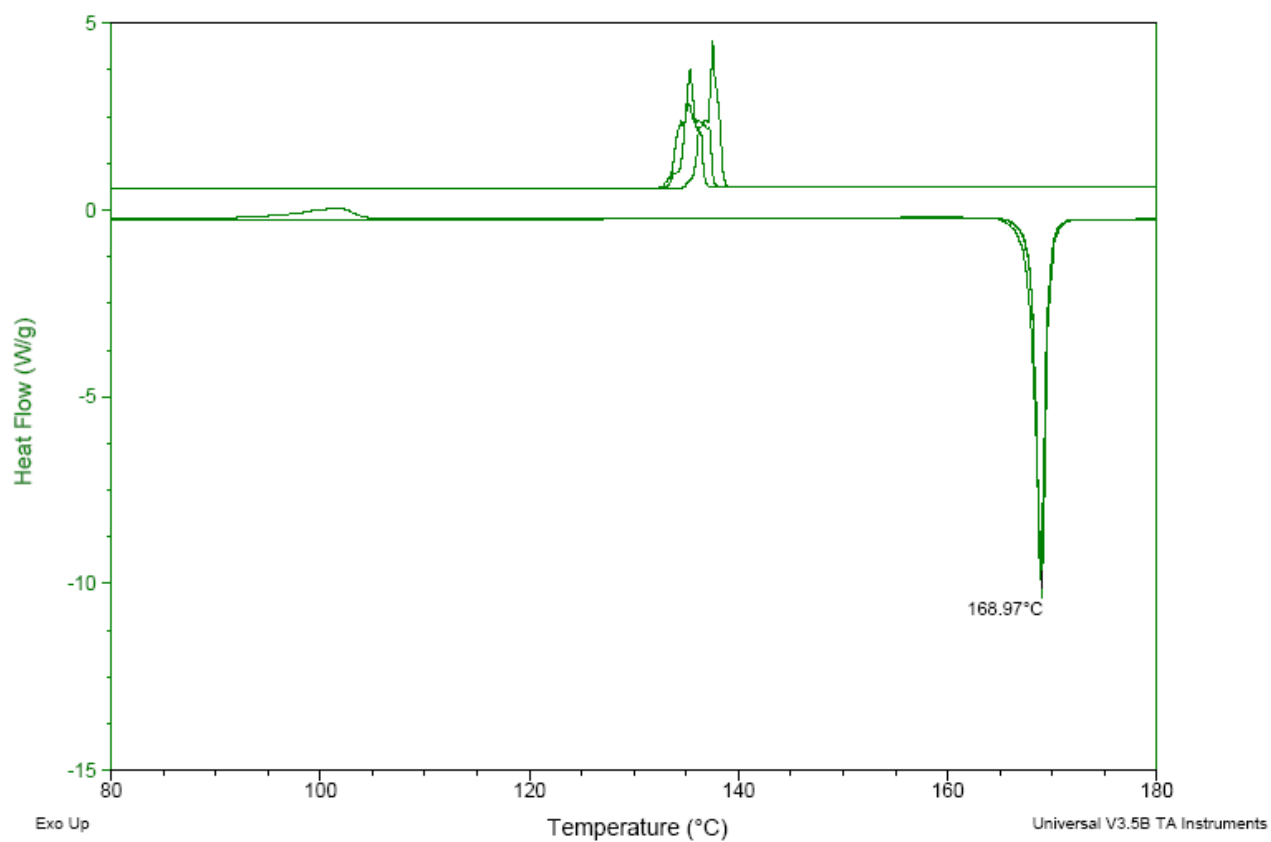


Figure S1. DSC Trace for compound **2a** over three heating and cooling cycles.

Sample: KM-V-60
Size: 1.7760 mg
Method: Ken

DSC

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Run Date: 22-Sep-05 10:47
Instrument: DSC Q1000 V7.3 Build 249

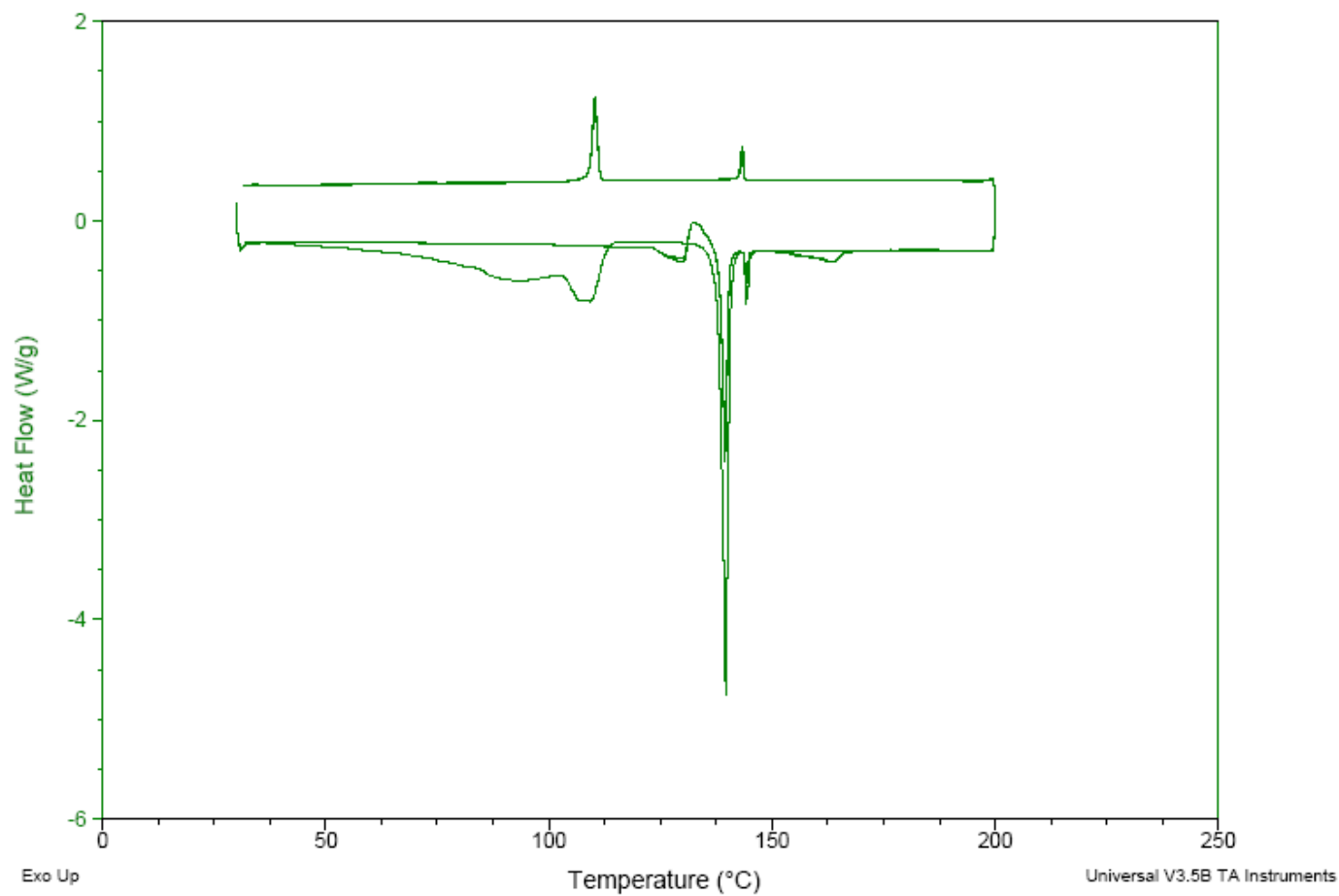


Figure S2. DSC Trace for compound **2b** over three heating and cooling cycles.

Sample: KM-V-132
Size: 1.7320 mg
Method: Ken

DSC

File: C:\DSC\2006\Jan 2006\Ken\KM-V-132.001
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Instrument: DSC Q1000 V7.3 Build 249

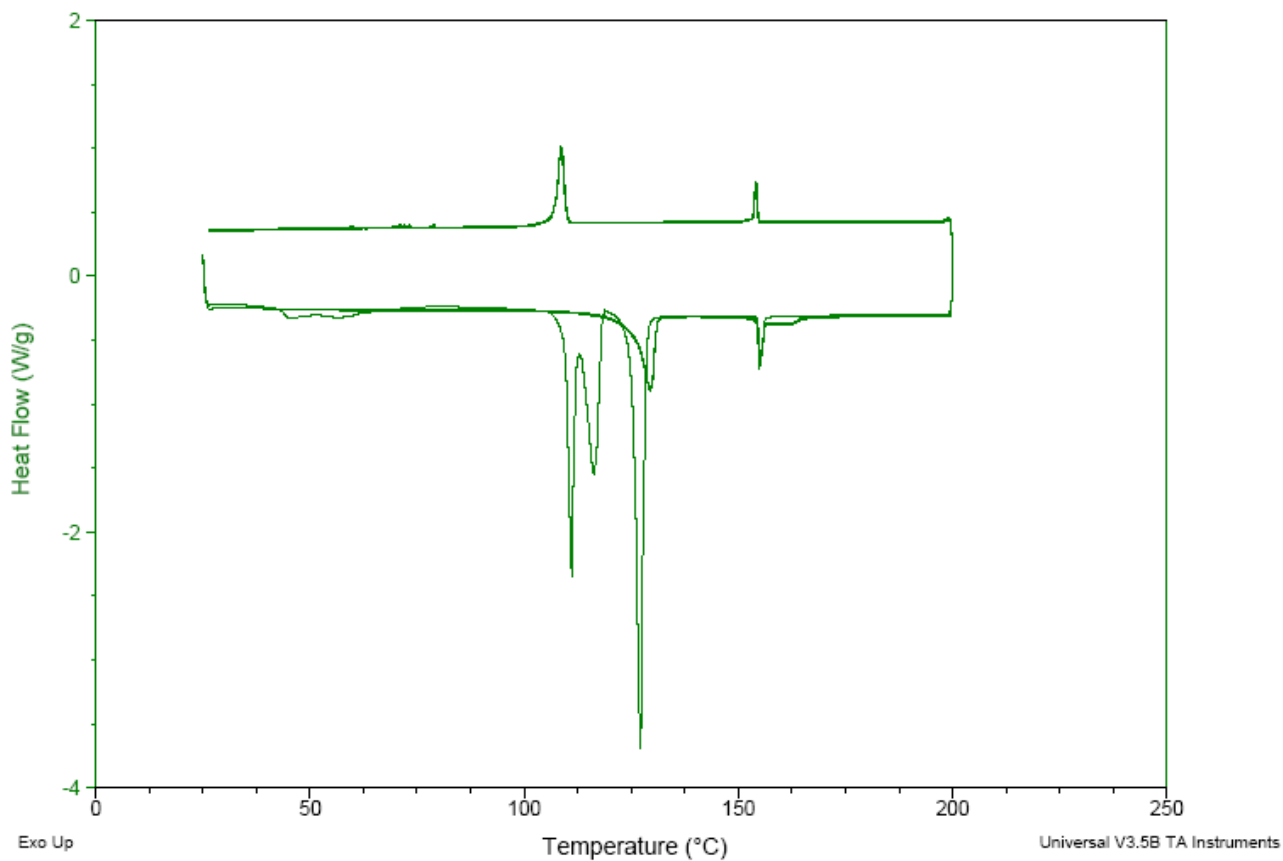


Figure S3. DSC Trace for compound **2c** over three heating and cooling cycles.

Sample: KM-V-242
Size: 1.2030 mg
Method: Ken

DSC

File: C:\2006\Mars 2006\Ken\KM-V-242.001
Operator: ED
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Instrument: DSC Q1000 V7.3 Build 249

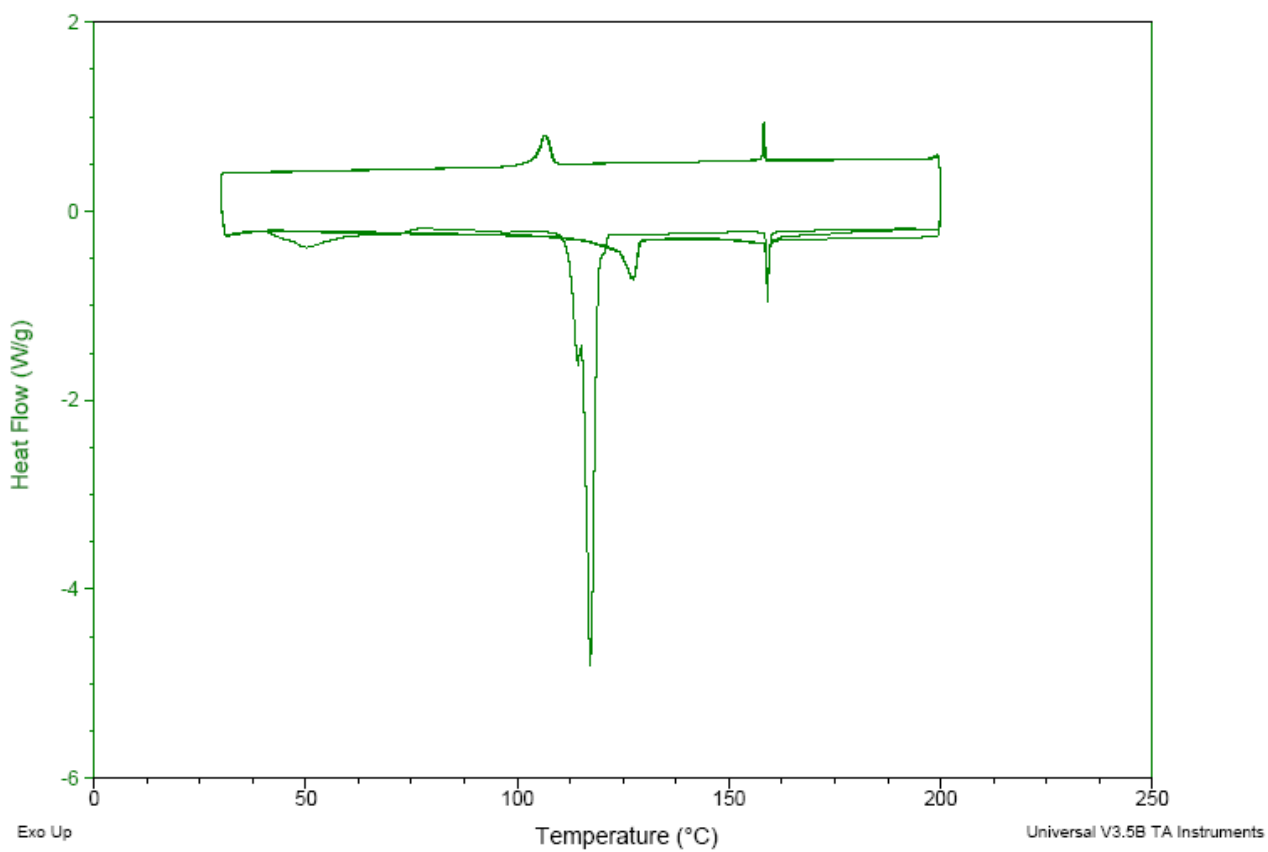


Figure S4. DSC Trace for compound **2d** over three heating and cooling cycles.

Sample: KM-V-192
Size: 0.9630 mg
Method: Ken

DSC

File: C:\...2006\Mars 2006\Ken\KM-V-192.003
Operator: ED
Run Date: 21-Mar-06 18:54
Instrument: DSC Q1000 V7.3 Build 249

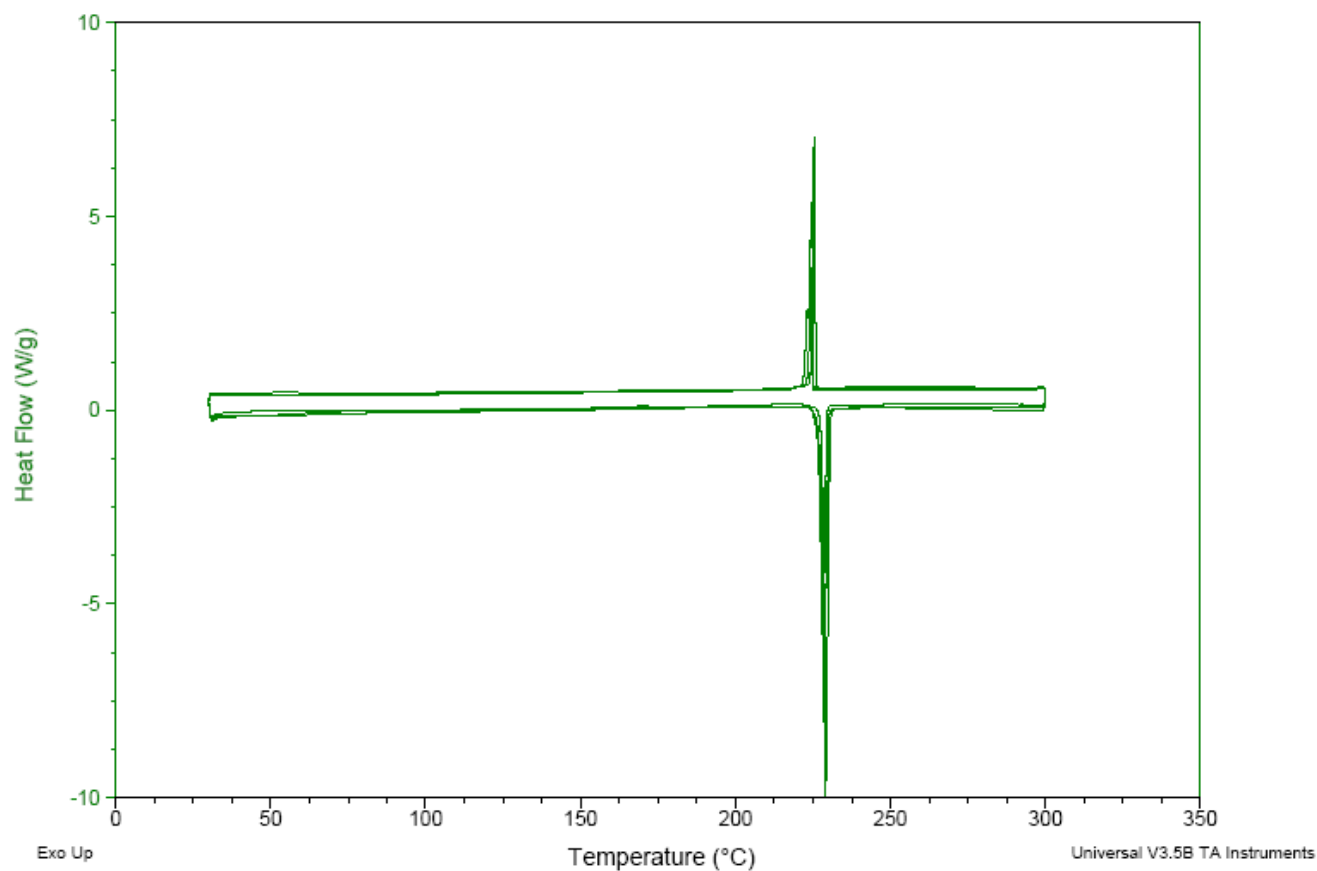


Figure S5. DSC Trace for compound **3** over three heating and cooling cycles.

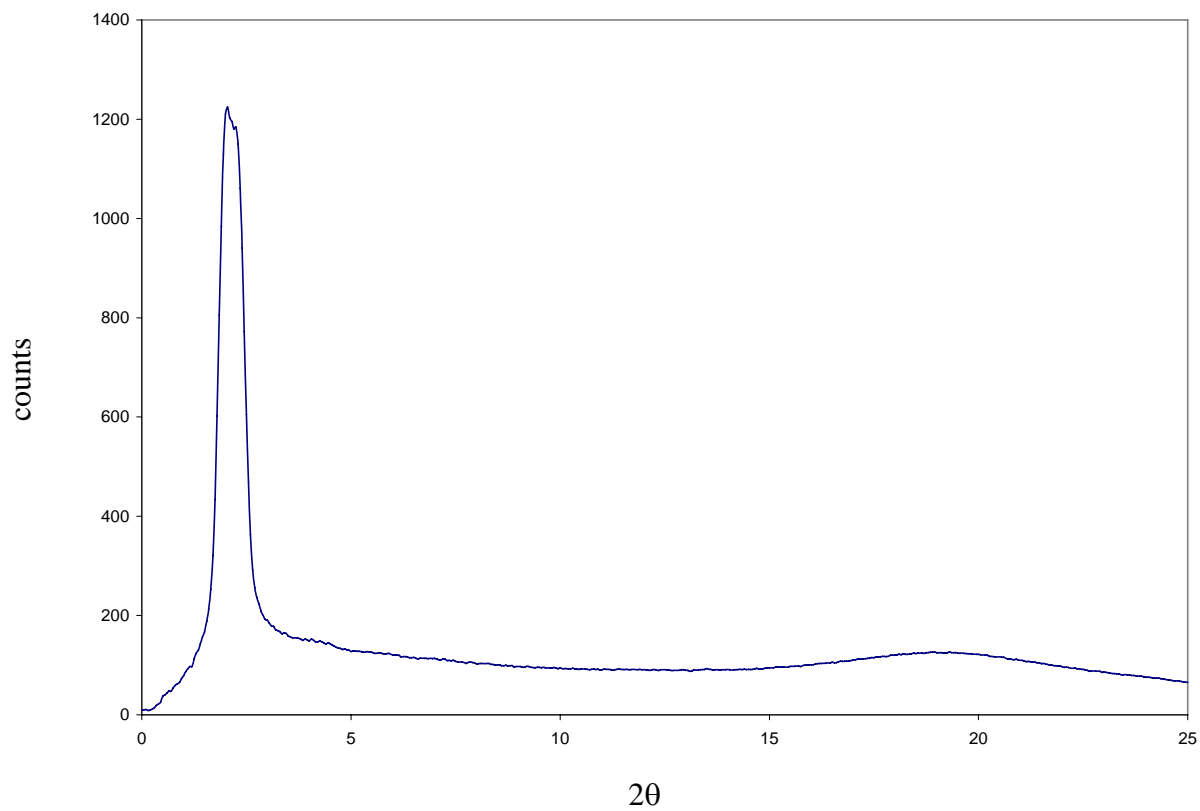


Figure S6. X-Ray diffractogram for compound **2c** at 132 °C.

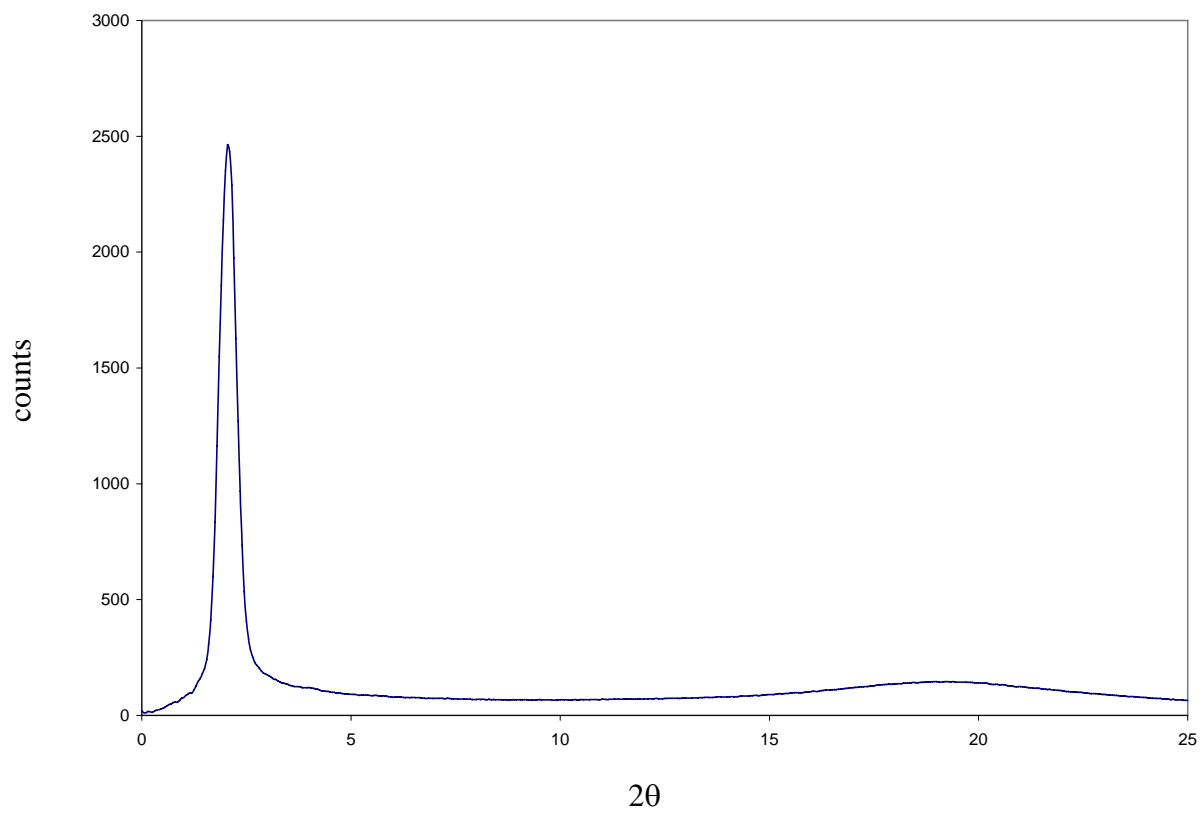


Figure S7. X-Ray diffractogram for compound **2d** at 132 °C.

Calculation of Lattice Parameters and Estimation of Density

The lattice parameters (a) for compounds **2b-d** were calculated from the observed (100) reflections using the following equation: $a = 2(d_{100})/\sqrt{3}$. The unit cell volume was calculated using the following equation: $V = (\sqrt{3}/2)a^2c \times 10^{-24}$, where V is the unit cell volume in cm^3 , and a and c are the lattice parameters in Angstroms. The value of c was assumed to be 3.7 \AA , which is a reasonable estimate for the distance between molecules in a columnar stack and corresponds to values observed for similar compounds.¹ The mass of each unit cell was calculated assuming six molecules per unit cell.

Table S1. Observed spacings from X-Ray measurements, and the corresponding lattice parameters and calculated densities.

Compound	R =	Observed Spacing (1 0 0) Reflections (\AA)	Lattice Parameters (\AA)	Calculated density (g/cm^3)
2b	C_8H_{17}	$d_{100} = 39.1$	$a = 45.1$	0.80
2c	$\text{C}_{10}\text{H}_{21}$	$d_{100} = 41.1$	$a = 47.4$	0.80
2d	$\text{C}_{12}\text{H}_{25}$	$d_{100} = 42.9$	$a = 49.5$	0.80

1. J. Barberá, L. Puig, P. Romero, J. L. Serrano, T. Sierra, *J. Am. Chem. Soc.* 2005, **127**, 458-464.