Electronic Supplementary Information for

Magnetic behaviour of bent-core mesogens derived from the 1,4-dihydrobenzo[*e*][1,2,4]triazin-4-yl

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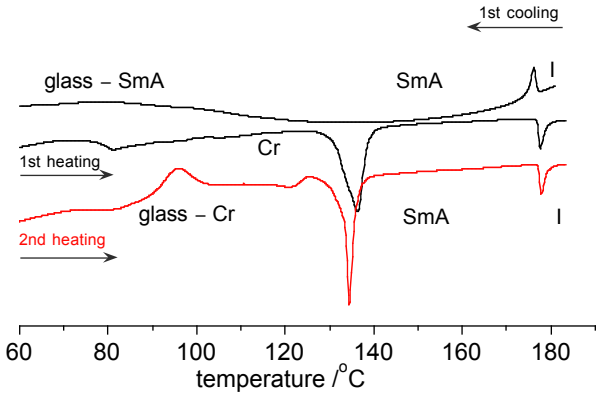
Table of Content:

1. Additional DSC data

Table S1. Thermal properties of **1[m,n]**, **2[4,6][6,n]** and triazine **12[6,6]**.

Compound	Phase behaviour[a] *T* /°C
1[12]	Cr 135 (*29.4*) I
2[6,4]	Cr 134 (*13.4*) SmA 178 (*1.4*)[b] I
2[6,6]	Cr 111 (*6.6*) SmA 174 (*0.8*) I
2[6,8]	Cr 104 (*13.3*) SmA 164 (*1.3*) I
2[6,10]	Cr 109 (*9.7*) SmA 158 (*1.6*) I
2[4,6]	Cr 113 (*10.3*) I
2[4,8]	Cr 103 (*6.5*) I
3[4,6][6,6]	Cr 112 (*10.7*) SmA 127 (*0.8*) I
3[4,6][6,8]	Cr 110 (*14.9*) SmA 116 (*0.4*) I
12[6,6]	Cr 201 (*16.0*) SmX 259 (*8.5*) SmA 294 (*4.6*) I

[a] Peak temperature on first heating. Heat of transition listed in the ESI. Cr-crystal, SmA-Smectic A phase, I-isotropic. [b] Enthalpy of transition in parentheses (kJ mol^{-1}).



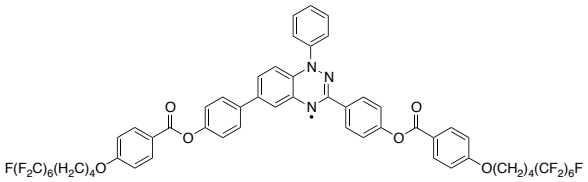
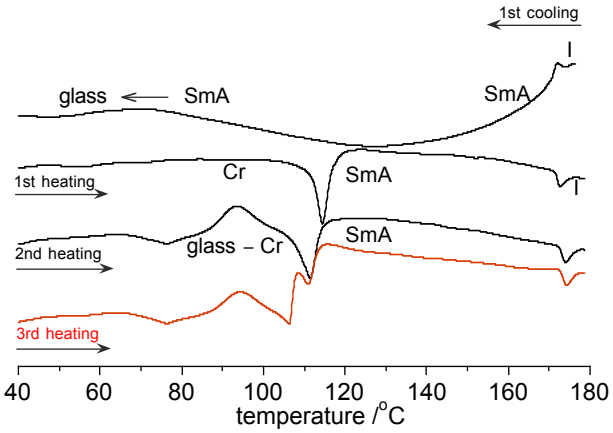


Fig. S1. DSC traces of **2[6,4]**. The heating and cooling rates are 10 K min^{-1}.



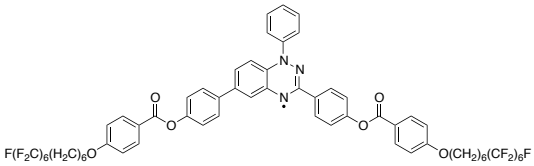
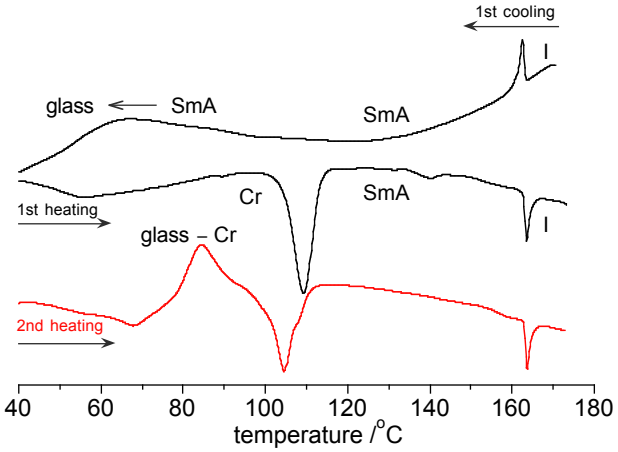


Fig. S2. DSC traces of **2[6,6]**. The heating and cooling rates are 10 K min^{-1}.



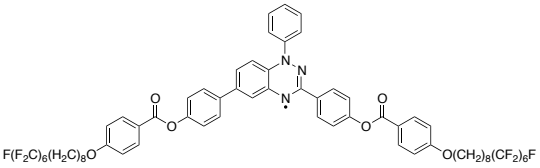
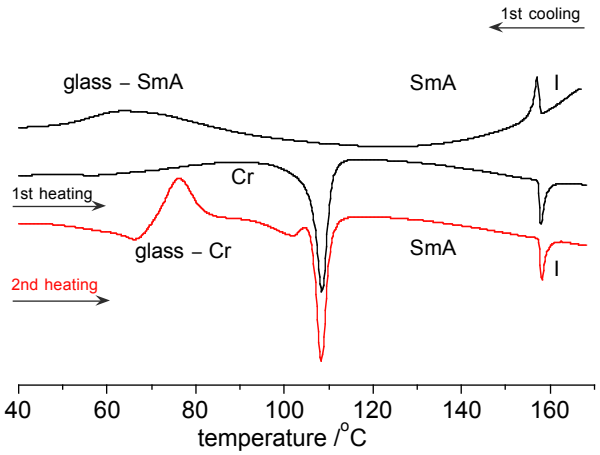


Fig. S3. DSC traces of **2[6,8]**. The heating and cooling rates are 10 K min^{-1}.



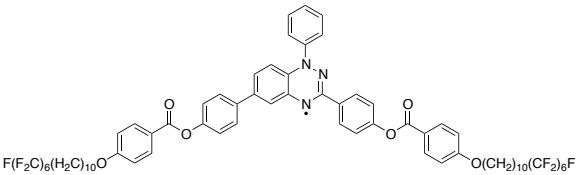
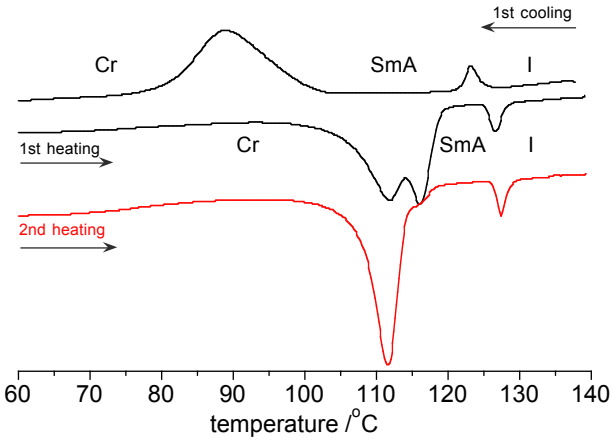


Fig. S4. DSC traces of **2[6,10]**. The heating and cooling rates are 5 K min^{-1}.



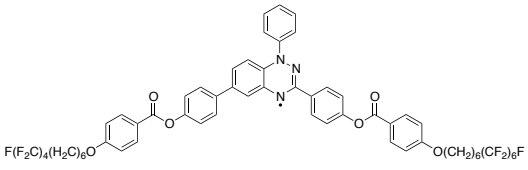
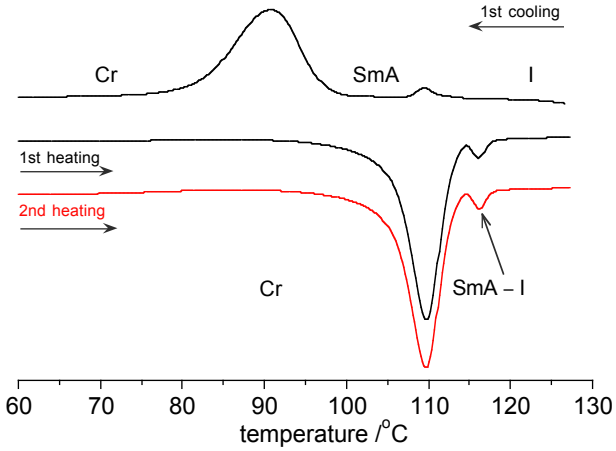


Fig. S5. DSC traces of **3[4,6][6,6]**. The heating and cooling rates are 5 K min^{-1}.



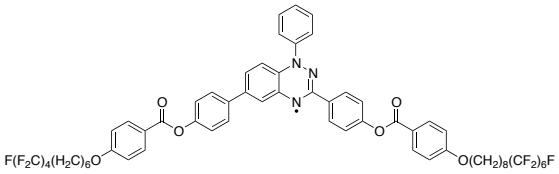
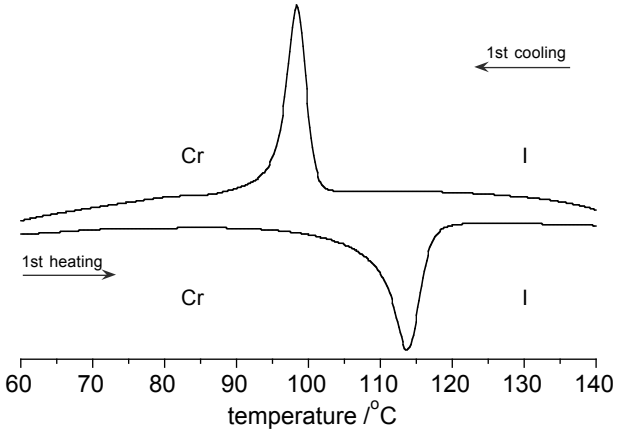


Fig. S6. DSC traces of **3[4,6][6,8]**. The heating and cooling rates are 5 K min^{-1}.



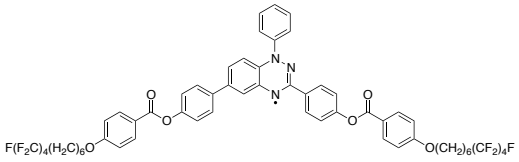
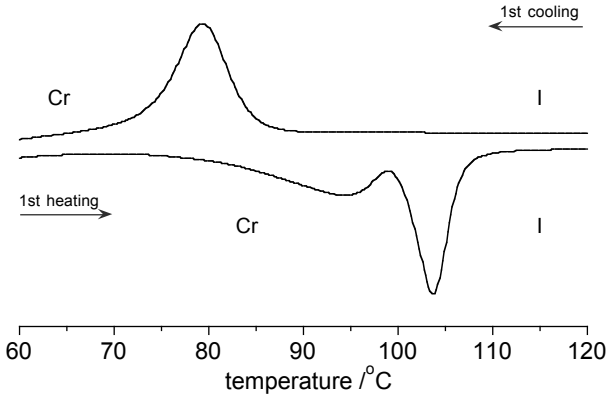


Fig. S7. DSC traces of **2[4,6]**. The heating and cooling rates are 10 K min^{-1}.



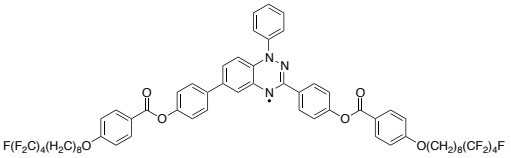
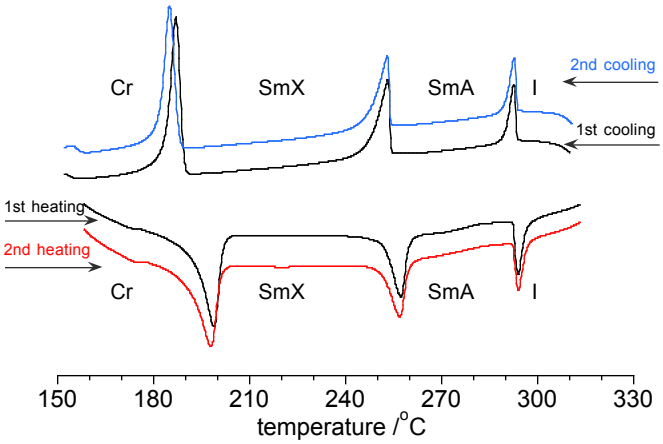


Fig. S8. DSC traces of **2[4,8]**. The heating and cooling rates are 10 K min^{-1}.



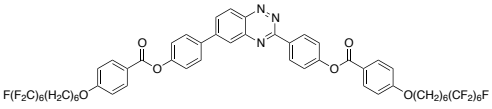


Fig. S9. DSC traces of benzo[*e*][1,2,4]triazine **12[6,6]**. The heating and cooling rates are 10 K min^{-1}.

2. Powder XRD measurements

X-ray diffraction experiments in broad angle range were performed with Bruker D8 GADDS (Cu Kα radiation, Göbel mirror, point collimator, Vantec 2000 area detector) equipped with a modified Linkam heating stage. For small angle diffraction experiments Bruker Nanostar system was used (Cu Kα radiation, cross-coupled Göbel mirrors, three pinhole collimation, Vantec 2000 area detector). Samples were prepared in a form of a thin film or a droplet on a heated surface. The X-ray beam was incident nearly parallel to sample surface. Results are shown in Fig. S10 – S16.

Analysis demonstrated that the temperature dependence for **2[6,n], 3[4,6][6,n]** is well described by a litear function, e.g. $d_{01} = a \bullet T + b$. For comparison purposes, thermal expansion coefficients are obtained from fitting of the $d_{01}(T)$ data to the linear function $d_{01} = a \bullet T + b$.

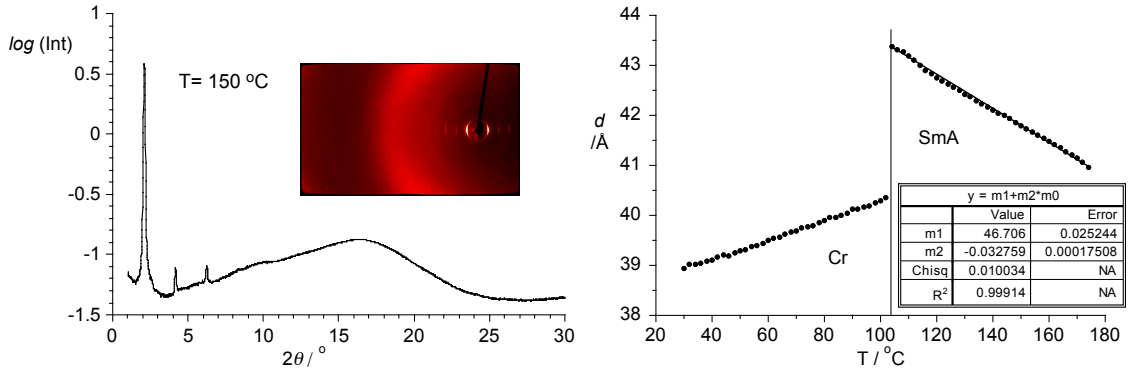


Fig. S10. Left: X-ray diffractogram for **2[6,4]** obtained by integration of the 2D pattern at 150 °C. Right: Layer thickness d_{01} as a function of temperature; fitting the SmA datapoints in a range of 174 °C – 104 °C to the function $d_{01} = a \bullet T + b$

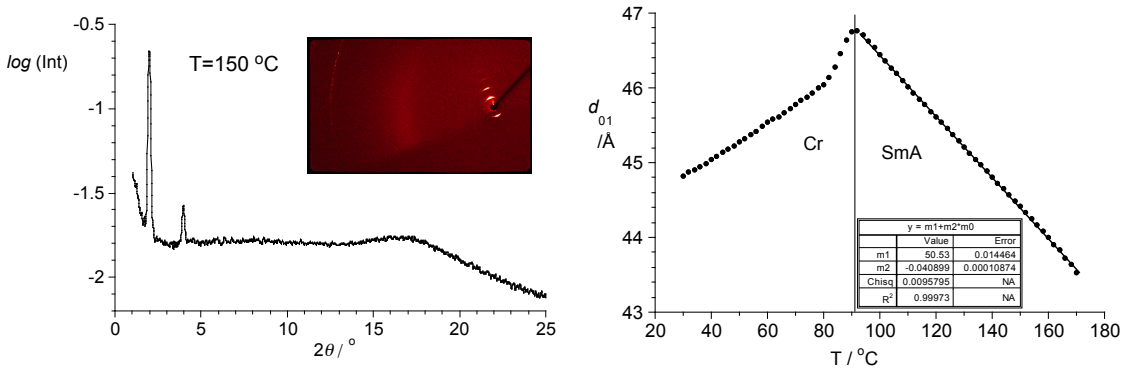


Fig. S11. Left: X-ray diffractogram for **2[6,6]** obtained by integration of the 2D pattern at 150 °C. Right: Layer thickness d_{01} as a function of temperature; fitting the SmA datapoints in a range of 170 °C – 92 °C to the function $d_{01} = a \bullet T + b$

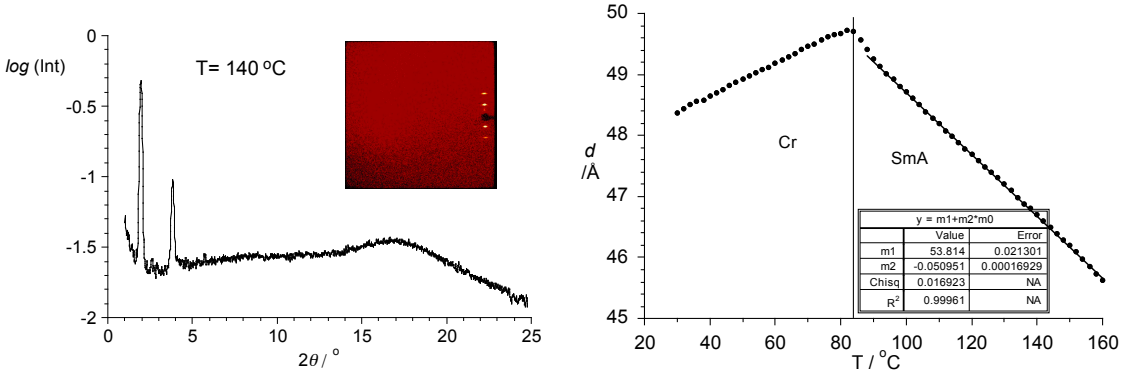


Fig. S12. Left: X-ray diffractogram for **2[6,8]** obtained by integration of the 2D pattern at 140 °C. Right: Layer thickness d_{01} as a function of temperature; fitting the SmA datapoints in a range of 160 °C – 90 °C to the function $d_{01} = a \bullet T + b$

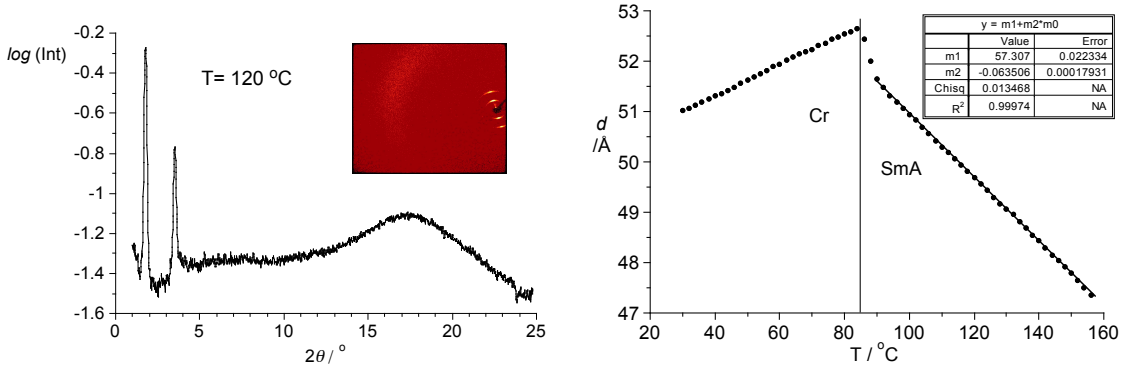


Fig. S13. Left: X-ray diffractogram for **2[6,10]** obtained by integration of the 2D pattern at 120 °C. Right: Layer thickness d_{01} as a function of temperature; fitting the SmA datapoints in a range of 156 °C – 90 °C to the function $d_{01} = a \bullet T + b$

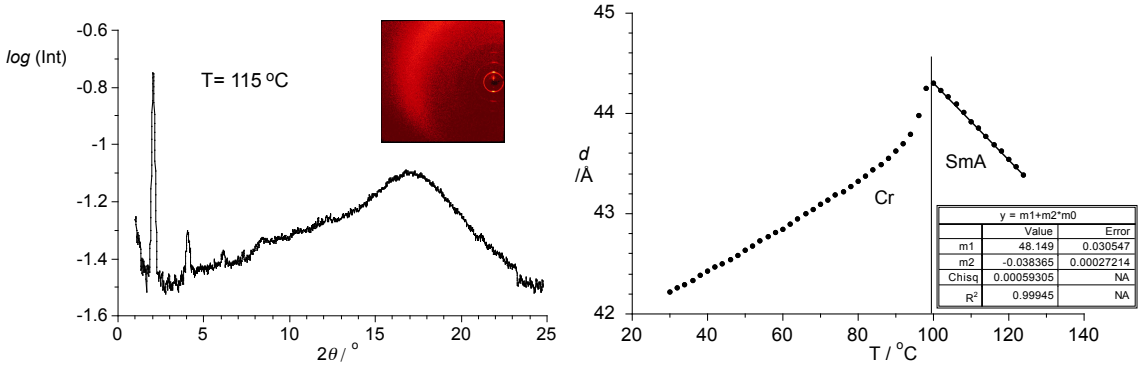


Fig. S14. Left: X-ray diffractogram for **3[4,6][6,6]** obtained by integration of the 2D pattern at 115 °C. Right: Layer thickness d_{01} as a function of temperature; fitting the SmA datapoints in a range of 124 °C – 100 °C to the function $d_{01} = a \bullet T + b$

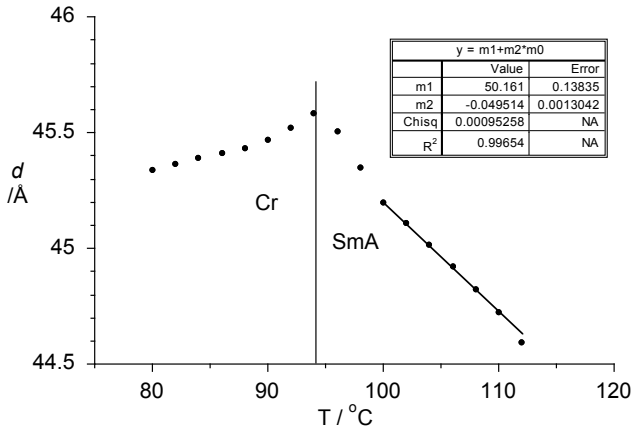


Fig. S15. Layer thickness d_{01} for **3[4,6][6,8]** as a function of temperature; fitting the SmA datapoints in a range of 112 °C – 100 °C to the function $d_{01} = a \bullet T + b$

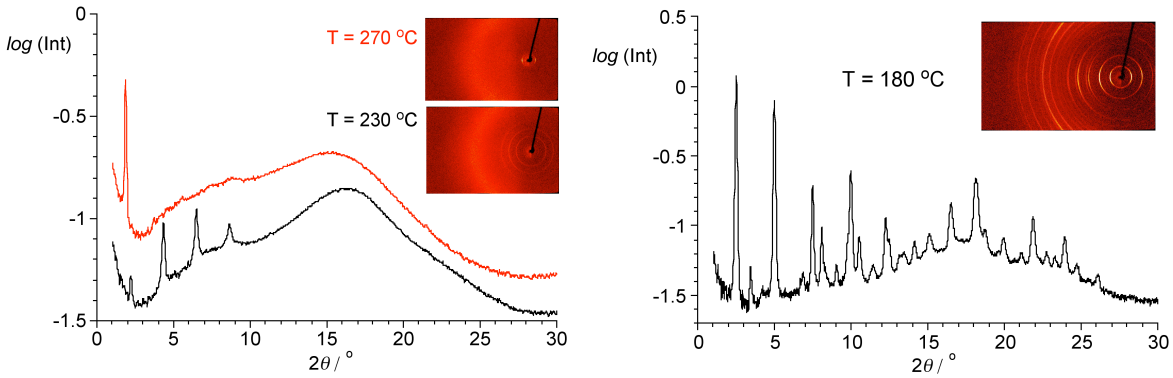


Fig. S16. X-ray diffractogram for **12[6,6]** obtained by integration of the 2D pattern at 270, 230 and 180 °C.

3. Additional textures

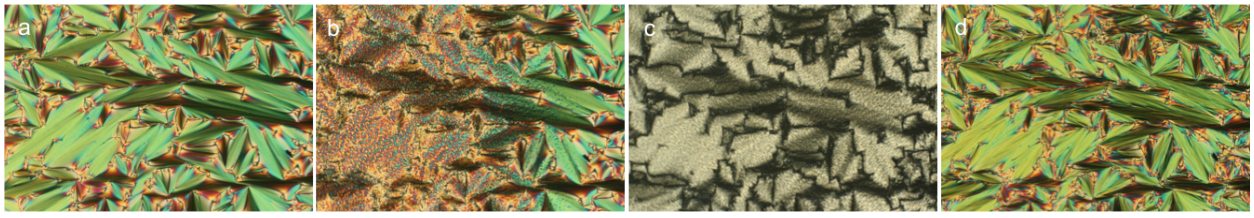


Fig. S167 Optical textures obtained on cooling from the isotropic phase of **12[6,6]**: a) SmA at T = 290 °C, (b) SmA–SmX transition at T = 265 °C, (c) SmX at T = 255 °C, and (d) SmA upon reheating to T = 270 °C.

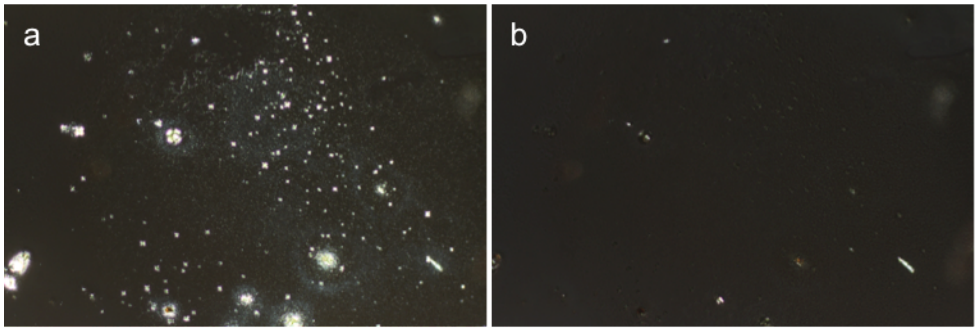


Fig. S18. Optical textures obtained by cooling from the isotropic phase of **12[6,6]** without the top cover glass: a) T = 280 ºC, (b) T = 240 ºC.

4. EPR spectroscopy

Solution EPR spectrum for radicals **3[4,6][6,8]** was recorded using an X-band EPR spectrometer at RT in dilute and degassed solutions in CH_2Cl_2. The microwave power was in a range of 5-70 mW with a modulation frequency 100 kHz, a modulation amplitude of 1.0 G_{pp} and spectral width of 80 G. Accurate g-values were obtained using solid DPPH as internal standard (g = 2.0036). Simulations were performed with the PEST program (EPR-WinSim.2002 version 0.98 for Windows; available at:

http://www.niehs.nih.gov/research/resources/software/tox-pharm/tools/index.cfm using DFT results for **3[4,6][6,8]** as the starting point for the simulation. The resulting *hfcc* values were perturbed until the global minimum for the fit was achieved using the LMB1 algorithm of WinSim.[5]

Simulation parameters:

DG = 0.22 G, LS=78.0 (78% Lorentzian, 22% Gaussian), r = 0.985

Experimental and simulated spectra are shown in Figure S19 and resulting *hfcc* are listed in Table S2.

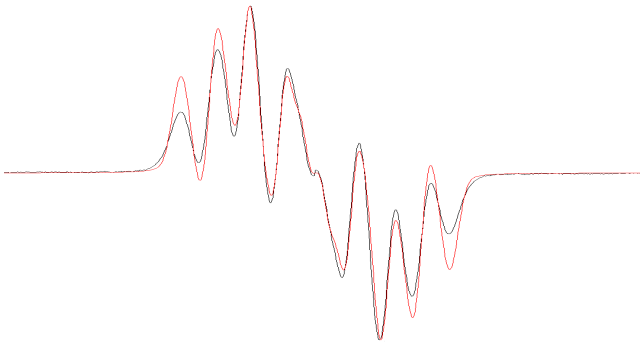


Figure S19. Experimental (black) and simulated (red) spectra for **3[4,6][6,8]** recorded in CH_2Cl_2 a 23 ºC

Table S2. Experimental hyperfine coupling constants (G) for for **3[4,6][6,8]** in CH_2Cl_2 at 23 ºC.

N	7.606	
N	4.748	
N	4.736	
H	1.869	
H	0.933	
H	0.398	
H	0.791	
H	0.104	(x2)
H	0.988	
H	0.838	
H	0.696	
H	0.473	
H	0.431	
H	0.180	(x2)
H	0.304	
H	0.738	

Temperature dependent EPR spectra for neat **3[4,6][6,8]** (about 2 mg) were recorded using an X-band Bruker spectrometer typically every 2–3 K on cooling allowing for 1–2 min of stabilization. The samples were not degassed. The line width was measured as a difference in position of the maximum and minimum of the EPR signal. The double integral was obtained using Kaleidagraph software in two steps. First, the original curve was integrated, the slope was removed from the resulting function, and shifted to $y = 0$ line. Subsequently, the area under the curve was integrated in the range of 3300 G to 3400 G. The formula for the slope was obtained by fitting the linear portions of the integrated curve (on both sides of the peak) to a line.

5. Magnetization measurements and data analysis.

Experiments were conducted using SQUID magnetometer (Quantum Design MPMS-XL-7T). Analysis of the magnetic data was performed using χ•T vs T plots (eq 1).

$$\chi \bullet T = \left(\chi_p + \chi_{dia}\right) \bullet T = C + \chi_{dia} \bullet T \quad \text{(eq 1)}$$

where C = 0.375 cm^3 K mol^{-1} for an ideal paramagnet.

A sample of **2[4,6][6,8]** (*m* = 8.49 mg, 6.22×10^{-6} mol, M_w= 1365.07 g mol^{-1}) was placed in a polycarbonate capsule fitted in a plastic straw. The sample was heatd (2 K → 400 K) and then cooled from the isotropic phase (400 K → 2 K) at a rate 0.8 K min^{-1} in a magnetic field of 0.1 T. The total molar susceptibility of the sample, χ, as a function of temperature is shown in Figure S20 and a χ•T *vs* T plot in Figure S21.

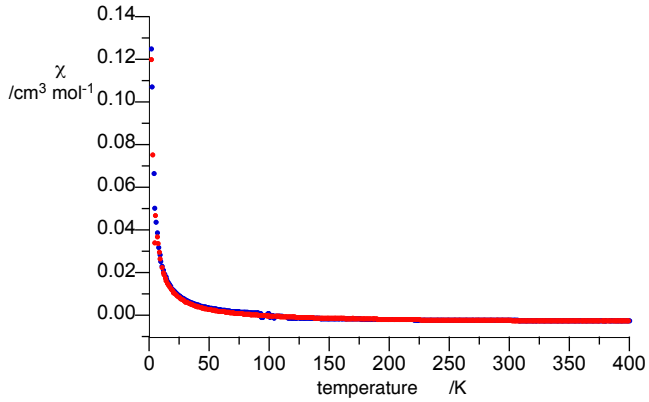


Figure S20. Molar magnetic susceptibility χ *vs* T obtained for **2[4,6][6,8]** on heating 2 K → 400 K (red) and then on cooling 400 K → 2 K (blue) at 0.1 T. Cooling and heating rates are 0.8 K min^{-1}.

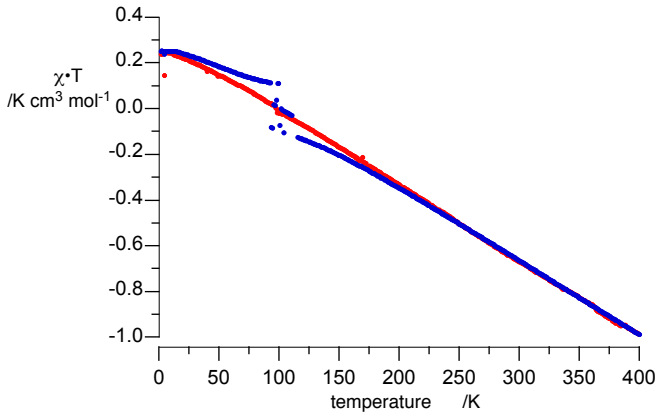


Figure S21. A χ_{tot}•T *vs* T plot of molar magnetic susceptibility of **2[4,6][6,8]** obtained on heating 2 K → 400 K (red) and then on cooling 400 K → 2 K (blue) at 0.1 T. Cooling and heating rates are 0.8 K min^{-1}.

The diamagnetic correction, χ_{dia}, was determined from a linear portion of the χ•T *vs* T plot in the temperature range 300 K – 400 K (Figure S22) for data obtained on cooling. The diamagnetic correction, χ_{dia} = –0.003242 cm^3mol^{-1}, obtained for the flat portion of the heating curved was applied to both the heating and cooling χ•T curve. The resulting χ_p(T) and χ_p•T(T) curves are shown in Figures S23 and S24, respectively.

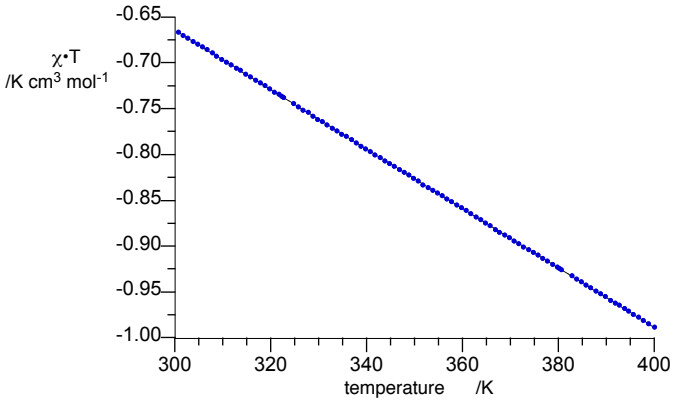


Figure S22. A linear portion of the χ•T *vs* T plot for **3[4,6][6,8]** on heating (Figure S21) in a range of 400 K → 30 K. Best fit line: χ•T = –0.003242(1)•T +0.3082(5), r^2 = 0.9999.

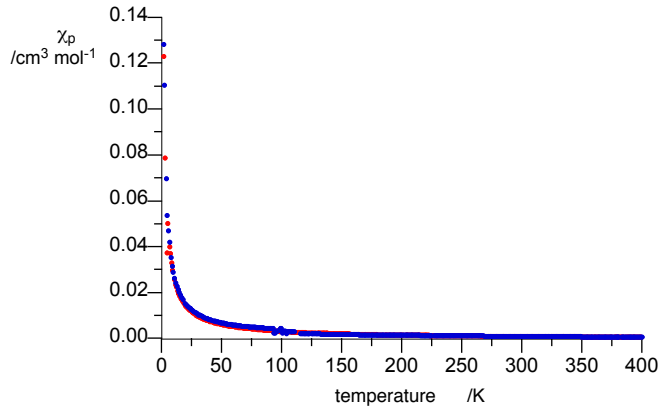


Figure S23. A χ_p *vs* T plot of molar magnetic susceptibility of **3[4,6][6,8]** obtained on heating 2 K → 400 K (red) and then on cooling 400 K → 2 K (blue) at 0.1 T. Cooling and heating rates are 0.8 K min^{-1}.

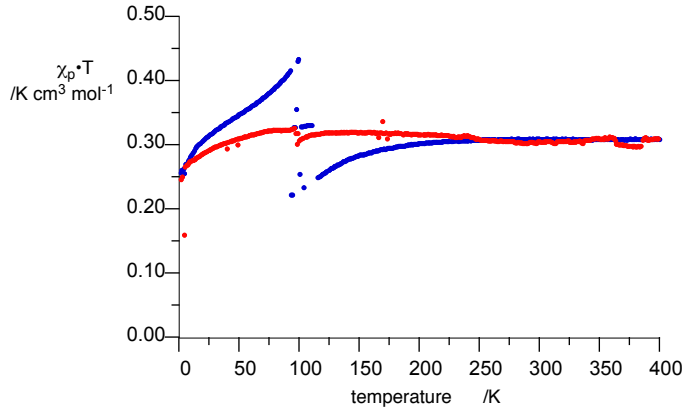


Figure S24. χ_p•T *vs* plots T for **3[4,6][6,8]** after diamagnetic correction χ_{dia} = –0.003242 cm^{3}mol^{-1}, determined in Figure S20. Applied field 0.1 T and the cooling rate 0.8 K min^{-1}.

The discontinuity around 100 K is due to magnetization crossing 0 (see Figure S24).

6. Computational details

Quantum-mechanical calculations were carried out using Gaussian 09 suite of programs. Geometry optimizations for unconstrained molecules were undertaken at the B3LYP/6-31G* level of theory using default convergence limits. The alkoxy chains were set at the all-trans conformations coplanar with the benzene ring.

7. Archive for DFT results

2[6,4]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2[6,6]

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2[6,8]

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2[6,10]

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3[4,6][6,6]

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@

3[4,6][6,8]

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