

Supporting Information

The first examples of discotic radicals: the columnar mesomorphism in spin-carrying triphenylenes

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Synthetic procedure and molecular structural characterization data for the **3,6,7,10,11-pentapentyloxy-2-hydroxytriphenylene:**

1,2-Dipentyloxy benzene (70.04 mmol, 1 equiv) was dissolved in a solution of 2% H₂SO₄ in dry dichloromethane (88 ml). To this solution, anhyd. FeCl₃ was added in portions over a period of 30 min. The reaction mixture (RM) was stirred at room temperature (RT) for 1 h. Then the RM was cooled in ice. To this solution, precooled methanol was slowly added. The yellow precipitate appeared was filtered and washed with little cold methanol (170 ml). The yellow solid turns bluish. The solid containing the mixture of hexapentyloxy triphenylene and monohydroxy triphenylene was purified by column chromatography on neutral alumina using 30 % MDC-hexanes as eluent and were isolated respectively in 66 % and 8 % yields. 3,6,7,10,11-Pentapentyloxy-2-hydroxytriphenylene: R_f = 0.38 (50% CH₂Cl₂-hexanes); a black solid; IR (KBr pellet): $\nu_{\max}$ in cm⁻¹ 3544, 2954, 2230, 2859, 1616, 1595, 1519, 1450, 1438, 1389, 1262, 1171, 1074, 1054, 1031, 1015, 909, 849, 836, 768, 732 and 650; ¹H NMR (CDCl₃, 400 MHz): δ 7.96 (s, 1H, Ar), 7.83(m, 4 H, Ar), 7.77 (s, 1H, Ar), 5.9 (s, 1H, OH), 4.26 (m, 10H, OCH₂), 1.95 (m, 10H, 5 $\times$ CH₂), 1.37-1.56 (m, 20H, 10 $\times$ CH₂), 0.97 (t, 15H, 5 $\times$ CH₃); ¹³C NMR (CDCl₃, 100 MHz): 149.1, 149, 148.8, 145.8, 145.3, 123.9, 123.6, 123.2, 123, 107.6, 107.4, 107.3, 106.5, 104.3, 69.9, 69.6, 69.1, 29.1, 28.3, 22.5, 14.1; MS (FAB⁺): m/z for C₄₃H₆₂O₆, Calculated:674.95, Found: 675; Anal. calcd for C₄₃H₆₂O₆: C, 76.52; H, 9.26. Found: C, 76.23; H, 9.4.

3,6,7,10,11-Pentahexyloxy-2-hydroxytriphenylene:

Procedure followed is same as in the case of 3,6,7,10,11-pentapentyloxy- 2-hydroxytriphenylene; quantities of the reagents used are: 1,2-dihexyloxy benzene (58.8 mmol, 1 equiv.), Anhyd.FeCl₃ (176.9 mmol, 3 equiv.), 2% H₂SO₄ in dry dichloromethane (74 ml), methanol (150 ml). Hexapentyloxy triphenylene and monohydroxy triphenylene were isolated respectively in 61 % and 6 % yields. 3,6,7,10,11-Pentahexyloxy-2-hydroxytriphenylene : R_f = 0.40 (50% CH₂Cl₂-hexanes); a black solid;; IR (KBr pellet): $\nu_{\max}$ in cm⁻¹ 3544, 2953, 2229, 2860, 1617, 1596, 1520, 1451, 1439, 1390, 1263, 1172, 1075, 1055, 1032, 1016,

908, 850, 835, 769, 733 and 651; ^1H NMR (CDCl_3 , 200 MHz): δ 7.96 (s, 1H, Ar), 7.83(m, 4 H, Ar), 7.77 (s, 1H, Ar), 5.9 (s, 1H, OH), 4.26 (m, 10H, OCH_2), 1.95 (m, 10H, $5 \times \text{CH}_2$), 1.37-1.56 (m, 30H, $15 \times \text{CH}_2$), 0.97 (t, 15H, $5 \times \text{CH}_3$); MS (FAB+): m/z for $\text{C}_{48}\text{H}_{72}\text{O}_6$, Calculated: 745.08, Found: 745; Anal. calcd for $\text{C}_{48}\text{H}_{72}\text{O}_6$: C, 77.38; H, 9.74. Found: C, 77.2; H, 9.6.

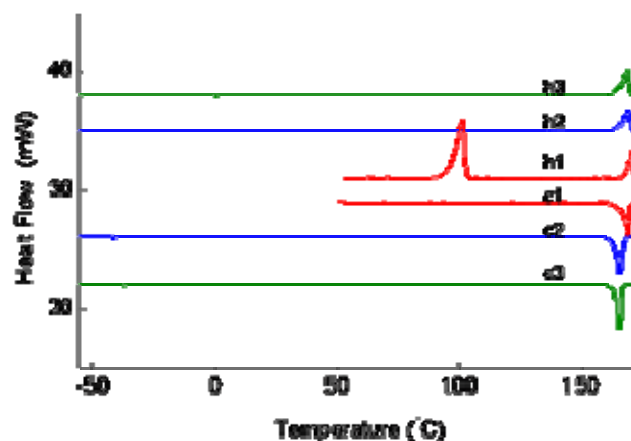


Figure S1: DSC thermograms obtained, during the 1st heating (**h1**)-cooling (**c1**), 2nd heating (**h2**) - cooling (**c2**) and 3rd heating (**h3**) -cooling (**c3**) cycles, for compound **1a**. It can be seen that the Col phase exists for a very wide thermal range and mesophase does not reverts to solid state once melted.

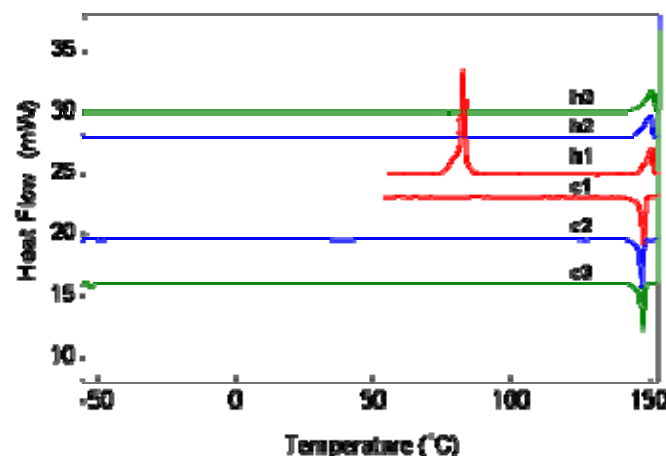


Figure S2: DSC thermograms obtained, during the 1st heating (**h1**)-cooling (**c1**), 2nd heating (**h2**) and cooling (**c2**) and 3rd heating (**h3**) and cooling (**c3**) cycles, for compound **1b**. In this case also, as can be seen, the Col phase exists for a very wide thermal range and freeze into glassy state

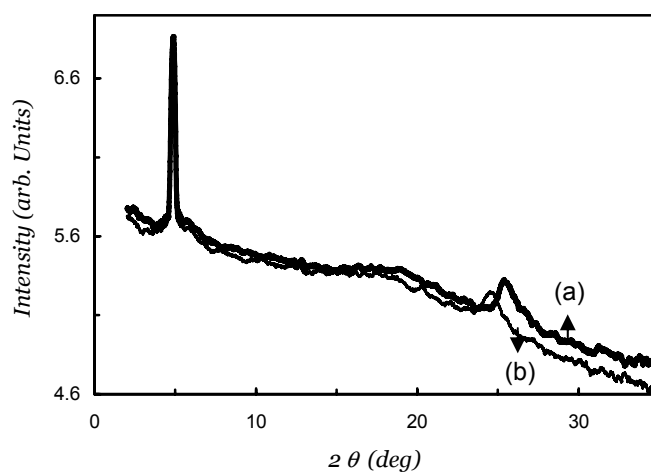


Figure S3. Intensity vs 2θ profile derived from the 2D XRD pattern of Col_h phase (a) at 150 °C and frozen Col_h phase (b) at 30 °C for compound **1a**

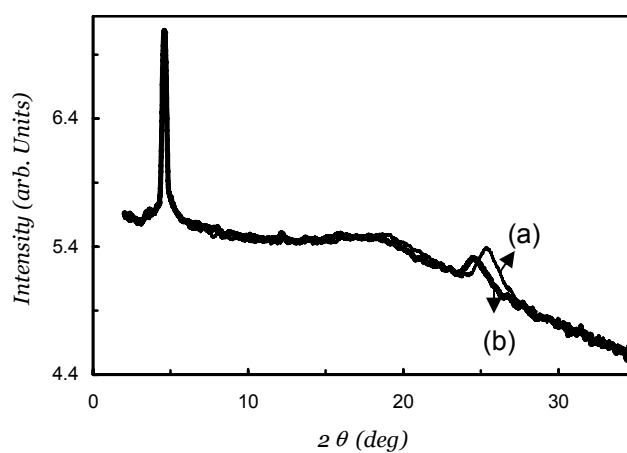


Figure S4. Intensity vs 2θ profile derived from the 2D XRD pattern of Col_h phase (a) at 140 °C and frozen Col_h phase (b) at 30 °C for compound **1b**