

Generation of a Chiral Mesophase by Achiral Molecules: Absolute Chiral Induction in the Smectic C Phase of 4-Octyloxyphenyl 4-Octyloxybenzoate.

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Supporting Information

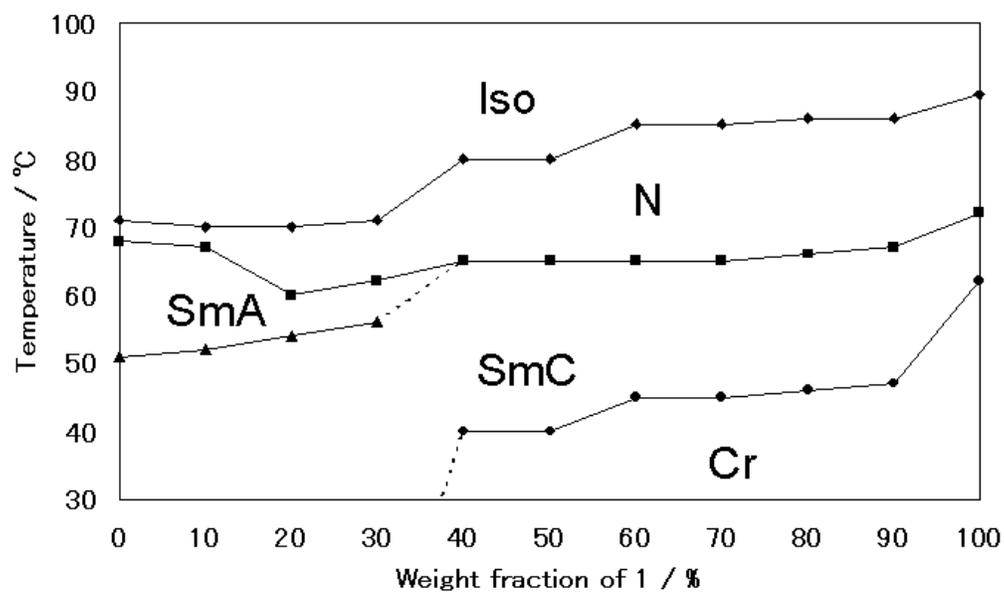


Figure S1. Plots of the phase transition temperatures against the content of **1** in the mixture of **1**, **2**, and **3** (**2** : **3** = 1:1).

A synthesis 4. 4-octyloxyphenol (0.13 g, 0.57 mmol) was added to a 100 mL-round-bottom flask, and 4-citronellyloxybenzoyl chloride (0.20 g, 0.68 mmol), 4-(*N,N*-dimethylamino)pyridine (0.14 g, 1.14 mmol), and THF (50 mL) were added. The mixture was stirred at room temperature for 24 h. To the solution was added ethyl acetate (50 mL), and the solution was washed with aqueous solution of NaHCO₃ (100 mL) and dried over MgSO₄. The solvent was evaporated under reduced pressure, and a yellow oil was obtained as the residue. The crude product was purified by silica gel chromatography (chloroform) to give **4** as an oil (0.11 g, 40.7 %).

4: yield 40.7 %; oil; IR (NaCl) 2923, 2855, 1728, 1606, 1510, 1258, 1195, 1169, 1076, 1008, 850, 765 cm⁻¹; ¹H NMR (500 MHz, CDCl₃) δ 0.89 (t, 3H, *J* = 7.0Hz), 0.97 (d, 3H, *J* = 6.4Hz), 1.22-1.34 (m, 10H), 1.44 (t, 2H, *J* = 7.1Hz), 1.61 (s, 3H), 1.65 (t, 1H, *J* = 6.7Hz), 1.69 (s, 3H), 1.78 (t, 2H, *J* = 7.6Hz), 1.88 (t, 2H, *J* = 6.7Hz), 2.01 (t, 2H, *J* = 7.1Hz), 3.95 (t, 2H, *J* = 6.6Hz), 4.08 (t, 2H, *J* = 7.3Hz), 5.11 (t, 1H, *J* = 1.4Hz), 6.91 (d, 2H, *J* = 8.9Hz), 6.96 (d, 2H, *J* = 8.9Hz), 7.09 (d, 2H, *J* = 9.2Hz), 8.12 (d, 2H, *J* = 9.2Hz); ¹³C NMR (125.65 MHz, CDCl₃) δ 14.11, 17.69, 19.55, 22.67, 25.45, 25.73, 26.05, 29.25, 29.30, 29.37, 29.50, 31.83, 35.95, 37.10, 66.61, 68.45, 114.27, 115.09, 121.73, 122.47, 124.58, 131.48, 132.22, 144.40, 156.80, 163.42, 165.36; Anal. Calcd for C₃₁H₄₄O₄: C, 77.46, H, 9.23, Found: C, 77.74, H, 9.06, N, 0.14.

The CD measurement of pure 1. Compound **1** was sandwiched with two quartz plates (size of the quartz plate: 25mm×50mm (thickness: 1mm), sample area size: 15mm×15mm, sample thickness: about 4μm). The quartz plates were heated and the sample became the isotropic liquid. After cooling of the sample to room temperature (the temperature of the room was kept at 22°C), the quartz plates were set in the chamber in the CD spectroscopy, in which the beam direction was perpendicular to the quartz plate plane. The CD spectra were measured under nitrogen atmosphere (the beam diameter: φ1mm). The homeotropically alignment of the sample was confirmed by polarized optical microscopy.

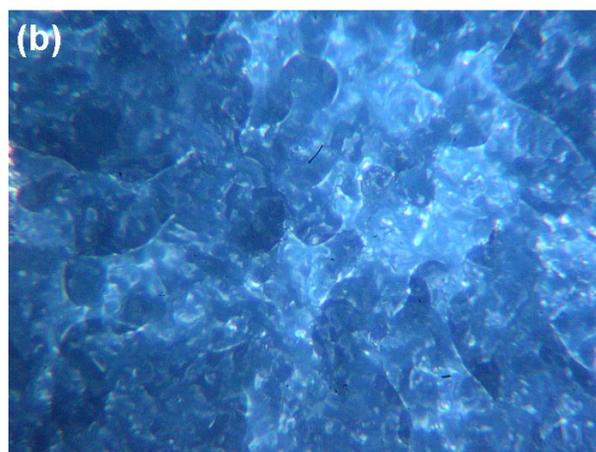
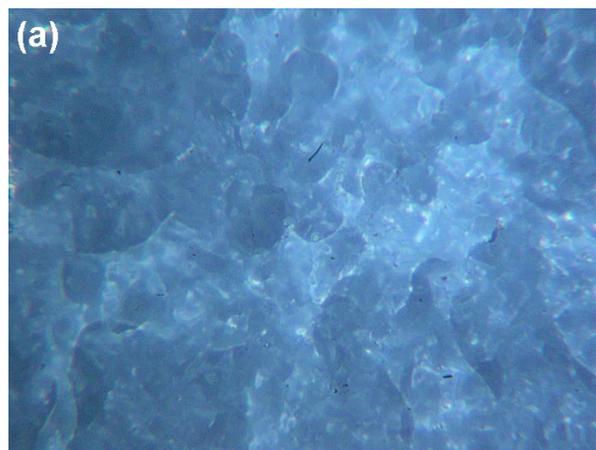


Figure S2. POM in the smectic C phase of **1** doped with 5% of **4** with at 50°C with the 5°-clockwise (+5°, (a)) and 5°-counterclockwise (-5°, (b)) rotations from the cross-polarization position.