Supporting Information for Chiral Random Grain Boundary Phase of Achiral Hockey-stick Liquid Crystals

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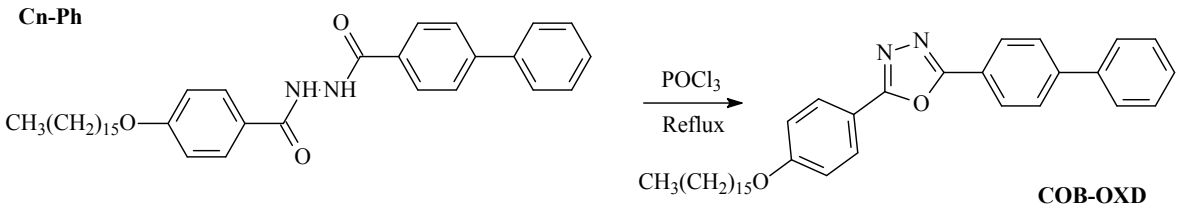
Synthesis of 2-(4-cetyloxyphenyl)-5-biphenyl-1,3,4-oxadiazole (COBOXD)

COBOXD was derived by intramolecular dehydration cyclization of dihydrazide derivative, *N*-(4-cetyloxybenzoyl)-*N*'-(4'-biphenyl carbonyl) hydrazine (C16-Ph) [1], with $POCl_3$ under reflux condition (Scheme 1), and the coarse product was further purified by repeated recrystallization from ethanol for the ^1H NMR, FT-IR spectroscopic characterization and elemental analysis. ^1H NMR (500 MHz, $CDCl_3$), (ppm, from TMS): 8.20 (d, 2H, J=8.3Hz); 8.09 (d, 2H, J=8.8Hz); 7.76 (d, 2H, J=8.4Hz); 7.66 (d, 2H, J=7.3Hz); 7.49 (t, 2H, J=7.6Hz); 7.41 (t, 1H, J=7.3Hz); 7.03 (d, 2H, J=8.8Hz); 4.04 (t, 2H, J=6.5Hz); 1.83 (m, 2H); 1.48 (m, 2H); 1.36 (m, 2H); 1.26 (m, 24H); 0.88 (t, 3H, J=6.9Hz). FT-IR (KBr disk, cm^{-1}): 3089, 3059, 3040, 2954, 2918, 2849, 1616, 1586, 1498, 1483, 1472, 1449, 1409, 1573, 963, 1464, 1427, 1394, 1307, 1258, 1176, 1160, 1129, 1104, 1079, 1025, 963, 843, 823, 767, 740, 727, 720, 708, 697, 688. Anal. Calcd for $C_{36}H_{46}N_2O_2$: C, 80.26%; H, 8.61%; N, 5.20%. Found C, 80.47%; H, 8.73%; N, 5.47%. Yields >80%



Scheme S.1: The synthesis route for COBOXD.

Characterization methods

^{1}H NMR spectra were recorded with a Bruker Avance 500MHz spectrometer, using $CDCl_3$ as solvent and tetramethylsilane (TMS) as an internal standard. FT-IR spectra were recorded with a Perkin-Elmer spectrometer (Spectrum One B).

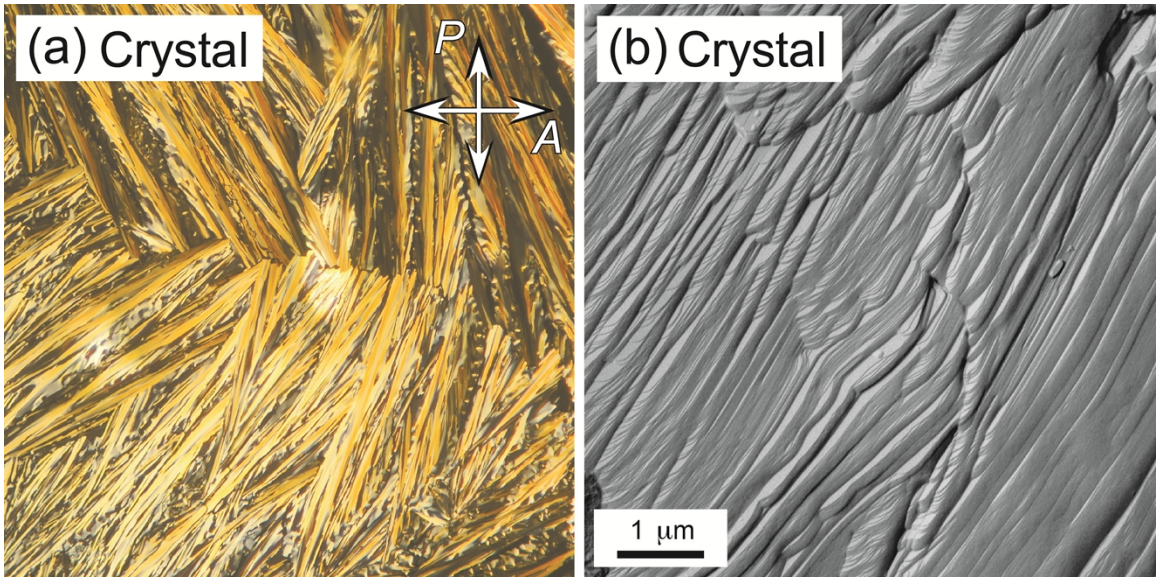


Figure S.1: The crystal phase of the achiral, hockey-stick molecule COBOXD. (a) Optical texture of the crystal phase showing birefringent domains. (b) Free-surface TEM image of the crystal phase at the air/liquid crystal interface, quenched at T=90°C. In contrast to the RGB phase, the crystal phase shows a structure with long-range order.

Reference

[1] D. M. Pang, H. T. Wang, and M. Li, *Tetrahedron*, **61**, 6108-6114 (2005).