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Title:	Phase Behavior of a New Class of Anthraquinone-Based Discotic Liquid Crystals
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Keywords:	Physical and chemical processes Mesostructures Electrical conductivity
Issue Date:	2017
Publisher:	ACS Publications
Citation:	Langmuir, 33(48)
Abstract:	<p>Five novel columnar liquid crystalline compounds (4.1–4.5) consisting of a central anthraquinone core carrying four alkoxy chains (R = n-C₆H₁₃, n-C₈H₁₇, n-C₁₀H₂₁, n-C₁₂H₂₅, and 3,7-dimethyloctyl) with two diagonally opposite 1-ethynyl-4-pentylbenzene units were synthesized, and their phase transitions were investigated between changes in the molecular structure and their self-assembly into the columnar mesophases. Small and wide-angle X-ray scattering (SAXS/WAXS) studies were performed to deduce the exact nature of the mesophases, and their corresponding electron density maps were derived from the intensities of the peaks observed in the diffraction patterns. A comparison of compounds with different alkoxy chains indicated that the soft crystal columnar rectangular (Crcolrec) phase was stable at lower temperature for the shortest peripheral alkoxy chain (4.1; R = n-C₆H₁₃) and was found to exhibit the columnar hexagonal (Colh) phase and then the discotic nematic (ND) phase with increasing temperature. In contrast, increasing the peripheral chain length to n-C₈H₁₇ or the branched one (4.2 and 4.5) stabilized the Colh phase at lower temperature and showed the ND phase at higher temperature. Further increase in chain length (4.3 and 4.4; n-C₁₀H₂₁, n-C₁₂H₂₅) demonstrated the formation of the ND phase. Conductivity measurement in the Colh mesophase was found to be almost 10 times higher in magnitude than the corresponding Crcolrec phase. The HOMO–LUMO band gap of all the compounds was found to be in the range from 2.79 to 2.82 eV, which is quite less and comparable with the optical energy band gap.</p>
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