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Supplementary Materials

Optical and Geometrical Characterizations of Non-Linear Supramolecular Liquid Crystal Complexes

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Characterizations

Supramolecular complex formation was confirmed by TA Instruments Co. Q20 Differential Scanning Calorimeter (DSC; USA), polarized-optical microscopy (POM, Wild, Germany) and FT-IR (Nicolet iS 10 Thermo scientific) spectroscopic analysis.

FT-IR spectra for structural characterization were recorded by using a diamond tip Perkin Elmer ATR spectrometer. All spectra ranging between wave numbers 4000 and 400 cm^{-1} were recorded with Fourier transform infrared spectroscopy. All spectra were collected at room temperature and the base line corrected and vector normalized. Number of scan and spectral resolution were 32 scan and 4 cm^{-1}; respectively

Calorimetric measurements were carried out using a PL-DSC of Polymer Laboratories, England. The instrument was calibrated for temperature, heat and heat flow according to the method recommended by Cammenga, et. al. [1]. Measurements were carried out for small samples (2–3 mg) placed in sealed aluminum pans. All measurements were conducted at a heating rate of (10 °C/min) in an inert atmosphere of nitrogen gas (10 mL/min). For DSC, the sample was heated from room temperature to 280 °C at heating rate of (10 °C/min) under nitrogen atmosphere and then cooled in the cell to 0 °C. All weighed samples were made using an ultra-microbalance, England, with accuracy ±0.0001.

Transition temperature for the complexes (**I/II** and **I/III**) was investigated by DSC in heating and cooling cycles. The type of the mesophase was identified using a standard polarized-optical microscopy POM (Wild, Germany), attached with Mettler FP82HT hot stage. Measurements were made twice, and the results were found to have accuracy in transition temperature and enthalpy within ± 0.2.

Computational methods and calculations

The theoretical calculations for the investigated compounds were carried out by Gaussian 09 software [2]. DFT/B3LYP methods using 6-31G (d, p) basis set was selected for the calculations. The geometries were optimized by minimizing the energies with respect to all geometrical parameters without imposing any molecular symmetry constraints. The structures of the optimized geometries had been drawn with Gauss View [3]. Moreover, the calculated frequencies were carried out using the same level of theory. The frequency calculations showed that all structures were stationary points in the geometry optimization method with none imaginary frequency. Conformer

selections have been considered for the present complexes are based on the steric hindrance point of view according to the least energy conformers [4–12].

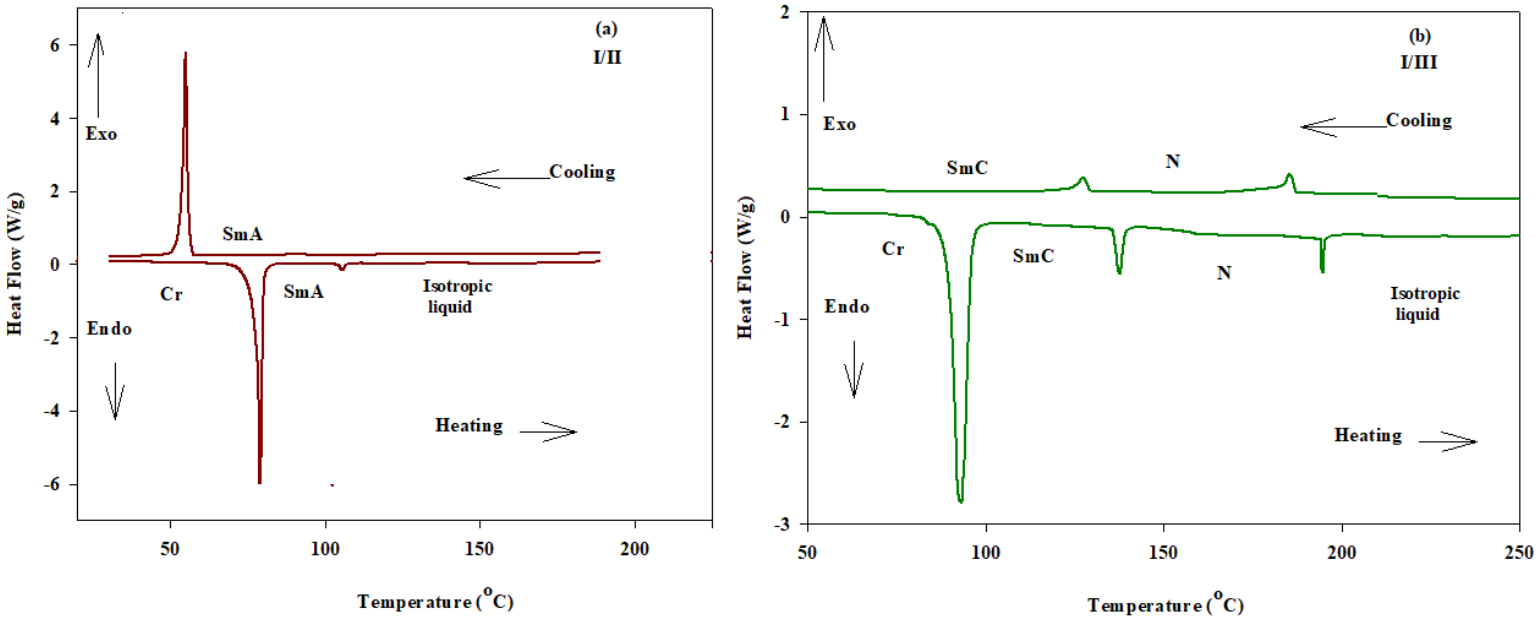

Figure 1. DSC thermograms of 1:1 SMHBCs (**a**) **I/II** and (**b**) **I/III** at heating rate 10 °C/min upon heating and cooling cycles.

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