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Polymesomorphism in a smectic SmC* phase in a comb-shaped liquid crystalline stereoregular cyclolinear methylsiloxane copolymer with the 4,4'-bisphenylene fragment at terminal lactic acid derivative in mesogenic group

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Experimental

^{1}H and ^{29}Si NMR spectra were recorded using an AV-400 spectrometer (Bruker) at 20°C in $CDCl_3$ + CCl_4 or C_6D_6 solutions. Infrared (IR) spectra were recorded on a Specord M-82 spectrophotometer (Carl Zeiss Jena, Germany) in KBr pellets. The temperatures and enthalpies of phase transitions were measured by differential scanning calorimetry (DSC) using a DSC-7 calorimeter (Perkin-Elmer, USA). The heating rate was 20 K min^{-1} (T_g is the glass transition temperature, and T_i is the isotropisation temperature). DSC scans were recorded after cooling from the isotropic melt at a rate of 20 K min^{-1}.Mesomorphic properties were studied by optical polarization microscopy using an Axiolab Pol microscope (Carl Zeiss, Germany) equipped with a hot stage (Linkam, UK). The samples as thin films about 10 μm thick placed between two cover glasses.

X-ray diffraction patterns in small and wide angle scattering regions were obtained using a *S3-Micropix* system (*Hecus*), CuK_α radiation, $\lambda = 1.5406$ Å with a *Xenocs Genix* source (the working voltage and current were 50 kV and 1 mA, respectively). A *Pilatus* 100K detector and a linear *PSD* 50M gas detector (Ar/Me mixture at $8 \cdot 10^5$ Pa) were employed,. A *Fox* 3D pinhole collimation system with Kratky collimation slits of 0.1 and 0.2 mm widths was used, allowing the stable measurements in a wave vector interval from $s = 0.003$ Å^{-1} to $s = 1.9$ Å^{-1} where $s = 4\pi\sin\theta/\lambda$, and 2θ is the scattering angle. To get rid of the scattering of X-rays on air molecules, Goebbel mirrors and scattering path were evacuated at 2.6 ÷ 5.0 Pa. Exposure times were varied from 600 to 5000 s. Temperature behavior of samples was studied using Peltier and Joule attachments at low (-5 - 120˚C) at Joule and high (23 - 300˚C) temperatures, respectively. Transmission X-ray diffraction patterns at wide angles were also recorded on a *Bruker* D8 *Advance* powder diffractometer (CuK_α radiation, $\lambda = 1.5406$ Å, a *Vantec* 2D detector).

The Accelrys Materials Studio® program set was employed for the molecular modeling of the test compounds. We used two sets of potentials for taking into account non-covalent interactions of mesogenic groups in liquid-crystalline mesophases: COMPASS (Condensed-phase Optimized Molecular Potentials for Atomistic Simulation Studies) and UFF (Universal Force Field). The COMPASS set is suitable for modeling isolated molecules and condensed phases; it also allows one to parameterize partial charges and valence *ab initio* with the subsequent system optimization. To prove the results of modeling, we applied UFF potentials, used for calculation of geometry of organic molecules containing metal-organic complexes, as well as it does not have any limitation on the chemistry of compounds involved.