X-ray diffraction, DFT theoretical, and IR polarized spectroscopic studies of the crystal-like E-mesophase of 4'-hexyloxy-isothiocyanatotolane (6OTOLT).

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Streszczenie

The dynamics of 6OTOLT molecules was analyzed based on IR absorption spectra and DFT calculations. Of particular interest was the mode ascribed to the ν_{as}(NCS) vibrations, the transition dipole moment of which is directed along the long axes of the molecules. Polarized IR spectra in the region of this mode allowed a characterization of the ordering of molecules in the analyzed phases. In a case of the smectic E phase, a random distribution of molecules aligned laterally in two-dimensional space between KRS-5 windows was found. The crystals of 6OTOLT were successfully grown and are characterized by an interesting Pc space group. The molecules are parallely arranged in layers and cross the adjoining ones underneath at an angle of 86.04°. The distance between the ring planes is 3.48 Å. The packing of molecules indicates a tendency to maintain short contacts between NCS groups and alkyl chains. The crystals grown do not correspond to the ordering of the smectic E phase and thus to the solid state obtained after cooling the smectic phase. Calculations of the interaction energy for three possible arrangements of dimeric species show a predominance of the core-to-core units. It was also shown that in this case an increase in ν_{as}(NCS) frequency should be expected, in good agreement with experimental data.

Słowa kluczowe

Isothiocyanatotolanes 6OTOLT, Liquid crystal, X-ray diffraction, Polarized IR spectra, DFT calculations

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