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Structural studies of 4-n-pentylphenyl-4'-n-heptyloxythiobenzoate (7OS5)

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Compounds from the homologous series of 4-n-pentylphenyl-4'-n-alkoxybenzoates $C_nH_{2n+1}-O-C_6H_6-COS-C_6H_6-C_5H_{11}$, denoted as nOS5, known of creating liquid crystalline phases, are the subject of our recent studies. Some results for crystalline and liquid crystalline phases of 4-n-pentylphenyl-4'-n-heptyloxythiobenzoate (denoted as 7OS5), studied with differential scanning calorimetry (DSC), polarization microscopy (PM) and X-ray diffraction (XRD), will be presented.

DSC (DSC 8000 Perkin Elmer calorimeter, 6 K/min.) and PM (Nikon Eclipse LV100POL microscope, 6 K/min.) measurements deliver information about the phase sequences at heating and cooling as well. 7OS5 occurs in two liquid crystalline phases and polymorphism in a crystalline phase is also observed. In our DSC and PM measurements the following sequence of the phase transitions was observed: *isotropic liquid* \rightarrow *nematic* \rightarrow *smectic C* \rightarrow *crystal 1* while cooling and *crystal 1* \rightarrow *crystal 2* \rightarrow *crystal 3* \rightarrow *nematic* \rightarrow *isotropic liquid* upon heating. In the simultaneous XRD-DSC measurements (SmartLab 9kW, Rigaku, $CuK\alpha$, 2 K/min.) only one crystal phase during the first heating but two different crystal phases during the second heating were visible and no smectic order was detected while cooling. Single crystal X-ray analysis (SuperNova, Agilent Technologies, $CuK\alpha$, 90 K) enabled us to solve the structure of 7OS5 in the crystalline phase. The compound crystallizes in an orthorhombic system (space group $Pca2_1$) with the cell parameters $a = 54,285(5)\text{ \AA}$, $b = 5,5843(3)\text{ \AA}$, $c = 14,8411(10)\text{ \AA}$.

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