Spectroscopic features of low-temperature phase transitions for 5CB liquid crystal

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4-n-pentyl-4'-cyanobiphenyl (5CB) is one of the most studied liquid crystal materials, since it has an available nematic phase near room temperature and a simple molecular structure. These facts allow using this compound as a suitable model substance in the investigations of the physical behaviour of the simple nematics. substantial efforts have been devoted to the investigations of structural transformation, intermolecular order, and orientational molecular dynamics in the isotropic and nematic phases of 5CB liquid crystal. Up to now, little information is available from the low temperature phase transformations.

Luminescence measurements of bulk 5CB were carried out and analyzed in detail in 4.2 – 300 K temperature and 320 – 520 nm spectral ranges. The results obtained are discussed in the terms of different types and amounts of monomers and excimers formed at different temperatures, which correspond to the different phases of 5CB. The analysis of the luminescent spectra allowed to detect three phase transitions, occurred for the 5CB at temperatures 80, 140 and 220 K. This can be connected with an existence of several 5CB crystal states, where different conformers of its molecules and dimers are realized. The most prominent spectral changes were observed for the last transition, suggesting the formation of the 5CB glassy state above 220 K.

Structural re-alignments in the crystalline state of 5CB at the temperatures mentioned were also confirmed by the IR-spectroscopic measurements, made at the same temperature range and in the 400 – 4000 cm^{-1} spectral region. The significant changes in the spectral peak position and intensity of the CN-group stretching vibration band (at 2226 cm^{-1} in the case of the dimer structure), Q(CN), and the intensity redistributions for the deformation γ(CCN) (at 555 and 567 cm^{-1}), δ(CCN) (at 840 cm^{-1}), γ(CCC) (at 638 cm^{-1}) vibration bands were observed at the 5CB phase transition points. The conclusions about the 5CB possible molecular structure and conformers were made at different temperatures of the region studied.