

Structures and phase transitions in neat 4,4'-di-*tert*-butyl-2,2'-bipyridyl and in its molecular complexes with either bromanilic or iodanilic acid.

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Streszczenie

Using the DSC method the structural phase transitions have been found at 165 and 219 K for 4,4'-di-*tert*-butyl-2,2'-bipyridyl (dtBBP), whereas for its complex with iodanilic acid (dtBBP-IA) - at 331 K. For the other molecular complex described, with bromanilic acid, dtBBP·BRA, no phase transitions have been disclosed between the liquid nitrogen temperature and a temperature of the crystal decomposition. The crystal structures of the neat dtBBP have been determined at 130, 190 and 250 K, whereas for its molecular complexes with brom- (BRA) at 150 K and iodanilic acid (IA) - at 293 and 345K. The crystal structure of neat dtBBP is characterized by layers of molecules, which are grouped by their *t*-butyls. The structures of dtBBP·BRA and dtBBP·IA are analogous one to the other and consist of the infinite chains of the alternating acid and base molecules linked by the hydrogen bonds. On the basis of the structural, dielectric and spectroscopic results (infrared and Raman) the mechanisms of the phase transitions have been proposed for dtBBP and dtBBP·IA. The ¹H NMR spin-lattice relaxation times for all compounds under study, as well as the second moment for the neat dtBBP in a wide temperature, have been measured. The anomalies in the temperature dependent infrared spectra together with the NMR results support a supposition that for dtBBP the dynamics of *tert*-butyl groups is responsible for the mechanism of the phase transitions found. The dynamics of the molecules in the crystals presented is related to the rotation both of the methyl and *tert*-butyl groups.

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