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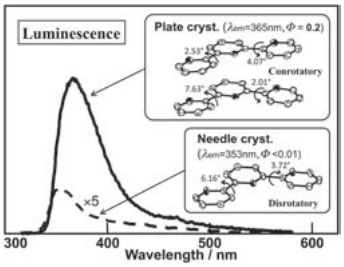
2,2':6',2''-Terpyridine (tpy), which is practically non-fluorescent (Φ <0.01) in organic solutions, in an amorphous solid and a needle crystal ($P2_12_12_1$, Z=4), was found to show an efficient solid-state luminescence (365 nm, Φ =0.2) upon formation of a plate crystal ($P2_1/c$, Z=8). Furthermore, effective on-off switching of this solid-state luminescence was realized by heat-mode interconversion between the plate and needle crystals. It was shown that the rate constant of the non-radiative relaxation of the needle crystal (k=1.2x10^{9}s^{-1}) was an order of magnitude larger than the plate crystal, while that of the emissive process were comparable (k~10^{7}s^{-1}). In contrast to a frozen solution, both polymorphs did not exhibit phosphorescence at 77 K, suggesting that the triplet state might not be involved in the non-radiative process. Comparing both polymorphs, tpy molecules were in different conformation, conrotated and disrotated, which might be due to a different molecular packing. Relation between the difference in the crystal structure and the solid-state luminescence property was further studied.



Keywords: luminescence, polymorphism, heterocyclic compounds

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Polymorphism of chlorpropamide: Structure and transitions

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The importance of the polymorphism of drugs can hardly be over-estimated. Detailed structural studies not only allow to identify a selected form reliably, but also provide a valuable insight into the structure-properties relations, especially, when combined with vibrational spectroscopy, thermal analysis and calorimetry. Chlorpropamide an atidiabetic drug, has been known to be highly polymorphic since a very long time, but the crystal structures of all the claimed forms but the one produced commercially remained unsolved. Structure of only one polymorph was known when we started our investigation. We solved three new ones . The molecule is very flexible and different parts of the molecule can freely rotate and bend. Having crystal structure data, we defined quantitatively the values of torsion angles and variations in hydrogen bonds among them. Motif of hydrogen bonds is really the same, and the polymorphism results mainly from the difference in intramolecular (conformational polymorphism). Packing of neibouring molecules in the structure is similar for all polymorphs but one (beta). Hydrogen bonds in that polymorph differ from those in the rest ones. We investigated polymorph transitions near the melting point by using DSC, IR spectroscopy, and X-ray powder diffraction. All the polymorphs are proved to transform into the fifth polymorph, epsilon, which melts then. Kinetics of polymorph transition is inhibited for beta polymorph. This work was supported by the grants from BRHE (RUX0-008-NO-06/BP2M08, Y3-C-08-01), Innovation Project "Education" from the Russian Ministry of Education and Science #456, and Integration Projects #49 and #110 of SB RAS.

Keywords: polymorphism, drug structures, hydrogen bonds

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Structure formation effects on electro-optics of montmorillonite clay-5CB liquid crystal composites

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Nanomaterials based on liquid crystals (LCs) and montmorillonite (MMT) clay are perspective due to their applications in the information record and storage devices, etc. The nematic LC, pentyl-cyanobiphenyl (5CB) was used in our composites. The MMT was modified with octadecylbenzyldimethylammonium chloride (OBDM) and dioctadecyldimethylammonium chloride (DODM), which leads to the better chemical affinity of the clay to LCs and increase of MMT basal spacings for the penetration of 5CB dimers to the interlayer space. The nature of the surfactant is responsible for chemical affinity between the clay and LC, affecting the structure formation in the composites. These properties explain their different electro-optical (EO) characteristics. In the case of OBDM-MMT, well separated small clay particles are uniformly distributed in the 5CB medium. Under applied electric field, this mobile system is easily oriented along the field direction resulting in significant increase in optical transparency, when the applied voltage increases. Due to the fairly strong molecular interactions between the composite components, the field-induced alignment of 5CB domains remains the same even when the electric field is removed (considerable EO memory). Contrary, due to the smaller affinity of DODM to 5CB molecules, DODM-MMT particles are only partially covered by LC layer, which allows them to aggregate. These aggregates form a stable colloidal network with 5CB dimers. In EO measurements, when an electric field is applied to the composite, its transparency increases, but less, than for the former one. So the EO memory of the composite with DODM-MMT is low, but the contrast is high. These investigations will assist in the development of the composites with desired optical characteristics.

Keywords: LC-clay composites, X-ray diffraction, electro-optical properties

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Crystal structure of metastable cubic B_1-phase of the $La_2Mo_2O_9$ single crystal

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