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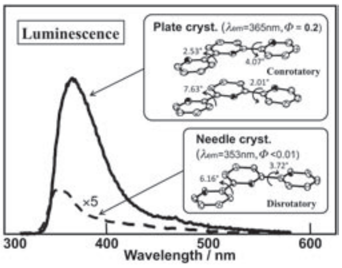
2,2’:6’,2’’-Terpyridine (tpy), which is practically non-fluorescent (Φ <0.01) in organic solutions, in an amorphous solid and a needle crystal ($P2_12_12_1$, Z=4), was found to show an efficient solid-state luminescence (365 nm, Φ =0.2) upon formation of a plate crystal ($P2_1/c$, Z=8). Furthermore, 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=1.2x$10^9$$s^{-1}$) was an order of magnitude larger than the plate crystal, while that of the emissive process were comparable (k~$10^7$$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 un-solved. 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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LAMOX, the new family of oxide conductors, obtained on the basis of $La_2Mo_2O_9$ compound with the use of different substitutions is the object for intensive studies. In 2005 year single crystals of the anionic conductor $La_2Mo_2O_9$ were grown by crystallization from the nonstoichiometric flux [1]. Their polymorphism, domain structure and temperature dependences of conductivity and permittivity were studied [1]. Conductivity of these crystals at 750-600 °C reaches 10^{-1}-10^{-2} $Om^{-1}sm^{-1}$. It was established that in dependence of the cooling rate and of the admixture content, these crystals can exist at the room temperature as stable monoclinic A-phase or metastable cubic B_1-phase or as their mixture. Obtaining of the most complete and precise structural data about the crystals of cubic metastable B_1-phase from X-ray experiment was the purpose of the present study. It is important that these studies were done for the first time for single crystals. Cubic cell with a=7.158(1)Å, which was found for the studied single crystal, allowed to index about 84% of measured reflections. While solving the structure (in sp.gr. $P2_13$) it was established that La and Mo atoms are shifted from the threefold axes. Occupation of three positions of La and Mo atoms was found to be equal to 100%. Two of the three independent oxygen positions in this crystal are not fully occupied, have quite large thermal parameters and are located at the short distances from each other. Concluding R-factor for this structure was 2.46%. The work was done with the partial support of the grant RFBR No.07-02-00180, Grant for the Leading Scientific Schools NSh-2192.2008.5 and "Russian Science Support Foundation".

[1]. Voronkova V.I., Yanovskii V.K., Kharitonova E.P. Crystallography Reports. 2005. V.50. No.5. P.940.

Keywords: conducting materials, crystal structure analysis, structure-properties relationships

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Pulse laser deposition of $AgInSe_2$ films

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High quality $agInSe_2$ (AIS) films were grown on Si and glass substrates by the ultra-high-vacuum pulsed laser deposition technique from the AIS target synthesized from high-purity materials. The X-ray diffraction and microscopic studies of the films show that films are textured in (112) direction. The effect of substrate temperature on growth on Si and glass substrates was observed. The substrate temperature appears to influence the properties of films. The films prepared on Si show more crystallinity than on glass showing good lattice matching. Chalcopyrite phase (112) is dominant up to 3000 ℃. The optical studies of the films show that the optical band gap is about 1.24 eV, which also show change with change in temperature. This shows that AIS films are very good absorber material for solar cell technology.

Keywords: pulse laser deposition, thin films, optical properties

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Modified 6-deoxyclitoriacetal and their crystal structures as anticancer agents

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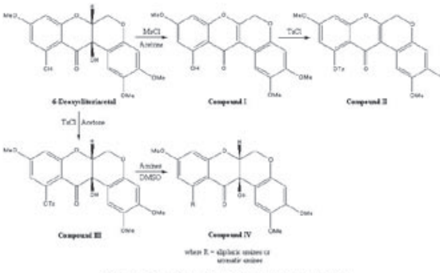
6-Deoxyclitoriacetal is a substance extracted from the dried roots of *Stemona collinsae* Craib. It has been known to have a cytotoxic activity against various types of human carcinoma possibly due to by its ability to intercalate with DNA as evidenced *in vitro* assay. In order to enhance its activity, 6-deoxyclitoriacetal was derivatised to contain a functional group with more flexible and can be participated hydrogen bonding with DNA. The derivatives of 6-deoxyclitoriacetal were prepared as shown in scheme 1. In this work, we studied the relationship between crystal structures, hydrogen bonding and cytotoxic activity of 6-deoxyclitoriacetal and its derivatives based on spectroscopic and X-ray crystallographic techniques.



Scheme 1 Synthesis of compound I, compound II, compound III and compound IV.

Keywords: 6-deoxyclitoriacetal, hydrogen bonding, cytotoxic activity

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Using electron microscopy techniques studies in microstructure of NdFeCoAl-(B,C) based alloys

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Magnetic materials on basis of the NdFeAl alloys have been intensively studied because of their interesting physical properties and application potential. The magnetic measurements reveal that the samples exhibit hard-magnetic characteristics quite good at room temperature. However, the relationship between hard magnetic properties and microstructure in these alloys are still not well understood. We present here the results of studies on the microstructure of some NdFeCoAl-(B,C) alloy system by the electron microscopy techniques as TEM, HRTEM, SEM, SAED, EDX and EBSD. Rods and ribbons of the NdFeCoAl-(B,C) alloys were prepared from the pure elements Nd, Fe, Co, Al, B and C by rapid-quenching methods. We used a Philips CM20-FEG TEM and a FEI NovaNanoSEM 200 SEM to characterize the microstructure of these alloys. We found the different crystalline phases in the alloys. In the NdFeCoAlB samples, the tetr. $Nd_2(Fe,Co)_{14}B$ (2:14:1), fcc Nd rich, hcp Nd, alpha-Fe and in the NdFeCoAlC samples, the tetr.