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The First All-Russian Conference on Liquid Crystals (Ivanovo, 2012)................................................................. 99
HYBRID LUMINESCENCE MATERIALS BASED ON LYOTROPIC LANTHANIDE–CONTAINING MESOPHASES

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The templating method based on sol-gel technology for creation hybrid silicate materials with effective luminescence was described. The lyotropic liquid-crystalline (LC) system containing Eu$^{III}$ ions – $\text{C}_{12}\text{H}_{25}\text{O(CH}_{2}\text{CH}_{2}\text{O})_{10}\text{H/Eu(NO}_3\text{)}_{3}\cdot6\text{H}_{2}\text{O/H}_{2}\text{O}$ was used as a template. Conditions of the synthesis were established. The role of the liquid-crystalline template was shown. Evaluation of the changes of the surface topography of the film during the transition to the LC template in comparison to simple silicate matrix was carried out. The influence of composition on the luminescence properties of hybrid films was investigated.

Key words: lyotropic liquid crystal, sol-gel technology, lanthanide, luminescence.

(P. 5 – 12)

CHIRAL MESOGENIC NANOMATERIALS.
NEW MOLECULAR PARAMETERS FOR PROGNOSIS OF CHIRAL MESOMORPHISM OF DISCOTIC MESOGENS

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A series of 55 discotic mesogens of different chemical structure with chiral centers was investigated. 35 out of 55 compounds exhibit chiral mesomorphism, while the other 20 form achiral structures. The modeling of molecular structures for these compounds was carried out using the HyperChem software package. Calculation and analysis of the molecular parameters introduced in order to isolate a subclass of chiral discotic mesogens from the class of discotic mesogens were performed. We analyzed the information content of the parameters, and on the basis of this analysis we offered two new the most informative parameters that allow to predict the formation of twisted supramolecular structures of discotic mesogens of various chemical classes with the reliability $\geq$ 70%.

Key words: chiral discotic mesogens, molecular parameters, prognosis of mesomorphism. (P. 13 – 20)
Yu. N. Timoshin, E. A. Kirsanov

ANALYSIS OF COEFFICIENTS OF THE GENERALIZED FLOW EQUATION

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Behavior of rheological equation coefficients is discussed in the framework of the generalized flow model of structured systems under change of physical and chemical characteristics of the system. The dependence of the coefficients on temperature, viscosity of dispersion medium and ζ – potential is explained.

Key words: generalized flow model, rheological equation, characteristics of the dispersed system. (P. 21 – 30)


INVESTIGATION OF Pt-PORPHYRIN COMPLEXES LUMINESCENCE QUenchING IN POLYMERIC MATRIX

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Platinum complexes of 5,10,15,20-tetrakis(4’-hexadecyloxyphenyl)porphin (1) and octaethylporphin (2) have been synthesized. Their luminescent properties in polymeric matrix are studied.

Key word: synthesis, luminescence, porphyrin complexes of platinum. (P. 31 – 41)

A. M. Parshin, V.A. Gunyakov,V. Ya. Zyryanov, V.F. Shabanov

NEMATIC DOMAIN STRUCTURES ON POLYMER SURFACE

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The ordering of MBBA and 5CB nematic liquid crystals on the surface of polycarbonate is studied. On films prepared from the solutions of polycarbonate in dichloromethane or chloroform were visualized domains that grow in nematic liquid crystals on the background of the initial thread-like or schlieren texture over time, depending on time
of exposure of the film before applying a liquid crystal to it. By optical methods using birefringence effects and optical probing, it was found that the nematic director within domain forms a radial structure. In the nematic droplets the temperature transition from planar to homeotropic orientation and to isotropic state with intermediate sloping degenerated states the director is found. It is shown that the transition occurs in a thin initial layer of liquid crystal and it is a result of the competitive forces near the surface.

Key words: liquid crystal, polymer structure, domains. (P. 42 – 51)

O.A. Denisova, A.N. Chuvyrov*

RELAXATION OF DIRECTOR AT LIQUID CRYSTALS AZIMUTHAL INSTABILITY

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The relaxation processes in thin layers of homeotropically oriented nematic liquid crystals under the action of a periodic low-frequency shift (frequency of exposure of ~ 100 Hz) is experimentally investigated. It is found that the relaxation processes are described by an exponential time dependence and take dozens of seconds.

Key words: nematic liquid crystal, relaxation of director. (P. 52 – 58)

E. Yu. Tyunina

VOLUME EFFECTS IN SUBLIMATION ENTHALPIES OF AMINO ACIDS AND N-ACETYLAMIDES OF AMINO ACIDS

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The effects of molecular shape, crystal density and free space in thermodynamic properties of the organic crystals were investigated on the basis of the experimental data analysis on thermodynamic (enthalpy of sublimation, heat capacity) and structural characteristics of 20 crystalline amino acids and 7 N-acetylamides of amino acids. Multiparameter correlations between enthalpy of sublimation and molecular descriptors of compounds were proposed. Using the form of the multi-parameter equations, the estimation of volume, electrostatic and hydrogen bond factors to the enthalpy of sublimation for the studied compounds was carried out.

Key words: amino acids, N-acetylamides of amino acids, enthalpy of sublimation, crystal volume factors, multi-parameter equations. (P. 59 – 68)
S.M. Pestov, R.S. Shamsiev, B.A. Belyaev

SURFACE TENSION OF MESOGENS. CALCULATION METHODS

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Surface tension of nematic liquid crystals (LC) was measured by the Wilhelmy plate and ring methods. A possibility to estimate surface tension of individual LC and their mixtures basing on the minimum information (molecular structure) was demonstrated. The group-contribution scheme basing on the parachor was suggested.

Key words: liquid crystals, surface tension, Wilhelmy plate, ring method, estimation, parachor. (P. 69 – 72)

T. R. Prosochkina, R. G. Shestakova, E. A. Kantor, K.G. Kichatov

MOLECULAR ORDERING OF 2,5-BIS-(4-BUTYLPHENYL)PYRAZINE
AT PHASE TRANSITION TEMPERATURES – COMPUTER SIMULATION

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The computer simulation of 2,5-bis-(4-butilphenyl)pyrazine is executed. The probability of each configuration of dimers (stacking, in-plane and terminal) is defined on the bases of values energy of intermolecular interaction. It is established that the sliding one molecule over the other in dimers of 2,5-bis-(4-butilphenyl)pyrazine it is energetically allowed for a small range of distance, which provided the preservation of orientation of molecules in a mesophase. The relationship between the translation rigidity of molecules in dimers and shown liquid crystal properties is revealed.

Key words: mesophase, computer simulation, intermolecular interactions, dimmers, quantum chemistry, translation rigidity. (P. 73 – 81)
Physiological and Physical Properties of Multiwall Carbon Nanotubes – Polymer Composite

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The influence of multiwall carbon nanotube dispersion on exploitation properties of dispersion medium – high-pressure polyethylene is investigated in this work. Important for practical application physical and physical-mechanical data are analyzed.

Key words: multiwall carbon nanotubes, high-pressure polyethylene, tensile strength, elongation at break, electrical surface resistance, abradability and oxygen index. (P. 82 – 87)

Investigation of Influence of Cholesteric Additives and Carbon Nanotubes on Properties of Cutting Oils

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The influence of cholesteric additives or carbon nanotubes on the properties of lubricants under drilling is studied. The use of the X-15 additive at optimal concentration significantly improves lubricating properties. The effect of low concentrations of carbon nanotube additives on the lubrication ability was not found.

Key word: liquid crystals, additives, cutting oils, drilling. (P. 88 – 91)