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S. A. Pikin

ABOUT EXISTENCE OF MODULATED FLEXOELECTRIC STRUCTURE IN SMECTICS C

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It is shown that the necessary conditions for existence and observation of the periodic flexoelectric modulations in smectics C are the planar initial orientation of smectic layer, rather small dielectric anisotropy, high inclination of molecules, relatively low threshold in the electric field. Comparisons with other mechanisms of the advent of modulated structures in smectics are done.

Key words: smectic C phase, modulated flexoelectric structure, threshold electric field, width of domains, inclination of molecules in the smectic layer. (P. 6 – 13)

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STRUCTURAL INVESTIGATIONS OF IRON COMPLEX IN BULK SAMPLES, FLOATING LAYERS AND LANGMUIR-BLODGETT FILMS

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Comparative investigations of both volumetric and film structures of complex [Fe(L)₂]⁺X(PF₆)⁻ were carried out by X-ray scattering, electrons diffraction and a scanning probe microscopy. The analysis of phase transformations in Langmuir monolayers based on the complex was fulfilled and magnetic field effect was fixed during their formation.

Key words: metal complex, Langmuir monolayers, multilayer films, structure. (P. 14 – 22)
CRYSTALLINE STRUCTURE AND MESOMORPHIC PROPERTIES OF 4-(\(\omega\)-HYDROXY)OCTYLOXY-4’-CYANAZOBENZENE

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The molecular packing in the crystalline phase of 4-(\(\omega\)-hydroxy)octyloxy-4’-cyanazobenzene is studied by X-ray-structural analysis method. It is shown, that determined influence on the molecular packing is putting up H-bond of compete intermolecular interactions. Mesophase properties of the compound are studied by polarization thermomicroscopy and differential scanning calorimetry methods. The enantiotropic nematic phase presence is established.

Key words: liquid crystals, H-bond, mesophase properties, X-ray-structural analysis, molecular packing in the crystalline phase, polarization thermomicroscopy, differential scanning calorimetry. (P. 23 – 31)

PECULIARITIE OF BANANA-SHAPED MESOGEN PHASE STRUCTURE ACCORDING TO COMPUTER CALCULATIONS

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To determine the supramolecular organization of the banana-shaped compound – bis\{-3,4,5-tri\{4-(4’-nonyloxybenzoyloxy)benzoylamino\}-1,3-phenylene – numerous experiments were carried out by the method of molecular dynamics with molecular mechanics in the MDsimGrid program. The possible packings of the banana-shaped molecules in different phase conditions were discussed. The obtained data were compared to research results of the phase structure using synchrotron radiation method.

Key words: banana-shaped mesogen, structure, synchrotron radiation, molecular dynamics with molecular mechanics, MDsimGrid program. (P. 32 – 40)
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ESTIMATION OF MESOGENIC PROPERTIES OF LANTHANUM ADDUCTS ACCORDING TO QUANTUM-CHEMICAL CALCULATIONS

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The article introduces the result of the integrated theoretical investigation of the liquid-crystalline adducts of lanthanides by the methods of molecular simulation. The correlation between the geometrical parameters and liquid-crystalline properties, the influence of the ionic radius and alkyl substituents on the anisometry of the molecules were investigated. The anisometry values, within which the liquid-crystalline phase exists, were established to be 2.5±3.5.

Key words: liquid crystals, lanthanides, adduct, quantum-chemical calculations. (P. 41 – 49)

G. M. Zharkova, A. P. Petrov, S. A. Streltsov, V. M. Khachaturyan

STRUCTURIZATION OF POLYMER-LIQUID CRYSTAL DISPERSIONS BY OPTICAL METHODS

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Evolution of optical properties of polymer-liquid crystal dispersions on the basis of acrylate monomers and nematic liquid crystals generated by photopolymerization method with use of principles of holography is experimentally investigated. It is shown that optical (holographic) methods allow creating structures from traditional polymer-dispersed scattering systems to periodic, showing diffraction properties gratings.

Key words: Structurization, polymer-dispersed liquid crystals, holography. (P. 50 – 58)
UDK 532.783

E. M. Averyanov

LOCAL FIELD AND POLARIZABILITY OF BIOMOLECULES IN ANISOTROPIC MEDIA

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Using the data on dispersion of the refractive indices in the visible range for anisotropic films composed of polyglutamate and DNA macromolecules, the experimental values of the components $L_j$ for the Lorentz tensor and the components $f_j$ for the tensor of the local field of a light wave were obtained for the first time for such media. These local-field parameters correspond to limitations from below on the mean value $\gamma$ and anisotropy $\Delta \gamma$ of the polarizability of macromolecules in the film. The limitations reflect the change of the polarizability tensor due to anisotropic intermolecular interactions in anisotropic film relative to isotropic solution. The obtained results have been compared with consequences of the local-field models used in literature for anisotropic biomolecular media.

Key words: anisotropic biomolecular media, local field, intermolecular interactions, polarizability of biomolecules. (P. 59 – 68)

UDK 532.783

S. A. Znoiko, V. E. Maizlish, G. P. Shaposhnikov, V. V. Bykova*, N. V. Usoltseva*

MESOMORPHISM OF OCTASUBSTITUTED PHTHALOCYANINES, COMBINED BENZOTRYAZOLYL AND ARYLOXY-GROUPS ON PERIPHERY

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The research results of the nature influence of the functional substituents in ortho-position to benzotryazolyl fragment in octasubstituted phthalocyanines, on their physical and chemical properties, in particular – spectral and mesomorphic, are generalized.

Key words: synthesis, phthalocyanines, mesomorphism. (P. 69 – 79)

FUNCTIONAL SUPRAMOLECULAR SYSTEMS BASED ON AMPHIPHILIC AND POLYMER COMPOUNDS

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The possibility of the formation of functional supramolecular systems based on dicationic (gemini) surfactants with a high solubilizing capacity and controllable catalytic effect during the process of ester’s bonds cleavage has been demonstrated.

Key words: dicationic surfactants, micelle, electrolyte, nonionic polymer, aggregation, solubilization, kinetics, catalysis, hydrolysis, ester. (P. 80 – 89)

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EFFECTS OF COUNTER-ION SPECIFICITY IN SALT-AQUEOUS SOLUTIONS OF DODECYLSULFATES OF ALCALI METALS

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New experimental data are presented for aqueous solutions of sodium, potassium and cesium dodecyl sulfates containing salt additives; the latter are chlorides having the same cations as the surfactants, the salt concentration spans 0 – 30 mmol/l. The information obtained includes the critical micelle concentrations, the aggregation numbers, concentrations of sphere-to-rod transitions, degrees of counter-ion binding, thermodynamic functions of aggregation (at 40°C and 45°C): data on the Krafft boundary. Counter-ion effects are analyzed from the standpoint of ions specificity towards water structuring in their micro-environment. In the proposed version of the quasi-chemical model the specific contribution to the Gibbs aggregation energy is described through parameters of the counter-ions adsorption on the micelle surface. The results of model estimations are in a satisfactory agreement with the experiment and conform to the concept of ions chaotropy or cosmotropy.

Key words: ionic surfactants, micellization, effects of salt additives, counter-ion specificity, molecular-thermodynamic modeling. (P. 90 – 102)
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ION FORMING ADDITIVES INFLUENCE ON ELECTRICAL PROPERTIES OF PARAFFIN DISPERSED SYSTEMS ON BASIS OF TECHNICAL OILS

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Ion forming additives significantly affect the formation of micelles dispersed in paraffin wax medium. Like many surfactants, they also affect the structure of colloidal suspensions hydrocarbons of melting at high temperature. Investigation of the mechanism of such effects on the processes of nucleation and crystal growth has both theoretical and practical interest. This paper presents the results of dielectric, optical and X-ray diffraction studies of ion forming additives influence on equilibrium processes in these dispersed systems.

Key words: paraffin dispersed systems, the crystallization of paraffin, permittivity, optical microscopy, X-ray analysis. (P. 103 – 109)

E. A. Kirsanov

RHEOLOGY OF LIQUID CRYSTALS

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We consider various theoretical perspectives on the flow of unoriented liquid crystals as thermotropic and lyotropic. Generalized flow equation is used for describing of the characteristic properties of liquid crystals as structured systems. The importance of thixotropic properties of liquid-crystal systems was shown.

Key words: generalized flow model, rheology, liquid crystals. (P. 110 – 119)
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SOLVENT-INDUCED MESOMORPHISM IN CALAMITIC COMPLEXES OF SILVER(I)

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Calamitic stilbazole complexes of silver(I) containing a tetradecyl sulfate anion have been studied. The thermotropic behaviour of these materials shows the presence of nematic, SmC, SmA, S\textsubscript{4} and cubic phases. On addition of solvent, three types of behaviour can be discerned: apolar solvents associate with the ligand terminal chains and promote phases with curved interfaces; small dipolar, aprotic solvents associate with the core and favour mesophases that do not possess curved interfaces, while short-chain alcohols hydrogen bond with the ionic core of the complexes to form ribbon-like structures that organise into chromonic phases. This solvent-induced behaviour is compared with the solvent-induced behaviour of analogous polycatenar complexes of silver(I) and with more conventional, calamitic organic compounds with hydroxy-terminated chains.

\textbf{Key words:} calamitic mesogens, metallomesogens, solvent-induced mesomorphism, silver. (\textit{P. 120 – 128})