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A B S T R A C T S

**D.N. SERGEEV, V.B. MOTALOV, M.F. BUTMAN, D.A. IVANOV, A.M. DUNAEV, L.S. KUDIN
VAPOR COMPOSITION OF SAMARIUM, EUROPIUM AND YTTERBIUM HALIDES
AT CONDITION OF DISPROPORTIONATION AND DECOMPOSITION**

The review of studies of a vapor phase composition of Sm, Eu, and Yb di- and trihalides is presented. Many of these compounds are thermally unstable. This fact leads to incongruent evaporation and complex vapor composition. Within high-temperature mass spectrometry technique, approaches to mass spectra interpretation were developed. These approaches based on a joint analysis of ionization efficiency functions, temperature and time dependences of the ionic currents in the electron ionization and thermionic emission modes allow establishing the molecular and ionic composition of a vapor at different steps of evaporation.

Key words: lanthanide halogenides, vapor composition, thermal instability, mass-spectrometry

T.A. KALININA

COPPER COMPLEXES OF DIAMINODIIMIDS OF ASPARTIC ACID

The paper presents the study of structure and properties of copper complexes of stereo isomeric diaminodiimids of aspartic acid by methods of infrared spectroscopy and ESR-spectroscopy. The protonization constants of the ligands' and stability constants of copper complexes were calculated with the potentiometric titration.

Key words: diaminodiimides, complexation, composition, structure, protonation constants, complexes stability constants

E.V. RUMYANTSEV, S.N. ALYOSHIN, Yu.S. MARFIN

**QUANTUM CHEMICAL MODELING INITIAL STEPS OF PROTOLYTIC DISSOCIATION
OF BORON DIFLUORIDE COMPLEX OF DIPYRROLYLMETHENE**

The energy profiles of the two theoretically possible initial steps of the protolytic dissociation of boron fluoride complex of dipyrrolylmethene were calculated using quantum-chemical methods. The structural and energy characteristics for the corresponding transition states were obtained. The protonation of the heterocyclic ligand was shown to be energetically less favorable than protonation of the fluorine ligands, which is consistent with experimental data. The observed difference in the mechanisms of bodipy and complexes with d-metals dissociation explains the anomalously high kinetic stability of the bodipy in acidic media.

Key words: bodipy, protolytic dissociation, quantum-chemical calculation, energy profile

**O.V. DOBROKHOTOV, D.V. LUFERENKO, I.G. ABRAMOV, Zh.V. CHIRKOVA, S.I. FILIMONOV
DEVELOPMENT OF SYNTHESIS METHOD OF 9H-CARBAZOL-3-YL-AZOPHTALONITRILES**

The article is devoted to new approach to synthesis of novel 9H-carbazol-3-yl-azophthalonitriles. Due to a low solubility of 9H-carbazoles in aqueous solutions there is difficulties in synthesizing of targeted compounds under classical conditions. The solvents influence on azocoupling reaction was studied. The best result was achieved under using THF:Water solution in 1:2 ratio.

Key words: non-linear optical properties, 4-aminohtalonitrile, diazotization, azocoupling, 9H-carbazol-3-yl-azophthalonitrile

T.A. BOBOVA, A.V. KOLOBOV, K.L. OVCHINNIKOV

**SYNTHESIS OF ANHYDRIDES OF GETARYLSUCCINIC ACIDS CONTAINING FRAGMENT
OF PYRIDAZINONE OR PHTALAZINONE AND THEIR DERIVATIVES**

The conditions for carrying out the dehydration reaction of substituted succinic acid containing fragments of pyridazinone or ftalazinone were developed. Corresponding amides and imides were synthesized by reacting obtained anhydride with aromatic amines

Key words: substituted succinic anhydride, phtalazinone derivatives, pyridazinone derivatives, dicarboxylic acid, amide, imide

**A.D. KOTOV, D.A. BAZLOV, M.A. PROKAZNIKOV, V.Yu. ORLOV, E.A. ANTONOVA
THEORETICAL STUDY OF STRUCTURE OF 2,5-BIS(4-NITROPHENYL)-1,3,4-OXADIAZOLE**

The optimized molecular geometry and nuclear charges for 2,5-bis(4-nitrophenyl)-1,3,4-oxadiazole were calculated by different methods. Comparison of results of calculations by the semi-empirical PM3 method, Hartree-

Fock methods (with different basic sets), Møller-Plesset, the density functional theory with Single-crystal X-ray diffraction data was carried out. The analysis of Mulliken charges was made. On the basis of molecular geometry and the analysis of Mulliken charges intermolecular interactions were identified.

Key words: quantum-chemical modeling, 2,5-bis(4-nitrophenyl)-1,3,4-oxadiazole, X-ray diffraction analysis

A.A. IBRAGIMOV, V.P. MESHALKIN, L.A. PANCHIKHINA, M.N. RAKHIMOV
**INFLUENCE OF BRANCHING ALKANES ON PROCESS OF *n*-HEXANE ISOMERIZATION
IN SUPER ACID IONIC LIQUID**

Influence of catalytic activity of super acid ionic liquid in a process of isomerization of *n*-hexane on the yield and selectivity of formation of iso-components was studied. It was established that the mono substituted alkanes attending in pentane-hexane fractions can initiate the process of isomerization of *n*-alkanes in the medium of ionic liquids.

Key words: isomerization, ionic liquid, super acid, initiator, isopentane

A.L. LOBACHEV, N.V. FOMINA, I.V. LOBACHEVA, E.V. REVINSKAYA
ENSURING CORRECTNESS OF MEASUREMENT OF IDENTIFICATION PARAMETERS OF OIL

Methods of ensuring correctness of determination of standard indicators of oil quality in accordance with GOST R 51858-2002 for the purpose of their further use as identification parameters of oil were studied.

Key words: oil, oil products, identification, identification parameters, correctness

L.A. KOCHERGINA, A.I. LYTKIN, O.N. KRUTOVA, K.V. DAMRINA
STANDARD ENTHALPIES OF FORMATION OF *L*-CYSTEINE IN AQUEOUS SOLUTION

The heat effects of dissolutions of crystalline *L*-cysteine in water at 298.15K were determined by direct calorimetry. The standard enthalpies of formation of *L*-cysteine solution at various dilutions were calculated. The standard enthalpy of formation of *L*-cysteine in the hypothetical non-dissociated state at infinite dilution was determined.

Key words: thermodynamics, amino acid, solutions, calorimeter, enthalpy

D.O. KORPATENKOV, A.A. KOMAROV, A.A. MERKIN, O.V. LEFEDOVA
**CATALYTIC HYDROGENATION OF 2-NITROANIZOLE IN WATER-ORGANIC SOLVENTS
ON SKELETAL NICKEL**

The liquid phase catalytic hydrogenation is effective method for obtaining aromatic amines having practical importance. In given article the kinetics of hydrogenation of 2-nitroanizole in water and water-alcohol solvents with addition of sodium hydroxide was considered under different temperatures.

Key words: liquid phase hydrogenation, solvents, skeletal nickel, 2-nitroanizole

E.G. KHOMUTOVA, V.A. ZAGORODNIKOVA, S.A. ZAGORODNIKOVA, E.V. KOPYLOVA
**IRIDIUM COMPOUNDS SOLUTIONS CATALYTIC ACTIVITY IN INDICATOR CATALYTIC
REACTION OF SULFARSAZENE OXIDATION BY POTASSIUM PERIODATE**

Catalytic activity of 10^{-4} - 10^{-5} M solutions of complex chlorides of Ir(III) and Ir(IV) in an indicator reaction of sulfarsazene oxidation by potassium periodate was studied by spectrophotometric and kinetic methods. The preparation recommendations of iridium comparison solutions were given for catalytic method.

Key words: test-method, catalytic reaction, iridium determination

V.Kh. FEDOTOV, N.I. KOLTSOV
**FUZZY LOGIC USE FOR CONSTRUCTION OF ADEQUATE KINETIC MODELS
OF CHEMICAL REACTIONS**

Application of fuzzy logic for building kinetic models of chemical reactions taking into account the error of experimental data was described. Fuzzy analogs of kinetic equations were formulated for the simple model (in the form of the law of mass action) reaction and complex (in the form of the equations of Langmuir-Hinshelwood) hydrochlorination reaction of acetylene. The application of fuzzy logic was shown to allow constructing kinetic models which are adequately described experimental data.

Key words: fuzzy logic, kinetic models, chemical reactions, adequacy, experimental data

Yu.K. SUNTSOV, M.V. VLASOV
**VOLUME AND REFRACTOMETRIC PROPERTIES OF BINARY SOLUTIONS
OF BUTANOL - ALIPHATIC KETONES**

The obtained experimental data on density and index of refraction of binary mixtures formed by common component, *n*-butanol, and members of homologous series of aliphatic ketones have allowed to reveal a linear relation of molar volume and a molar refraction for the given systems and to propose the equations describing properties in a temperature range from 318K to 338K.

Key words: molar volume, molar refraction, linear relation, operative check

S.I. LAZAREV, I.V. KOTELNIKOVA

INFLUENCE OF TREATMENT METHODS ON EFFICIENCY OF REVERSE OSMOTIC PURIFICATION OF INDUSTRIAL SOLUTIONS AND DRAINS FROM ANILINE

In this paper, the methods of improving the efficiency of cleaning solutions and industrial drains from aniline by modification of the membrane surface, acidification of the initial solution and applying a dc electric field on the membrane – solution system are considered. All methods of treatment increase the detention coefficient, reduce sedimentation on the membranes and increase the service life of reverse osmotic semi-permeable membranes.

Key words: membrane, detention coefficient, solvent specific flux

A.S. VYSOKOVSKIY, I.S. KOROTNEVA

STUDY OF INTERACTION OF SURFACTANTS IN MICELLE SOLUTIONS OF MIXTURES OF SODIUM SALT OF ETHER OF ALKYLPHENOL SULFATE AND SODIUM ALKYLARYLSULPHONATE AND THEIR USE FOR SYNTHESIS OF GRAFT-COPOLYMER LATEXES

The interaction in the binary anionic surfactant systems was researched. The interaction parameter was calculated and its independence on emulsifiers mixture composition was shown. Synthesis of graft-copolymer latexes was performed with utilization of surfactant researched combinations.

Key words: interaction parameter, mixed micelles, synergism, graft-copolymers

N.G. VILKOVA, S.I. ELANEVA

INFLUENCE OF HYDROPHOBICITY OF SILICA PARTICLES ON FOAMS AND FOAM FILMS STABILITY

The properties of foam films stabilized by silica particles of different sizes and degrees of hydrophobicity were investigated. The properties of the foams produced from suspensions of aerosil and ludox with the addition of hexylamine were studied. It was shown that the thick (up to 200 μm) films and very stable foams are formed from suspensions of aerosil with the mass content of solids in the initial suspensions of 2-6% and the degree of hydrophobicity of the particles corresponding to the values of the contact angle of $\theta = 52^\circ$. Insulated foam films, obtained from 20% of the sol ludox and hexylamine with the concentration of 11-44 mmol/L have bilayer structure and are quickly destroyed. Gel formation in an isolated foam film at hexylamine concentrations of more than 44 mmol/L corresponds a stability of thin layers of the foam.

Key words: silica, hexylamine, dispersion, gel-formation, stability

S.V. FEDOSOV, M.V. AKULOVA, M.V. TANICHEV, R.V. SLATSHCHYOV, D.A. SHUTOV
DIRECT CURRENT GLOW DISCHARGE TREATMENT INFLUENCE ON ADHESION AND HYDROPHILIC PROPERTIES OF VLIESELINE

The influence of the direct current air glow discharge treatment on the adhesion and hydrophilic properties of vlieseline in the ranges of discharge current of 20-100 mA, pressure of 50-200 Pa, treatment time of 15-120 s was studied. The plasma treatment was shown to result in the increase in the water absorption and in the decrease in wetting time of material. Also plasma treatment increases the material adhesion to concrete and wood surface at a glue deposition onto material.

Key words: glow discharge, air plasma, treatment, vlieseline, adhesion, hydrophilic properties

I.A. VERSHININA, O.V. GORNUKHINA, A.A. GLADYSHEVA, O.A. PETROV, O.A. GOLUBCHIKOV
TETRA-(4-TERT-BUTYL)-TETRABENZOPORPHYRAZIN: ACID-BASE PROPERTIES AND APPLICATION

The features of the acid-base interaction of tetra-(4-tert-butyl)-tetrabenzoporfirazin with nitrogen-containing bases in dimethylsulfoxide were investigated. Complex materials such as polymer type – tetra-(4-tert-butyl)-tetrabenzoporphyrazin were obtained. The modified polymeric materials were shown to have the sorption activity in relation to the nitrogenous bases.

Key words: acid-base interaction, tetrabenzoporphyrazin, polymeric materials, polypropylene, polyethylene-terephthalate, sorption activity

M.V. SOLOVSKIY, N.V. ZAKHAROVA, E.B. TARABUKINA, M.S. BORISENKO, E.N. VLASOVA, P.E. ALEKSEEVA
SYNTHESIS OF 6-CROTONOILAMINOCAPROIC ACID AND ITS COPOLYMERS WITH N-VINYLPYRROLIDONE

New monomer, 6-crotonoilaminocaproic acid, was synthesized. Its ability to react with N-vinyl-pyrrolidone through the reaction of radical co-polymerization was found out. The structure of water soluble copolymers of N-vinylpyrrolidone and 6-aminocaproic acid obtained with the yield of 38-40 % was confirmed by means of IR spectroscopy. The composition and molar mass characteristics of the copolymers were determined.

Key words: N-vinylpyrrolidone, 6-crotonoilaminocaproic acid, co-polymerization, polymer composition, molar mass

M.S. SOLODOV, A.S. SOLODOV, E.S. SOBOLEVA, S.G. KOSHEL

ELECTROCHEMICAL SYNTHESIS OF POLYANILINE COMPLEXES WITH MOLYBDATE ANION

The electrochemical synthesis of polyaniline in the presence of molybdate anions was carried out. The influence of the concentration of molybdate anion on the polymerization rate of aniline was studied. Using the cyclic voltammetry and spectroscopy the molybdate anion effect on the properties of polyaniline complexes was established.

Key words: polyaniline, molybdate anion, electron spectrum, morphology

N.A. LEZHINA, A.O. KARANETS, M.E. SOLOVYEV

MODELING DYNAMICS OF CHAIN FRAGMENTS OF BUTADIENE-NITRILE RUBBER

In this work the possibility of calculation of short relaxation times was estimated by means of molecular simulation with Langevin dynamics method for chain fragments of butadiene-nitrile rubber. The distribution of relaxation times was found to have a non-linear behavior. Thus, the dependence of relaxation properties on strain qualitatively corresponds to equilibrium transitions for macromolecule states such as globule-coil and coil - stretched chain.

Key words: molecular simulation, relaxation times, Langevin dynamics, viscoelastic properties

E.V. BORZOVA, E.P. GRISHINA, A.M. PIMENOVA, N.O. KUDRYAKOVA

IONIC LIQUIDS – SALTS OF 1-BUTYL-3-METHYLIMIDAZOLIUM AS ELECTROLYTES FOR ENERGY CAPACITIVE STORAGE

Temperature dependencies of specific conductivity in the range from -65°C to 85°C and sparking voltage were obtained and discussed for three ionic liquids namely 1-n-butyl-3-methylimidazolium hexafluoro-phosphate, trifluoromethanesulfonate and bis(trifluoromethylsulfonyl)imide. Also, the effect of temperature (25-85°C) on “electrochemical window” of these ionic liquids and anodic behaviour of aluminium in them were investigated. Conclusion on possibility of investigated ionic liquid application in low voltage aluminum electrolytic capacitors operating at the temperature below (-5 -15°C) was made from experimental data.

Key words: ionic liquids, “electrochemical window”, specific conductivity, sparking voltage, aluminium, anodic oxidation

M.K. KOTVANOVA, S.S. PAVLOVA, N.N. EFREMOVA

NANO-SIZE CRYSTALS OF OXIDE BRONZES OF TITANIUM, MOLYBDENUM AND TUNGSTEN AS COMPONENTS OF ANTICORROSIVE COATS

Conductive nanomaterials based on oxide bronzes of titanium, molybdenum, tungsten were obtained by means of the self-propagating high-temperature synthesis and the mechano-chemical interaction. The method of improvement of corrosion resistance of the conducting machine details was proposed by means of deposition of protective coats containing nano-powders of oxide bronzes.

Key words: nanoparticles, oxide bronzes, self-propagating high temperature synthesis, mechano-chemical interaction, corrosion resistance, electrical conductivity

A.S. KRUCHININ, M.P. TSYGANKOV

PARAMETRICAL CONSOLIDATION OF MEASUREMENTS DATA OF CARBON BLACK YIELD

Questions of parametrical consolidation of the statistic measurements data of the carbon black yield are considered. The universal way of the estimation of dependence of the yield on properties of used raw materials for various marks of carbon black is offered.

Key words: carbon black, raw materials distribution, raw mix, optimization, statistic data, parametrical consolidation, regression dependence

A.I. BALUNOV, V.P. MAIYKOV

CALCULATION OF DISTILLATION PRODUCTS COMPOSITION FOR COMPLEX RECTIFICATION SYSTEMS BASED ON MAXIMUM ENTROPY PRINCIPLE

The calculation close to thermodynamic one of separation products of multi-component mixtures in multi-products rectification systems is considered. The method is based on information approach of entropy maximum. Features and advantages of the proposed method are discussed. The calculation results are shown for products composition for project and verification tasks.

Key words: rectification, complex system, flow products compositions, entropy maximum principle

A.D. POLYANIN, A.V. VYAZMIN

HEAT AND DIFFUSION EQUATIONS WITH FINITE RELAXATION TIMES. STATEMENT OF PROBLEM AND SOME SOLUTIONS

Heat and diffusion equations with finite relaxation times, which give a finite velocity of perturbations propagation, are considered. For the heat flux the model of Cattaneo–Vernotte is used. An exact solution of the differential-difference equations of Stocks problem without initial conditions (with any periodic boundary conditions) was

found. The statement of initial value problems of heat-transfer with finite relaxation times is discussed. Several exact solutions of linear and non-linear heat differential-difference equation were found.

Key words: Kattaneo-Vernotte model, relaxation time, heat-conductivity difference-differential equation, exact solutions, boundary tasks, non-linear difference-differential equations exact solution

A.B. KAPRANOVA, A.A. PETROV, A.I. ZAIYTSSEV
INVESTIGATION OF PHASE OF SHOCK INPUT OF SINGLE PARTICLE TO FIXED LAYER OF BULK MATERIAL

The functional relationship between the velocity of a spherical particle in a fixed layer of bulk material with grains of the essentially smaller solid skeleton and extending the range of the funnel with the porosity and thickness of the compacted layer in the contact area with the incident particle on the basis of the mechanics of heterogeneous systems was obtained.

Key words: shock interaction, spherical particles, fixed layer of bulk media, disperse phase, porosity, compaction, contact area, movement velocity, expanding funnel radius

V.M. NIKOLSKIY, M.V. SIMONOVA, S.N. GRIDCHIN, A.N. SEMENOV, A.A. YAKOVLEV
SYNTHESIS AND CONSTANTS OF STEPWISE DISSOCIATION OF HEXAMETHYLENEDIAMINE-N,N'-DISUCCINIC ACID

For the first time, the new prospective complexone, hexamethylenediamino-N,N' disuccinic acid, was synthesized. Protolytic equilibria of this compound in an aqueous solution were studied by potentiometric titration. Constants of stepwise dissociation were determined at 25 °C and at solution ionic force of 0.15 (KNO₃).

Key words: complexones, aminopolycarbonic acids, synthesis, dissociation stepwise constants, potentiometry

I.K. GARKUSHIN, M.A. DYOMINA, E.M. BEKHTEREVA
PHASE EQUILIBRIA IN STABLE TETRAHEDRON OF LiF-Li₂MoO₄-KCl-KBr OF Li,K||F,Cl,Br,MoO₄ QUINARY RECIPROCAL SYSTEM

Phase equilibria in the stable tetrahedron of LiF-Li₂MoO₄-KCl-KBr of Li,K||F, Cl, Br, MoO₄ quinary reciprocal system were studied by the differential thermal analysis. Volumes of crystallizable phases were marked off. The composition of crystallizing phases in volume of tetrahedron was confirmed by the X-ray diffraction analysis.

Key words: differential thermal analysis, T-x-diagram, phase equilibria, solid solutions continuous series

A.V. RUKHOV
BASIC PROCESSES OF SYNTHESIS OF CARBON NANOTUBES WITH METHOD OF CHEMICAL GAS-PHASE DEPOSITION

The new approach to developing and research of the basic processes of carbon nanotubes synthesis by a method of chemical deposition from a gas phase on metallic catalyst surface was offered at thermal decomposition of substances containing carbon. The analysis of interconnections of the basic processes of carbon nanotubes synthesis was carried out. On the basis of the offered approach the mathematical model which has shown a divergence with experimental data less than 10 % was developed.

Key words: carbon nanotubes synthesis, gas-phase chemical deposition, mathematical modeling

O.V. ROMANKEVICH, O.A. GARANINA, N.A. BARDASH
WETTING THERMODYNAMICS OF POLYMERS

The analysis of wetting thermodynamics with the interphase region presentation in a form of limited thickness layer with constant thermodynamic properties in the bulk layer was carried out. The value of the relative change in the free energy of interfacial layer upon wetting (ΔG_{rel}) was introduced. It allows estimating the change in the thermodynamic properties of the surface.

Key words: wetting, interfacial layer, surface tension, wetting contact angle, free energy change at wetting