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(inorganic and organic substances.
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*V.K. ABROSIMOV, A.V. KRASNOV, Yu.A. ZHABANOV, E.V. IVANOV***MOLECULAR STRUCTURE AND SUBLIMATION ENTHALPY OF 2,4,6,8-TETRAMETHYL-GLYCOLURIL – DRUG «MEBICARUM»**

Using a combination of the mass-spectrometry and Knudsen effusion methods, the standard molar enthalpy of sublimation of 2,4,6,8-tetramethylglycoluril (drug «Mebicarum») was determined to be $\Delta_{\text{sub}}H^\circ(298) = 108 \pm 3$ kJ/mol. The structural parameters of 2,4,6,8-tetramethylglycoluril molecule were computed using quantum chemical methods.

Key words: 2,4,6,8- tetramethylglycoluril, fusion point, fusion heat, sublimation standard enthalpy, structure-molecular parameters

*S.V. MARUTYAN, A.L. NAVASARDYAN, L.A. NAVASARDYAN***INFLUENCE OF X-RADIATION ON FLUORESCENCE PARAMETERS OF DNA OF YEASTS IRRADIATED AT DIFFERENT TEMPERATURES**

Isolation of DNA from yeast cells *Candida guilliermondii* and investigation of changes of its fluorescence parameters under influence of X-radiation of yeast cells at different temperatures was carried out. It has been shown that the irradiation of yeast cells at 0°C results in more damages in double stranded structure of DNA than irradiation at the room temperature. In a case of repaired DNA the further increase in damages of radiated DNA was observed.

Key words: DNA, X-radiation, repair, fluorescence

*G.I. EGOROV, D.M. MAKAROV, A.M. KOLKER***EXCESS THERMODYNAMIC CHARACTERISTICS OF WATER + ETHYLENE GLYCOL MIXTURE UP TO 100 MPa**

The variations of excess molar thermodynamic characteristics: Gibbs energy $\Delta_{P_o \rightarrow P} G_m^E$, entropy $\Delta_{P_o \rightarrow P} S_m^E$, and enthalpy $\Delta_{P_o \rightarrow P} H_m^E$ of the mixture of water (1) + ethylene glycol (2) were calculated in the temperature range of 278.15-323.15 K and pressures up to 100 MPa. Dependences of $\Delta_{P_o \rightarrow P} G_m^E$, $\Delta_{P_o \rightarrow P} S_m^E$, and $\Delta_{P_o \rightarrow P} H_m^E$ versus mole fraction of ethylene glycol (x_2) are characterized by the presence of extrema at all pressures studied. A good correlation between the phase diagram and $\Delta_{P_o \rightarrow P} S_m^E = f(x_2)$ function was found.

Key words: water, ethylene glycol, non-electrolytes mixtures, high pressure, excess thermodynamic properties, mixing enthalpies

M.B. BEGIEVA, L.R. PASHTOVA, V.V. KHASANOV, L.G. GRINEVA, S.I. PAKHOMOV, M.Kh. LIGIDOV
SYNTHESIS REACTIONS AND RADICAL POLYMERIZATION OF N-ALKYL-N,N-DIALLYLAMINE AND THEIR DERIVATIVES

Monomers of N-alkyl – N,N- diallylamine derivatives were obtained and the radical polymerization in an aqueous and water-organic solutions was studied. New polymers with $M_w = (14 - 96) \cdot 10^3$ were received.

Key words: radical polymerization, N-alkyl-N, N-diallylamines, poly-N-alkyl-N, N-diallylamines

*V.G. SOLOMONIK, A.N. SMIRNOV, Y.V. STAROSTIN***A NONEMPIRICAL STUDY OF YTTERBIUM DIHALIDE MOLECULES**

The molecular structures, vibrational frequencies, infrared intensities, electric dipole moments, and thermochemical properties of ytterbium dihalides YbX_2 (X = F, Cl, Br, I) were studied at the coupled-cluster singles, doubles, and perturbative triples CCSD(T) level of theory using a series of large all-electron basis sets and the complete basis set extrapolation technique. All the molecules are found to possess equilibrium geome-

try of C_{2v} symmetry. Small energy barriers to intramolecular rearrangement $C_{2v} \rightarrow D_{\infty h} \rightarrow C_{2v}$ in $YbBr_2$ and YbI_2 indicate structural nonrigidity of the molecules. The second-order spin-orbit coupling effect on atomization energy of YbI_2 is shown to be significant.

Key words: coupled-cluster method, core-valence correlation, complete basic set limit, ytterbium dihalides, atomization energy, vibrational frequencies, IR intensities, second-order spin-orbit coupling

S.M. BUTRIM, T.D. BILDYUKEVICH, N.S. BUTRIM, T.L. YURKSHTOVICH

MODIFICATION OF POTATO STARCH BY ACTION OF HYDROGEN PEROXIDE SOLUTIONS

The oxidation reaction of potato starch by the action of the hydrogen peroxide depending on suspensions pH, oxidizer concentration, time, a catalyst kind ($FeSO_4$, $CuSO_4$, $CoCl_2$, $NiCl_2$) was studied. It was shown, that at oxidation an insignificant accumulation of carboxyl (max. 0,11%) and carbonyl (max. 0,21%) groups takes place as well as the reduction of molecular weight appearing in an essential reduction of viscosity of starch water pastes. The mode optimization for reception of the oxidized potato starch suitable for surface sizing of paper was carried out.

Key words: potato starch, hydrogen peroxide, catalyst, oxidation, dynamic viscosity, surface sizing

S.A. KOKSHAROV

ON APPLICATION OF DYNAMIC LIGHT SCATTERING METHOD FOR ESTIMATION NANOPARTICLE SIZES IN TWO-COMPONENT HYDROSOL

The possibility of changing for typical setup of the measuring computer program DLS instruments to increase of sensitivity to the presence of small dispersion fractions was showed considering the limitations of using for the method of dynamic light scattering to estimate of the nano-objects mixture condition connected with influence of effect of reflexion for large particle.

Key words: hydrosol, nano-particles, size estimation, dynamic light scattering method

E.V. MAKAROVA, Yu.V. POLENOV, E.V. EGOROVA

KINETIC MODEL OF PROCESS OF NICKEL IONS REDUCTION BY THIOUREA DIOXIDE IN WATER-AMMONIA SOLUTION

The kinetics of reduction of nickel ions by thiourea dioxide was studied in a water-ammonia solution at different temperatures and concentrations of ammonia. The parameters of the individual steps of the process were determined by solving the inverse kinetic problem on the basis of the data obtained. Analysis of the obtained results has allowed drawing a conclusion on the adequacy of the proposed kinetic model to experimental data.

Key words: kinetics, nickel ions, thiourea dioxide, rate constants

Yu.V. KUSMANOVA, S.A. KUSMANOV, A.R. NAUMOV, P.N. BELKIN

ANODE PLASMA ELECTROLYTIC CARBONITRIDING OF STEEL IN AQUEOUS ELECTROLYTE BASED ON ACETONITRILE

The possibility of using acetonitrile as the nitrogen- and carbon-containing component of the electrolyte for the anode plasma electrolytic carbonitriding of steel was shown. The composition and structure of the surface layer consisting of oxide and diffusion layers were revealed. The mechanism of saturating components transport from electrolyte to steel includes evaporation and thermo destruction of acetonitrile, its adsorption and reduction on anode surface, formation of ammonia as nitrogen source, adsorption of ethanol and ammonia on the anode, and formation of carbon monoxide as carbon source. The influence of concentration of electrolyte components and processing conditions on the thickness of oxide and diffusion layers, distribution of micro-hardness of the surface layer and the surface roughness were established.

Key words: anode plasma electrolysis, diffusion saturation, carbonitriding, micro-hardness, roughness

E.V. GANEBNIKH, A.V. SVIRIDOV, G.I. MALTSEV

NICKEL EXTRACTION FROM SOLUTIONS WITH FINE MODIFIED ALUMINOSILICATES

The nickel adsorption isotherms from solutions with natural and modified montmorillonite were obtained. It was shown that adsorption processes can be described by Langmuir and S-shaped isotherms the form of which is defined both the surface properties of the sorbent and forms of nickel existence in aqueous solutions. Intercalation of sodium montmorillonite with the modifiers can sharply increase the extreme nickel ions adsorption, as well as can extend the range of pH values corresponding to high degree of nickel extraction.

Key words: montmorillonite, aluminosilicates, nickel, sorption, intercalation

A.A. LIPIN, A.G. LIPIN, A.V. SHIBASHOV

POLYACRYLAMIDE SYNTHESIS USING POLYMERIZATION-DESORPTION PROCESS

Experimental studies of polyacrylamide two steps synthesis were accomplished. At the first step, the acrylamide polymerization initiated by the redox system is carried out in concentrated water solutions under isothermal conditions. The second polymerization step was combined with product drying. The conditions under which the polymerization advances of water removal from the reaction system were determined.

Key words: acrylamide, polyacrylamide, polymerization, solution, drying

A.V. BABKIN, E.M. ERDNI-GORYAEV, A.V. SOLOPCHENKO, A.V. KEPMAN

INFUSION BISMALEIMIDE RESINS FOR POLYMERIC COMPOSITE MATERIALS

Various composition binders based on bismaleimide resins were investigated. Composition and curing mode for the infusion resin was developed. The physical and mechanical properties of the polymer matrix and composite material based on the developed bismaleimide resin were studied.

S.A. VSHIVKOV, A.G. GALYAS, T.S. SOLIMAN

RHEOLOGICAL BEHAVIOR OF HYDROXYPROPYL CELLULOSE - ETHYLENE GLYCOL SYSTEM IN MAGNETIC FIELD

The phase transitions, rheological properties and relaxation nature of the rheological behavior of the hydroxypropyl cellulose solutions in ethylene glycol were investigated. The magnetic field was shown to increase in the viscosity and concentration dependence of the magnetic field influence is described by the curve with a maximum. The energies of mechanical and magnetic fields stored by solutions under shear were calculated.

Key words: phase liquid-crystal transitions, rheological properties, relaxation, ester cellulose solutions

O.G. VOLOKITIN, V.I. VERESHCHAGIN, V.V. SHEKHOVTSOV

MELTING PROCESSES OF SILICA SAND IN LOW-TEMPERATURE PLASMA TECHNOLOGY

This work presents methods for the production of quartz glass using low-temperature plasma (LTP) to obtain a melt and glass from quartz raw materials.

Key words: silica sand, silicate melt, electro-plasma device, quartz ceramics

E.A. ALEKSEEV, B.A. GOLOVUSHKIN, A.N. LABUTIN, E.V. EROFEEVA

MODELING PROCESS OF POLYAMIDE-6 PRODUCTION

Improved mathematic model of polyamide-6 production process was obtained. The simulation model was created. The digital experiment was carried out.

Key words: polyamide-6, mathematic model, simulation modeling

S.P. RUDOBASHTA, G.A. ZUEVA, N.A. ZUEV

HYGROSCOPIC PROPERTIES OF SEEDS

The results of experimental studies of hygroscopic properties of typical colloid-porous materials – seeds of white mustard and bulb onion – were given and analyzed. The comparison of hygroscopic properties of these materials with the hygroscopic properties of other colloid capillary-porous materials of phytogenous – grain – was given.

Key words: equilibrium, drying, seeds, desorption isotherm, colloid capillary-porous materials, white mustard, bulb onion

E.S. SLIVCHENKO, A.P. SAMARSKIY, V.N. ISAEV, V.N. BLINICHEV

CLASSIFICATION OF CRYSTALLIZATION SYSTEMS ON THEIR ABILITY TO PHASE FORMATION

Theoretical and experimental evaluations of the crystallization systems ability to phase formation are summarized. The analysis of influence of crystalline substance and solvent nature on the position and magnitude of extremes rates of formation and growth of crystals and their activity was made in order to determine the systems classification identity.

Key words: crystallization system, complete mixing cell, overcooling, rate of crystals formation, rate of crystals growth, grain size measure, classification

S.V. NATAREEV, E.A. DUBKOVA, T.E. NIKIFOROVA, O.S. NATAREEV, A.A. BYKOV
**ION-EXCHANGE EXTRACTION OF IONS OF BIVALENT METALS IN PLATE COLUMN
WITH SUSPENDED LAYER OF CATION EXCHANGER**

The mathematical description of the process of solution purification from divalent metal ions by means of ion exchange in a plate column was proposed. Adequacy of the mathematical model developed was established using the solutions purification from zinc and calcium ions on the sulfonic acid cation exchanger KU-2-8 as an example.

Key words: ion exchange, plate column with overflow glasses

I.I. SHEPELEV, N.N. BOCHKOV, N.V. GOLOVNYKH, A.Yu. SAKHACHEV
**CHEMICAL-TECHNOLOGICAL FEATURES OF RESOURCES-SAVING PROCESSES
AT UTILIZATION OF SOLID METALLURGICAL WASTES**

Involvement in production of industrial wastes of iron-titanium production and wastes of fireclay brick lining, which characterized by a higher content of alumina, reduces the harmful effects on the environment and provides the additional recovery of valuable components, while achieved increasing output of commercial products and raw materials savings. At using gypsum-anhydrite wastes of aluminum fluoride production in the technology of soda products the increase in yield of potassium sulfate and the decrease in the consumption of limestone is achieved.

Key words: energy saving technologies, alumina, soda products, sludge of iron-titanium production, waste of firebrick, gypsum-anhydrite wastes

S.V. FEDOSOV, V.E. RUMYANTSEVA, N.S. KAS'YANENKO, I.V. KRASILNIKOV
**NON-STEADY MASS TRANSFER IN CORROSION PROCESSES OF SECOND KIND OF CEMENT
CONCRETE. LOW VALUES OF FOURIER NUMBERS WITH INTERNAL MASS SOURCE**

This article is devoted to mathematical modeling the corrosion processes of reinforced concrete constructions proceeding according to the mechanism of the second kind. Mass conductivity boundary problem is presented as well as its solution in the Laplace transform. The results of calculations by expressions obtained for low values of Fourier number indirectly indicate that concrete corrosion is determined by physical and chemical processes occurring in the surface layers.

Key words: corrosion, concrete, mass transfer, internal mass source, concentrations profile

S.V. FEDOSOV, V.E. RUMYANTSEVA, I.V. KRASILNIKOV, N.L. FEDOSOVA
**STUDY OF DIFFUSION PROCESSES OF MASS TRANSFER AT LIQUID CORROSION
OF FIRST KIND OF CEMENT CONCRETE**

The mathematic model of corrosion process of the first kind of cement concrete was given. The mathematic task of mass transfer was presented for close system of liquid-vessel at existence internal source of mass in a solid phase. The obtained solutions of task were given. These solutions describe dimensionless concentrations of component on concrete thickness and in a liquid phase. Solutions allow calculating the dynamics and kinetics of process. The method of determination of mass-transfer coefficients and power of internal mass source is described.

Key words: liquid corrosion, mathematic model, internal mass source, concentrations profile

R.F. SHEKHANOV, S.N. GRIDCHIN, A.V. BALMASOV, K.E. RUMYANTSEVA
PROMISING ELECTROLYTES FOR OBTAINING GALVANIC ALLOYS OF ZINC AND NICKEL

Electrodeposition processes of zinc-nickel alloys from sulfamate, chloride, oxalate, pyrophosphate and alkaline electrolytes have been investigated. The possibility of obtaining the good-quality electroplating has been shown at current densities from 0.5 to 5.0 A/dm².

Key words: electroplates, galvanic alloys, nickel, zinc

V.E. RUMYANTSEVA, K.E. RUMYANTSEVA, V.S. KONOVALOVA
**INFLUENCE OF ACCELERATORS OF PHOSPHATING PROCESS AND INHIBITORS
OF CORROSION OF REINFORCED-CONCRETE CONSTRUCTIONS ON DESTRUCTION
OF REINFORCEMENT AND CONCRETES**

The inhibitory effect of nitrates and nitrites of metals on the corrosion of the reinforced-concrete constructions was considered. Corrosion indicators were calculated and conclusion on the optimal amount of inhibitors in phosphating solutions and concrete was made.

Key words: corrosion, phosphate coating, concrete, reinforcing steel, inhibitors, reinforced concrete

D.A. FILIMONOV, T.F. YUDINA, I.V. BRATKOV, M.I. BAZANOV, T.V. ERSHOVA
**CYCLIC VOLTAMMETRY METHOD FOR STUDY OF OXIDIZED GRAPHITE
IN ALKALINE SOLUTION**

By the method of cyclic voltammetry the study of electrochemical and electrocatalytic properties of oxidized graphite in alkaline solution was carried out. The data of choosing the experimental conditions were presented. The estimation of catalytic activity for the reaction of molecular oxygen reduction in an alkaline solution was carried out. The effective number of electrons for given process was determined.

Key words: oxidized graphite, cyclic voltammetry, alkaline medium

E.Yu. TYUNINA, M.D. CHEKUNOVA
**ELECTROCONDUCTIVITY OF SOLUTIONS OF LiAsF_6 IN APROTIC SOLVENTS
WITH DIFFERENT PERMITTIVITY**

The electroconductivity of solutions of LiAsF_6 in N-methyl-2-pyrrolidone (MP) was determined at temperatures of 253.15, 263.15, 273.15, 283.15, 293.15, 303.15, 313.15, 323.15 and 333.15 K in the concentration range of 0.1 - 1.1 mol/kg. The comparison of values of activation energy for conductivity in a system under consideration with analogous magnitudes of earlier investigated solutions of LiAsF_6 in propylene carbonate (PC), γ -butyrolactone (γ -BL), tetrahydrofuran (THF), methyl acetate (MA) was carried out. The mechanism of charge transfer in systems LiAsF_6 – high-polar aprotic solvents (PC, γ -BL) was shown to be the ion migration one, and high electroconductivity of solutions of LiAsF_6 in low-polar aprotic solvents (THF, MA) can be conditioned by additional contribution from charge transfer by ionotropic mechanism.

Key words: lithium hexafluoroarsenate, N-methyl-2-pyrrolidone, aprotic solvents, electroconductivity, activation energy, ion migration mechanism, ionotropic mechanism