A B S T R A C T S

A.V. VOLKOVICH, V.I. ZHURAVLEV, V.V. NIKOLAEV, M.V. SIGAYLOV

ACTIVITY COEFFICIENTS OF CALCIUM IN LIQUID ALLOYS WITH ALUMINUM AND LEAD

The values of activity coefficients of the calcium have been calculated on the base of measurements of potentials of liquid alloys of calcium-lead and calcium-alumina. The activity coefficients of calcium have been established to increase in temperature and under a transition from lead alloys to alumina alloys.

Key words: liquid alloy, calcium, lead, aluminum, coefficients of activity

M.V. SOLODKOVA, V.I. ZHURAVLEV, A.V. VOLKOVICH

SOLUBILITY OF CALCIUM, STRONTIUM AND BARIUM OXIDES IN CHLORIDE AND CHLORIDE-FLUORIDE MELTS

The solubility of calcium, strontium and barium oxides was obtained by a method of isotherm saturation of chloride and chloride-fluoride molten salts. The factors influencing on solubility of alkali-earth metals oxides in molten salts were established.

Key words: calcium, strontium, barium, oxides, solubility, salt melts

K.S. LEBEDEV

NEW COMPUTER METHODS FOR CHEMICAL STRUCTURE DETERMINATION OF ORGANIC COMPOUNDS USING LOW RESOLUTION MASS SPECTRA

Two new computer methods for chemical structure determination of organic compounds using low resolution mass spectra are considered. Both methods use the results of spectral similarity search in a mass spectral database. The first method is based on extraction from selected structures the maximal common fragments while the second is based on decomposition of those fragments for the purpose of fragment extraction confirmed by primary processes of molecules fragmentation under the action of electron impact.

Key words: organic compound structure, mass-spectrometry, computer methods

A.N. NOVIKOV

SYSTEM OF STANDARD VALUES OF HEAT CAPACITY AND VOLUME OF IONS IN N-METHYLPYRROLIDONE AND SOME REGULARITES

The standard values of heat capacity $\overline{C^o_{P\,i}}$ and volume $\overline{V^o_i}$ of ions in N-methylpyrrolidone (MP) at 298.15 K were calculated on the base of theory being developed by author. The dependences of $\overline{C^o_{P\,i}}$ and $\overline{V^o_i}$ on radius, charge and chemical nature of ions were considered.

Key words: heat capacity, ion volume, N-methylpyrrolidone

N.F. KIZIM, E.N. GOLUBINA

STRUCTURIZATION IN $ErCl_3$ - H_2O- DI-(2-ETHYLHEXYL)PHOSPHORIC ACID - C_7H_{16} SYSTEM

The organogel in the system $ErCl_3$ – H_2O – di-(2-ethylhexyl) phosphoric acid (D_2EHPA) - C_7H_{16} at D2EHPA concentration of 0.01 – 0.1 M, Er (III) 0.01 – 0.1 M, (pH ≈ 5,3) depending on the conditions of its formation has different properties. In the static systems at [D2EHPA]/[Er(III)]=2 the jelly-like mass is formed. Further that mass transforms to solid mass with amorphous and crystal sites of polymers $(ErR_3)_n$. In systems with a free interface the extract represents weakly structured disperse system with coagulation - thixotropic structure.

Key words: gel formation, $ErCl_3$ – H_2O – di-(2-ethylhexyl)phosphoric acid - C_7H_{16} system

E.V. PRONIN, N.F. KIZIM, O.M. ROSLYAKOVA

ELECTRIC CONDUCTIVITY OF SOLUTIONS OF DI-(2-ETHYLHEXYL) PHOSPHORIC ACID AND ITS SALTS IN ALIPHATIC ALCOHOLS

Isotherms of conductivity for solutions of di-(2-ethylhexyl) phosphoric acid (D2EHPA) and also its salts (Fe(III), Ce(III), Cu(II)) in aliphatic alcohols (n-butanol, n-hexanol and n-octanol) were obtained. Transfer numbers for hydrogen ions and also D2EHPA anions in butanol were measured and their limiting electrical mobilities were calculated. Tempera-

ture dependencies of electric conductivity for D2EHPA and its salts in aliphatic alcohols were studied; activation energies of electric conductivity and micelle formation were calculated.

Key words: electric conductivity, transfer numbers, mobilities

S.V. DOBRYDNEV, G.I. KAPAEV, O.V. ZAMURUEV, V.S. BESKOV

THERMOLYSIS FEATURES OF HYDRATES OF HYDROXYCARBONATES OF NICKEL (II), COPPER (II) AND ZINC (II)

The thermolysis of hydrates of hydroxycarbonates of the nickel (II), copper (II) and zinc (II) of non-stoichiometrical structure of general formula $xMeCO_3 \cdot yMe(OH)_2 \cdot zH_2O$ has been studied with the methods of gravimetry, gas-volumetric and thermogravimetric analysis. Features of physical and chemical transformations of compounds mentioned above at thermal decomposition have been established.

Key words: thermolysis, hydrates, hydroxycarbonates of the nickel (II), copper (II) and zinc (II)

V.A. AVERYANOV, N.M. NOSOVA, K.S. LEBEDEV

ROLE OF ALCOHOLS AS NUCLEOPHILIC AGENTS IN HYDROCARBOALKOXYLATION REACTIONS. PROBLEM OF ACCOUNTING OF SOLVATION PROPERTIES INFLUENCE OF COMPONENTS OF REACTION MEDIUM ON REACTION RATE

The concentration influence of three nucleophilic reagents (m-cresol, methanol and cyclohexanol) on the rate of the cyclohexene hydrocarboalkoxylation at the catalysis by the $Pd(PPh_3)_2Cl_2$ – PPh_3 – p-toluenesulfonic acid system has been studied. On the base of the comparison of reaction ability of these nucleophilic reagents itself and conditions of competitive hydrocarboalkoxylation with account of influence on reactions of the tozylate-anion the conclusion has been done about contribution in this reaction rate of three factors – nucleophilic activity, specific solvation and ligand exchange. The role of latter has been confirmed by linear dependence of reaction rate on donor and acceptor properties of solvents.

Key words: hydrocarboalkoxylation, cyclohexene, catalysis, reaction rate, alcohol

V.N. FILIMONOV, S.I. SIRITSO

PARAMETERS OF HYDROPHOBICY FOR FORECASTING OF RETENTION OF WATER-SOLUBLE VITAMINS BY A NON- POLAR SORBENT AT CONDITIONS OF REVERSED-PHASE HPLC

Calculation methods the parameters of hydrophobicy H and logP have been determined. The possibility of forecasting of retention of water-soluble vitamins by non- polar sorbent on the basis of their hydrophobicy has been shown. Dependences between energy characteristics of studied systems and H analytes have been established.

Key words: hydrophobic parameters, vitamins, retention, sorbent

S. V. DOBRYDNEV

STUDY OF FLOW VELOCITY OF AQUEOUS SOLUTIONS THROUGH POROUS MATERIALS

Both the scheme of experimental set up and method of flow velocity measurement of aqueous solutions through the porous materials have been offered. The flow velocities of aqueous solution of calcium chloride through a powder of calcite and aqueous solutions of the hydrochloric acid through the porous glass have been measured. In the isoelectrical conditions of the surface of the porous body the flow velocities of aqueous solutions have been established to be maximal. The explanation of the observable phenomenon with application of structural model of double electric layer of Stern is given.

Key words: porous materials, liquid flow velocity

A.V. YANKOV

OBTAINING COMPLEX CARBAMIDE –CONTAINING FERTILIZER FROM KOVDOR'S APATITE CONCENTRATE

The study of Kirov's apatite concentrate exchange on Kovdor's one by some authors showed on the decrease of shop productivity and existence of some difficulties. Using the experiment planning method the influence of some parameters on P2O5 various forms has been established. The carbamide addition influence on phase composition of carbonitrophoska has been studied. The mechanism of carbonitrophoska formation has been given.

Key words: apatite concentrate, P2O5 forms, carbamide

T.A. VOROBYEVA, A.V. YANKOV

THERMODYNAMICS AND KINETICS OF CHEMICAL TRANSFORMATION UNDER INTRODUCTION IN AMMONIUM NITRATE FUSION CAKE THE POWDER OF CAUSTIC MAGNESITE

The calculation results of thermodynamic parameters and studies of possible chemical transformation kinetics under introduction of the caustic magnetite powder (MgO – main substance) with components of fusion cake of ammonium nitrate are given. In the temperature range of 448-468 K the magnesium oxide has been established to react with ammonium nitrate fusion cake forming magnesium nitrate, water and ammonia.

Key words: kinetics, thermodynamics, magnesium oxide, ammonia nitrate, fusion

L.Y. RASSOKHINA, N.P. BELOVA, V.T. LEONOV

ABOUT POSSIBILITY OF COMPLEX FERTILIZERS PRODUCTION FROM PHOSPHORITE OF KIMOVSK DEPOSIT

There is phosphate row deposit on a territory of Tula region. Both the phosphorite composition and its physical and chemical properties have been determined. Studies on concentrating have been carried out. The process of obtaining the complex fertilizers has been studied.

Key words: phophate row, complex fertilizers ontaining

M.M. MOISEEV, E.V. BUDEYKINA, I.D. MOISEEVA

STUDY OF AMMONIA DECOMPOSITION CATALYSTS FOR PROTECTIVE ATMOSPHERES PRODUCTION AND ECOLOGICAL PURPOSES

The results of ammonia cracking catalysts studies for a gas and ventilating exhausts purification and also for production of protective atmospheres and hydrogen are presented. The high efficiency of studied compositions of catalysts for the process of ammonia decomposition at the temperature higher 800°C and flow rate of 5000 h-1 has been shown. The oxygen presence in gas emissions containing ammonium excludes the purification accomplishing by means of catalytic cracking due to the formation of the nitric oxides.

Key words: catalyst, cracking, ammonium, gas purification, hydrogen

A.M. KOZLOV, G.V. MESHERYAKOV

CO-PRODUCTIONS: METHANOL-HYDROGEN AND METHANOL-AMMONIA

Possibility and necessity of creation of co-productions of methanol-hydrogen and methanol-ammonia have been proved. The analysis of existing schemes of methane conversion for their use in co-productions has been carried out. Variants of co-productions have been offered at use of various schemes of conversion. Technical parameters of offered schemes are given.

Key words: methanol, hydrogen, ammonium, joint production, methane conversion

V.M. POMOGAEV, A.V. VOLKOVICH, I.V. PETROCHENKOVA, A.E. SHUVAKIN

INFLUENCE OF ELECTROLYSIS CONDITIONS ON DIFFUSING ABILITY OF CHROMIUM-PLATING ELECTROLYTES

The diffusing ability on current and on metal of chromium-plating electrolytes has been measured with standard method. The diffusing ability on current of chromium-plating electrolytes has been shown to decrease whereas on metal to increase. Experimental results agree satisfactorily with calculation results. Equations obtained allow to calculate the diffusing ability on current and on metal for electrolytes containing chromium three oxide and sulfuric acid.

Key words: diffusion ability, chromium-plating, electrolyte composition

V.I. ZHURAVLEV, A.V. VOLKOVICH, I.S. TROFIMOV

PHASE FORMATION OVERVOLTAGE AT ELECTROLYTICAL OBTANING OF DOUBLE-PHASE ALLOYS OF ALKALI–EARTH METALLS

The existence of phase overvoltage on zinc cathode at the calcium, strontium and barium inter-metal compounds formation has been established with galvanostatic method. Parameters of phase polarization have been determined.

Key words: zinc cathode, polarization, calcium, strontium and barium inter-metal compounds

O.V. IVANOVA, B.A. KHORISHKO, N.F. KIZIM, I.V. MEKAEVA, A.D. DAVYDOV, S.A. KHORISHKO

REGULARITIES OF CATHODE PROCESSES ON MAGNETITE IN ACID MEDIA

On the basis of potentiostatic and spectrophotometric researches some aspects of dissolution kinetic of magnetite at cathode polarization in aqueous solutions of acids: H_2SO_4, HCl, HNO_3, CH_3COOH, $HClO_4$ at (pH= -0.5 ÷ 4), temperatures of 278÷363 K and pressure of 101325 Pa have been discussed. The magnetite cathode dissolution has been established to form ions of Fe^{2+} mainly. The influence of potential on activation energy and on order of process have been shown.

Key words: magnetite, dissolution kinetics, cathode polarization, acid solutions

Yu.N. ZHIRKOVA,V.I. ZHURAVLEV, A.V. VOLKOVICH

DISTRIBUTION OF CURRENT DENSITY AND POLARIZATION ON ALUMINUM–NICKEL COMPOSITION POWDER CATHODE AT NICKEL ELECTRODEPOSITION

The model of current density distribution on the composition aluminum–nickel powder cathode has been proposed. By means of probe method the values of polarization have been measured on different levels of such cathode. The results of calculations of current density distributions and experimental measurements of polarization distributions agree satisfactory.

Key words: powder cathode, modeling of current density distribution, polarization

B.A. KHORISHKO, A.D. DAVYDOV, A.I. ERMAKOV, A.L. TRAVIN, O.V. IVANOVA, I.V. MEKAEVA

INFLUENCE OF PH ON INTERACTION IN SYSTEM OF MAGNETITE – AQUEOUS MEDIUM

The magnetite behavior in solution of 0.5M Na_2SO_4 in absence of external polarization has been studied and discussed with quantum-chemical, gravimetric, spectrophotometric, voltamperometrical, pH-metric and microscopic methods. An adequacy of earlier proposed conceptual model of interaction in system of magnetite – aqueous medium has been experimentally confirmed. The participation of water oxygen in new chemical bond formation of Fe-O with cation sublattice of oxide has been shown and forecasted.

Key words: magnetite, water medium, quantum-chemical model, chemical bond, molecular cluster

V.M. POMOGAEV, A.V. VOLKOVICH, A.E. SHUVAKIN

ABOUT PECULARITIES OF PERIODICAL CURRENT INFLUENCE ON DIFFISING ABILITY OF ELECTROLYTE OF COPPER COATING

It has been shown that the application of pulsed current does not allow to increase the uniformity of coating and diffusing ability of electrolyte for copper plating with the polarization curve in the form of half-wave. The method of the increase of cover uniformity by imposing a current pulse on direct current has been proposed. The application of proposed current form and electrolysis parameters as comparing with direct current allows increasing by 10-25% the diffusing ability of electrolyte at the same average rate of cover deposition.

Key words: pulse current, copper coating electrolyte, diffusion ability, cover uniformity

B.A. KHORISHKO, YU.D. ZEMLYAKOV, K.V. STANISLAVCHIK, O.V. IVANOVA, I.V. MEKAEVA, S.A. KHORISHKO

CORROSION STABILITY OF MAGNETITE IN SULPHATE MEDIA

The corrosion behavior of magnetite in aqueous solutions of sodium sulphate in the absence of external polarization has been studied by spectrophotometric and microscopic methods. The corrosion stability of magnetite in studied media has been estimated an according to State Standard 13819-68

Key words: magnetite, aqueous media, pH, uniform corrosion, corrosion stability

G.A. AFONINA, W.G. LEONOV, O.N. POPOVA

PHASE COMPOSITION AND MORPHOLOGY OF $MgO–SiO_2$ SOL-GEL POWDER

The phase composition and morphology of magnesium- silicate system has been studied in the range of SiO_2 content from 32 to 70%. Using X-ray, spectroscopic and microscopic analysis the sol-gel method with application of inorganic precursors has been established to provide the decrease in synthesis temperature of the forsterite and the enstatite.

Key words: phase composition, magnesium- silicate system, morphology

V.V. VOROBYEVA, V.G. LEONOV

FILTERING ALUMINOSILICATE CERAMIC FOR BAROMEMBRANE PROCESSES OF PURIFICATION OF WATER SYSTEMS

The results of several-year's studies in the field of porous penetrable ceramics for micro and ultra filtration process are presented. Parameters of porous structure of aluminum-silicate filtering ceramic based on natural raw resources as well as on anthropogenic components which weren't previously used for ceramic filter production have been studied. The "composition-structure-property" relationship has been analyzed for penetrable multi-component ceramics.

Key words: porous ceramics, penetration, micro and ultra filtration

G.V. MESHERYAKOV

REACTOR OF METHANOL SYNTHESIS

The design of methanol synthesis reactor of low pressure 5 MPa with higher yield of methanol than in the existing schemes has been proposed. The results of calculation of material balance of column for methanol synthesis with four layers of catalyst are shown. The review of existing and being worked out reactors for methanol synthesis is given.

Key words: low pressure reactor, methanol, synthesis

E.I. KOSTYLEVA, T.I. RYBKINA, I.M. KOSTYLEV, V.M. KOPYLOV

SYNTHESIS AND PROPERTIES OF NEW METAL-CONTAINING ORGANOSILICON COMPOUNDS

The process of interaction of acetylacetonates of some s,p,d-elements and silicon-hydrides of various functionality has been studied. The synthesis method of mono and poly functional compounds by hydrosilization reaction has been developed. The reaction products have been studied with various physical-chemical methods. Obtained chelate silicon-organic compounds are completely dissolved in silicon-organic liquids of PMS type. The important operating parameters of polydimethylsiloxanes can be essentially changed by means of addition of compounds obtained.

Key words: synthesis, acetylacetonates, s,p,d-elements, silica-containing organic compounds

R.V. RODIONOVA, V.A. BALASHOV

SYNTHESIS OF NANODISPERSED SYSTEMS BASED ON STYRENE AND UNSATURATED SURFACTANTS

Nanodispersed systems with the chemical localization of stabilizer on the particles surface on the base of styrene and unsaturated surfactants have been synthesized. The hydration of latex particles has been studied at various degrees of surface hydrophylization. The main role in stability of nano-dispersed system stabilized with unsaturated surfactants has been established to play a particles hydration.

Key words: nano-dispersed system, synthesis, styrene, unsaturated surfactants, hydration

A.A. ALEKSEEV, E.V. ORDINA, V.S. OSIPCHIK, E.A. KIRICHENKO

BEHAVIOUR OF BEADED STYRENE COPOLYMER WITH ACRILONITRILE IN WATER SOLUTION OF SODIUM HYDROXIDE

The treatment of beaded statistical copolymer SAN containing 30 % on mass of the acrylonitrile by NaOH solutions with concentration of 0, 10, 20, 30 and 40 % is accompanied with partial hydrolysis of nitrile groups of surface macromolecules to amide and carboxyl groups. Obtained at that treatment the bead variants look like the mixtures of initial and chemically modified SAH for production of goods with improved mechanical parameters

Key words: copolymer, acrylonitrile, hydrolysis, imide and carboxyl groups

A.A. ALEKSEEV, T.V.PETUKHOVA, V.S. OSIPCHIK, E.A.KIRICHENKO

PLASTICIZATION OF BUTADIENE-STYRENE BLOCK COPOLYMER OF RADIAL STRUCTURE BY INDUSTRIAL OIL

The properties of current consignments of industrial oils of the trademark I-12A, I-20A, I-40A and I-50A, being of interest of their application as plasticizers for polymer have been studied. The possibility of the using industrial oils as molecular plasticizers for butadiene-styrene block copolymer has been shown.

Key words: industrial oil, plasticizer, butadiene-styrene block copolymer

V.A. AVERYANOV, S.A. BATASHEV, N.T. SEVOSTYANOVA

KINETIC MODEL OF CYCLOHEXENE HYDROCARBOMETHOXYLATION CATALYZED BY SYSTEM $Pd(PPh_3)_2Cl_2$ – PPh_3 – p-TOLUENESULFONIC ACID

On the basis of earlier founded kinetic regularities of cyclohexene hydrocarbomethoxylation catalyzed by the system $Pd(PPh_3)_2Cl_2$ – PPh_3 – p-toluenesulfonic acid the kinetic model of this process has been proposed. The model parameters estimation has been made. Discovered statistic insignificance of the one from parameters allowed to simplify the model form. The independent test experiments have demonstrated good correspondence of experimental and calculated reaction rates.

Key words: cyclohexene, hydrocarbomethoxylation, kinetic model

V.I. ZHURAVLEV, A.V. VOLKOVICH, I.S. TROFIMOV

ESTIMATION OF DIFFUSION COEFFICIENTS OF ALKALI–EARTH METALS IN LIQUID ALLOYS ON DATA OF CATHODE CHRONOPOTENTIOMETRY

The diffusion coefficients of the calcium, strontium and barium have been calculated on the base of data of chronopotentiongrams analysis for liquid cadmium, lead, tin and aluminum cathodes in melts containing chlorides of alkali–earth metals.

Key words: cadmium, lead, tin and aluminum cathodes, diffusion coefficients, melt

V.Yu.VOLKOV, V.V. BATYSHKINA

PROBLEMS OF COGNITIVE APPROACH APPLICATION FOR CREATION OF INTELLECTUAL SYSTEM OF ECOLOGICAL MONITORING AND CONTROL

Basic problems concerning the development of intellectual systems of ecological monitoring and control (ISEMC) based on ISEMC with various degrees of pollution of the atmospheric air conducted in real time mode have been considered in the city of Novomoskovsk. In order to solve the problem, the modern method based on "soft-computing" principle and, in particular, cognitive modeling is proposed. It has been shown how the method mentioned above can be applied for ISEMC of Novomoskovsk.

Key words: ecological monitoring, intellectual system

I.V. EMIROVA, A.A. ALEKSEEV

NEW ANTICORROSIVE PIGMENTS

The protective coating film forming from the composition PF-115 with the newest non toxic anticorrosive pigment “Pigmentan” was investigated.

Key words: protective non toxic cover, anticorrosive cover

A.I. ERMAKOV, E.M. KAZAKOVA

QUANTUM-CHEMICAL CALCULATIONS OF COMPLEXES OF SMALL IRON CLUSTERS FeN (n = 1 - 4) WITH MOLECULES OF WATER, METANE AND BENZENE

The geometrical structure and Gibbs energy of complexes of small iron clusters Fe_n (n = 1 - 4) with molecules of methane, benzene and water have been studied by PBE/3z method of density functional theory. Complexes are characterized by presence of chemical bonds of iron with hydrogen and carbon or oxygen. The increase in the sizes of iron clusters results in the monotonically increase of stability of its compounds with the water molecules. The iron clusters in structure of the considered molecules reduce the Gibbs energy of their homolytic dissociation with hydrogen formation.

Key words: quantum-chemical calculations, iron clasters, structure, Gibbs energy

Yu.A. KRUTOV, V.S. BESKOV, V.T. LEONOV

RESOURCE –ENERGY- SAVING TECHNOLOGY FOR RECYCLING NITROGEN OXIDES FROM EXHAUST GASES OF CONTINUOUS AND LOCAL PROCESSES AND SUDDEN EMISSIONS

The technology of recycling nitric oxides from exhaust gases of various manufactures with application of fluorine fibre has been developed. The recycling mechanism of nitrogen oxides to nitric acid and the sorbent self-regeneration in high-speed reactor has been found. The process scheme is closed and resource-energy saving. The clearing reactor is simple in service and allows returning nitric acid in a production cycle.

Key words: nitrogen oxides, exhausted gases, utilization

V.Yu. VOLKOV, ALI MANSOOR

APPLICATION OF BAYESIAN TECHNOLOGIES IN SYSTEMS OF ECOLOGICAL MONITORING OF CHEMICAL ENTERPRISES

Maintenance of stable, non-life threatening ecological environment to human populations in regions with high number of chemical infrastructure facilities is of a great importance. For monitoring of the atmospheric air conditions in such regions, intellectual system based on Bayesian technological approach has been proposed. An integrated approach for task solution allow getting the optimal decisions for reducing air pollution in real time regime.

Key words: monitoring of atmosphere air, intellectual system of controling

S.I. SIDEL'NIKOV, S.V.GOLIKOV

DEVELOPMENT OF SITUATION ADVISING SYSTEM OF RECTIFICATION COLUMN SEWAGE CONTROL

The development of local open-source expert system has been suggested for prevention the exceeding of methanol maximum allowed concentration in the sewage of rectification column. The comparative analysis of inaccuracy has been performed for models based on various mathematical applications. It has been shown that the lowest inaccuracy was found for hybrid neuronic networks. Fuzzy mathematical model of rectification process sewage has been built. It was suggested to solve the problem of forecasting of object state based on results of control decision by means of fuzzy control model.

Key words: rectification, methanol, modeling, control

D.S. ERMAKOV, T.I. RYBKINA

TRAINING OF CHEMISTRY TEACHERS IN CHEMICAL TECHNOLOGICAL UNIVERSITY

The features of training of chemistry teachers for the secondary school in the chemical technological university have been analyzed. The structure of curriculum, the content of separate disciplines has been considered.

Key words: training, chemistry teachers, curriculum, disciplines