ИЗВЕСТИЯ ВЫСШИХ УЧЕБНЫХ ЗАВЕДЕНИЙ

Т 57 (12) ХИМИЯ И ХИМИЧЕСКАЯ ТЕХНОЛОГИЯ 2014

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A B S T R A C T S

N.N. SMIRNOV, A.P. ILYIN, D.N. SMIRNOVA, S.P. KOCHETKOV, A.V. POPOVA

PURIFICATION OF EXTRACTION PHOSPHORIC ACID AND SIMULTANEOUS EXTRACTION OF RARE EARTH ELEMENTS ON CARBON ADSORBENTS

The analysis of methods for producing purified phosphoric acid indicates that the main problem is the decomposition and removal of soluble complex compounds of fluorine with metals. The required product quality is achieved by using universal methods of complex purification of extraction phosphoric acid by applying carbon adsorbents. The efficiency of the proposed method of production of purified phosphoric acid was shown to achieve by combination of venting stapes of fluoride compounds, adsorption purification and simultaneous extraction of rare earth elements.

Key words: extraction phosphoric acid, purification, fluorine compounds, carbon adsorbents, defluorination, rare earth elements extraction

M.A. YUROVSKAYA, N.P. GERASIMOVA, E.M. ALOV, A.S. DANILOVA, E.I. FILIMONOVA, L.M. SOBOLEVA

CHLOROSULFONYLATION OF METHACRYLIC ACID AND METHYL METHACRYLATE

The addition reaction of aromatic sulfonyl chlorides to methacrylic acid and methyl methacrylate was investigated. It was shown that the reaction leads to adducts without their simultaneous dehydrochlorination. Convenient conditions for dehydrochlorination of sulfonyl chloride and methacrylic acid adducts without isolating them in a pure form were chosen. Herewith, vinyl or allylic sulfones are selectively formed.

Key words: chlorosulfonylation, adducts, methacrylic acid, methyl methacrylate, vinilic and allylic sulfones

M.V. KARUNNAYA, E.R. KOFANOV, V.V. SOSNINA, G.G. KRASOVSKAYA, A.S. DANILOVA

SYNTHESIS OF 3-(3-NITROPHENYL)-5-STYRYLE-1,2,4-OXADIAZOLE

The reaction of 3-(3-nitrophenyl)-5-styryle-1,2,4-oxadiazole obtaining from 3-nitrobenzeneamidooxime and chloranhydride of cinnamic acid was considered.

Key words: 3-nitrobenzeneamidooxime, cinnamic acid chloranhydride, 3-(3-nitrophenyl)-5-styryle-1,2,4-oxadiazole

N.I. GIRICHEVA, A.A. ISHCHENKO, V.I. YUSUPOV, V.N. BAGRATASHVILI, G.V. GIRICHEV

VIBRATIONAL SPECTRA OF METHANE HYDRATES

Calculations of the vibrational spectra of $H_2O[5^{12}]$, $H_2O[6^25^{12}]$, $CH_4{\cdot}H_2O[5^{12}]$, $CH_4{\cdot}H_2O[6^25^{12}]$ clusters were implemented by the DFT (LC-wPBE/6-311+G(d,p)) method. It was shown that the model of small and large frames can be successfully used to interpret the experimental vibrational spectra of methane hydrates. It was found that the frequency shift of the O-H stretching vibrations in related water molecules to longer wavelengths, as compared with the vibrations of the free molecule, due to the formation of intermolecular hydrogen O···H bonds requiring to a lengthening of the intramolecular O-H bonds, reduction of the $f_{O\text{-}H}$ force constants and respectively, the frequency of stretching vibrations, and the frequency shift of the deformation vibrations in the short wavelength region, due to the increase in the deformation force constants, which is due to the interaction between neighboring water molecules, stabilizing the structure of the water framework. It was noted that with decreasing size skeletons H_2O $[5^{12}]$ and H_2O $[6^25^{12}]$ marked trends are enhancing. In contrast to the frequency of stretching vibrations of skeleton molecules, stretching vibration frequencies of the guest CH_4 molecule are increase with the decreasing size of the frame, which can be explained by the repulsive part of the host-guest interaction.

Key words: methane hydrates, vibrational spectra, structure, clathrates, quantum-chemical calculations, vibration frequencies

V.G. SOLOMONIK, A.N. SMIRNOV, O.A.VASILIEV, E.V. STAROSTIN, I.S. NAVARKIN

NONEMPIRICAL STUDY ON THE ELECTRONIC STRUCTURE OF CERIUM, PRASEODYMIUM, AND YTTERBIUM TRIHALIDE MOLECULES

The molecules LnX_3 (Ln = Ce, Pr, Yb; X = F, Cl, Br, I) are studied at the multireference configuration interaction MRCISD+Q level of theory with an accounting for relativistic effects. The species are shown to possess a manifold of low-lying electronic states. A significant spin-orbital coupling effect on the molecular properties is emphasized.

Key words: lanthanide trihalide molecules, low electronic states, multireference configuration interaction, spin-orbital interaction

E.M. KUVSHINOVA, A.V. RODIONOV, V.E. MAIZLISH, S.A. SYRBU, O.A. GOLUBCHIKOV

SYNTHESIS AND COORDINATION PROPERTIES OF TETRA-4-TERT – BUTYLPHTHALOCYANINE AND ITS NITRO DERIVATIVES

Tetra (4-tert-butyl) phthalocyanine (I) and nitro-tetra (3-nitro-5-tert-butyl) phthalocyanine (II) and tetra (4 - tert-butyl-5-nitro) phthalocyanine (III) were synthesized. The kinetics of complexation reactions of phthalocyanines I-III with acetates of copper, cobalt and manganese in a mixed solvent of pyridine and acetic acid (9:1) was studied. The influence of the structure of phthalocyanines I-III on the kinetic parameters of the formation of metal complexes was established.

Key words: synthesis, phthalocyanines, complexation, kinetics, metal-complexes, 3d metals acetates

Z.M. MUKHTAROVA

PHYSICAL-CHEMICAL ANALYSIS OF SmTe-Sm_5Ge_3 SYSTEM

The state diagram of Ge-Te-Sm system was studied using DTA, X-ray and microstructure methods, and measurements of micro hardness. The SmTe-Sm_5Ge_5 system was established to be an eutectic type. Eutectics coordinates are found to be 52 mol% of SmTe at 1600 K.

Key words: phase diagram, eutectic, thermogram, quasi-binary sections, non-quasi-binary sections, microhardness

I.M. BORISOV, Z.Sh.GAZIZOVA, G.R. SHAYAKHMETOVA, I.S. FAIYZRAKHMANOV

KINETICS OF PEROXYDE OXIDATION OF OIL SULPHIDES IN PRESENCE OF MOLYBDENUM ACID AND MOLYBDENUM OXIDE (VI)

The kinetics of reaction of peroxide oxidation of oil sulphides up to sulfoxides was studied in the presence of catalytic system of molybdenum acid- molybdenum oxide (VI). The scheme of occurring reactions was proposed.

Key words: oil sulfides, oxidation, hydrogen peroxide, molybdenum acid, molybdenum oxide (VI), kinetics

M.D. PLOTNIKOVA, N.A. MEDVEDEVA, A.B. SHEIN

INVESTIGATION OF ELECTRICAL AND KINETIC PROPERTIES OF INHIBITORS "FLEK" IN NEUTRAL MEDIA

Results of investigation of electrical and kinetic properties of inhibitors "FLEK" are presented. The influence of particles size as well as of their charge on the inhibitive effect on mild steel in a neutral media containing hydrogen sulfide was estimated. ζ-potential of steel surface in solutions under study was determined.

Key words: corrosion, inhibitor, micelle, ζ-potential

A.A. ZALUTSKIY

DETERMINATION OF DIFFUSION COEFFICIENTS OF MOSSBAUER IRON ATOMS IN WATER FILMS ADSORBED ON SURFACE OF NANOCLAY

Parameters of diffusion movement and data on geography of iron exchange complexes on aluminum silicate surface of clay are presented. The data were obtained using original method based on Mossbauer spectroscopy. Analyzed phycival reasons of temperature behavior of dynamic Mossbauer parameters allow determining the character of atoms movement using the different models of diffusioin movement. For iron atoms adsorbed to inter box space of mineral the uneven progressive diffusion is typical. It allows determining the size of fluctuation cavity($r \approx 0.16$ nm) which is require for atoms diffusion. The anisotropic character of diffusion was established for inter layers and surface iron atoms due to structural anisotropy of clay substrate and

structure of iron complexes itself. The surface dissusion of iron dimers takes place in limited area (L ≈ 0.25 nm) and has rotational character.

Key words: Mossbauer spectroscopy, diffusion, nanoclays

O.M. SHABANOV, R.T. KACHAEV, L.A. KAZIEVA, S.I. SULEIYMANOV

HIGH-VOLTAGE PHENOMENA IN MELTED AND SOLID ELECTROLYTES. 3. ACTIVATION OF SUPERIONIC CONDUCTORS AND THEIR MELTS

Experimental data on the dependence of the electrical conductivity of halide super ionic conducting electrolytes and of their melts on the electric field are presented, as well as the phenomenon of their activation by the action of microsecond pulses. An abnormally long relaxation of some electrolytes in non-equilibrium state with increased electrical conductivity was discovered.

Key words: super ionics and their melts, Veen's effect, activation, long relaxation

A.L. GABOV, A.A. KHRENOVA, N.A. MEDVEDEVA, N.E. SKRYABINA, D. FRUSHART, E.F. KUZNETSOVA

INFLUENCE OF METHODS AND CONDITIONS OF INTENSIVE PLASTIC DEFORMATION ON ELECTROCHEMICAL HYDROGENATION OF MAGNESIUM

The influence of different methods of plastic deformation (forging, isochannel angle pressing, rolling) on sorption of electrolytic hydrogen with magnesium was studied. The equivalent electric scheme of impedance was chosen for materials under study. The limiting step of hydrogen evolution reaction was shown to be the step of electrochemical desorption. The formation of non-equilibrium material structure promotes to the increase in its sorption capacity. Magnesium forging results in the structure inclined to high reversible parameters of sorption/desorption of hydrogen.

Key words: magnesium, intensive plastic deformation, hydrogen electrochemical sorption, hydrogen energetics

S.V. FILIMONOV, O.N. SHORNIKOVA, A.P. MALAKHO, V.V. AVDEEV

INFLUENCE OF PRODUCTION METHOD ON HEAT CONDUCTING PROPERTIES OF COMPACTED EXPANDED GRAPHITE

The graphite nitrate of the first step was obtained by anodic oxidation of natural graphite in the 90% solution of nitric acid. Structural, heat-conducting properties of compacted expanded graphite were studied. It was shown that both the plenty of structural defects and low critical density allow to obtain material with reduced thermal conductivity up to 0.4 W/(mK).

Key words: graphite anodic oxidation, compacted expanded graphite, critical density, heat conductivity, high temperature heat insulation

O.A. GOLUBCHIKOV, A.V. LARIONOV, V.E. MAIYZLISH, A.V. BALMASOV

PHTHALOCYANINE MODIFIERS OF NICKEL-PLATING ELECTROLYTE

Phthalocyanine tetrasulfoacid, its cobalt and nickel complexes as well as phthalocyanine disulfoacid inserted in standard sulfuric acid electrolyte for nickel-plating at content of 10 – 50 mg/l is decreased the roughness of electrodeposited coating. Ligand possess of brightener effect at that.

Key words: electrochemical nickel-plating, water soluble sulfophthalocyanines

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

INVESTIGATION OF INFLUENCE OF WATER PRESENT ON CHROMIUM PLATING PROCESS FROM IONIC LIQUID

The influence of water content was studied on the electrical conductivity of ionic liquid based on choline chloride and chromium chloride hexahydrate. The influence of water on the nature of the polarization dependency of chromium plating process was established. The properties of the chromium coatings obtained from the ionic liquid containing trivalent chromium were studied.

Key words: chromium-plating, polarization studies, conductivity, ionic liquid, viscosity

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

STUDY OF ANTICORROSIVE PROPERTIES OF CHROMIUM COATNGS DEPOSITED FROM IONIC LIQUID

The polarization study was carried out for anticorrosion properties of chromium coatings deposited from ionic liquid based on choline chloride and chromium chloride hexahydrate. The effect of electrodeposition conditions on the corrosion currents of steel with chrome plating was determined. The effect of the additional processing the chromium coatings on their anti-corrosive properties was established.

Key words: chromium-plating, corrosion protection, corrosion current, ionic liquid

M.M. SYCHYOV, O.A. CHEREMISINA

INTERCONNECTION OF ACID-BASE PROPERTIES OF FILLER SURFACE AND DIELECTRIC CONSTANT OF POLYMER COMPOSITES BASED ON IT

We have studied the relationship of acid-basic properties of the surface of ceramic materials with the processes of structure formation in their polymer composites with polar and non-polar polymer binders, as well as the electrical properties of the obtained dielectric films. Modified Lichtenecker equation was proposed to approximate concentration dependences of films dielectric constant.

Key words: surface properties, rheological properties, ferroelectric materials, dielectric constant, composit

P.B. RAZGOVOROV, R.S. NAGORNOV, M.P. RAZGOVOROVA

UTILIZATION OF BLUE CLAY FOR SEPARATION OF IMPURITIES FROM LINSEED OIL

The possibility of using blue clay of different composition to separate the impurity bioactive ingredients from linseed oil under standard conditions was shown. Natural sorbent composition, particularly the presence of kaolin, effects positively on the extraction of aliphatic acids, in particular, ω-3 from the oil-containing media.

Key words: blue clay, linseed oil, acid number, peroxide number, color number

M.B. BEGIEVA

POLYMERS AND COPOLYMERS ON BASIS OF N,N-DIALLYLAMINOETHANE ACID

The conditions of synthesis of new monomer - N, N-diallylaminoethane acid were discussed. By radical polymerization reaction a new polymer poly-N, N-diallylaminoethane acid was obtained. By the reaction of radical co-polymerization of N, N-diallylaminoethane acid and vinylacetate in the water environment and the water- organic environment (a mix of methanol- water in a ratio of 70:30 mol. %) polymers of statistical nature were obtained. It was established that vinylacetate possesses higher reactionary ability in comparison with N, N-diallilaminoethane acid. Kinetic regularities of reactions were investigated and the copolymer structure was established.

Key words: radical polymerization, polymer, monomer, monomer- N,N-diallylaminoethane acid, poly-N,N- diallylaminoethane acid, copolymer, copolymerization, kinetics

A.P. ALESHINA, I.A. BALAGUROV, V.E. MIZONOV, V.A. OGURTZOV

NON-LINEAR CELL MODEL OF VIBRATION SCREENING KINETICS

A non-linear cell mathematical model of the kinetics of fine fraction extraction into the sub-grid product of a vibration screen was proposed. The model takes into account the dependence of the rate of fine fraction migration to the screen surface on its content in a material layer of material located lower. Results of numerical experiments showed that it is important to take into account this non-linearity.

Key words: vibration screen, segregation, Markov chain, extraction degree

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

MODELLING ACRYLAMIDE POLYMERIZATION IN CONCENTRATED WATER SOLUTIONS

The mathematical model of acrylamide polymerization in concentrated water solutions taking into account the change in an initiation efficiency and chain termination rate with the growth in viscosity of the polymerization system is presented. The model predicts the degree of monomer conversion and molecular weight of synthesized polyacrylamide.

Key words: mathematical model, polymerization, solution, acrylamide, polyacrylamide

I.D. LUCHEYKO

MATHEMATICAL MODELING SYSTEM "MIXING FLOW REACTOR + REACTION $A_1 \leftrightarrow \alpha A_2$" AT CONDITIONS OF CATALYST DEACTIVATION

The problem of the description of a non-stationary operating mode of a perfect-mixing flow reactor caused by deactivation of the solid catalyst with a simple reversible reaction is analytically solved. It was established that the relative deviation ε_η of the product yield from nominal value is defined by an algebraic difference between a simplex of rates of the catalyst deactivation and a simplex of nominal reaction rates. The existence of effect of self-regulation ($\varepsilon_\eta = 0$) of stationary mode was proved. In the case of first order reaction the nomogram for determination of rational exploitation time of the industrial catalyst on maximum-admissible value $\left|\varepsilon_\eta\right|^{adm}_{max} \ll 1$ is given.

Key words: perfect-mixing flow reactor, simple reversible reaction, solid catalyst deactivation, catalyst lifetime, mathematical modeling

A.I. BALUNOV, V.P. MAIYKOV

EXTENDED PRINCIPLE OF MAXIMAL ENTROPHY FOR DESCRIPTION OF PROCESS OF PHASE TRANSFORMATIONS IN ATHERMAL SYSTEM

The paper presents the extended principle of maximum entropy that uses entropy of a complex experiment as the plausibility criterion. The extended version was used to describe the non-equilibrium processes of the phase transitions during the evolution of the athermal system toward the thermodynamic equilibrium. It is shown, that taking into account the athermal mixture properties in general formulation and solving of the problem leads to relations in which there are the activity coefficients in typical for thermodynamics form. The relations for ideal systems can be reproduced as a special case of the method. An example of calculation that illustrates the technique of the consideration of the athermal mixture properties is shown.

Key words: athermal system, phase transformations, maximal entrophy principal, complex experiment entrophy, conditional probability, entrophy activity coefficient

A.A. VOLINA, K.S. KRAVCHUK, A.A. RUSAKOV, A.S. USEINOV

USING EXTREMELY SHARP PYRAMID INDENTERS FOR STUDY OF MECHANICAL PROPERTIES AND SURFACE TOPOGRAPHY

Three pyramidal indenters with different apex angles were tested for suitability of their use to obtain the surface topography by scanning probe microscopy and measurement of hardness by indentation. Sharp indenters enable obtaining images of the surface topography comparable with atomic force microscopy and allow measuring the mechanical properties of thin coatings more correctly with less influence of the substrate.

Key words: indentation, indenter, diamond-like coating, scaning probe microscopy, durometer

A.S. ANTONOVA, T.N. KROPACHEVA, V.I. KORNEV

COMPLEXONS AS REAGENTS FOR REMEDIATION OF NICKEL-CONTAMINATED SEDIMENTS

The use of various complexones for extraction of nickel from contaminated sediments containing Fe (III) hydroxides was shown. The influence of some complexones on Ni (II) cations sorption by goethite (α-FeOOH) in a wide pH range was studied. For the reducing Ni (II) mobility (immobilization)) the use of EDTMP and NTMP is efficient (pH = 3-5). Conversely, for Ni(II) remobilization the best chelating agent is EDTA (pH = 2-10). Goethite demetallization under the action of complexones was studied. The desorbing effect of complexones on Ni(II) is reduced in the order: EDTA >> NTA > IDA > NTMP ≈ EDTMP > Glycine.

Key words: sediments remediation, heavy metals, sorption, goethite, complexones

Kh.A. PAVLOVA, A.A. ZUEV, M.E. SOLOVIEV

QUANTUM CHEMICAL MODELING INITIATION REACTIONS OF CHLOROPRENE RUBBER OXIDATION

The quantum-chemical method DFT B3LYP/6-31G** was used for calculation of enthalpies of hydrogen and chlorine abstraction from chain units of polychloroprene in various configurations, as well as reactions of oxygen addition and the formation of hydroperoxides. A significant role in a thermal oxidation of chloroprene rubber was shown to play the mechanism associated with elimination of chlorine from chloroprene units in 1,2 configuration.

Key words: chloroprene rubber, quantum-chemical calculations, thermal oxidation

S.G., ALEKSEEV A.V. PISHCHALNIKOV, N.M. BARBIN

DEPENDENCE OF FLASH TEMPERATURE ON STORAGE CONDITIONS OF WATER–ETHANOL SOLUTIONS

The influence of storage temperature conditions was studied on the flash temperature of water–ethanol solutions.The flash temperature of the ethanol-water system was shown to be sensitive to this action. This effect is caused by the presence of hydrated clusters of ethanol in a vapor phase.

Key words: ethanol, solution, flash point, fire hazard

V.G. SOLOMONIK, A.N. SMIRNOV, I.S. NAVARKIN

MOLECULAR STRUCTURE, VIBRATIONAL SPECTRA, AND ATOMIZATION ENTHALPY OF ZINC, CADMIUM, AND MERCURY DIFLUORIDES

The geometries, vibrational frequencies, and atomization enthalpies of MF_2 molecules (M = Zn, Cd, Hg) have been calculated at the complete basis set coupled cluster CCSD(T) level of theory. The results are in excellent agreement with the available experimental data.

Key words: molecular properties, zinc difluoride, cadmium difluoride, mercury difluoride, coupled cluster CCSD(T) method, complete basis set limit, second-order spin-orbital coupling effect