ИЗВЕСТИЯ ВЫСШИХ УЧЕБНЫХ ЗАВЕДЕНИЙ

Т 57 (9) ХИМИЯ И ХИМИЧЕСКАЯ ТЕХНОЛОГИЯ 2014

C O N T E N T S

C H E M I S T R Y
(inorganic, organic, analytical, physical, colloid and high-molecular compounds)

C H E M I C A L T E C H N O L O G Y
(inorganic and organic substances. Theoretical fundamentals)

A B S T R A C T S

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

STRUCTURE AND ELECTRON ENERGY CHARACTERISTICS OF METHANE HYDRATES BY QUANTUM CHEMICAL CALCULATIONS

Methane hydrates are highly present in sea-floors and in other planets and their moons. Hence, these compounds are of great interest for environment, global climate change, energy resources, and Cosmo chemistry. The knowledge of stability and physical–chemical properties of methane hydrate crystal structure is important for evaluating some new green becoming technologies such as, strategies to produce natural gas from marine methane hydrates and simultaneously store CO_2 as hydrates. However, some aspects related with their stability, spectroscopic and other chemical-physical properties of both hydrates are not well understood yet. This paper analyzes the changes in the energy of hydration shells formation in H_2O [5^{12}] and H_2O [$6^2 5^{12}$] structures and hydrogen bonding energy dependence on the shells size changes and other similar characteristics of the methane clathrates. Energy dependence on their size of the H_2O [5^{12}], $CH_4 \cdot H_2O$ [5^{12}] and, for the first time, of H_2O [$6^2 5^{12}$], and $CH_4 \cdot H_2O$ [$6^2 5^{12}$]] were analyzed by ab initio quantum chemical calculations. The optimal geometric parameters of the clusters were determined.

Key words: methane hydrates, clathrates structure, hydration shells formation, quantum chemistry

A.I. LYTKIN, N.V. CHERNYAVSKAYA, A.S. CHERNOV, V.E. LITVINENKO

THERMODYNAMIC CHARACTERISTICS OF COMPLEXATION OF Gd^{3+} WITH ETHYLENEDIAMINE-N,N/-DISUCCINIC ACID IN AQUEOUS SOLUTIONS AT 298.15K

The enthalpies of complexation of ethylenediamine - N, N /-disuccinic acid (H_4Y) with Gd^{3+} ion were determined by calorimetric method at 298.15 K and ionic strength of 0.5; 1.0; 1.5 (KNO_3). Thermodynamic characteristics of complex formation of GdY and GdHY were calculated at fixed and zero ionic strength. The obtained results were interpreted.

Key words: complexation, thermodynamic parameters, calorimetry

I.A. DMITRIEV, G.A. PRIGORELOV, A.A. BARANETS

STUDY OF BIOLOGICAL ACTIVITY OF NEW TETRAPHENYLPORPHYRINE FLUORALKYLIC DERIVATES

The synthesis of new compounds belonging to a class of fluorinated tetraphenylporphyrine derivatives are realized and explored some indicators of their biological activity. It was found that chemical compounds are substances with low toxicity. Also, the article presents the results of study of the cytotoxic action of new substances on the various types of peripheral blood cells (erythrocytes and leucocytes) of mice. These compounds were shown to have a high affinity to the outer plasmatic membranes of red blood cells causing osmotic shift which can lead to the destruction of these cells. Probably the same mechanism lays at the basis of the white blood cells injury as a result in an action of toxic doses of fluorinated tetraphenylorphyrine derivatives.

Key words: fluorinated tetraphenylporphyrine, biological activity, cell membranes

A.V. KOLESNIKOV, P.A. NIKOLAIYCHUK

INVESTIGATION OF REACTION OF GRAPHITE GASIFICATION IN PRESENCE OF ACTIVATION DOPANTS

The results of calculation of kinetic constants of graphite gasification reaction counting heat- and mass-transfer processes at temperatures of 900-1200^{o}C are presented. The calculation was performed for the reaction in presence of magnesium, calcium and strontium oxides, strontium carbonate, metallic iron as well as iron di- and tri-oxide. The graphs of linear dependencies of pre-exponential factors on activation energy for the dopants of compounds of calcium, strontium and iron were plotted. Isokinetic temperature for C+CO_2 reaction in the

presence of strontium compounds was calculated, which equals to 1204±60°C. The mechanism of activating influence of dopants was considered.

Key words: graphite gasification, pre-exponential factor, activation energy, compensation effect, isokinetic temperature, activating additions, kinetic constants, active sites

R.N. YASTREBINSKIY, O.V. KUPRIEVA, N.I. CHERKASHINA

STRUCTURAL-PHASE CHARACTERICTIC OF BOROSILICATE COVERAGE

The work presents the results of a study of the structural-phase characteristic of individual borate and combined coating on the basis of borosilicate oligomer heat-treated at temperature interval of 150-500 °C. To establish the phase composition, structure and morphology of coverings on the basis of boric acid and oligomeric sodium borosilicate, the spectra of x-ray fluorescence analysis, IR spectroscopy and electron micrographs of coatings were studied. The analysis of the infrared spectrum of borosilicate cover indicates a well-formed crystal structure of matter and the presence of amorphous silicate matrix.

Key words: silicates, borosilicate, heat treatment, X-ray phase analysis, IR-spectra

Yu.A. RODICHEVA, N.V. BELOV, V.A. BURMISTROV, T.G. SHIKOVA

ACTION OF LOW-TEMPERATURE PLASMA ON CATALYTIC ACTIVITY OF MODIFIED POLYMER FIBERS

Polyimide and polypropylene fibers modified with cobalt phthalocyanines were obtained by electro flow turning method from a solution and melt. The treatment of polymer fibers was carried out with low-temperature plasma in air and argon.

Key words: polypropylene and polyamide fibers, electro flow turning, plasma, catalytic activity, specific capacity

D.V. OVSYANNIKOVA, O.Yu. SOLOVYEVA, M.E. SOLOVYEV, A.O. KARANETS

QUANTUM-CHEMICAL EVALUATION OF REACTIONS THERMODYNAMICS OF OXIDATION PRODUCTS OF POLY ISOPRENE WITH SILICA-ACID FILLER

Silicon-acid fillers condition a number of behavior peculiarities of rubber mixtures in a course of curing, specifically the viscosity increasing in an induction period. The aim of this paper is comparative evaluation the thermodynamic probability of different chemical reactions proceding in a system of oxidized rubber-silicon-acid filler using quantum-chemical calculations. The most probable reaction was shown to be the interaction between silicon fragment and modeled molecule of isoprene unit containing carboxylic groups.

Key words: 1,4-cis-isoprene, silica-acid filler, quantum-chemical modeling of the reactions, oxygen-containing groups, thermodynamic parameters

V.A. STRIGINA, I.S. YAKOVLEV, V.Yu. DOLUDA, M.G. SULMAN, E.M. SULMAN

FURFURAL CATALYTIC HYDROGENATION

Furfural hydrogenation reaction was studied in the H_2 environment on Pd-containing catalysts deposited on various carbon carriers at H_2 pressure of 60 atm and in a temperature range from 343 to 473 K. The main products were found to be furfuryl and tetrahydrofurfuryl alcohols. The maximum conversion was obtained on 5% Pd/active carbon catalyst at 453 K and 60 atm and it was 15.72% under selectivity of 87%.

Key words: furfural, hydrogenation, catalyst, biomass

S.M. ROMANOVA, L.A. FATYKHOVA

REACTIVITY OF FUNCTIONAL GROUPS OF ESTERS OF CELLULOSE NITRATE

The interaction of cellulose nitrate with chloranhydride of acetic acid was studied. As a result of physicochemical studies the most probable path ways of the reactions were established.

Key words: cellulose nitrite, chloranhydride, nitrate groups substitution, chemical modification

M.A. YUROVSKAYA, N.P. GERASIMOVA, E.M. ALOV, A.S. DANILOVA, S.V. KRASNIKOV, N.V. KAMKINA

CHLOROSULFONYLATION OF 4-ISOPROPENYL- AND 4-(1-CYCLOHEXENYL)-BENZOIC ACIDS

The reaction of 4-isopropenyl- and 4-(1-cyclohexenyl)-benzoic acids with sulfonyl chlorides was investigated. It was found that the sulfonyl chloride addition to these alkenes is accompanied by simultaneous dehydrochlorination of adducts and unsaturated sulfones of allylic structure are formed.

Key words: chlorosulfonylation, unsaturated sulfones, alkenylbenzoic acids

A.E. KISELEV, L.S. KUDIN, A.P. ILYIN

STUDY OF IRON OXIDE CATALYST $K_2O \cdot nFe_2O_3$. III. HIGH TEMPERATURE REDUCTION OF CATALYST

The experimental results of reduction of $K_2OnFe_2O_3$ catalysts synthesized by mechanochemical activation (MCA) are presented on data of study of the evaporation of K_2O promoter in a field of heterogeneous reduction of Fe_2O_3. The effect of vapor composition change in course of solid phase reduction at vacuum annealing was revealed. The calculation method of K_2O and K partial vapor pressures during the reduction period of Fe_2O3 up to Fe_3O_4 was developed and tested. For the first time changing in the vapor composition was used to assess the degree of catalyst reduction.

Key words: high temperature reduction, vacuum annealing, vapor phase composition, alkali promoter, mass spectrometry, mechanochemistry

A.G. TITOVA, M.A. KRESTYANINOV, A.M. ZAICHIKOV

THERMODYNAMIC AND STRUCTURAL CHARACTERISTICS OF SELF-ASSOCIATED AMINOALCOHOLS

Thermodynamic characteristics of aminoalcohols self-associated by hydrogen bonds were calculated. Specific and nonspecific components of the total energy of intermolecular interactions were determined. It was established that the most part of the studied aminoalcohols belongs to solvents with H-bonds networks in which there is an intensifying of nonspecific interactions with the temperature rise, and to solvents with chained self-association where the contribution of these interactions practically don't depend on temperature. The aminoalcohols obtained by the substitution of nitrogen atom protons of monoethanolamine by alkyl radicals belong to group of solvents similar aprotic ones at which nonspecific interactions are weakened with the temperature rise.

Key words: amino alcohol, internal pressure, intermolecular interaction, thermodynamic and structural characteristics

A.A. VORONINA, A.S. VASHURIN, N.A. LITOVA, M.V. SHEPELEV, S.G. PUKHOVSKAYA

ASSOCIATION OF SULFODERIVATIVES OF Co(II) AND Cu(II) PHTHALOCYANINE IN PRESENCE OF CREATININE

The associative state of Cu(II) and Co(II) complexes with tetrasulfo-substituted phthalocyanine in water solution was considered in the paper. An addition of creatinine to Co(II) tetrasulfo-substituted phthalocyanine solution results in a formation of sandwich-type dimer due to coordination of creatinine by two macrocyclic molecules. Monoligand molecular complexes only are formed in reactions of Cu(II) complexes with tetrasulfo-substituted phthalocyanine.

Key words: phthalocyanine, water solution, self- association, molecular complex, creatinine

V.F. SMIRNOV, E.P. KOMOVA, E.V. SKOROBOGATOVA, A.P. ARBATSKY

COORDINATION INTERACTIONS OF SYSTEM GLYCOSAMINE HYDROCHLORIDE – GLYCOSAMINE WITH d-METAL IONS

Coordination interactions of ions Co^{2+}, Ni^{2+}, Zn^{2+}, Cd^{2+}, Cu^{2+} in system "glycosamine - glycosamine hydrochloride - water" at pH 7.8 were studied with electronic and IR-spectroscopy, pH-metric and conductometric methods. Glycosamine complexes (27% for studied system) received in situ at interaction with sodium hydroxide, and ions of abovementioned metals have composition from 1:1 to 1:4, thus amino groups, oxygen atoms of hydroxyl groups and carbohydrate skeleton participate in a coordination. The composition of complexes depends on a type of ion, the salts maintaining constancy of ionic force ($NaClO_4$, NaCl), pH solution and a ratio of initial concentration of reagents. Unlike it, complexes of glycosamine hydrochloride are formed only with Cu^{2+} and Zn^{2+} ions.

Key words: coordination complexes, d-metal ions, glycosamine hydrochloride, glycosamine

N.S. BORISOVA, G.G. KUTLUGILDINA, Yu.S. ZIMIN, A.R. GIMADIEVA, A.G. MUSTAFIN

OXIDIZING DESTRUCTION OF ARABINOGALACTAN AND ITS COMPLEX FORMATION WITH URACILS

On the basis of studying the kinetics of oxidizing destruction of arabinogalactan the conditions for obtaining polysaccharide's oxidized fractions with an average molecular weight of 25 kDa were choosen. The complex formation of obtained fraction of arabinogalactan with uracil and its derivatives was studied. The composition of complexes was estabiliched and their stability constants were determined. As the example, for

complex of arabinogalactan and 6-methyluracil the temperature dependence of stability constants was studied and thermodynamic parameters of complex formation were determined.

Key words: arabinogalactan, oxidative destruction, arabinogalactan oxidated fraction, complexation, uracil and its derivatives, stability constants, thermodynamic parameters

A.E. ZAVADSKIY, S.Yu. VAVILOVA, N.P. PROROKOVA

X-RAY ANALYSIS OF CRYSTALLITES BIMODAL STRUCTURE OF POLYPROPYLENE THREADS

The method of x-ray analysis of the content of crystallites with the c- and a*-axis orientation in polypropylene complex threads (PCT) was developed. It was established, that increasing the apparent jet spinning of threads from 1400 to 16300% substantially decreases the ability to form a*-oriented lamellaes in which molecular chains are directed across an axis of threads.

Key words: polypropylene, complex threads, x-ray analysis, texture, crystallites, bimodal structure

E.A. POLYAKOVA, I.S. KOROTNEVA, B.S. TUROV, K.A. MYAGKOVA

SELECTING POLYMER BINDER FOR CREATION OF BIODEGRADABLE POLYMER COMPOSITION

The choice of polymer binder based on aqueous dispersions of carboxyl-containing butadiene-methylmethacrylate copolymers to create bioavailable composition, ensuring the best quality of material for decorative molding, was arried out.

Key words: polymer composition, copolymer composition, plasticizer, tensile strength

S. USMANOV, U.M. TOIYPASOVA, G.T. OMAROVA, E.B. KOZYBAKOVA, Sh.H. BAIYBASHCHAEVA, Z.S. ASHIMKHANOVA

RESEARCH OF TECHNOLOGY OF OBTAINING NEW FORMS OF BIOFERTILIZERS CONTAINING PHOSPHORUS

In given article the principal technological scheme was proposed for receiving fertilizer containing phosphorus on the basis of a phosphorite flour of phosphorites of Karatau, the biopreparation №1 and phosphormobilizing bacteria. Researches were done to determine: durabilities of granules; hygroscopicities and commodity properties of biofertilizers; life function of the phosphormobilizing microorganisms at storage.

Key words: technology, phosphorite flour, ammonium nitrate, phosphormobilizing bacteria, fertilizer marketability

E.P GRISHINA, A.M. PIMENOVA, E.V. BORZOVA, N.O. KYDRYAKOVA, L.M. RAMENSKAYA

CORROSION RESISTANCE OF HIGH-CAPACITY ALUMINIUM FOIL IN IMIDAZOLIUM IONIC LIQUIDS

The specific capacity dynamics of condenser foil from aluminum being in a long time contact with corrosive ionic liquid medium of 1-N-butyl-3-methylimidazolium Br-, Cl-, BF_4^-, PF_6^-, $[(CF_3SO_2)_2N]^-$, $[CF_3SO_3]^-$ and $[CF_3COO]^-$ was studied by means of impedance technique at ambient temperature and 85°C. The correlation between specific capacity C_s and interelectrode space electroconductivity G_{el} was determined. On a base of optical microscopy method it was found that in the absence of microscopic corrosion destruction the linear dependence Cs versus G_{el} was observed. In the presence of corrosion proceeding on the foil face, there was the deviation from linearity on Cs - G_{el} plot.

Key words: aluminum foil, specific capacity, corrosion, ionic liquid

A.L. SMIRNOV, S.Yu. SKRIPCHENKO, V.N. RYCHKOV, M.G. SHTUTSA, S.Yu. SYRTSOV, A.I. POLYANSKIY, A.M. PASTUKHOV

PROCESSING OF SPILLAGE SOLUTIONS OF URANIUM TETRAFLUORIDE PRODUCTION

The processes of mutual neutralization of acid and carbonate spillage solutions of uranium tetrafluoride production were investigated. The effect of temperature, air blowing, mutual neutralization pH and alkaline neutralization pH, presence fluoride ions in solution on the degree of uranium precipitation and sodium hydroxide consumption is shown.

Key words: spillage solutions, extraction raffinates, carbonate uranium-containing solutions, chloride-fluoride uranium-containing solutions, neutralization, uranium tetrafluoride

O.V. NEYELOVA

SILICONE-ORGANIC COMPOSITION FOR PROTECTION OF DEVICES OF ELECTRONIC TECHNICS WITH IMPROVED ADHESIVE PROPERTIES AND THERMO- AND FROST RESISTANCE OF COVERINGS

The receipt of silicone-organic composition of low temperature curing with the high adhesion of polymeric covering to various constructional materials both under normal climatic conditions and at the conditions of influence of hard climatic factors was developed. The covering is efficient in the range of temperatures from -70 to +250^{0}C, possesses high dielectric characteristics (including the micro wave range), lack of corrosion action in relation to aluminium and to copper, high moisture resistance properties, combines high elasticity with durability. The composition is applied to protection of active elements and boards of micro-wave devices of electronic technics.

Key words: silicone dielectric polymeric materials, adhesion, thermo-and frost resistance, protection of devices of electronic technics

V.M. SEDELKIN, L.N. POTEKHINA, E.V. OLEIYNIKOVA

RHEOLOGICAL PROPERTIES OF POLYMER SOLUTIONS WITH SOLID FILLERS BASED ON WASTE OF PLANT CULTIVATION FOR MANUFACTURING NANOSTRUCTURATED FILTRATION MEMBRANES

Results of research are given for rheological properties of polymeric solutions with solid fillers from thermo treated waste of millet thrashing. The influence of fillers on the solutions viscosity was shown. The universal dependence for calculation of effective viscosity of the filled solutions was obtained.

Key words: cellulose diacetate, polymeric solution, solid filler, millet thrashing waste, nano structurated membranes

N.A. LEZHNINA, A.O. KARANETS, M.E. SOLOVIEV

NUMERICAL MODELING OF RUBBER PLATE DYNAMICS UNDER IMPACT LOADING

Technical rubber plates are used in many industries. Many products made from rubber plates operate in a dynamic mode, specifically, they are undergone to pressure pulses. Therefore, it is important to study the influence of parameters of nonlinear elastic and viscoelastic properties of the plate material on the nature of its dynamic behavior under load. The numerical calculation was carried out by finite element method. It was found that the nonlinear viscoelastic properties of the material parameters significantly affect both on deformation distributions and on the dependence of the fraction of dissipated energy on a time. Numerical calculation allows varying these parameters to formulate technical requirements for materials depending on the nature of pulse loading.

Key words: computer modeling, rubber plate, viscosity-elactic properties

P.A. ZERNOV, D.Yu. MURZIN, O.I. PARPUTS, N.V. KUZICHKIN

PROCESS MODELING OF ISOBUTANE ALKYLATION WITH BUTYLENES IN CATALYTIC DISTILLATION UNIT

An energy-efficient scheme of alkylation process using catalytic distillation was proposed. Simulation of scheme using flow reactors and single separation unit of alkylate, and scheme with using catalytic distillation was carried out by Aspen HYSYS software. Based on the simulation results a comparison of two schemes of process carring out was conducted

Key words: alkylation, isobutane, olefins, high-octane components, solid phase catalyst, modeling, reaction-rectification technology

A.B. KAPRANOVA, M.N. BAKIN, A.E. LEBEDEV, A.I. ZAIYTSEV

EVALUATION OF FACTOR HETEROGENEITY OF GRAINY MIXTURE IN VOLUME OF DRUM-TAPE DEVICE

On the basis of the stochastic approach the method of estimation the heterogeneity coefficient of the granular mixture in a working volume of the drum-tape device was proposed using simulated differential distribution functions of the components on the angle of their atomization after the collapse of the flexible elements from the rotary drum.

Key words: bulk material, mixing, drum-tape device, grainy mixture quality, differential distribution function, atomization angle