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A B S T R A C T S

L.B. KOCHETOVA, M.V. KLYUEV
REDUCTIVE ACYLATION OF NITROARENES

The literature data on effect of conditions of nitro compounds reductive acylation on the yield of target products and kinetic investigations of the reductive acylation on palladium catalysts were considered. Results of quantum chemical simulation of reaction mechanism of reaction of lidokaine synthesis and solvation of molecules participating in reaction were discussed.

Key words: reductive acylation, nitro compounds, catalysis

N.I. GIRICHEVA, A.A. ISHCHEENKO, V.I. YUSUPOV, V.N. BAGRATASHVILI, G.V. GIRICHEV
ELECTRONIC STRUCTURE OF METHANE HYDRATES

Based on the NBO-analysis of electron density distribution (LC-wPBE/6-311 + G (d, p)), the specificity of the geometric and electronic structure of $\text{CH}_4 \cdot \text{H}_2\text{O}$ [5^{12}] and $\text{CH}_4 \cdot \text{H}_2\text{O}$ [6^25^{12}] clathrates, as well as their hydration shells, H_2O [5^{12}] and H_2O [6^25^{12}] was shown. The energies of the intermolecular hydrogen bonds in the four types of clusters that are ~ 6.5 kcal / mol, and are practically independent on the size and shape of the hydration shells, and the presence or absence of the guest molecule, CH_4 in a cluster were evaluated. In $\text{CH}_4 \cdot \text{H}_2\text{O}$ [5^{12}] clathrate succeeded in isolating the weak interaction between the donor orbital of one atom of oxygen LP (O) of the hydration shell and acceptor antibonding orbital σ^* (C-H) of the CH_4 guest molecule. The analysis of the composition and energy of the frontier orbitals of clusters, which allows estimating the ionization energy and comparing their redox properties was accomplished. The analysis of the "host-guest" interaction suggests that changes in the properties of gas hydrates at different depths of the bottom of their occurrence, are mostly determined by changes in the geometric dimensions of $\text{CH}_4 \cdot \text{H}_2\text{O}$ [5^{12}] than $\text{CH}_4 \cdot \text{H}_2\text{O}$ [6^25^{12}] fragments.

Key words: clathrates, methane hydrates, electronic structure, hydrogen bonding, donor-acceptor interaction, quantum-chemical calculations, NBO-analysis

E.A. DANILOVA, Yu.V. BUTINA, T.V. KUDAYAROVA, M.K. ISLYAIKIN
SYNTHESIS OF MACROHETEROCYCLIC COMPOUND BASED ON DIAMINE P

Macroheterocyclic compound consisting of 8 small cycles were synthesized by the interaction of the dimer or trimeric products derived from diamine P and phthalonitrile. The compounds were characterized by mass-spectrometry, ^1H NMR, UV-vis, IR spectroscopy and elemental analysis.

Key words: diamine P, macroheterocyclic compounds, synthesis, properties

A.N. VINOGRADOV, V.O. KOZMINYKH, E.N. KOZMINYKH
SYNTHESIS AND TAUTOMERIC TRANSFORMATION OF 2-[(AMINOCARBONYL)-HYDRAZONO]-5,5-DIMETHYL-4-OXOHEXOATES

The «one pot» three-components condensation of pinacolone with dialkyl oxalates and hydrochloric hydrazinecarboxamide, which leads to 2-[(aminocarbonyl)hydrazono]-5,5-dimethyl-4-oxohexanoates was studied. The ring-chain tautomerism of synthesized compounds is discussed on the basis of IR and NMR ^1H spectroscopy.

Key words: ring-chain tautomerism, 2-[(aminocarbonyl)hydrazono]-5,5-dimethyl-4-oxohexanoates, pinacolone, hydrochloric hydrazinecarboxamide

R.N. SHAKHMAEV, A.U. KASHIPOVA, N.V. EMYSHAeva, A.V. YUDINA, V.V. ZORIN
SYNTHESIS OF 2-METHYLENE ALLOBETULONE

The synthesis of 2-methylene allobetulone was carried out by condensation of allobetulone with paraformaldehyde. The starting allobetulone was obtained by isomerization of betulin in the presence of Amberlyst 15 and subsequent oxidation of allobetulin by sodium hypochlorite.

Key words: betulin, allobetulin, allobetulone, 2-methylene allobetulone, triterpenoids

Yu.E. ROMANENKO, A.A. MERKIN, O.V. LEFEDOVA
**MODELING AZOXYBENZENE HYDROGENATION IN AQUEOUS 2-PROPANOL MEDIA
ON RANEY NICKEL**

Hydrogenation of azoxybenzene as a nitrobenzene liquid-phase reduction intermediate was modeled. Process constants were computed and compared with the complex modeling results.

Key words: Raney nickel, 2-propanol, sodium hydroxide, acetic acid, kinetic modeling

L.A. KOCHERGINA, V.G. BADELIN, O.N. KRUTOVA, V.V. CHERNIKOV, K.V. DAMRINA
**STANDARD ENTHALPIES OF FORMATION OF DL- α -ALANYL - DL-NORLEUCIN
AND HIS DISSOCIATION PRODUCTS IN AQUEOUS SOLUTION**

The heat effects of dissolutions of crystalline DL- α -alanyl - DL-norleucin in aqueous solutions of potassium hydroxide at 298.15K were determined by direct calorimetry. The standard enthalpies of formation of DL- α -alanyl - DL-norleucin and its products dissociation in aqueous solution were calculated.

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

M.A. SAVENKOVA, N.P. VASSEL, I.V. MARDIROSOVA, A.I. KOROLYOVA, S.A. VOLYANIK
STATE DIAGRAM OF Mg(PO₃)₂-Pb(PO₃)₂ SYSTEM

The interaction in Mg(PO₃)₂ - Pb(PO₃)₂ system was studied both on the interface and in a solid phase with the methods of physical-chemical analysis. The formation of compound of 1:1 composition was revealed. The type of anion of double phosphate of MgPb(PO₃)₄ was identified. Some physical-chemical properties of new phase in crystal and glassy states were established.

Key words: system state diagram, metaphosphates, anion ring structure, crystals, glass

S.A. BYCHKOVA, N.B. CHERNYAVSKAYA, M.S. KORNILOVA
COMPLEX FORMATION OF L-ASPARTIC ACID Hg(II) IN AQUEOUS SOLUTION

By the method of potentiometric titration the complex formation of L-aspartic acid and Hg²⁺ ions was studied in a wide range of concentration ratios at t = 298 K and I=0.1 моль/л (KNO₃).

Key words: L-aspartic acid, stability constant

I.M. BORISOV, Z.Sh. GAZIZOVA, G.R. SHAYAKHMETOVA, I.S. FAIYZRAKHMANOV
**KINETICS OF PEROXIDE OXIDATION OF OIL SULFIDES IN PRESENCE OF MOLYBDENUM
AND TUNGSTEN ACIDS**

Kinetics of reaction of peroxide oxidation of oil sulfides to sulfoxides in the presence of catalytic system "molybdenum acid+tungsten acid" was studied. The reactions scheme was proposed.

Key words: oil sulfides, oxidation, hydrogen peroxide, molybdenum acid, tungsten acid, kinetics

I.S. KOVAL, A.V. VOLKOV, T.V. KUDAYAROVA
**STANDARD ENTHALPIES OF COMBUSTION AND FORMATION OF 2,5-DIMERCAPTO-1,3,4-
THIADIAZOLE AND 2,5-DIAMINO-1,3,4-THIADIAZOLE IN CRYSTALLINE STATE**

Energies of combustion of 2,5-dimercapto-1,3,4-thiadiazole and 2,5-diamino-1,3,4-thiadiazole were determined using oxygen bomb calorimetric method. The standard enthalpies of combustion and formation were calculated for 2,5-dimercapto-1,3,4-thiadiazole: $\Delta_c H^\circ = -1930.1 \pm 3.3$ kJ/mole, $\Delta_f H^\circ = 32.6 \pm 3.3$ kJ/mole and for 2,5-diamino-1,3,4-thiadiazole: $\Delta_c H^\circ = -1956.5 \pm 3.6$ kJ/mole, $\Delta_f H^\circ = 301.2 \pm 3.6$ kJ/mole, respectively. The values are given for the studied substances in a crystalline state at the temperature of 298.15 K.

Key words: thiadiazoles, burning calorimetry, standard burning enthalpy, standard formation enthalpy

O.M. SHABANOV, S.M. GADHZIEV, A.O. MAGOMEDOVA
**HIGH-VOLTAGE PHENOMENA IN MOLTEN AND SOLID ELECTROLYTES.
1. VIEN EFFECT IN MOLTEN SALTS**

The electrical conductivities of molten electrolytes are increased with the increasing the electrical field strength and reach the limiting values. The limiting high-voltage electrical conductivities of molten salts obey the Nernst-Einstein and Stocks-Einstein relations, and additivity rule.

Key words: conductivity, melt, electrolyte

O.M. SHABANOV, S.I. SULEIYMANOV, L.A. KAZIEVA, A.O. MAGOMEDOVA
**HIGH-VOLTAGE PHENOMENA IN MOLTEN AND SOLID ELECTROLYTES.
2. ACTIVATION OF CHLORIDE MELTS**

Under the influence of high voltage micro second pulses the molten electrolytes pass into a non-equilibrium state with the intensification of the electrochemical properties and elimination of light scattering peaks. The pro-

longed relaxation of non-equilibrium melts with the reduction of their characteristic electrochemical properties and Raman spectra is observed.

Key words: molten electrolytes, high-voltage pulses, activation, relaxation

V.V. OPENKO, D.Zh. N. KONSHINA, Z.A. TEMERDASHEV, V.V. KONSHIN
SORPTION STUDY OF Co(II), Cd(II), Ni(II), Cu(II) AND Zn(II) ON SILICA GEL WITH CHEMICALLY IMMOBILIZED 1-(2-PYRIDYLAZO)-2-NAPHTHOL

The sorption material based on silica gel with a covalently immobilized 1-(2-pyridylazo)-2-naphthol was obtained. Dependences of the equilibrium sorption capacity on the equilibrium concentration of Cu(II), Zn(II), Cd(II), Co(II), Ni(II) in a solution were determined. The values of maximum sorption capacity of mono molecular layer and the equilibrium constant for all metals were calculated. The possibility of using the obtained sorbent for the concentration of zinc (II) from solutions followed by X-ray fluorescence determination in the concentrate was estimated.

Key words: silica gel, 1-(2-pyridylazo)-2-naphthol, sorption, concentration, X-ray fluorescence determination

T.S. KORNIENKO, L.P. BONDAREVA, E.A. ZAGORULKO, A.A. GAPEEV, N.N. GAIYVORONSKAYA
DIFFUSION COEFFICIENTS DETERMINATION OF METAL IONS AND AMINO ACIDS IN PHASE OF MACRO POROUS COMPLEXING ION EXCHANGER

The method for determining the effective diffusion coefficients (Dsol) of organic and inorganic ions in the grains of macroporous ion exchange sorbents based on the analysis of the process kinetics and the use of a one-dimensional model of capillary flow was proposed. The values of the diffusion coefficients of copper (II), nickel (II), glycine and alanine ions in protonated and deprotonated forms of aminophosphonic exchanger Purolite S950 were obtained. It was found that Dsol of copper ions (II) in the deprotonated form of the ion exchanger is much higher than in the protonated, some difference of Dsol of bipolar ions of amino acids is explained with the influence of their size.

Key words: diffusion coefficient, ion exchange, one-dimensional model of capillary flow

A.A. ILYIN, A.B. ZHUKOV, R.N. RUMYANTSEV, I.V. BABICHEV
SYNTHESIS AND RHEOLOGICAL PROPERTIES OF IRON-MOLYBDENUM CATALYSTS MASS

The process of joint mechanical activation of α -Fe₂O₃ and MoO₃ oxides to produce iron molybdate Fe₂(MoO₄)₃ was studied by means of X-ray, simultaneous thermal analysis and Mössbauer spectroscopy. The data on the structural and mechanical properties of the catalyst masses with different atomic ratio of Mo: Fe were obtained by the rheometer with parallel-moving plate.

Key words: mechanical activation, iron molybdate, structural and mechanical properties, extrusion molding

A.S. SOLODOV, M.S. SOLODOV, E.S. SOBOLEVA, S.G. KOSHEL
INVESTIGATION OF INFLUENCE OF RATIO OF IONIC LIQUID COMPONENTS ON CHROMIUM ELECTRODEPOSITION

The chromium electro deposition was conducted from the ionic liquid based on choline chloride and chromium chloride hexahydrate at different molar ratios of components. The influence of the ionic liquid on its conductivity was studied. Using voltammetry the process of electro deposition of chromium ionic liquids of different compositions was studied.

Key words: choline chloride, molar ratio, conductivity, ionic liquid, electro deposition

E.A. KURGANOVA, A.S. FROLOV, A.S. DANILOVA
JOINT SYNTHESIS OF 3,4-XYLENOL AND ACETONE BY LIQUID PHASE OXIDATION OF ISOPROPYL-O-XYLENE

The regularities of oxidative method of 3,4-xylene obtaining based on o-xylene were studied. Method includes the steps of synthesis of individual isopropyl-o-xylene, its liquid phase oxidation to hydro peroxide followed by acid decomposition of last to 3,4-xylene along with acetone.

Key words: oxidation, 2,5-xylene, hydroperoxydes

I.A. VERSHININA, O.V. GORNUKHINA, O.A. GOLUBCHIKOV
CELLULOSE MATERIALS WITH SURFACE ANTIMICROBIAL PROPERTIES

The experimental results of surface modification of cellulose materials with medicinal preparations of cefazolin and dioxynium are presented. Modified materials were shown to have clearly defined antimicrobial and anti-inflammatory activity. They can be recommended for the creation of new suture material for veterinary science.

Key words: cellulosic materials, surface modification, immobilization, antimicrobial properties, drugs

L.N. OVCHINNIKOV, N.L. OVCHINNIKOV
NUMERICAL AND EXPERIMENTAL INVESTIGATION OF SECOND PERIOD OF CONVECTIVE DRYING OF SORBENT GRANULES BASED ON PEAT AND CLAY

The calculation method of the second period of drying of granulated sorbents based on peat and clay was proposed. The experimental equation for determination of material moisture content as a function of its temperature as well as the criterion equation of heat exchange including mass exchange was obtained.

Key words: peat, clay, sorbents, granules, drying, heat and mass transfer

A.E. LEBEDEV, A.I. ZAYTSEV
STUDY OF FORMATION PROCESS OF DISPERSED FLOW IN CENTRIFUGAL MIXER

Using a probabilistic approach the mathematical description of the process of formation of rarefied flows of bulk materials in a new centrifugal mixer of channel type was developed. The expression was obtained for the differential distribution function of the particles number on the scattering angles. The comparative experimental and theoretical studies were carried out.

Key words: process, mixing, flow, scattering angle, mixture, probability, particle

M.N. BAKIN, A.B. KAPRANOVA, A.I. ZAITSEV
INVESTIGATION OF MIXING BULK MATERIALS IN DEVICE WITH MOBILE TAPE AND FLEXIBLE WORKING ELEMENTS

The studies on influence of operational and design parameters of device on the coefficient of mixture heterogeneity at step by step introduction into mixture one of the component were carried out on the pilot set-up with movable tape and flexible working elements.

Key words: mixer, bulk material, mobile tape, flexible working elements, heterogeneity coefficient, deformation, flexible beats

M.A. YUROVSKAYA, D.E. SMIRNOV, A.V. SUGAK, V.K. LEONTIEV
EXPERIMENTAL STUDIES OF COLLECTOR-CLASSIFIER OF DUST

A operation of the new dust collector-classifier was studied experimentally. The influence of geometric parameters of the apparatus and operating conditions on the dust collection efficiency was established.

Key words: dust collector-classifier, dust collection efficiency, median size of trapped particles

M.E. KOSTICHEV, A.V. SUGAK, D.E. SMIRNOV, L.V. CHEKALOV
DEVELOPMENT AND INVESTIGATION OF CHARACTERISTICS OF HIGH-EFFICIENT ELECTROSTATIC FILTER

The design of an electrostatic filter for high-efficient purification of gases from suspended fine particles was proposed. Experimental tests of apparatus under various operational and geometrical characteristics which influence the most strongly on gas purification efficiency were carried out.

Key words: electrostatic filter, fine particles, experimental set-up, efficiency gas cleaning

E.S. BOBKOVA
ATMOSPHERIC PRESSURE DISCHARGE AS SOURCE OF ACTIVE SPECIES FOR WATER PURIFICATION FROM ORGANIC POLLUTANTS

On the base of kinetic model of atmospheric pressure DC discharge in air with water cathode proposed before the calculations of entering rates of main active species into liquid phase were carried out. The comparison of these rates with the decomposition rates of dissolved pollutants allows analyzing the processes mechanisms proceeding in a liquid phase. The calculation results explain some experimental data on the formation processes of hydrogen peroxide and nitrophenols in water under the discharge action on it.

Key words: plasma, gas discharge, water purification, organic pollutants, processes mechanisms

Yu.A. DMITRENKO, O.V. STAROSVITSKIY, A.V. MAMCHENKO
OBTAINING DRINKING WATER OF FULL VALUE PHYSIOLOGICALLY WITH HELP OF SAPONITE

It was found that at water treatment with saponite it can be possible not only effectively to remove fluoride ions, but also to provide water conditioning with respect to ions of hardness

Key words: saponite, fluoride ions, hardness ions

E.P. ROZHKOVA, E.A. VENEDIKTOV
FORMATION OF SILVER NANOPARTICLES IN ALIPHATIC EPOXY RESINS

The Ag nanoparticles were obtained by means oligooxypropylenetriol glycidyl ether (Laprosid 603) and AgNO₃.

Key words: epoxy-oligomer, nano particles, synthesis