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A B S T R A C T S

S.V. DUSHINA, V.A. SHARNIN, V.V. ALEKSANDRIYSKIY
NEW OPPOTUNITIES OF SOLVATION-THERMODYNAMIC APPROACH TO DESCRIPTION
OF SOLVENT ROLE FOR COMPLEXATION REACTIONS

The development of the solvation-thermodynamic approach as a tool for interpretations of complexation thermodynamic data is presented in following directions: 1. A ligand donor centre solvation contribution and 2. A metal ion coordination centre; 3. accounting the central ion solvate formation equilibrium in the equation of a complex particle stability constant ; 4. A solvent transfer thermodynamic characteristic change in the ratio of solvation reagents contributions.

Key words: thermodynamics, complexation, solvation, nicotinamide, enthalpy, Gibbs's energy

M.S. CHERKALIN, T.A. BOBOVA, A.V. KOLOBOV
SULFONYLCHLORIDES OF ARILPYRIDAZINONES AND SULFONYLAMIDES ON THEIR BASE

Novel sulfonylchlorides and sulfonylamides derivatives containing pyridazinon fragment were obtained.

Key words: aldol condensation, Friedel-Crafts acylation, pyrinazinon, sulfochlorination

A.A. ZHANSITOV, A.I. MARTYNENKO, N.I. POPOVA, M.P. FILATOVA, S.YU. KHASHIROVA,
N.A. SIVOV

STUDY OF STRUCTURE PECULIARITIES OF GUANIDINE CONTAINING-MONOMERS
BY NMR SPECTROSCOPY

New methacrylate monomer derivatives: methacrylate guanidine, methacryloyl guanidine and its hydrochloride as well as a number of model methacrylate compounds (corresponding acid, sodium salt and amide, methacryloyl chloride, methylmethacrylate, guanidine and its hydrochloride) were investigated by NMR spectroscopy method. The structure of synthesized monomers was determined, and dependence of spectral characteristics on structure of investigated compounds and used solvent was shown.

Key words: NMR spectroscopy, methacryloyl guanidine, methacryloyl guanidine hydrochloride, methacrylate derivatives, deuterated solvents

N.M. REPKIN, T.N. NESTEROVA, YU.A. DRUZHININA, S.V. LEVANOVA, V.S. SARKISOVA
IDENTIFICATION OF THERMAL DECOMPOSITION PRODUCTS OF SOME ALKYLBIIPHENYLS

The identification of products of thermal decomposition of 4-methylbiphenyl, 4,4'-di-methylbiphenyl and 4-tert-butylbiphenyl was carried out using chemical methods and chromatography-mass spectrometry.

Key words: alkylbiphenyl, chromatography-mass spectrometry, identification

Yu.B. RUMYANTSEVA, E.A. KURGANOVA, A.A. IVANOVA, G.N. KOSHEL,
V.V. KHRENOVA, N.N. KIRILLOVA

LIQUID PHASE OXIDATION OF ISOPROPYLTOLUENE ISOMERS MIXTURE
TO HYDROPEROXIDES

The reaction of liquid phase oxidation of isopropyltoluene isomers to isopropyltoluene hydroperoxides in the presence of initiator – isopropylbenzene hydroperoxide and nitrogen-containing catalyst was studied.

Key words: liquid phase oxidation, *m*-, *p*-, *o*-, isomers of isopropyltoluene, isopropylbenzene hydroperoxide, N-hydroxyphthalimid, isomerization

L.A. KOCHERGINA, A.V. EMELIANOV, O.N. KRUTOVA
STANDARD ENTHALPY OF L- ALANINE FORMATION AND ITS DISSOCIATION PRODUCTS IN
AQUEOUS SOLUTION

The heat effects of dissolution of crystalline *L*-alanine in water and solutions of potassium hydroxide at 298.15K were determined by direct calorimetry. The standard enthalpies of *L*-alanine formation and its products dissociation in aqueous solution were calculated.

Key words: thermodynamics, amino acid, dipeptides, solutions, *L* –alanine, calorimeter

NGUYEN THI THU HA, A.A. MERKIN, A.A. KOMAROV, O.V. LEFEDOVA
KINETICS OF HYDROGENATION OF SUBSTITUTED NITROBENZENES ON HETEROGENEOUS CATALYSTS IN AQUEOUS SOLUTIONS

The rate of hydrogenation of substituted nitrobenzenes on heterogeneous catalysts in aqueous solutions of 2-propanol was established to depend on the alcohol content. Depending on the mole fraction of 2-propanol, a monotonic change in the solubility of nitro compounds and the shift of K-bands in their EAS is observed. It is significant that the dependence between these characteristics and kinetic parameters of hydrogenation of substituted nitrobenzenes keeps linear one. The transition from water-alcohol media to water solutions of alcohols containing additives of acid or base results in disturbance of these linear relations.

Key words: nitrobenzene, hydrogenation, 2-propanol, rate, adsorption, acetic acid, sodium hydroxide, skeletal nickel

A.A. ISAKINA, D.A. SHUTOV, A.S. KONOVALOV, A.V. BORISOV, E.S. BOBKOVA, V.V. RYBKIN
DESTRUCTION OF SULFONOL IN LIQUID CATHODE OF DIRECT CURRENT DISCHARGE AT ATMOSPHERIC PRESSURE

The kinetics of the sulfonol (sodium alkylbenzene sulfonate) decomposition in water solution at the atmospheric pressure direct current air discharger action was investigated. Effect of the discharge current and initial solution concentration on the destruction rate of the sulfonol was studied. On the base of the IR spectra analysis of the treated solutions some assumptions on the sulfonol decomposition products were supposed.

Key words: sulfonol, liquid cathode discharge, decomposition kinetics

A.A. ILIYN, YU.M. KOMAROV, N.N. SMIRNOV, A.P. ILIYN, A.N. ZHELEZNOVA
PROCESS STUDY OF Al-Zn-Cu CATALYSTS FORMATION, THEIR ACTIVITY AND SELECTIVITY IN REACTION OF CARBON OXIDE CONVERSION WITH WATER VAPOR

The possibility of mechanochemical synthesis of Al-Zn-Cu catalysts by mechanochemical activation of copper and zinc oxides with ammonium carbonate followed by addition of γ -Al₂O₃ was shown. The influence of promoter additions, hydrothermal and thermal treatments of the mass was studied. The activity and selectivity of the samples in the conversion reaction of CO with water vapor to hydrogen were investigated.

Key words: Al-Zn-Cu catalysts, mechanochemical synthesis, carbon monoxide conversion reaction

M.S. SOLODOV, A.S. SOLODOV, E.S. SOBOLEVA, S.G. KOSHEL
STUDY OF INFLUENCE OF ACID-DOPANT ON CORROSION PROPERTIES OF POLYANILINE

Corrosion studies were carried out of polyaniline doped with inorganic and organic acids. Corrosion currents were determined for the polyaniline coatings. The influence of acid-dopant on corrosion properties of polyaniline was established.

Key words: polyaniline, corrosion, corrosion potential, corrosion current, dual protective mechanism

N.M. BEREZINA, M.I. BAZANOV, DO NGOK MIN, A.S. SEMEYKIN
ELECTROCHEMICAL PROPERTIES OF 5-(3'-PYRIDYL)-2,3,7,8,12,18-HEXAMETHYL-13,17-DIETHYLPORPHIN AND ITS COMPLEXES WITH Cu(II), Co(II) AND Fe(III)

The comparative investigation of electrochemical and electrocatalytic properties of 5-(3'-pyridyl)-2,3,7,8,12,18-hexamethyl-13,17-diethylporphyrin (H₂mono-Py[3]P) and their complexes (M(mono-Py[3]P)), where M = Cu(II), Co(II) и Fe(III) was carried out using the cyclic voltammetry method in 0.1 M KOH. The influence of quantity of pyridyl fragments and the metal nature on character of cyclic I,E-curves, values of redox potentials and electrocatalytic activity of compounds in reaction of ionisation of molecular oxygen was established.

Key words: voltammetry, porphyrins, electroreduction, molecular oxygen

O.N. SHCHERBININA, N.O. LYSENKO, F.S. FEDOROV
DURATION INFLUENCE OF MAGNETIC FIELD IMPACT UPON BISMUTH SOLUTION AT ELECTROCHEMICAL ALLOYS FORMATION ON BASE OF COPPER AND LEAD

Impact of preliminary treatment duration of bismuth salt solution in constant magnetic field upon kinetic of formation of Bi-Cu, Bi-Pb, Bi-Pb-Cu, Bi-Cu-Ca, Bi-Pb-Ca, Bi-Pb-Cu-Ca alloys by the method of electrochemical intercalation was studied. Diffusion-kinetic characteristics of penetration process were calculated. The stability of forming phases was determined.

Key words: copper and lead alloys with bismuth and calcium, intercalation, kinetics, diffusion, magnetic field

*A.A. IVANOVA, E.A. KURGANOVA, Yu.B. RUMYANTSEVA, A.V. TARASOV, G.N. KOSHEL,
Yu.A. PETRENCHUK*

**ISOLATION OF HYDROPEROXIDE OF *p*-CYMENE FROM PRODUCTS OF LIQUID-PHASE
OXIDATION OF *p*-CYMENE WITH EXTRACTION METHOD**

A possibility of isolation of hydroperoxide of *p*-cymene (HPC) and *p*-cymene from products of its liquid phase oxidation with efficiency more than 95 % by liquid extraction with a solution of a water-methanol with concentration of 80 % was established. The isolated *p*-cymene is undergone to repeated oxidation without essential change of process parameters.

Key words: extraction, *p*-cymene, *p*-cymene hydroperoxide, distribution factor

D.A. KAZAKOV, V.V. VOL'KHIN, I.S. BOROVKOVA

**INFLUENCE OF AQUEOUS SOLUTION IONIC COMPOSITION ON RATE OF HETEROGENIC
REACTION LIMITED BY GAS-LIQUID MASS TRANSFER IN PRESENCE OF INTERFACIAL
TRANSPORT ACTIVATORS**

The influence of aqueous solution ionic composition on the rate of heterogenic reaction of sulfite ions oxidation limited by gas-liquid mass transfer in the presence of interfacial transport activators was investigated. The possibility to predict the effect of electrolytes on the reaction rate on the base of data on their influence on water structure and the solubility of O₂ was shown.

Key words: heterogenic reaction, gas-liquid system, interfacial transport activators, oxygen, structure-forming ions, structure-breaking ions

I.I. DRIGANOVICH, N.N. YELIN, V.E. MIZONOV, N.R. LEZNOVA

CELL MODEL OF ION EXCHANGE IN SPHERICAL INONITE BEAD

A cell mathematical model of the process of ion exchange in a spherical ionite bead was proposed. The process was reduced to the spherically symmetric problem of diffusion with the step change of diffusion coefficient on the bead surface. The rules of constructing the transition matrix for the problem were proposed. Some examples of the ion exchange kinetics at different ratio of impurity diffusion coefficients in solution and inside the bead are presented.

Key words: ion exchange, spherical ionite bead, impurity concentration, diffusion, reaction kinetics, state vector, transition probabilities matrix

A.A. MUKOVNIN, V.M. TALANOV

**DESCRIPTION OF PHASE DIAGRAM AND ORDER PARAMETER OF Ni_xFe_{1-x}Cr₂O₄
SOLID SOLUTION**

In the frame of phenomenological theory of second-kind phase transitions for thermodynamic potential which is invariant with respect to the group of transformations C_{3v} (3m), the shape of temperature and concentration dependencies of components of order parameter was predicted for Ni_xFe_{1-x}Cr₂O₄ system.

Key words: phase diagram, phase transition, order parameter

A.I. KOROLYOVA, V.M. TALANOV, M.A. SAVENKOVA

COMPLEXATION IN DOUBLE SYSTEM RbPO₃ – Bi₂O₃

The components interaction of RbPO₃ – Bi₂O₃ system on interface melt-solid phase and in solid phase was studied by the methods of physical-chemical analysis. The formation of new compounds 2RbPO₃ – Bi₂O₃ melting with decomposition and RbPO₃ – Bi₂O₃ melting congruent was established. According to results of IR spectroscopy and chromatography the anions of isolated compounds refer to chain metaphosphates.

Key words: metaphosphates, bismuth oxide (III), phase diagram, complexation, anions linear structure, metaphosphates glasses

A.S. VYSOKOVSKIY, I.S. KOROTNEVA, V.G. KURBATOV, I.V. GOLIKOV

**SURFACTANT COMBINATIONS FOR CARRYING OUT EMULSION GRAFT-
COPOLYMERIZATION**

The use of surfactant synergy combinations at the obtaining the seed copolymer lattices was established to be the most preferable. For carrying out the graft copolymerization in emulsion it is necessary to take into account both the surfactant synergetic combination efficiency and different ability of the specific components of the mixture to adsorb on the surface of polymer particles.

Key words: graft-copolymers, mixed micelles, synergism, latex particles diameter

S.Yu. SMIRNOVA, M.E. SOLOVYOV

QUANTUM-CHEMICAL INVESTIGATION OF HYDROGEN DETACHMENT REACTION IN HYDROCARBON RADICALS OF POLY-UNSATURATED FATTY ACIDS

The quantum-chemical method DFT B3LYP/6-31G* was used for calculation of thermodynamic functions of hydrogen detachment reaction in the hydrocarbon radical of fatty acids of different unsaturation. The influence of position of the reactionary center with respect to double bonds and to conformation of bisallylic group on the reactivity of the compounds in reaction under consideration was analyzed.

Key words: DFT B3LYP/6-31G*method, polyunsaturated fatty acids, pentadienil radical, reaction energy, reaction enthalpy

S.V. SHORIN, N.V. KSANDROV, G.V. PASTUKHOVA, A.V. SOLDATOV

OBTAINING GRANULATED COMPLEX FERTILIZERS ON BASE OF CARBAMIDE AND AMMOPHOS IN HIGH-SPEED DRUM GRANULATOR

The process of obtaining granulated complex fertilizers was considered. The mechanical-and-physical and chemical properties of the obtained fertilizers were studied.

Key words: carbamide, ammophos, granulating, drum granulator, mineral fertilizers

T.V. KONKOVA, M.B. ALEKHINA, T.F. SADYKOV, M.A. NIKIFOROVA A.I. MIKHAIYLICHENKO, E.Yu. LIEBERMAN

HETEROGENEOUS FENTON CATALYSTS FOR WASTE WATER PURIFICATION FROM ORGANIC DYES

Cobalt and cerium oxides applied on the aluminium oxide, silica gels, and amorphous aluminosilicate were investigated in process of catalytic oxidation of methyl orange by hydrogen peroxide in aqueous solutions. The greatest activity and stability in conditions under study showed the catalyst on the base of aluminum oxide that allow recommending it for the further researches of processes of waste water treatment from organic compounds.

Key words: liquid phase catalytic oxidation, hydrogen peroxide, transition metals oxides, dyes

L.N. OVCHINNIKOV, N.L. OVCHINNIKOV

DIGITAL AND EXPERIMENTAL STUDIES OF PREPARING ORGANIC-MINERAL SORBENTS ON PEAT BASE

Results of experimental – statistical modeling and optimization of technological conditions for obtaining the effective granulated sorbents on the base of peat and mineral additives – clay and gypsum are given.

Key words: peat, clay, sorbents, optimization, granulation, drying

L.N. MOROZOV, S.V. RUMYANTSEV, A.V. BUROV, A.L. KOLOSOVSKIY

SIMULATION OF RUNNING REGIMES OF RECYCLING SCHEME OF AMMONIA SYNTHESIS

The numerical simulation of recycling scheme of ammonia catalytic synthesis was carried out using operating parameters of real industrial unit. The effect of pressure, temperature of ammonia condensation as well as the effect of catalytic activity on unit productivity and the degree of nitrogen-hydrogen mixture processing into a final product was shown.

Key words: ammonia synthesis, recycling schemes, feedback

V.E. MIZONOV, S.V. KRUPIN, K.A. SHELATONOVA, E.A. BARANTSEVA

OPTIMAL SET-IN OF FEED OF SEGREGATING COMPONENT TO CONTINUOUS MIXER

A mathematical model of formation of mixture quality at the outlet of a continuous mixer with the feed of segregating component to an intermediate cross section of the mixer is proposed. It is shown that there is the optimal position of this cross section that provides the maximum mixture quality at the outlet. The position of the optimal cross section depends strongly on the segregation velocity and only slightly depends on the macro-diffusion coefficient.

Key words: continuous mixer, segregation, cell model, transition matrix of probabilities, mixture quality

S.P. RUDOBASHTA, S.Yu. MAHMUD

MATHEMATICAL MODELLING MEMBRANE DISTILLATION PROCESS

The mathematical model taking into account the effects of temperature and concentration polarization and steam depression over solution was presented. The steam conductivity coefficient for film membranes MFFK2, MFFK 3, MFFK4 was experimentally determined and analyzed. The equations for temperature calculation of hot and cold membrane surfaces were obtained which are necessary to consider for calculation the temperature polarization effect. The modified equation for steam conductivity in which the effect of depression of steam over a solution and concentration polarization is considered was offered. The parameter reflecting given effect was experimentally determined for sea water membrane distillation. The engineering calculation technique of membrane distillation was developed.

Key words: membrane distillation, sea water, kinetics, temperature and concentration polarization, steam depression

A.N. LABUTIN, V.Yu. NEVINITSYN

SYNERGETIC SYNTHESIS OF CHEMICAL REACTOR CONTROL SYSTEM

The paper deals with the analytical synthesis of synergetic control system of chemical reactor with a complex series-parallel exothermic reaction. Control laws synthesis is based on the analytical design of aggregated regulators approach. Proposed nonlinear control system solves the task of stabilization of target component concentration at reactor outlet and allows passing to new productivity of reactor operation automatically.

Key words: chemical reactor, synergetic control system, analytical design of aggregated regulators, invariant manifold, attractor, computer simulation

A.N. LABUTIN, M.A. CHESHINSKIY

GAS-LIQUID PROCESS OPTIMIZATION OF ALCOHOLS OXYETHYLATION

The problem of optimizing the gas-liquid process of alcohols oxyethylation was formulated and was solved using mathematical modeling. An algorithm for the calculation was offered. The results of the optimization were presented.

Key words: reactor, absorber, target product, simulation, optimization

A.B. KAPRANOVA, Yu.V. NIKITINA, A.E. LEBEDEV, A.I. ZAIYITSEV

MODELING CURVILINEAR BLADE PROFILE FOR CENTRIFUGAL SPRAYER OF VISCOUS LIQUID

The method of estimation of angle characteristic for the centrifugal set-up's blade for the fluid spraying at conditions for liquid uniform flow through the chamber. The calculation was carried out taking into account the medium sliding along the curvilinear blade and functional dependence for the Newtonian viscous fluid's velocity at reactor outlet on reactor parameters in the polar coordinate system.

Key words: centrifugal sprayer, curvilinear blade, isothermal Newtonian viscous fluid, polar coordinate system, set-up's parameters, slip coefficient

A.B. KAPRANOVA, Yu.V. NIKITINA, A.E. LEBEDEV

METHOD OF EVALUATION OF "BREAKING" VELOCITY OF VISCOUS FLUID AT CHAMBER OUTLET OF CENTRIFUGAL SPRAYER

The method of search of "breaking" velocity of liquid medium in the polar coordinate system was proposed for the Newtonian viscous fluid movement along the curvilinear blade at conditions of uniform outflow from a centrifugal sprayer chamber. The given method may be used under the designing the centrifugal set-up blade profile for the liquid dispersion.

Key words: centrifugal sprayer, curvilinear blade, isothermal Newtonian viscous fluid, movement model, polar coordinate system, device parameters

A.E. LEBEDEV, A.I. ZAIYITSEV, A.B. KAPRANOVA, A.A. PETROV

DETERMINATION METHOD OF COEFFICIENT OF HETEROGENEITY OF MIXTURE AT INTERACTION OF RAREFIED FLOWS

Using probabilistic approach the calculation method of coefficient of heterogeneity at interaction of dispersed flows of granular media was presented. The resulting expression for the coefficient of heterogeneity can be used for assessing the quality of mixture at mixing materials in a rarefied state.

Key words: process, mixing, flow, heterogeneity coefficient, concentration

*A.A. BAKANOVA, S.V. BAIYKOV, V.V. SOSNINA, G.G. KRASOVSKAYA,
A.F. BETNEV, E.R. KOFANOV*

**SYNTHESIS OF PHENYLCYCLOALKYLAMINOCARBOXYLIC ACIDS CONTAINING IMIDE
CYCLE**

The synthesis scheme of aminocarboxylic acids containing cycloalkyl, phenyl and imide cycles is presented.

Key words: aminocarboxylic acids, imides, cycloalkylcarboxylic acids

G.M. POLTORATSKIY, A.N. EVDOKIMOV, A.V. KURZIN

**VAPOR PRESSURES FOR METHANOL - TETRAMETHYLAMMONIUM AZIDE
AND METHANOL - TETRAETHYLAMMONIUM AZIDE SYSTEMS**

The vapor pressure of methanol in the binary methanol - tetramethylammonium azide and methanol - tetraethylammonium azide systems was measured at different salt concentrations in the temperature range of 281.79 – 327.17 K.

Key words: vapor pressure, methanol, tetramethylammonium azide, tetraethylammonium azide

E.V. ZOLOTUKHINA, T.V. GUBANOVA, I.K. GARKUSHIN
THREE-COMPONENT SYSTEM KF–KBr–KVO₃

The phase equilibria in three-component system KF–KBr–KVO₃ were studied by differential thermal analysis (DTA). The eutectic compositions was revealed (mol. %) KF 21,25 %, KBr 15 %, KVO₃ 63,75 % with melting point of 429 °C and enthalpy of melting of 184.94 J/g. Fields of crystallization of phases were differentiated.

Key words: differential thermal analysis, state diagram, phase equilibria, melting temperature

V. M. TALANOV

**RHYTHM- CASCADES IN PERIODIC TABLE. TEACHING EXPERIENCE
OF THEORY OF PERIODIC LAW**

The principles of rhythm-cascads in the periodic system of D.I. Mendeleev allowing ordering conceptions on multiform dependencies "ordinal number of elements – the physical and chemical properties of atoms and chemical compounds» were formulated. The experience of teaching the theory of the periodic law based on the proposed principles is discussed.

Key words: rhythm-cascads, periodic table, elements, teaching

Yu.N. USHAKOVA, L.A. KALININA, T.A. GOLOVANOV

**ORGANIZATION OF INDIVIDUAL WORK OF STUDENTS OF CHEMICAL FACULTY
IN VYATKA STATE UNIVERSITY**

The transition of higher education to two-level system of training raises before higher education the new challenges. The present level of requirements to graduate dictates the need for such an approach to the educational process in which a student and teacher collaboration forms a creative person who has the necessary competence and independence. Proper organization of independent work greatly helps to gain knowledge and skills necessary for future employment and career growth.

Key words: two-level system of education, competence-based approach, module-rating system of knowledge, students' independent work, self study, employer, student

V.A. NEBOL'SIN

**ON EXPERIENCE OF MODERN EXPENSIVE EQUIPMENT OF CENTRE FOR COLLECTIVE USE
AT LABORATORY WORKSHOP ON INORGANIC CHEMISTRY IN TECHNICAL UNIVERSITY**

The usage of modern precision and expensive equipment of multi-access center was shown to influence positively on motivation of students for learning chemical disciplines during laboratory courses.

Key words: collective use center, equipment, inorganic chemistry