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## A B S T R A C T S

*B.D. BEREZIN, O.V. MAL'TSEVA, D.B. BEREZIN***ELECTRONIC AND STERIC EFFECTS IN COORDINATION SPHERE OF METAL 3d - COMPLEXES. *Trans*- AND *cis*-INFLUENCE OF LIGANDS**

The article is the experimental and theoretical development of some important ideas of the theory of mutual influence of atoms and atomic groups in complex molecules of inorganic and organic origin. The coordination theory of A. Verner as a result of development of classical theory of A.M. Butlerov (1861) was foundation of stereochemistry of *trans*-influence of I.I. Chernyaev in metal complex compounds of platinum groups and Co(III). Authors of given article study the *trans* influence in coordination sphere of solvate complexes of 3d-metals salts in reactions with the complex micro cyclic ligands of aromatic nature and its influence on kinetics and mechanism of formation of macro cyclic complexes of porphyrines. The data obtained together with literature data are discussed in given paper.

**Key words:** porphyrines, *trans*-influence, indicator reactions, complexation

*E.K. AMINOVA, A.N. KAZAKOVA, M.V. PROSKURNINA, S.S. ZLOTSKIY***SYNTHESIS OF CYCLIC ACETALS CONTAINING *gem*-DICHLOROCYCLOPROPANE FRAGMENT**

Possible ways of synthesis of substituted 4-(*gem*-dichlorocyclopropyl)-1,3-dioxolanes from commercially available reagents - 1,3-butadiene and isoprene were studied.

**Key words:** epoxydation, *gem*-dichlorocyclopropanes, 1,3-dioxolanes, oxyranes, dichlorocarbenes, interphase catalysis

*P.A. AGATIEV, A.V. TARASOV, Yu.A. MOSKVICHEV***CHLOROSULFONATION OF 3-METOXYBENZOIC ACID AND ITS METHYL ESTER**

It was found that chlorosulfonation of 3-methoxybenzoic acid leads to selective introduction of sulfo group in ortho position with respect to carboxylic group. The ortho-sulfochloride of methyl ester of 3-methoxy benzoic acid was obtained with the subsequent sulfo chlorination of methyl ester of 3-methoxy benzoic acid. This ester is a convenient product for synthesis of 5-methoxy-1,2-benzothiazole-3(2N)-one-1,1-dioxide.

**Key words:** chlorosulfonation, 2-sulfobenzoic acid derivatives, anhydride, sulfonamide, saccharine derivatives

*L.A. ALAKAEVA, A.K. TKHAMOKOV***ETHERS OF SULFOSALICYLIC ACID DERIVATIVES AS NEW LUMINESCENT REAGENTS FOR TERBIUM**

By means of synthesis the new ethers of sulfosalicylic acid derivatives were obtained. Those esters give the bright luminescent reactions with terbium ions. Optimum conditions of complexation were found and high-sensitivity methods of terbium determination were proposed for various objects.

**Key words:** sulfosalicylic acid derivatives, reagent, structure, luminescence, terbium

*E.G. KHOMUTOVA, E.V. KOPYLOVA***CATALYTIC TEST-METHOD FOR DETERMINATION OF IRIIDIUM MICRO AMOUNTS ON BASE OF SULFARSAZENE OXIDATION REACTION WITH POTASSIUM PERIODATE**

The test-method for the determination of iridium, which is based on carrying out the catalytic indicator reaction of oxidation of sulfarsazena with the potassium periodate on paper carrier was offered. Determination is possible in a wide range of iridium concentrations from 0.2 to 2.0 µg/ml. The detection limit is 0.02 µg/ml, the error does not exceed  $Sr = 0.20$ . The validity of the method was confirmed by the "introduced-found" method.

**Key words:** test-method, catalytic reaction, iridium determination

*O.S. KUNDIY, A.M. ZAIYCHIKOV***THERMODYNAMIC AND STRUCTURAL CHARACTERISTICS OF AQUEOUS SOLUTIONS OF APROTIC AMIDES**

Thermodynamic characteristics of aqueous solutions of aprotic amides were calculated. On its base the regularities of structural properties change of mixtures under study were established. The correlation of entrop-

ic and enthalpic characteristics of aqueous amide systems with excess packing coefficient indicates that universal interactions define structural and energetic properties of aqueous solutions of tertiary amides including hexamethylphosphoric triamide. The extremal shape of concentration dependences of solvation enthalpy of noble gases in aqueous mixtures of aprotic amides is caused by destruction of H-bond network of water and formation dense packed solutions in this area.

**Key words:** internal pressure, intermolecular interactions, thermodynamic and structural characteristics, aqueous solutions, water, aprotic amides

***Yu.E. ROMANENKO, A.A. KOMAROV, M.A. BUDANOV, O.V. LEFEDOVA***  
**KINETIC MODEL OF REACTIONS OF INTERMEDIATES HYDROGENATION  
OF NITROGROUP REDUCTION**

The kinetics of liquid-phase hydrogenation of products of incomplete nitro group reduction in 2-propanol aqueous solutions on skeletal nickel was studied. Kinetic description of the liquid phase hydrogenation of phenylhydroxylamine, azobenzene and azoxybenzene were proposed. Model calculations have shown the correspondence of calculated values of reaction participants concentration to experimental ones.

**Key words:** liquid-phase hydrogenation, skeletal nickel, 2-propanol aqueous solutions, azobenzene, azoxybenzene, phenylhydroxylamine, aniline, kinetic model

***D.S. KOSYAKOV, M.V. PANFILOVA, N.S. GORBOVA, K.G. BOGOLITSYN***  
**ACIDITY OF PHENOLS OF SYRINGYL SERIES IN BINARY MIXTURES OF WATER  
WITH 1,4-DIOXANE AND ACETONITRILE**

Using the methods of spectrophotometric and potentiometric titration the acidity constants of syringylic phenols were determined in the system water – 1,4-dioxane and water – acetonitrile. The effects of solvent and phenol structure on protolytic properties of p-derivatives of 2,6-dimethoxyphenol were considered.

**Key words:** 1,4-dioxane, acetonitrile, mixed solvents, phenols, acidity constants

***N.M. BEREZINA, D.R. KARIMOV, M.I. BAZANOV, D.B. BEREZIN***  
**INFLUENCE OF FUNCTIONAL SUBSTITUTION ON ELECTROCHEMICAL CHARACTERISTICS  
AND ELECTROCATALYTIC ACTIVITY OF MESO-TRIPHENYLCORROLE  
AND ITS COMPLEXES WITH Cu(III) AND Mn(III)**

The comparative investigation of electrochemical and electrocatalytic properties of meso-triphenylcorrole and its para-substituted [ $H_3(ms-p-R-Ph)3Cor$ ], containing electron donor ( $R = OMe$ ) and electron acceptor ( $R = NO_2$ ) substituents in phenyl ring, as well as their complexes with Cu(III) and Mn(III) was carried out using cyclic voltammetry method in 0.1 M KOH. On I,E-curves of nitro-derivative of corrole and their complexes the transition corresponding electroreduction of nitro-groups was found. Electrocatalytic activity of investigated compounds in reaction of reduction of molecular oxygen was increased in the series: ligand < copper (III) complex < manganese(III) complex, as well as under the growth of an electron-donor ability of substituents in phenyl rings of macrocycles.

**Key words:** meso-substituted corrole, voltammetry, molecular oxygen electroreduction, copper (III) and manganese (III) complexes

***V.G. PRYAZHNIKOVA, O.V. KOZLOVA, F.Yu. TELEGIN***  
**RELATIONSHIP BETWEEN STRUCTURE AND TECHNICAL PROPERTIES OF SURFACTANTS**

The relationship between chemical structure of ethoxylated surfactant and technical results of solvation pre-treatment of textile materials was shown by the use of software for molecular modeling.

**Key words:** structure, surfactants, hydrophobic-lipophilic balance

***R.N. RUMYANTSEV, A.A. ILYIN, A.P. ILYIN***  
**MECHANOCHEMICAL SYNTHESIS OF IRON OXIDE BY MEANS OF INTERACTION  
OF METAL POWDERS WITH WATER**

The investigations of oxidation of metallic iron powders and cast iron in their mechanochemical interaction with water were carried out. The composition of formed phases of oxides was established by the methods of differential dissolution and Mössbauer spectroscopy. The main kinetic regularities of valence state of iron at various steps of mechanical activation were determined. The basic parameters of the kinetics of dispersion were established.

**Key words:** mechanical activation, oxidation, iron oxides, metal powders

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

**DECREASE IN NITROGEN OXIDES EMISSION AND NITRIC ACID CONSUMPTION  
AT LEACHING OF URANIUM CONCENTRATES**

The processes of leaching of uranium oxide (VI)-diuranium (V) and metal uranium with the nitric acid with and without addition of ammonium nitrate were investigated. The effect of concentration of ammonium nitrate, temperature, concentration of nitric acid and weight ratio of uranium concentrates on the degree of reduction of nitrous gases and acid consumption was shown.

**Key words:** leaching, triuranium octoxide, metal uranium, ammonium polyuranate, ammonium nitrate, nitrogen oxides, nitric acid

*R.M. SHLENEV, N.A. NOZHIN, Yu.A. MOSKVICHEV*

**INVESTIGATION OF REACTION OF N-SUBSTITUTED NITRILES OF AMINOPROPIONIC ACID  
WITH THIOSEMICARBAZIDE IN PRESENCE OF POLYPHOSPHORIC ACID**

The possibility of synthesis of 5-aminoalkyl derivatives of 2-amino-1,3,4-thiadiazoles by reaction of N-substituted nitriles of aminopropionic acid with thiosemicarbazide in polyphosphoric acid medium was investigated. The influence of the reaction temperature, time and molar ratio of nitril: polyphosphoric acid on yield of target compounds was studied. The best reaction conditions of reaction accomplishing were determined. The target compounds were obtained with a yield of not less than 40%.

**Key words:** substituted nitriles of aminopropionic acid, thiosemicarbazide, polyphosphoric acid, derivatives of 1,3,4-thiadiazoles

*V.V. TUZOVA, S.V. FILIN, P.P. GLADYSHEV*

**LUMINESCENT POLYMER COMPOSITE MATERIALS ON BASE OF ACRYLIC CO-POLYMERS AND  
ORGANIC PHOSPHORS OF CUMARINE AND 6 AND 5-DIMETHYLAMINO-4'-NITRO TOLUYLENE**

Study deals with obtaining the luminescent polymer composite materials on the base of acrylic copolymers with organic phosphors in process of photo-initiated polymerization and study of their spectral parameters. The influence of composition of polymer composition and the time of photo-initiation on optical properties of materials being obtained was shown.

**Key words:** acrylic co-polymers, oligourethanemethacrylate, photo polymerization, cumarine-6, 4-dimethylamino-4'-nitro toluene

*V.Yu. DOLUDA, G.N. DEMIDENKO, M.G. SULMAN, N.V. LAKINA, V.G. MATVEEVA, E.M. SULMAN*  
**INVESTIGATION OF NITROBENZENE CATALYTIC HYDROGENATION OVER Pd-  
CONTAINING CATALYSTS IN SUPERCRITICAL CARBON DIOXIDE MEDIA**

In given article the results of study of catalytic hydrogenation of nitrobenzene with the use of Pd-containing catalysts in supercritical carbon dioxide and in solvent 2-propanol and without solvent are presented. The essential acceleration of nitrobenzene hydrogenation rate in supercritical carbon dioxide media was shown.

**Key words:** supercritical carbon dioxide, nitrobenzene, aniline, catalysis, reaction rate, hydrogenation

*A.T. GALIMOVA, A.A. SAGDEEV, F.M. GUMEROV*

**RESEARCH OF SOLUBILITY OF SUBSTANCES DEACTIVATING CATALYST OXIDE  
OF ALUMINUM POSSESSING ACTIVITY IN SUPERCRITICAL CARBON DIOXIDE**

The results of solubility research of styrene, methylphenylcarbinol in supercritical carbon dioxide are given with the use of dynamic (flowing) method. The obtained data were described in the frame of Peng – Robinson equation.

**Key words:** styrene, methylphenylcarbinol, supercritical carbon dioxide, solubility, dynamic method, Peng – Robinson equation

*E.V. UDORATINA, M.A. TORLOPOV*

**PARTIAL DESTRUCTION OF CELLULOSE IN WATER AND IN ACETIC ACID IN PRESENCE  
OF HETEROPOLYACIDS**

The process of partial degradation of cellulose was studied in the presence of heteropolyacids. The degradation of cellulose catalyzed with phosphormolybdenic and phosphortungsten acids in acetic acid medium were shown to proceed more efficiently than in aqueous media. Products of partial destruction (cellulose powders) were obtained. The basic physical and chemical properties of cellulose powders such as the degree of polymerization, crystallinity index, functional and fractional composition were analyzed.

**Key words:** cellulose destruction, heteropolyacids, powder cellulose, submolecular structure

*E.E. ERGOZHIN, B.E. BEGENOVA, T.K. CHALOV, T.V. KOVRIGINA, N.V. OSTAFEIYCHUK,  
D.U. KALIEVA*

#### **IONITES ON BASIS OF GLYCIDYL DERIVATIVES OF QUINONES AND POLYAMINES**

Polyelectrolytes on the basis of glycidyl derivatives of quinones and polyamines were synthesized. The proposed method for the synthesis of ion exchangers does not require complex manufacturing equipment. The process is carried out under mild conditions. An advantage of these polymers is the ability to use them not only in the reactions of ion exchange but also in the process of oxidation-reduction. The obtained sorbents are promising for the adsorption of rare, scattered and noble metals.

**Key words:** p-benzoquinone, p-naphthoquinone, epichlorohydrin, polyamine, quinone glycidyl derivative, polyelectrolyte, ionite, anionite, sorption, metal ions

*S.Yu. VASILYEVA, D.L. KOTOVA, T.A. KRYSANOVA, V.A. KRYSANOV*

#### **SOLID - PHASE EXTRACTION OF $\alpha$ - TOCOPHEROL FROM VEGETABLE OILS**

Regularities of  $\alpha$  - tocopherol adsorption on clinoptilolite tuff activated with 4.0 M HCl from solutions of ethanol, hexane and acetic ether were studied. The activated sorbent was established to possess increased affinity to vitamin E molecules in ethanol solution and it can be used for  $\alpha$ -tocopherol extraction from vegetable oils.

**Key words:** clinoptilolite tuff, vitamin E, adsorption, solvent nature

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

#### **STUDY OF IMPACT MIXING SOLID DISPERSION MEDIA AT PARTICLES SECONDARY COLLISIONS**

On the base of stochastic approach the complex differential functions of distribution on particle diameter and on spray angle were obtained for mixing friable components at the use of the impact interaction with inclined baffle.

**Key words:** dispersed solid material, mixing, impact interaction, baffle, secondary collision, phase space, distribution differential function, particle diameter, spray angle

*L.V. KOROLEV, D.O. BYTEV*

#### **RANDOM TRANSPORT IN POROUS SORBING MEDIUM**

A continuous random walks model taking into account the particle sorption is used to describe transport processes of particles in porous sorbing medium. The influence of the particle residence time on macroscopic process behavior and the medium transmitting efficiency was investigated.

**Key words:** porous medium, continuous random walks, subdiffusion

*A.E. LEBEDEV, A.A. PETROV*

#### **STUDY OF MIXING PROCESS OF BULK MATERIALS IN CENTRIFUGAL MIXER OF CHANNEL TYPE**

The process of mixing the bulk materials was studied in new centrifugal mixer of channel type. On the base of probabilistic approach the mathematical description of particle movement in flow was created. The effect of shift of spray channels on a factor of mixture heterogeneity was examined.

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

*A.G. LAPTEV, T.M. FARAKHOV*

#### **MASS TRANSFER MODEL IN GRANULAR AND PACKED LAYER**

For determination of mass-transfer coefficients the boundary layer model of Prandtl was considered. Equations for calculation of transfer coefficients of impulse and mass were obtained. Examples of calculations of Sherwood number in a column filled with elements of fine packing were shown. Comparisons of obtained results with results of other researchers are given.

**Key words:** boundary layer, hydrodynamic analogy, energy dissipation, mass transfer coefficient, disordered attachments

*A.Yu. DONCHENKO, Yu.G. GOGOLEV*

#### **MODELING OF PROCESS OF VOLUME DESUBLIMATION IN DEVICES WITH VERTICAL ENTRY AT OBTAINING FINE DISPERSED MATERIALS**

In given paper the mathematical model of desublimation process for producing the ultra-fine materials in volume type device was proposed. On the base of modeling results the influence of separate factors on the

process proceeding is analyzed. The proposals on efficient organization of resublimation at obtaining the target product are given.

**Key words:** desublimation, fine-disperse materials, heterogeneous nucleation, supersaturation

*A.G. LAPTEV, M.M. BASHAROV*

#### **DETERMINATION OF GAS PURIFICATION EFFICIENCY FROM DISPERSE PHASE WITH VORTICAL ELEMENTS**

On the base of use of the theory of particles turbulent migration and mass-transfer equation the expressions were obtained for calculation of gas purification efficiency with the vortical elements. Calculation results of separation efficiency of disperse phase were presented. Conclusions on variant of application of vortical units were done.

**Key words:** aerosols, turbulent migration, vertical units, gas purification, efficiency calculation

*V.E. MIZONOV, I.A. BALAGUROV, V.A. ZAIYTSEV*

#### **CELL MODEL OF CONVECTIVE DIFFUSION IN COMPLEX PLANE DOMAIN WITH PARTITIONS**

A cell mathematical model to describe the evolution of concentration distribution at convective diffusion in a complex plane domain with partitions was proposed. The domain is presented as 2D Markov chain, in which transition probabilities are separated into symmetrical parts related to pure diffusion, and non-symmetrical part related to convection transition. It was shown how complex borders of domain and various partitions can be taken into account in the matrix of transition probabilities using the form matrix of the domain on the basis of universal computational algorithm. An example of calculation of concentration distribution evolution was presented.

**Key words:** convective diffusion, cell model, Markov chain, state vector, concentration distribution

*A.O. KARANETS, M.E. SOLOVOYV*

#### **APPLICATION OF COMPOSITION-PROPERTIES MODELS FOR AUTOMATION DESIGN OF RUBBER GOODS**

The method of calculation of rubber goods using composition-properties model based on general purpose rubbers and application this model at computer-aided design of rubber shock absorbers was proposed. The developed method was implemented to the software system to automate design of rubber goods.

**Key words:** design automation, rubber shock absorbers, Legendre polynomials, properties prediction

#### ***L.N. SKVORTSOVA, L.N. CHUKHLOMINA, G.M. MOKROUSOV, V.N. BATALOVA, O.A. TURCHINA* CATALYTIC DEGRADATION OF PHENOL AND INTERMEDIATE PRODUCTS OF ITS OXIDATION WITH USE OF IRON-CONTAINING COMPOSITIONS OF SILICON NITRIDE**

Conditions for the deep degradation of phenol using iron-containing compositions based on silicon nitride at ozonization combined with UV irradiation were determined. The catalytic activity of Si-N-Fe compositions under UV irradiation in the presence of oxalic acid was shown to be photoactive ferric-oxalate complex, which is formed in solution. In other words, a combination of heterogeneous and homogeneous catalysis takes place. GC-MS was used to establish degradation products of phenol. Catalytic composites were tested for the phenol-containing waste water treatment at different Tomsk companies.

**Key words:** phenol, ferric-oxalate complex, catalytic ozonation, dissolved organics photooxidation, silicon nitride

*A.A. KOLESNIKOV, M.O. MESNIK*

#### **BEAM DISTRIBUTION OF ELECTRON ACCELERATOR ON IRRADIATION DEEP OF POLYMERIC MATERIALS**

The distribution of electron beam on deep of elastomeric artificial leathers and rubber-technical goods with electron accelerator was considered at beam different energies.

**Key words:** electron accelerators, absorbed irradiation doses