

A B S T R A C T S

*A.D. KOTOV, E.V. SNEZHKOVA, D.A. BAZLOV***SYNTHESIS AND QUANTUM-CHEMICAL MODELING OF 2,3-BIS(2-CYANOPHENYL)-2,3-DIPHENYLSUCCINAMIDE**

The 2,3-bis(2-cyanophenyl)-2,3-diphenylsuccinamid has been synthesized by an interaction of phthalonitrile with phenylacetone in the NaOH/DMSO system. The molecular structure of synthesized compound has been studied by means of quantum-chemical modeling (by the MP3 semiempirical method). The number of stable conformations has been revealed.

Key words: quantum-chemical modeling, nucleophilic aromatic substitution, 2,3-bis(2-cyanophenyl)-2,3-diphenylsuccinamid

*V.Yu. ORLOV, A.D. KOTOV, A.V. TSIVOV***REGULARITIES AND MECHANISM OF ARYLACETONITRILES INTERACTION WITH NITROARENES**

The basic regularities of arylacetone nitriles interaction reactions with nitroarenes have been considered. On the base of data analysis of preparative and kinetic studies as well as preliminary results of quantum chemical modeling the steps of mechanism of given reaction have been proposed.

Key words: nucleophilic substitution, arylacetone nitriles, nitroarenes, reaction mechanism, quantum chemistry modeling

*A.A. BOGOMAZOVA, R.V. KUNAKOVA, S.S. ZLOTSKIY***O-ALKYLATION OF PHENOL AND ALCOHOLS WITH ALLYL BROMIDE AND 1,2,3-TRIGALOGENPROPANS**

The O-alkylation of phenol and alcohols with the allyl bromide and 1,2,3-trihalogenpropanes has been investigated. It has been established that the phenol is active in one order of magnitude than allyl alcohol and 3 times more active than the benzyl alcohol. In the salicylic alcohol the phenolic hydroxyl group by a factor 5-7 more active than benzyl one at the reaction with allyl bromide and 1,2,3-trihalogenpropanes.

Key words: alkylation, phenol, benzyl alcohol, salicylic alcohol, allyl alcohol, allyl bromide, 1,2,3-trihalogenpropanes

*V.V. ZHANDAREV, M.E. GOSHIN, S.I. FILIMONOV, V.N. KAZIN,**T.N. ORLOVA, E.M. PLISS, V.V. PLAKHTINSKIY***SYNTHESIS AND ISOMERISM OF 4-R-METHYLENE-5-MORPHOLINE-4-YL-2,4 DIHYDROPYRAZOLE-3-ONE DERIVATIVES**

Aromatic nitro compounds containing pyrazolone cycle have been synthesized. An isomerism of substituted compounds has been studied. Appropriate amino compounds have been obtained by afterhydrogenation.

Key words: synthesis, structure, pyrazolone derivatives, isomerism, hydrogenation

*E.A. KIRILLOVA, P.P. MUKOVOZ, A.N. VINOGRADOV, V.O. KOZMINYKH, O.N. DVORSKAYA***SYNTHESIS, STRUCTURE PECULIARITIES AND TAUTOMERISM OF 1,6-DISUBSTITUTED OF 3,4-DIHYDROXY-2,4-HEXADIENE-1,6-DIONES**

With the Claisen reaction of methyl ketones with diethyl oxalate in the presence of sodium or sodium hydride the disodium 1,6-dioxo-2,4-alkadiene-3,4-diolates have been obtained. At acidation of products obtained the 3,4-dihydroxy-2,4-alkadiene-1,6-diones have been isolated. Chain and ring-chain tautomeric equilibria in solutions of 1,3,4,6-tetracarbonyl compounds have been investigated. The structure peculiarities of synthesized compounds have been studied by spectral methods of analysis.

Key words: 1,3,4,6-tetracarbonyl compounds, Claisen reaction, ring-chain tautomeric equilibria

*A.A. DAVLYATSHINA, S.A. PIVOVARENOK, A.V. DUNAEV, A.M. EFREMOV, V.I. SVETTSOV***RADIATION OF HYDROGEN CHLORIDE PLASMA**

The analysis of the HCl plasma emission spectrum was carried out under the conditions of the direct current glow discharge. The change in gas pressure ($p = 40-200$ Pa) at a constant discharge current has been

shown to results in the change in the excitation conditions for both chlorine and hydrogen atoms. The possibility of control of the relative changes of atom densities using the ratio of their emission intensities was investigated.

Key words: plasma, emission, intensity, excitation, concentration

D.R. KARIMOV, V.P. BARANNIKOV, O.V. MAL'TSEVA, R.S. KUMEEV, D.B. BEREZIN
UNACCOMPLISHED ACID-BASIC INTERACTIONS OF CORROLES
WITH ELECTRON-DONOR SOLVENTS

Factors determining a chemical activity of NH-bonds in corrole molecules as well as its influence on a reactivity of compounds are discussed. Investigation has been carried out by methods of spectrophotometric titration, fluorescence spectroscopy, thermogravimetric analysis, ¹H-NMR spectroscopy and quantum-chemical calculations. The meso-substituted corrole ability to a formation of H-associates with organic solvents has been found to be higher as comparing with the β-substituted compound. A composition of H-associate meso-triphenylcorrole – DMF (1-1) and interaction energy of its components in solid state has been determined. An H-associate composition in a solution depends on a medium polarity. The decreasing medium polarity results in increasing solvent molecules number.

Key words: corroles, aromaticity, solvent activation of NH bonds, absorption and fluorescence spectra, Stokes shift, NMR spectroscopy, thermogravimetry, composition of proton transfer complexes, evaporation enthalpy

N.V. TUKUMOVA, T.R. USACHEVA, CHAN TKHUAN, V.A. SHARNIN
INFLUENCE OF COMPOSITION OF AQUEOUS-ETHANOL SOLVENT ON STABILITY
OF COMPLEXES OF MALEIC ACID AND NICKEL (II) IONS

A composition and stability of nickel (II) ions has been determined for aqueous- ethanol solutions with various ethanol content ($X_{EtOH} = 0 - 0.7$ mol.d.) by means of potentiometric titration at 298 K and $I=0.1$ (NaClO₄). The increase in ethyl alcohol content in solution results in the increase in complexes stability. The results obtained have been compared with the literature data on related compounds.

Key words: coordination compounds, stability constants, solvation contribution, maleic acid

Yu.V. POLENOV, E.V. EGOROVA, A.V. NIKOLAEV
REDUCTION KINETIC OF 4- NITROSODIPHENYLAMINE BY SODIUM HYDROXYMETHANE-
SULFINATE IN BYNARY SOLVENT DIMETHYLSULFOXIDE – WATER

The kinetic of reaction of interaction between 4- nitrosodiphenylamine and sodium hydroxymethanesulfinate in bynar solvent dimethylsulfoxide - water has been investigated. An order of reaction on the 4- nitrosodiphenylamine and reaction rate has been discovered to change at a changing solvent composition. At DMSO content higher 0.3 mole fraction in the binary solvent the kinetics of reaction under study has been shown can describe in the frame of method of quasy-stationar approach.

Key words: 4- nitrosodiphenylamine, 4- aminodiphenylamine, sodium hydroxymethanesulfinate, dimethylsulfoxide, kinetics

A.A. YAKOVLEVA, M.A. BOCHAROVA
INFLUENCE OF SOME SURFACTANTS ON STABILITY OF TALK SUSPENSIONS

Quantitative parameters of process of precipitate forming in the talc-sodium oleat, talk-Penta 416 systems are presented. The influence of surfactants both on the precipitate height and sedimental stability of talk suspensions has been shown. The analysis of surfactant action on the change of dispersion size has been presented.

Key words: talc, suspension, dispersive analysis, stability, optical characteristics, turbidimetry, turbidity, wave index n , surfactants

E.I. YARMUKHAMEDOVA, Yu.I. PUZIN, Yu.B. MONAKOV
RESEARCH OF METHYL METHACRYLATE POLYMERIZATION IN PRESENCE
OF 1,3,5-TRIMETHYL-HEXAHYDRO-1,3,5-TRIAZINE

The influence of 1,3,5-trimethyl-hexahydro-1,3,5-triazine on a radical polymerization of methyl methacrylate has been studied. Kinetic parameters of the process (orders, polymerization activation energy) have been determined. The triazine during polymerization has been shown to act as a slight chain transmitter and it interacts with initiator (benzoyl peroxide) forming initiating system. The polymer synthesized in the presence

of 1,3,5-trimethyl-hexahydro-1,3,5-triazine has been discovered to have a heightened content of syndio and isotactic sequences in macro molecule.

Key words: polymerization, methyl methacrylate, 1,3,5-trimethyl-hexahydro-1,3,5-triazine, polymer microstructure

N.Ch. MOVSUM-ZADE

CALCULATION DETERMINATION OF CYANO BOND LENGTH IN TRIMERYZATION REACTION

Six-member heterocyclic compounds (triazynes) to containing three atoms of nitrogen in cycle (1,3,5-triazine or s-triazine) was obtained by Neve in 1895 but a structure of this compound was established in 1953 only. In given study the initial substituted nitriles and triazines on their base was calculated with the semi-empirical method. For the first time, parameters of that substituted triazines were obtained.

Key words: 1,3,5-triazine, s-triazine, heterocyclic compounds, substituted nitriles, bond length, electrons pair, angles between atoms, triazines substitute

A.A. NIKITIN, M.E. KLUEVA

PROTONATION OF MONO- AND DI -ARYL SUBSTITUTED OKTAALCYLPORHPRINS IN BENZENE – ACETIC ACID MIXTURE

The protonation constants of monophenyl-octamethylporphyrin, monophenyl-octaethylporphyrin, diphenyl-octaethylporphyrin, diphenyltetramethyltetra-butylporphyrin, diphenyltetramethyltetra-butylporphyrin have been determined by means of spectrophotometric titration in the benzene – acetic acid medium under the temperatures of 288 – 318 K. The thermodynamic parameters of the processes have been calculated. The basicity sequence of studied porphyrins has been obtained.

Key words: porphyrins, protonation, basicity

R.D. GADZHIEV, I.I. ALIEV, M.B. BABANLY

STRUCTURAL STATE IN ALLOYS (Ti,Hf)₅₀ (Ni,Cu)₅₀ HARDENED FROM LIQUID STATE

Two series of alloys have been studied: A:Ti₃₂Hf₁₈Ni_{50-x}Cu_x (where x= 5; 15; 25 at.%) and B: Ti₃₅Hf₁₅Ni_{50-x}Cu_x (where x= 5; 10; 15 at. %). The temperature of martensite transformation (after crystallization) in four-component rapid hardened alloys (Ti,Hf)₅₀ (Ni,Cu)₅₀ has been established to be higher than in ternary TiNiCu alloys. The size and shape of forming martensitic crystals are largely determined by grain size of the initial phase.

Key words: amorphous alloys, crystallization, martensite transformation, shape memory effect, rapid hardened ribbons

N.T. SHAMILOV

PROMOTING EFFECT AND ROLE OF ANTIMONY IN OXIDATIVE DEHYDROGENATION OF ISO-BUTANE ON SUPPORTED V-Sb OXIDE CATALYSTS

This article describes the problems of the selectivity increase of supported V-Sb oxide catalyst and isobutylene yield as well as a stability of catalytic activity in an oxidative dehydrogenation of iso-butane. The addition of 10 atomic % of antimony to supported catalyst of vanadium oxide has been shown to prevent the coke formation and catalyst deactivation which is explained with formation of new forms of active oxygen on the VSbO/Al₂O₃ catalyst.

Key words: catalyst, isobutene, oxidative dehydrogenation, isobutane, hydrocarbons, catalytic activity

E.G. STEPANOV, M.A. ABRAMOV, D.V. KACHALOV, S.V. VASILIEV

INTERACTION OF LITHIUM CARBONATE WITH MECHANICAL ACTIVATED HEMATITE AT NON-ISOTHERMAL CONDITIONS

The influence of hematite mechano-chemical activation on the interaction process with lithium carbonate has been studied. Marked change in the phase composition of the solid phase synthesis products has been shown. Possible reasons of formation of metastable α -LiFeO₂ mainly are discussed.

Key words: hematite, lithium carbonate, reactivity, fine crystal structure

R.F. SHEKHANOV, S.N. GRIDCHIN

ELECTRODEPOSITION OF COBALT-NICKEL ALLOY FROM SULFATE-OXALATE ELECTROLYTE

The possibility of obtaining cobalt and nickel electrochemical alloys from sulfate-oxalate electrolytes of various compositions has been shown.

Key words: magnetic films, electrolysis, polarization curves

E. V. DOGADKINA, M.G. DONTSOV, V.I. PARFENYUK

TITANIUM CHEMICAL POLISHING. II. INFLUENCE OF SOLUTION CONCENTRATION OF CHEMICAL POLISHING ON PROPERTIES OF PHASE FILM ON TITANIUM SURFACE

The influence of dissolved titanium concentration on electrophysical properties of the phase layers forming on the titanium surface in the process of chemical polishing in solutions on the basis of acid fluorine ammonium and hydrochloric acid hydroxylamine has been investigated. Electrophysical properties of phase films on the titanium surface have been determined on the basis of photopolarization method and impedance spectroscopy. Forming surface phase films have been shown to play an important role in the process of the titanium chemical polishing.

Key words: chemical polishing, titanium, diffusion currents

I.G. ZHIKHAREVA, V.V. SHMIDT, M.A. SHESTAKOV, A.A. PERSHIN

CORROSION STABILITY OF COATINGS WITH INTERMETALLIDE Ni₅Zn₂₁ IN SALT SOLUTIONS

The mechanism of Zn-Ni alloys corrosion containing the γ - phase of intermetallide Ni₅Zn₂₁ and precipitated from chloride-ammine electrolytes in the presence of isomeric additions of amino-benzoic acid (ABA) has been considered. The 2% NaCl solution has been used as an aggressive media. The usage of homogeneous alloys Zn-Ni (γ - phase) has been shown to allow to increase by a factor 10 the corrosion - protective properties comparing with biphasic coatings (γ - phase + η - phase).

Key words: corrosion, structure, intermetallide, alloys

Yu.S. POLIKARPOVA, E.A. RASKATOVA

PHYSICAL AND CHEMICAL CHARACTERISTICS OF POROUS GLASS

In given study the physical-chemical parameters of porous glass such as pore radius, specific surface, and water desorption temperature with surface, change capacity, dissociation constant of silanole groups have been calculated.

Key words: porous glass, Mac-Ben set, potentiometry, derivatography, exchange capacity, adsorption capacity, isotherm, monolayer capacity, specific surface, Tomson equation

M.Yu. KUKIN, T.A. NIKIFOROVA

PHYSICAL AND CHEMICAL PROPERTIES AND OBTAINING FOOD ADDITIVE E329 – MAGNESIUM LACTATE

The article is devoted to studying the solubility and the temperature stability of L and DL-forms of magnesium lactate as well as to development of technology of its obtaining. The received experimental data are of interest because in the literature there are no materials on comparison of properties of L and DL-forms of magnesium lactate. In Russia the technology of magnesium lactate is developed for the first time. The application for the patent has been submitted.

Key words: lactic acid, magnesium, magnesium lactate, properties, obtainig

N.A. KORNILOVA, I.M. LIPATOVA

APPLICATION OF MECHANICAL ACTIVATION OF DRESSING SOLUTIONS AT RECEIVING TEXTILE MATERIAL WITH EXTENDED MEDICAL ACTION

The possibility of hydroacoustic action application implemented in the rotor-impulse devices at receipting chitosan dressing solutions containing a medicinal drug has been studied. Mechanical method of reception of such finishes has been shown to allow regulating a yield rate of drug by a variation of parameters of mechanical treatment of chitosan dressing solutions.

Key words: chitosan, medical drugs, hydroacoustic action, rotor-impulse apparatus

A.V. CHESHKOVA, T.N. BELYAKOVA, M.E. BLINOV

MODIFICATION OF A COTTON PEEL BY ENZYMES

On the base of the complex analysis of data on physical and chemical properties of the cotton peel modified with enzymes and results of spectrophotometry the enzymic hydrolysis of polysaccharides of cotton peel has been revealed to provide a liberation of painting substances of aromatic nature, and, also, fragments of lignine with developed chromophore system and diffusion them into a solution.

Key words: polysaccharide, lignin-polysaccharide complex, enzyme, lignin- carbohydrates complex, delignification, spectrophotometer

P.A. MUZALYOV, I.D. KOSOBUDSKIY, N.M. USHAKOV, D.M. KUL'BATSKIY
OBTAINING NANOCOMPOSITE MATERIALS WITH POLYHYDROXYETHYLMETHACRYLATE MATRIX (PHEMA) AND SILVER PARTICLES FOR OPTICAL COATINGS

Silver nanoparticles have been obtained in a polyhydroxyethylmethacrylate matrix by the photochemical reduction method. By X-ray diffraction it has been found out that the synthesis process results in metallic silver phase formation against the X-ray amorphous polymer matrix background. By the atomic-force and optical spectroscopy it has been confirmed that the coatings based on synthesized nanocomposites are characterized by high homogeneity and low light absorption and that coatings can be used in optics.

Key words: optical coatings, antireflection, polyhydroxyethylmethacrylate, silver, nanoparticle

I.V. POSTNIKOVA, V.N. BLINICHEV, S.G. FROLOV
CALCULATION OF PARTICLES MILLING PROCESS AT THEIR COLLISION IN COUNTERFLOW JETS

The process of solid material particle milling at their collision in counterflow two-phase high speed jets in a fluidized-bed layer is considered. The problem on particle collision probability in milling core has been analyzed in detail. The expression for determination of solid particle concentration for any cross-section of two-phase jet has been given. The algorithm of grain-size composition determination of particles after their milling at collision of two counterflow high speed two-phase jets is considered.

Key words: collision probability, milling probability, two-phase jet, jet torch, torch core, particle granulometric composition, matrix model

D.A. KIRILLOV, V.V. ELIZAROV, D.V. ELIZAROV
OPTIMIZATION OF DEGASSING PROCESS OF RUBBER CRUMB WITH METHOD OF RECONSTRUCTION OF UNIT INTERNAL DEVICE

The rubber crumb saturated with the methyl chloride and non-polymerized hydrocarbons is heterogeneously distributed on unit- disintegrator. Experimental results on rubber solid particle distribution in water medium for vessels of various constructions of mixing devices are given. The digital modeling methodology of turbulent mode hydrodynamics of dispersion phase in FLUENT program for vessels without reflective barriers has been described. The estimation of mass-transfer parameters of substance from crumb surface is given.

Key words: degasser, mass-transfer coefficient, rubber crumb, pseudo laminar boundary layer, methyl chloride

E.S. BOBKOVA, V.I. GRINEVICH, N.A. IVANTSOVA, A.A. ISAKINA, E.Yu. KVITKOVA, V.V. RYBKIN
COMPARATIVE STUDY OF DECOMPOSITION KINETICS OF PHENOL AND SOME SURFACTANTS IN AQUEOUS SOLUTIONS IN DIELECTRIC BARRIER DISCHARGE OF ATMOSPHERIC PRESSURE IN OXYGEN

The decomposition process of phenol, laurylsulphate and sulphonol in its aqueous solutions under the action of dielectric barrier discharge of atmospheric pressure in oxygen in a reactor of flow type has been studied. Kinetics dependencies of concentration of mentioned substances on residence time of solution with discharge zone as well as the same dependencies for concentrations of main destruction products have been obtained. On the base of that data the destruction process rates have been found. The decomposition efficiencies of substances have been compared.

Key words: decomposition kinetics, dielectric barrier discharge, oxygen, phenol, laurylsulphate, sulphonol

I.P. VERSHININA
RESEARCH OF RHEOLOGICAL PROPERTIES OF CELLULOSE NITRATE SOLUTIONS AT CONDITIONS OF COMPLEX STRESS SHEAR FLOW

The rheological characteristics of cellulose nitrate solutions have been studied on a rotational viscometer and on constant pressure capillary viscometer. The structural and mechanical characteristics, rheological constants and values of the slip coefficients have been determined.

Key words: rheological studies, cellulose nitrate solutions, structural and mechanical characteristics, rheological constants, near wall slipping, slip coefficient