

A B S T R A C T S

T.G. VOLKOVA, Ya.A. IVANENKOV, K.V. BALAKIN, N.A. MAGDALINOVA, M.V. KLYUEV
VIRTUAL SCREENING OF ORGANIC COMPOUNDS: THEORETICAL AND PRACTICAL BASES OF METHODOLOGY

The article shows the review of studies reflecting the modern state of studies in the field forecast of pharmaceutical properties of chemical compounds including an algorithms application allowing to analyze complex dependencies between compounds properties and their structural peculiarities.

Key words: biological activity, Schiff base, "structure - property" relationship

A.I. MOSKALENKO, A.Yu. CHASHCHIN, Yu.V. SHAPKIN, V.I. BOEV
SYNTHESIS OF N-ACYL AND N-SULFONYL-SUBSTITUTED 3-AZABICYCLO [3.3.1] NONAN-9 ONE

At treatment of N-tert-butoxycarbonyl-3-azabicyclo[3.3.1]nonane-9-one with saturated solution of hydrogen chloride in water-free dioxane the hydrochloride of 3-azabicyclo[3.3.1]nonane-9-one was obtained the interaction of which with anhydrides, chlorine anhydride of carboxylic and sulfo acids the N-substituted amides and sulfonylamides of 3-azabicyclo[3.3.1]nonane-9 one were formed.

Key words: synthesis, N-acyl and N-sulfonyl-substituted of 3-azabicyclo[3.3.1] nonan-9 one, amide, piperidine fragment, organic synthesis

Zh.V. CHIRKOVA, S.I. FILIMONOV, M.N. VORON'KO, I.G. ABRAMOV
SYNTHESIS OF 2-SUBSTITUTED BENZOXAZOL-5,6-DICARBONITRILES

Methods of synthesis of new aliphatic, aromatic and heterocyclic substituted of 2-R-benzoxazol-5,6-dicarbonitriles were developed and their structure was determined.

Key words: 4-amino-5-hydroxyphthalonitrile, amides, 2-R-benzoxazol-5,6-dicarbonitriles

Zh.V. CHIRKOVA, S.I. FILIMONOV, P.A. KHORN, I.G. ABRAMOV, S.I. FIRGANG, G.A. STASHINA
SYNTHESIS OF NOVEL SUBSTITUTED BENZOFURO [3,2-C]PYRIDINE-7,8-DICARBONITRILES

New substituted benzofuro [3,2-c]pyridine-7,8-dicarbonitriles and their N-oxides based on 3-substituted 2-dimethylaminovinylbenzofuran-5,6-dicarbonitriles were synthesized.

Key words: 3-substituted 2-dimethylaminovinylbenzofuran-5,6-dicarbonitriles, ammonia, hydroxylamine, benzofuro[3,2-c]pyridine N-oxides, benzofuro[3,2-c]pyridines

L.V. YEMELYANOVA, A.V. KALACH, V.F. SELEMENEV, V.Yu. KHOKHLOV

DETERMINATION OF PYRIDOXINE IN SOLUTION BY METHODS OF PIEZOELECTRIC MICRO WEIGHING AND UV-SPECTROSCOPY

The method for determination of pyridoxine in water solutions by the sensor method in the concentration range of 10^{-5} - 10^{-3} mol/dm³ is offered. Comparison of determination methods of pyridoxine by piezoelectric weighing method and UV spectroscopy was carried out.

Key words: pyridoxine, sensor, UV-spectroscopy

K.A. KULIYEV, N.A. VERDIZADE, U.B. ABASKULIYEVA
SPECTROPHOTOMETRIC STUDY OF TITANIUM (IV) COMPLEXES WITH 2,4-DITHIOL-4-TRET-BUTYLPHENOL AND AMINOPHENOLS

Different-ligand complexes (DLC) of titanium (IV) with 2,6-dithiol-4-tretbutylphenol (DTBPh) and aminophenols (APh) were studied with spectrophotometric method. The maximum extraction degree of different-ligand complexes was observed at pH 1.8-3.8. Optimal conditions for formation and extraction of different-ligand complexes were found. Optimal ratios of components were established. Methods of extraction-photometrical titanium determination were developed in metal aluminum and artificial mixture.

Key words: different-ligand complexes aminophenol, extraction, chloroform, titanium, solvent

S.A. SHAPOVALOV, Ya.A. SVISHCHOVA
HETEROGENEOUS ASSOCIATION OF ALIZARIN RED S ANIONS IN AQUEOUS SOLUTION

The formation of associates between one or two charged anion of alizarin red S and cation of cyanine dye pinacyanol was considered in aqueous solutions. The thermodynamical values of equilibrium constants of association were determined on the base of spectrophotometric data. The geometric and energetic parameters of associates were calculated. A destructive influence of ionic surfactants on the associates was established.

Key words: alizarin red S, association, solution, dye, pinacyanol, absorption spectra, formation enthalpy, ionic surfactants

V. Yu. ORLOV, A.D. KOTOV, A.V. TSIVOV, K.V. ANDREEVA
**QUANTUM-CHEMICAL MODELING CYCLIZATION STEP OF 2,1-BENZISOXAZOLE
FORMATION PROCESS**

The cyclization step of 2,1-benzisoxasolic cycle formation in a process of para-nitrochlorinebenzene interaction with phenylacetonitrile was investigated using non-empirical quantum chemical modeling methods both for isolated molecular structure and with consideration of solvent effect. On the base of obtained data the conclusion on the formation mechanism of mentioned heterocycle was done.

Key words: quantum-chemical modeling, hydrogen nucleophilic substitution, 2,1-benzisoxazole, limiting step, cyclization

E.K. KOPKOVA, P.B. GROMOV, E.A. SHCHELOKOVA
DENSITY, VISCOSITY AND SPECIFIC CONDUCTIVITY OF HYDROCHLORIC EXTRACTS OF MONOATOMIC HIGH-MOLECULAR ALIPHATIC ALCOHOLS IN HCl - C₅-C₁₀ ALCOHOLS-WATER SYSTEM AT 20 °C

The data on a equilibrium distribution of hydrochloric acid between water and organic phases in a process of hydrochloric acid extraction-reextraction with a monoatomic high-molecular aliphatic alcohols ROH (R=C₅-C₁₀) are presented. The density, viscosity and specific conductivity of saturated hydrochloric acid-alcohole extracts depending on the system composition were determined at 20°C.

Key words: hydrochloric acid, extraction, reextraction, monoatomic high-molecular aliphatic alcohol, density, viscosity, specific conductivity

G.I. ZAMALDINOVA, S.N. PARFYONOVA, A.I. GARKUSHIN, I.K. GARKUSHIN
ANALYTICAL DESCRIPTION OF CHARACTERISTICS OF LOW-MELTING COMPOSITIONS A NUMBER OF NaCl - MCl (M – K, Rb, Cs) AND CALCULATION OF EUTECTIC CHARACTERISTICS IN SYSTEM NaCl – FrCl

Temperatures and compositions changes of double systems a number of NaCl - MCl (M – K, Rb, Cs) are presented in analytical form as a function of crystal-chemical, thermodynamic and energetical parameters of M⁺ ions and chlorides. Calculation data of eutectic parameters are given for NaCl – FrCl system.

Key words: eutectic, chlorides, alkaline elements, correlation factor, calculation, forecast, root-mean-square deviation

M.M. GAFUROV, K.Sh. RABADANOV, M.B. ATAEV, A.R. ALIEV, S.A. KIRILLOV, V.D. PRISYAZHNIY
SPECTROSCOPIC INVESTIGATION OF STRUCTURAL AND DYNAMIC PROPERTIES AND SALVATION PROCESSES IN LiNO₃ – (CH₃)₂ SO₂ SYSTEM

Binary LiNO₃ – (CH₃)₂ SO₂ system was investigated by a vibrational spectroscopy method. Data on some structural-dynamic properties and salivation processes were obtained on the base of comparative analysis of vibrational bands profiles in Raman and IR absorption spectra. Correlations between composition and ion conduction of LiNO₃ – (CH₃)₂ SO₂ system were revealed.

Key words: ionic system, vibrational spectroscopy, molecular relaxation

A.K. FRIESEN, S.L. KHURSAN, Yu.B. MONAKOV
DFT STUDY OF INTERACTION BETWEEN TETRAPHENYLPORPHYRIN AND BENZOYL PEROXIDE

The interaction between tetraphenylporphyrin and free radical polymerization initiator – benzoyl peroxide – was investigated by means of density functional theory with PBE/3ζ method. The structure of charge-transfer complex formed was established and the reasons of the accelerating action of tetraphenylporphyrin upon the benzoyl peroxide decomposition were analyzed.

Key words: density functional theory, free radical polymerization, tetraphenylporphyrin, benzoyl peroxide, charge-transfer complex, methyl methacrylate

A.A. DURGARYAN, R.A. ARAKELYAN, N.A. DURGARYAN
SYNTHESIS AND INVESTIGATION OF amino-, azo- AND p-PHENYLENE GROUP CONTAINING POLYMERS

For the first time, polymers with different content of N-acetyl groups in the main chain were synthesized through classic methods, and were characterized by ¹H-nuclear magnetic resonance, UV-vis, ESR, Fourier transform infrared spectroscopy and electrical conductivity measurements. Poly(azo-1,4-phenylenimino-1,4-phenylene) was obtained by the reduction of 4,4'-dinitrodiphenylamine with zinc and poly(azo-1,4-phenylenacetylmino-1,4-phenylene) was synthesized by the diazotization of 4,4'-diaminodiphenylamine and subsequent coupling with N-acetyldiphenylamine.

Key words: azopolymers, N-acetylated polymers, azocoupling, reduction, electric conductivity, doping, ESR spectra

N.Ch. MOVSUM – ZADE
ESTIMATION OF TERMODINAMIC PARAMYTERS OF ACRYLONITRIL SYNTHESYS REACTION WITH QUANTUM-CHEMISTRY METHODS

Methods of synthesis of acrylonitril based on oxygen containing hydrocarbonss were presented. Early, syntheses of nitril derivatives were presented and parameters of these compounds were calculated by quantum-chemistry methods

[1-4]. Quantum-chemical methods with density functional using and basis set of program PRIOPDA [5,6] the thermodynamic parameters were determined. Comparisons of thermodynamic preferences of reactions of acrylonitril synthesis were carried out.

Key words: acrylonitrile, oxygen containing compounds, thermodynamic parameters, quantum – chemistry methods

R.Z. DEYANOV, A.A. ISHCENKO, A.I. KAMENEV, A.M. LEBEDEV, B.M. SCHEDRIN

NEW METHOD OF COMPONENTS DETERMINATION OF OVERLAPPING ANALYTICAL SIGNALS. I. INVERSION VOLTAMMETRY

New approaches to the modeling analytical signals based on combined Tikhonov regularization method and cumulant analysis of random non-Gaussian processes allowing selecting a background line, determining and refining parameters, and resolving overlapping peaks were proposed. The efficiency of the developed procedure for the analysis of inversion voltammetric measurements of analytical signals for Cd (II), Cu (II) and Pb (II) pollutants of natural water on mercury-graphite electrodes was demonstrated.

Key words: analytical signals, modeling, Tikhonov regularization method, cumulant analysis, inversion voltammetry, mercury-graphite electrodes

M.G. ABBASOV, G.Z. SULEYMANOV, A.A. MEDZHIDOV

COMPLEXES OF Ln(III) (Y, La, Ce, Nd, Sm, Er, Yb, Lu) WITH REDUCED SCHIFF BASES

The data on coordination compounds of Ln(III) with Schiff bases hydrogenated on azomethine group with N,N'-bis-(2-hydroxybenzyl) (H₂L¹), N,N'-bis-(2-hydroxy-5-bromobenzyl)(H₂L²)ethylenediamine, N,N'-bis-(2-hydroxybenzyl)-(H₂L³), N,N'-bis-(2-hydroxy-5-bromobenzyl)(H₂L⁴), N,N'-bis-(2-hydroxy-5-nitrobenzyl)(H₂L⁵), piperazineones are given. Obtained complexes were studied with IR and electron spectrometry, thermogravimetry and magnetochemistry.

Key words: hydroxybenzyl, lanthanide complexes, azomethine group, hydrogenated ligands

A.V. OKHLOBYSTINA, E.V. SHINKAR, A.O. OKHLOBYSTIN, N.T. BERBEROVA, V.F. ABDULAEVA

CATION-RADICALS OF *p*-PHENYLENE DIAMINES IN SULFURORGANIC COMPOUNDS SYNTHESIS

The usage ability of 1,4-phenylenediamine and N,N,N',N'-tetramethyl-1,4-phenylenediamine as electron transfer electromediators from hydrogen sulfide and thiols for reactivity rising and their syntheses with olefins and aromatic compounds was considered. N,N,N',N'-tetramethyl-1,4-phenylenediamine showed properties of effective electromediator whereas the 1,4-phenylenediamine irreversibly reacts with sulfurorganic compounds forming alkyl-thio-2,5diamino-benzenes in the case of thiols and 3,7-diaminophenothiazine in the case of hydrogen sulfide.

Key words: electron transfer, hydrogen sulfide, thiols, 1,4-phenylenediamine, N,N,N',N'-tetramethyl-1,4-phenylenediamine, electrochemical oxidation, 3,7-diaminophenothiazine, 1,4-phenylenediamine thioderivatives, radical-cation

E.S. BOBKOVA, V.I. GRINEVICH, A.A. ISAKINA, V.V. RYBKIN

KINETIC MODEL OF FORMALDEHYDE DESTRUCTION IN AQUEOUS SOLUTION IN DIELECTRIC BARRIER DISCHARGE OF ATMOSPHERIC PRESSURE IN OXYGEN

The decomposition kinetics of formaldehyde aqueous solution and main product of its decomposition (CO₂) was studied in flow reactor of dielectric barrier discharge of atmospheric pressure in oxygen. On the base of these data the processes scheme was offered. The calculation on proposed scheme describes well the data on formaldehyde decomposition kinetics and products formation kinetics.

Key words: formaldehyde, decomposition, dielectric barrier discharge, oxygen, modeling

N.V. GOLOVNYKH, V.A. BYCHINSKIY, K.V. CHUDNENKO, A.G. PIKHTOVNIKOV, I.I. SHEPELEV

THERMOCHEMICAL METHOD OF COMPLEX UTILIZATION OF GYPSUM-ANHYDRIDE WASTES IN PRODUCTION OF ALUMINA AND BY-PRODUCT

A resource-saving technology of mixture sintering allowing decreasing a limestone consumption at alumina production and increasing a production of by-product (potassium sulfate) was developed. The effect is reached due to a usage the gypsum-anhydride wastes of alumina production. This results in the decrease of wastes for store and in reducing hazardous impact on environment.

Key words: gyps-anhydrite wastes, alumina production, physico-chemical studies, limestone, industrial testing, potassium sulfate

S.V. LANOVETSKIY, V.A. TIKHONOV, V.Z. POIYLOV

STUDY OF HYDROLYSIS PROCESS OF TITANIUM CHLORIDE SOLUTION IN PRESENCE OF ORGANIC ADDITIVES

Features of hydrolysis process of titanium chloride solution in the presence of organic additives were studied. The influence of sedimentation pH, suspension ripening time, component initial concentrations and organic additives on phase-formation and structure of titanium hydroxide was established. The size control ways of titanium hydroxide particles as precursor of TiO₂ were determined.

Key words: titanium hydroxide, hydrolysis, titanium chloride solution, surfactants

R.N. SHAKHMAEV, A.U. ISHBAEVA, V.V. ZORIN
Pd-CATALYZED SYNTHESIS OF 1-[(2E, 4E)-DODECA-2,4-DIENOYL]PIPERIDINE

The stereoselective synthesis of natural alkaloid from Piper nigrum, 1-[(2E, 4E)-dodeca-2,4-dienyl]piperidine was developed utilizing the non-phosphine Heck reaction.

Key words: 1-[(2E,4E)-dodeca-2,4-dienyl]piperidine, Heck reaction, Piper nigrum

S.S. ROZHKOVA, K.L. OVCHINNIKOV, A.M. KURMANOV, A.V. KOLOBOV
ASSESSMENT OF ANTIOXIDANT ACTIVITY OF COMPOUNDS WITH QUANTUM-CHEMICAL MODELING

The possibility of using quantum-chemical methods for assessing the antioxidant activity of compounds was considered. The reliability of the results is confirmed by experimental verification of the effectiveness of antioxidants in mixtures with a rubber SKI-3.

Key words: polymers oxidation, antioxidants, quantum-chemical modeling

Yu.B. RUMYANTSEVA, E.A. KURGANOVA, G.N. KOSHEL, A.A. IVANOVA, A.A. ERSHOVA, V.V. KHRENOVA
INTENSIFICATION OF OXIDATION PROCESS OF CYCLOHEXYLTOLUENE TO HYDROPEROXIDES

The reaction of liquid phase oxidation of cyclohexyltoluene to hydroperoxide was studied in the presence of initiator –isopropylbenzene hydroperoxide and nitrogen-containing catalysts. It was found that at the use of N-hydroxyphthalimide in the temperature range of 110-140 °C the cyclohexyltoluene oxidation rate increases in 2.5-3 times at the hydrocarbon conversion up to 28-30 %. The selectivity of cyclohexyltoluene hydroperoxide formation was 93-95 %

Key words: liquid phase oxidation, cyclohexyltoluene, hydroperoxide cyclohexyltoluene, hydroperoxide isopropylbenzene, N-hydroxyphthalimide, cyclohexylbenzoic acid, selectivity, conversion

A.E. ZAVADSKIY
INFLUENCE OF INTENSIFYING ACTIONS ON MERCERIZATION KINETICS OF HYDROPHOBIC FABRICS

With methods of X-ray diffraction analysis and scanning electron microscopy the efficiency of preliminary processing raw cotton fabrics for increasing the rate of polymorphous transition of cellulose and uniformity of morphological changes of fibers across the volume of textile materials was shown. The process is based on the pre-treatment of cotton fabric in boiling water with subsequent cooling directly in solution of sodium hydroxide.

Key words: cellulose fibers, mercerization, X-ray diffraction analysis, scanning electron microscopy, polymorphous transition

O.I. BOYKOVA, N.V. ZAVYALOVA, S.M. SMIRNOV, S.G. ALEKSEEV, E.P. KHARITONOVA, Yu.M. ATROSHCHENKO, E.L. VULAKH, K.I. KOBRAKOV
SYNTHESIS OF 5(6)-AMINO-2-(4-AMINOPHENYL) BENZIMIDAZOLE WITH CYCLODEHYDRATION OF 2',4',4'-TRIAMINOBENZANILID IN WATER SULFURIC ACID

The possibility of creation of effective low-wasted technology of high purity 5(6)-amino-2(4-aminophenyl) benzimidazole production from 2',4',4'-triaminobenzanilide was studied by means of accomplishing cyclodehydration in water sulfuric acid with recycle of sulfuric acid solutions.

Key words: 5(6)-amino-2-(4-aminophenyl)benzimidazole, 2',4',4'-triaminobenzanilide, cyclodehydration, technology

O.V. MANAENKOV, A.A. KAMENCHSHIKOV, O.V. KISLITSA, Yu.V. STEPANENKO, M.G. SUL'MAN
RESEARCH OF CHITOSAN OLIGOMERS PRODUCTION POSSIBILITY VIA LOW-FREQUENCY ULTRASOUND

In this paper the data on investigation of the chitosan biologically active oligomers production possibility via low-frequency ultrasound treatment of polysaccharide solutions are presented. The dependence of chitosan macromolecules degradation degree on its solution concentrations, ultrasound intensity and time of ultrasonic treatment were considered.

Key words: ultrasound, chitosan, oligomers, macromolecules destruction

F.M. NASIRI, F.A. KULIYEV, A.D. EFENDI, R.S. SULTANOVA, T.A. ISMAILOVA, T.A. SHIKHLINSKAYA
MANIFESTATION OF PROPERTIES OF DITHIOCARBAMATE AND THIOAMIDE IN HYDROCARBONS OXIDATION PROCESS

With the aim of study of antioxidant action of dithiocarbamate (K_1) and thioamide (K_2) in the oxidation process their ability to chain interrupt was studied for the reaction with peroxide radicals. The antioxidative activity of interaction products of compounds under study with tertiary butyl-hydroperoxide was investigated. It was determined that the oxidation products were established to possess higher inhibiting properties than initial ones. In the process of oxidative transformations of initial compounds the new compounds which are more active acceptors of free radicals are formed. The f_k – parameter which characterizes the activity of inhibitor was studied.

Key words: thermo-oxidative degradation, carbamate and thioamide, antioxidant additives, alkylated phenols, aromatic amines, sulfur-organic compounds

D.I. MISYULYA

DETERMINATION OF PRESSURE LOSSES CONNECTED WITH ROTARY MOVEMENT OF FLOW AT CYCLONE OUTLET

In given article results of experimental researches of gas speeds distribution in an exhaust pipe of the most widespread types of cyclones CN-11 and CN-15 are given. On the base of these data theoretical calculations were carried out on determination of relative pressure losses connected with rotation of gas flow at arraratus outlet. For cyclones CN-11 and CN-15 these losses were 29–30% and 27–28% respectively from the general losses.

Key words: cyclone, pressure losses, hydraulic resistance, power inputs

V.E. MIZONOV, P.V. YAKIMYCHEV, V.A. ZAITSEV, N.N. YELIN

MODELING OF CONTACT UTILIZER OF HEAT OF EXHAUST DRYING AGENT

A cell mathematical model for calculation of distribution of heat carrier parameters in a contact heat exchanger in transient and steady- state regimes was proposed. The basic part of heat coming to heated water was shown to be the heat of moisture condensation from air-vapor mixture. The model operates on the universal algorithmic basis and allows solving various problems of contact heat and mass transfer.

Key words: cell model, heat and mass transfer, condensation, state vector, transition matrix

V.V. VLASOV, M.E. SOLOVYOV

SET-UP FOF RUBBER FRICTION PROPERTIES DETERMINATION OF LIQUID MEDIUM

The new method for estimation of rubber friction properties depending on test conditions was proposed on special set-up allowing to study rubbers parameters at friction on dry model surface, at friction on wet surface and at friction in water medium.

Key words: method, rubber, friction properties, contact pressure, friction coefficient

E.A. VERSHININA, D.G. KIM

UNUSUAL HALOGENOCYCLIZATION OF 2-(2-BROMOALLYLTHIO) QUINOLINE

Bromination of 2-(2-bromoallylthio) quinoline leads to 2-bromomethylthiazolo [3,2-a]quinolinium bromides.

Key words: 2-quinolinethione, 2,3-dibromine-1-ene, 2-(2-bromoallylthio) quinoline, 2-bromomethylthiazolo[3,2-a]quinolinium bromide

M.V. CHELNOKOVA, D.V. BELOV, T.N. SOKOLOVA, V.F. SMIRNOV, A.A. KALININA, V.R. KARTASHOV

GENERATION SUPEROXIDE ANION-RADICAL BY MICROSCOPIC FUNGI AND ITS ROLE IN CORROSION OF METALS

The ability of microscopic fungi to generation of superoxide anion-radical ($O_2^- \cdot$) which increases in series Alternaria alternata > Fusarium moniliforme > Penicillium ochro-chloron was revealed. Correlation between ability of microscopic fungi to emission in environment $O_2^- \cdot$ and their corrosion activity with respect to zinc is qualitatively established.

Key words: superoxide anion-radical, microscopic fungi, metals biocorrosion

E.E. FROLOVA, N.V. KAMKINA, S.V. KRASNIKOV, T.A. OBUKHOVA, A.F. BETNEV

SYNTHESIS OF DERIVATIVES BASED ON ACYLSUBSTITUTED AROMATIC CARBOXYLIC ACIDS

The method of synthesis of p-acylsubstituted benzoic acids based on liquid-phase oxidation reactions of p-acylsubstituted toluenes was developed. The ways of obtaining various derivatives which are interest as bio-active substancies on the base of the oxidation products are shown.

Key words: liquid-phase oxidation, p-acylsubstituted toluenes, p-acylsubstituted benzoic acid

G.I. KOSTRYKINA, T.N. SUDZILOVSKAYA, M.A. KOKOREVA, I.A. BORODIN

MODIFIERS OF ADHESION TO BRASS STEEL CORD WITH LOWERED CONTENTS OF COBALT

New adhesion modifiers were synthesized on the base of product GO with the lower contents of cobalt. In comparison with known modifiers the obtained modifiers have the best solubility in rubbers. They provide lower hysteresis losses of rubber and a high level of adhesion to brass steel wire cord.

Key words: modification, adhesion activators, viscoelastic and strength properties