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(inorganic, organic, analytical, physical, colloid
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CHEMICAL TECHNOLOGY

(inorganic and organic substances.

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A B S T R A C T S

*P.B. RAZGOVOROV***MODIFICATION OF WATER-SOLUBLE SILICATES BY ORGANIC ADDITIVES**

The actuality of studying the water-soluble silicate systems modified by introduction of organic additives was shown. Throughout last half a century the analysis of works of the domestic and foreign scientists studying questions of creation of new composite materials on the base of water-soluble silicates for the chemical industry and building industry was presented.

Key words: water-soluble silicates, liquid glasses, inorganic additives

*O.V. MATVEEVA, N.V. LAKINA, V.Yu. DOLUDA, E.M. SULMAN***CURRENT TRENDS OF APPLICATION OF OXYREDUCTASES IN INDUSTRY**

Oxydoreductases are the class of enzymes widely used in pharmaceutic, food and biotechnology industries, medicine and analytical chemical as efficient and environmentally friendly biocatalysts for oxidation-reduction reactions. In given review the current trends of application of laccases, peroxydases and glucooxydases were presented.

Key words: biocatalysts, oxydoreductase, biotechnological methods, immobilization

*G.Kh. KHODZHAEV***POSSIBILITY OF USE WITH CHELATE-FORMING GROUPS OF AMINO DERIVATIVES IN LIGAND-EXCHANGED REACTIONS WITH HEXACARBONYLE DERIVATIVES OF MOLYBDENUM AND CHROMIUM**

In this article the experimental data are given on the reaction study between the amine derivatives of 1-allyl-4-propargyl-oxybenzene, $\text{CH}_2=\text{CH}-\text{CH}_2\text{C}_6\text{H}_4\text{OCH}_2-\text{C}\equiv\text{C}-\text{CH}_2\text{NR}_2$ ($\text{R}=\text{CH}_3, \text{C}_2\text{H}_5$), and hexacarbonyles of molybdenum and chromium which reacting in CH_3CN medium result in a new mono nuclear mixed ligand-derivatives of these metals

The obtained complexes are characterized by ^1H NMR, IR, UV adsorption methods. Thus from the reactants only one molecule of the organic ligand is included to composition of forming complexes.

Key words: molybdenum and chromium hexacarbonyles, mononuclear metal-carbonyle complexes, mixed-ligand derivatives, chelate-forming ligand

*E.N. KRYLOV, E.A. ZUBANOVA, M.V. BELYAKOVA***QUANTUM-CHEMICAL DFT-INDEXES OF REACTIONARY ABILITY OF POLYMETHYLBENZENES AS DESCRIPTORS OF SELECTIVITY OF BROMINATION REACTION**

The analysis of reaction ability (substrat and position selectivity) was carried out for polymethylbenzenes within the framework of indexes theory of reactionary ability determining on the base of Fukui 's DFT- function as local parameter and global parameters electrophilicity, hardness and softness of aromatic compounds. Dynamic indexes were shown to describe adequately the dynamics of electronodonor ability of polymethylbenzenes in aromatic bromination reactions that corresponds to close to linear correlations of logarithmic anamorphoses of reaction ability (in a form of relative rate constants) and values of appropriated IRA.

Key words: benzene, polymethylbenzenes, bromination, relative reaction ability, Pearson's theory of hard and soft acids and bases, Fukui's function, hardness, electrophilicity, softness

*S.S. ROZHKOV, K.L. OVCHINNIKOV***SYNTHESIS OF ARYLAMIDES AND ESTERS OF (1,2,3,4-TETRAHYDRO-2- OXOQUINOXALINYL-3) ACETIC ACID BASED ON DERIVATIVES OF MALEIC ACID**

The method of synthesis of (1,2,3,4-tetrahydro-2-oxoquinoxaliny-3) acetic acid arylamides was improved. It was shown that the use of (Z)-4-oxo-4-arylamino-2-butene acids in contrast to N-aryl maleimides as starting compounds in these reactions allows to reduce the synthesis by one step and to increases in yield. The possibility of using monoesters of maleic acid for the synthesis of esters of (1,2,3,4-tetrahydro-2-oxoquinoxaliny-3) acetic acid was shown.

Key words: maleinamide, maleinimide, 1,2-phenylenediamine, activated double bond

E.E. ROZAEVA, A.A. ZAGULYAEVA, A.F. BETNEV, I.A. BAZHENOV, T.A. OBUKHOVA
OXIDATION OF TRANS-4-ALKYLCYCLOHEXYL-P-TOLYLKETONES. KINETICS. VALENCE
TRANSFORMATIONS OF CATALYST COMPONENTS. REACTION MECHANISM

The reaction of catalytic oxidation of trans-4-alkylcyclohexyl-p-tolylketones was investigated. The process kinetics was studied. The rate constants of oxidation were calculated. The valence transformations of catalyst components were investigated by a method of electronic spectroscopy.

Key words: liquid-phase oxidation, trans-4-alkylcyclohexyl-p-tolylketones, trans-4-alkylcyclohexanoylbenzoic acids, kinetics, catalyst components valence transformations, reaction mechanism

M.E. SOLOVIEV, E.A. KURGANOVA, Yu.B. RUMYANTSEVA, G.N. KOSHEL, A.S. FROLOV
ANALYSIS OF REACTION THERMODYNAMICS OF OXIDATION OF ETHYL
AND ISOPROPYLBENZENE IN PRESENCE OF N-HYDROXYPTHALIMIDE BY MEANS
OF QUANTUM-CHEMICAL CALCULATIONS

In order to base the role of N-hydroxyphthalimide in the process of oxidation of ethylbenzene and isopropylbenzene to hydroperoxides the quantum-chemical method of density functional theory DFT B3LYP/6-31** using software system Firefly the enthalpies of the reactions of initiation, the reactions of detachment of hydrogen atom from hydrocarbons with the N-oxypthalimide radical and the reaction of interaction of N-hydroxyphthalimide with peroxide radicals of hydrocarbons under study were calculated.

Key words: ethylbenzene, isopropylbenzene, liquid-phase oxidation, N-hydroxyphthalimide

M.A. SALNIKOVA, G.A. PRIGORELOV, S.A. SYRBU, O.A. GOLUBCHIKOV, A.S. SEMEIKIN
SYNTHESIS OF FLUOROALKYL DERIVATIVES OF TETRAPHENYLPORPHYRIN

Perfluoroalkyl substituted tetraphenylporphyrins were synthesized by reaction of tetraphenylporphyrin acylation with active groups in phenyl rings by perfluoroalkyl derivatives. Their spectral properties were studied

Key words: acylation, fluoroalkyl substituted tetraphenylporphyrins

O.A. MAZHAEVA, Yu.V. RUBLINETSAYA, V.V. SLEPUSHKIN, Yu. P. KOVRIGA
COULOMETRIC VERSION OF LOCAL VOLTAMMETRY OF LEAD-STIBIUM ALLOYS

Coulometric version of local voltammetry is considered for lead-stibium thermal alloys. The equation of the calibration curve of dependence of the quantity of electricity on the alloy composition was proposed. This equation was used for developing the standardless method of analysis of heterogeneous lead-antimony alloys.

Key words: local electrochemical analysis, lead-antimony alloy, quantity of electricity

A.S. KONOVALOV, S.A. SMIRNOV, V.V. RYBKIN
WATER MOLECULE INFLUENCE ON ELECTRONS PARAMETERS IN NON-EQUILIBRIUM
AIR PLASMA

The results of calculation of electron energy distribution functions, kinetic and transport parameters of electrons are considered for non-equilibrium air plasma with addition of water molecules. Water molecule additions were shown to influence strongly on electron parameters in a range of reduced electric field strengths E/N of $(1-4) \cdot 10^{-16} \text{ V} \cdot \text{cm}^2$ though then E/N is less than the influence degree is more. The increase in water content results in the decrease in rate constant of process with electron participation, in their average energy and drift velocity.

Key words: air plasma, electron energy function distributions, electron kinetic parameters

T.M. ZIYADOVA, V.A. BURMISTROV, A.S. SEMEIKIN, O.I. KOIFMAN
SPECTRAL MANIFESTATIONS OF COBALT (II) TETRAPHENYLPORPHYRIN OXIDATION
BY MOLECULAR OXYGEN

Oxidation of cobalt (II) tetraphenylporphyrin (Co(II)TPP) by molecular oxygen was studied by UV-Vis. The existence of three complexes in solution was confirmed: μ -peroxodimer (Co(III)TPP-O-O-Co(III)PP (D)), cobalt (II) tetraphenylporphyrin and cobalt (III) tetraphenylporphyrin (Co(III)TPP(Cl)). The absorption peaks of these compounds are 386, 411.8 and 427.4 nm, respectively.

Key words: axial coordination, metalloporphyrin, μ -peroxodimer

A.Yu. SAZONOVA, V.M. RAEVA, A.K. FROLKOVA
COMPARISON OF EXTRACTIVE AGENTS EFFICIENCY AT MIXTURE SEPARATION
OF ACRYLONITRILE AND WATER

For choice of separating agents of extractive rectification it was proposed to analyze diagrams of selectivity isolines. The comparison of extractive rectification was carried out for the mixture of acrylonitrile and

water in the presence of pure and binary agents using digital experiment. The energy consumption on separation including at pressure change was estimated.

Key words: acrylonitrile, water, glycerol, dimethylsulfoxide, extractive rectification, binary separating agent, relative volatility, isoselectivity, energy consumption

E.S. BOBKOVA, A.V. SUNGUROVA, N.A. KOBELEVA

MECHANISM OF PHENOL DECOMPOSITION IN AQUEOUS SOLUTIONS IN DIELECTRIC BARRIER DISCHARGE OF ATMOSPHERIC PRESSURE IN OXYGEN

The process of phenol decomposition in aqueous solution under the action of a dielectric barrier discharge in oxygen for a reactor of flow type was studied. On the base of these results the mechanism of process was proposed the calculations on which describe date on decomposition phenol and formation-loss of products of its transformation.

Key words: discharge, phenol, kinetics modeling

D.I. KIRDYANKIN, N.N. EFIMOV, V.D. DIDENKO, A.A. MELNIKOV, E.A. TYULYUMDZHIEV, E.V. BUSHEVA

PARAMAGNETIC PROPERTIES OF $Cd_{1-x}Zn_xCr_2S_4$ SOLID SOLUTION

The conditions of synthesis of semiconductor spinels $Cd_{1-x}Zn_xCr_2S_4$ were studied as well as a method for preparing their solid solutions was developed. Spinels were prepared on the base of ferromagnetic $CdCr_2S_4$ and antiferromagnetic $ZnCr_2S_4$. The magnetic properties of the samples measured over a wide temperature range (2 - 300 K) on the instrument PPMS-9 are discussed with respect to the paramagnetic region.

Key words: chalcogenide spinel, spin glass

Yu.V. TSAREV, Yu.O. PROKHOROVA, A.N. TROSTIN

RESEARCH OF SENSOR SENSITIVITY OF CARBON MATERIALS MODIFIED BY ZINC OXIDE

Catalysts on the base of carbon, activated coal and zinc oxide were investigated. The existence of minimum of catalyst conductivity was established at the temperature of 60-120°C. The adsorptive properties of carbon materials modified by zinc oxide were investigated. The estimation of the adsorptive characteristics of catalyst samples on the base of Dubinin-Astakhov's equation was carried out. The maximum sensitivity of the catalyst samples to acetone was 1.5.

Key words: gas sensors, conductivity, adsorptive characteristics, sensitivity

A.V. LINDIMAN, L.V. SHVEDOVA, A.P. KUPRIYANOVSKAYA, A.V. NEVSKY

INFLUENCE OF ALIPHATIC CARBOXYLIC ACIDS ON PHYTOEXTRACTION PROCESS OF LEAD AND CADMIUM FROM POLLUTED SOILS

Influence of aliphatic carboxylic acids (acetic, succinic, acrylic, maleic) on migratory ability of lead and cadmium in process of their phytoextraction from polluted soils was studied. It was shown that positive influence of this acids on vegetation stability of the investigated plants which were grown up on soils, contaminated by lead or cadmium, can be related with formation of inactive sedentary forms of lead and cadmium in soil. Rather probable in this case there is enhancement of compensatory effect in a process of plants vegetation, as response protective reaction on toxic action of heavy metals. The process of extraction of lead and cadmium from contaminated soil is influenced in a greater degree not by bond order in an acid molecule, but by carboxylic groups quantity.

Key words: aliphatic carboxylic acids, heavy metals migration, phytoextraction from soil

A.S. VASHURIN, A.A. VORONINA, S.G. PUKHOVSKAYA, I.A. KUZMIN, L.A. KUZMICHEVA, O.A. GOLUBCHIKOV

IMMOBILIZATION OF COBALT TETRASULFOPHTHALOCYANINE ON POLYMER MATRIXES

Hybrid materials containing in their structure cobalt tetrasulfophthalocyanine and polymeric matrix were obtained. The polypropylene matrix plasma chemical activation was shown to result in the immobilization of 80% of macrocycle. At immobilization of phthalocyanine into silicone matrix up to 65% of the macrocycle is fixed.

Key words: metallophthalocyanine, polymer matrixes, surface modification

O.G. TSIRKINA, M.B.ERMOLAEV, A.L. NIKIFOROV
**CLUSTER ANALYSIS OF TEXTILE MATERIALS DIELECTRIC PROPERTIES AT CHANGE
OF CONDITIONS OF THEIR TREATMENT IN FINISHING**

Dependence of dielectric indicators of cellulose-containing fabrics on composition of technological solutions, their components concentrations and initial humidity of materials was analyzed. By means of the cluster analysis the task of multi-dimensional classification was solved. The appropriate structure of task was revealed. For every cluster the mathematic model was created. This model allows to reveal the parameters most acting on dielectric parameters of materials and on efficiency of their heating in the field of currents of high frequency. The degree of action of this influence was determined.

Key words: dielectric properties, tangent of angle of dielectric losses, textile material, cluster analysis, mathematical model

Ya.O. MEZHUEV, S.V. OSADCHENKO, Yu.V. KORSHAK, M.I. SHTILMAN
**SYNTHESIS AND FILTRATION RANGE OF NEW HIGH-PERFORMANCE MEMBRANE
WITH SELECTIVE LAYER BASED ON POLYANILINE-POLY (N-VINYLPYRROLIDONE)**

The new high-performance membrane was synthesized. The chemical structure of selective layer was studied. The membrane filtration range was estimated.

Key words: membrane, nanofiltration, polyaniline, oxydative polymerization, poly-(N-vinylpyrrolidone)

M.Yu. KOLOBOV
ACTIVATION OF EMULSION POLYVINYLCHLORIDE IN DISINTEGRATOR

The results of experimental studies on the activation of the emulsion polyvinylchloride through high-speed loading way in a disintegrator were presented. At processing of PVC in the disintegrator it was shown to take place physical and chemical processes leading both to the increase and to the decrease in polymer viscosity in cyclohexanone. Optimization of processing modes of PVC-E allows acting on proceeding of these processes.

Key words: mechanical activation, emulsion polyvinyl chloride, disintegrator

Ya.O. MEZHUEV, Yu.V. KORSHAK, M.I. SHTILMAN, I.V. SOLOVYOVA, M.A. SALOP, I.Kh. NAGAEV
**KINETICS OF OXIDATIVE POLYMERIZATION OF ANILINE IN AQUEOUS SOLUTIONS
OF POLYETHYLENEGLYCOL**

The effect of polyethyleneglycol on the rate constants and on the activation energies of the steps of oxidative polymerization of aniline in aqueous solutions induced by ammonium persulfate was determined.

Key words: polyaniline, aniline, kinetics, polyethyleneglycol, rate constant, activation energy

V.A. PADOKHIN, Yu.V. KHOKHLOVA, G.A. ZUEVA, E.A. KALABIN
MARKOV MATRIX MODELS OF MECHANICAL DESTRUCTION OF HIGH-MOLECULAR SYSTEMS

On the base of the theory of Markov chains and discrete processes the matrix models of polymer degradation were constructed. An example of using Markov model of destruction for description of the starch macromolecules degradation in a process of its modification was given.

Key words: destruction, mechanodestruction, polymers, mathematical modeling, stochastic Markov process, Markov chains, matrix equations, molecular-weight distribution

E.M. KUVSHINOVA, A.S. SEMEIKIN, S.A. SYRBU, O.A. GOLUBCHIKOV
**SYNTHESIS OF NITRODERIVATIVES OF 5,15-
DIPHENYLTETRAMETHYLTETRAETHYLPORFIN AND FORMATION KINETICS
OF THEIR COMPLEXES WITH ZINC (II) IN ORGANIC SOLVENTS**

The synthesis of nitroderivatives of 5,15-diphenyltetramethyltetraethylporfin was carried out. Reactions of complexation of nitroderivatives of 5,15-tetraethyltetramethyl-diphenylporphyrin with zinc acetate in pyridine and mixed solvent acetic acid-benzene (7:3) were studied. Nitro group in the 5,15-tetraethyltetramethyl-diphenylporphyrin are in meso-positions of the tetrapyrrole macrocycle and (or) the para-positions of the phenyl rings. The rate of formation of zinc complexes in pyridine at the introduction of nitro groups in the 5,15-diphenyltetramethyltetraethylporfin was established to increase in the growth of the deformation degree of the tetrapyrrole macrocycle and the weakening its NH-bonds. In the binary solvent acetic acid-benzene (7:3) the effect of deformation of the macrocycle leads to the decrease in the rate of reaction due to the specific solvation of the reaction site of porphyrin by molecules of acetic acid.

Key words: 5,15-diphenyltetramethyltetraethylporfin nitroderivatives, zinc acetate, macrocycle, pyridine, acetic acid-benzene

T.A. VOROBYOVA, N.V. KOSTINA, D.A. SAVENKOV, A.V. SAVENKOV, A.V. YANKOV
RESEARCHES OF PHYSICAL - MECHANICAL PROPERTIES OF FERTILIZERS BASED
ON AMMONIUM SALPETRE WITH INORGANIC ADDITIONS

In this paper the possibility of introducing into melt ammonium nitrate dihydrate and calcium sulfate semi-hydrate produced of "Knauf Gypsum Novomoskovsk" is studied experimentally. The effect of different ratio of gypsum and semi-hydrate- dolomite on the fertilizer pH, hygroscopic point and the strength of the fertilizer granules was studied.

Key words: ammonium nitrate, gypsum, calcium sulfate semi-hydrate, physical, mechanical and chemical properties

B.R. KISELEV, N.I. ZAMYATINA
INFLUENCE OF GRAIN COMPOSITION OF MAGNESIUM HYDROSILICATE AS MODIFIER
OF LUBRICANT ON FRICTION OF STEEL COUPLE

The grain composition of magnesium silicate obtained with hydrothermal and zol-gel methods was studied. The influence of grain composition of magnesium silicates applying as modifiers of friction of metal plating for steel couple was established.

Key words: friction, lubricate, modifier, grain, steel, sliding coefficient

E.V. FESIK, V.I. ZARAZHEVSKIY, G.D. MALCHIKOV
RHENIUM-CONTAINING CATALYSTS OF NEUTRALIZATION PROCESSES OF EXHAUST
GASES OF CAR. III. FULL-SCALE (BLOCK) SAMPLES OF CATALYTIC CAR NEUTRALIZERS

Results of studies of full-scale samples of (Pd-Re, Pt-Re)-containing catalysts on engine test bench confirmed that efficiency of compositions mentioned above is not inferior to famous industrial samples on the base of Rh, Pt and Pd appropriating to Euro-3 standard. This fact indicates on theoretical possibility of the complete replacement of the expensive rhodium and the partial replacement of platinum and palladium by the cheaper component – rhenium. Composition of Pd-Re seems to us the most preferable from point of view of durability of use of catalyst.

Key words: rhenium, heterogeneous catalysts, platinum metals, catalytic automobile converter

V.I. ELIZAROV, D.V. ELIZAROV, S.G. DYAKONOV
APPROXIMATE METHOD FOR CALCULATING THEORETICAL AND ACTUAL STEPS
OF GAS MIXTURES SEPARATION IN ABSORPTION PROCESSES

A simple method is offered for the approximate calculation of the number of theoretical and the actual steps of gas mixtures separation in absorption processes. At the determination of number of the actual steps of separation the calculation method of step efficiency and device was used on the base of hydrodynamic analogy of processes of transfer of impulse and mass in a bubble layer. The given examples of the calculation of the theoretical and actual separation steps in processes of isothermal and non-isothermal absorption showed a satisfactory agreement of the results obtained with the known data.

Key words: absorption, separation step, efficiency

M.V. VOLKOV, M.YU. TARSHIS, A.I. ZAITSEV
RESEARCH OF GRAIN MATERIALS MIXER OF OPEN TYPE WITH WORKING BLADES

The process of mixing in a mixer of open type with mixing blades is investigated. The mechanisms of process are established. The obtained curves of mixing are approximated with the help of exponents.

Key words: mixer, research, criterion, homogeneity

A.V. VOROSHIN, O.V. CHAGIN, V.N. BLINICHEV
MATHEMATICAL DESCRIPTION OF RECTIFICATION OF BINARY SYSTEMS
IN DISTILLATION COLUMN WITH BATCH VORTEX NOZZLE

In given paper a mathematical description was proposed for the distillation process of water-ethanol mixture in a distillation column with a batch vortex nozzle.

Key words: rectification, mathematical modeling

E.A. DUBKOVA, S.V. NATAREEV, T.E. NIKIFOROVA, I.S. KHARCHENKO
MATHEMATICAL DESCRIPTION OF ION EXCHANGE EXTRACTION OF HEAVY METALS
ON NATIVE AND SYNTHETIC SORBENTS

The sorption of Cu^{2+} ions by native sorbents on the base of topinambour stalks core and linen fibers from CuSO_4 water solution was studied in horizontal device with a stationary adsorbent layer. The comparison

of sorption properties of cellulose-containing sorbents with cationite Lewatit S-100 was carried out. The mathematical model of ion exchange dynamics was proposed and its adequacy to real process was established.

Key words: ion exchange, cellulose-containing sorbent, cationite, output curves

A.V. MITROFANOV, V.E. MIZONOV, A.V. OGURTZOV

TWO-DIMENSIONAL CELL MODEL OF FLUIDIZATION IN NON-UNIFORM GAS FLOW

Two-dimensional Markov chain was used to simulate particles migration and concentration distribution in a fluidized bed. The two-dimensional statement of the problem allows taking into account gas velocity profile and crosswise mixing of material. These factors make it possible to describe internal particles circulation in a fluidized bed.

Key words: fluidized bed, state vector, transition probabilities matrix, concentration distribution, particles circulation

A.N. LABUTIN, V.Yu. NEVINITSYN, A.N. DEVETYAROV

CONTROL SYSTEM OF CHEMICAL REACTOR CASCADE FOR SERIES-PARALLEL REACTION REALIZATION

The paper deals with synergetic synthesis of nonlinear concentration control system of main product in continuous stirred-tank reactor cascade with partitioned feeding of common reagent to units. Concentration control algorithm synthesis is based on method of the analytical design of aggregated regulators.

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

E.P. ROZHKOVA, E.A. VENEDIKTOV

INVESTIGATION OF TEMPERATURE INFLUENCE ON VISCOSITY OF ED-20 EPOXY RESIN

The complex character of temperature dependence of viscosity of ED-20 epoxy resin was established. It was connected with the structural heterogeneity of resin.

Key words: epoxy resin, viscosity, activation energy

V.A. SIRENEK

STUDY OF RELAXATION NATURE OF MASS-TRANSFER IN METALS ON BASE OF DIFFUSION WAVE MODEL

The experimental data on study of diffusion processes kinetics for metals were treated on the base of hyperbolic equation (wave model) which takes into account the relaxation phenomena. Examples of calculation are given.

Key words: mass-transfer, diffusion, metals, wave model