T 55 (2)

#### ХИМИЯ И ХИМИЧЕСКАЯ ТЕХНОЛОГИЯ

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#### ABSTRACTS

## S.P. KOCHETKOV, N.N. SMIRNOV, A.P. ILYIN PROSPECTS OF NANOTECHNOLOGY USE IN PHOSPHATE INDUSTRY AND IN PRODUCTION OF CATALYSTS AND SORBENTS

Taking into account the changes in structure of world production and consumption of fertilizers, pure phosphoric salts as well as the catalysts and sorbent use on different steps of productions mentioned above the prospects of nano-techlogies and nano-compositions applications for such purposes were shown. The application of those technologies allows increasing the environmental and economic efficiency as well as a safety of production. The nano-methods analysis of production was given in the form of review of published papers and developments which were carried out by authors of given report.

**Key words:** mechanochemical synthesis, phosphate raw materials, extraction phosphoric acid, activated carbon, oxide catalysts, disperse-condensation method of production of nano-powder systems

#### S.S. ZLOTSKIY, N.N. MIKHAYLOVA

#### SYNTHESIS AND SOME REACTIONS OF ALKENYL-HEM-DICHLOROCYCLOPROPANES

The conditions of hem.-dichlorocyclopropanes synthesis and the reaction on the base of *hem.*-dichlorocyclopropanes proceeding with the carbocycle decomposition and halogen substitution were considered. The reactions of vinyl- *hem.*-dichlorocyclopropanes on the double bond without affecting the cyclopropane ring were studied. A prospect of application of such kind compounds for organic synthesis was shown.

Key words: hem.-dichlorocyclopropanes, dichlorocarbenation, carbens, hydrogenation, adducts

#### A.M. GRIGORYEV, A.A. MELNIK, L.V. RUDAKOVA CHROMATOGRAPHIC METHODS OF DROTAVERINE DETERMINATION AND IDENTIFICATION OF ITS DERIVATIVES AND METABOLITES IN BIOSAMPLES

Methods of drotaverine determination by GC-MS and HPLC in urine and tissue extracts including the sample preparation with liquid-liquid or solid-liquid extraction were proposed. A number of products of its oxidation and metabolites in biosamples were identified. UV, GC-MS and HPLC characteristics of these compounds are given. Detection limits of drotaverine are 9 and 2 ng/ml for the GC-MS and HPLC, respectively.

Key words: drotaverine, determination, oxidation, metabolites, GC-MS, HPLC, solid phase extraction

#### E.G. KHOMUTOVA, O.I. OSTANINA

# OSMIUM COMPOUNDS CATALYTIC ACTIVITY AT OSMIUM DETERMINATION ON OXIDATION REACTION WITH POTASSIUM BROMATE OF ARSENIT SODIUM AND NEUTRAL RED BY CATALYTIC METHOD

The catalytic activity of osmium solutions in the oxidation reaction of arsenic (III) and neutral red by potassium bromate was studied. It was found that the reaction is catalized as the osmium tetroxide as the potassium hexachlorosmate. The osmium determinition was possible in both forms, and at hexachlorosmate determinition it was not required of osmium separation from a matrix by osmium tetroxide distillation.

**Key words:** osmium, catalytic method, catalytic activity, flow-injection system

#### G.M. KUZ'MICHEVA, M.O. ANTONOVA, M.G. CHERNOBROVKIN, V.I. RUDENKO, D.V. MEL'NIKOV COMPOSITION DETERMINATION OF URINE AND URINARY STONES

### COMPOSITION DETERMINATION OF URINE AND URINARY STONES AND ESTABLISH RELATION BETWEEN THEM

Known methods of determining the composition of urine - biochemical (clinical), and chemical - are compared with each other, and application of urine complex analysis was proposed for the wide use in medical practice. On the base of comparison of urinary stones and urine composition some indicators were revealed showing their relationships and allowing to judge by separate ions about the possibility of stone formation.

**Key words:** urolithiasis, chromatographic methods, urine clinical analysis, chemical analysis, enzymatic analysis

#### O.V. SUROV, M.I. VORONOVA, N.Zh. MAMARDASHVILI, A.G. ZAKHAROV VAPOR PRESSURES OF MACROCYCLIC COMPOUNDS ON DATA OF KNUDSEN EFFUSION METHOD

For the first time the saturated vapor pressures of some macrocyclic compounds were determined with the Knudsen's effusion method in the wide temperature range. The average values of sublimation enthalpies and entropies for temperature ranges under study were calculated.

**Key words:** vapor pressure, sublimation thermodynamics, macrocyclic compounds

#### Yu.V. POLENOV, E.V. EGOROVA

### REDUCTION OF 4- NITROSODIPHENYLAMINE WITH THIOUREA DIOXIDE IN BYNARY SOLVENT DIMETHYLSULFOXIDE – WATER

The kinetic of reaction of interaction between 4- nitrosodiphenylamine (4-NDFA) and thiourea dioxide in bynary solution dimethylsulfoxide - water was investigated. Simultaneously with the reduction of 4-NDFA the interaction of reducer and the dissolved oxygen of air was revealed to proceed with appreciable rate. At the change in the solvent composition the reaction rate was established to change. It is connected with the change in concentrations of decomposition intermediats of thiourea dioxide.

**Key words:** 4-nitrozodiphenylamine, 4-aminodiphenylamine, thiourea dioxide, dimethylsulfoxide, kinetic

# E.N. KRYLOV, L.V. VIRZUM, T.V. SMELOVA, Yu.M. IVANOVA FUKUI FUNCTION AS INDEX OF REACTIVITY OF BENZENE MONOSUBSTITUTED COMPOUNDS IN REACTION OF AROMATIC NITRATION

The analysis of reactivity (substrate and positional selectivity) of benzene mono substituted derivatives was carried out in the frame of theoretical approaches based on the theory of density functional of reactivity index-Fukui function. The given index was shown to describe sufficiently the dynamics of electro donor ability of ortho, metha and para positions of ring that appropriates close to linear correlations of logarithmic anamorphosises of reactivity (in form of factors of partial rates and relative yield of isomeric products of nitration) and values of Fukui functions or their differences, respectively.

**Key words:** monosubstituted benzenes, nitration reactions, relative reactivity, isomer distribution, Fukui function

#### A.SH. TOMUYEVA, B.T. USUBALIEV, D.M. GANBAROV SYNTHESIS AND STRUCTURE-CHEMICAL STUDIES OF CLATRATE COMPOUNDS OF TEREPHTHALATES OF COPPER (II) AND CADMIUM (II)

On the base of complex compounds the clatrates of Cu (II) and Cd (II) with terephtalic acid were synthesized. The obtained crystals were undergone to X - ray, elemental, IR-spectroscopic and derivatographic analysis. On the results of analysis the chemical strutures of clatrate compounds were established.

Key words: complex compounds, terephthalates, synthesis, copper, cadmium

#### A.A. YAKOVLEVA, S.N. CHYONG

#### pH INFLUENCE ON SODIUM OLEATE ADSORPTION ONTO TALC OF ONOTSK DEPOSIT

The dependence of absorbing capacity of Onotsk deposit talc on the pH medium was investigated. A role of H<sup>+</sup> and OH<sup>-</sup> ions in differently characteristic mechanism of the sodium oleate adsorption from aqueous solutions onto this adsorbent was revealed.

Key words: pH action, adsorption, sodium oleate, Onotsk deposit talc, surface tension

### I.V. BRATKOV, N.N. SMIRNOV, T.V. ERSHOVA, N.Yu. BEIYLINA, T.F. YUDINA INVESTIGATION OF MECHANOCHEMICAL OXIDATION OF CARBON MATERIALS

The process of oxidation of graphitized coke was studied. Dependences of interplanar distances on the time and on the amount of inputted energy were established. The degree of graphitization and amount of amorphous carbon was determined.

**Key words:** mechanochemical oxidation, graphitized coke

#### V.V. KUZNETSOV, S.Yu. KLADITI

### PECULIARITIES OF ELECTROCHEMICAL BEHAVIOR OF DIOXYMANGANESE ANODES MODIFIED BY MOLYBDENUM OXIDES

The selective ability of  $MnO_2$ -anode materials containing manganese and molybdenum oxides with respect to the oxygen evolve reaction in chloride-containing solutions was investigated at pH range of 2.0 - 8.0.

The reasons of selective behavior of dioxidemanganase anodes modified with molibdenum oxides in chloride-containing media were dicussed at different pH values. In the presence of Br -ions in solution the MnMoO<sub>x</sub>-anodes were found to lose their selectivity with respect to reaction of oxygen evolving.

**Key words:** anodic behavior, oxide electrode materials, selectivity

#### E.V. KUVALDINA

### TOPOGRAPHIC AND CHEMICAL CHANGES KINETICS ON POLYPROPYLENE SURFACE UNDER ACTION OF ACTIVE OXYGEN

The study results of topographic and chemical changes kinetics on the film polypropylene surface under the action of individual active particles of low temperature plasma of oxygen are presented. The action of metastable oxygen molecules in the state  $O_2(a^1\Delta_g)$  results in both the formation of carbonyl groups in different environment and etching without relief substantial changes. Under the action of oxygen atoms the alcohol groups are formed and destruction occurs via pores formation resulting in the surface roughness increase. An efficiency of these active particles action is grown in the presence of UF - quanta and charged particles.

**Key words:** plasma, oxygen, active particles, polypropylene, topography, modification, infrared spectrum

### S.I. NIFTALIEV, L.V. LYGINA, Yu.S. PEREGUDOV, S.I. BOGUNOV, V.V. KHRIPUSHIN, Yu.V. BAKAEVA

### STUDY OF INFLUENCE OF CHEMICALLY PRECIPITATED CALCIUM CARBONATE DISPERSITY ON PROPERTIES OF POLYVINYLCHLORIDE COMPOSITIONS

The opportunity of a fine-dispersed calcium carbonate application as a filler for compositions on a base of plasticized polyvinylchloride was investigated. The influence of calcium carbonate dispersity and its mass fraction on the main physical-chemical parameters of developed compositions was studied.

**Key words:** chemically precipitated calcium carbonate, compositions on a base of plasticized polyvinylchloride, filler, dispersity

# V.G. STOKOZENKO, M.V. KONYCHEVA, Yu.V. NEMANOVA, A.P. MORYGANOV POSSIBILITY EVALUATION OF COMBINATION OF CHEMICAL MODIFICATION PROCESSES OF HEMP AND JUTE FIBERS AND THEIR DYEING WITH SULFUR AND VAT DYES

On the base of study of reduction properties of systems which are formed at an alkaline treatment of hemp and jute fibers the ground of combination possibility to single step of process of chemical modification and dvening with sulfur and vat dves was done.

**Key words:** hemp fiber, jute fiber, chemical modification, sulfur dye, vat dye

#### A.Yu. APPAZOV, N.V. PYKHALOVA, U.A. BALAMEDOVA

#### MANUFACTURE OF HIGH-QUALITY DIESEL FUELS BY LIQUID EXTRACTION METHOD

In given work, the extractive purification was proposed using N-methylpyrrolidone for refining diesel fuels. For this it is quite enough to subject to extraction the heavy part of initial wide diesel fraction followed by its mixing with appropriate light fraction to bring the value of cetane number, sulfur content and atomatic hydrocarbons in diesel fuel up to the requirements of Euro-3 class.

**Key words:** liquid extraction, diesel fuel, cetane number, aromatic hydrocarbons, sulfur content, N-methylpyrrolidone

### S.V. KAZAK, L.YA. TSARIK, A.V. ROKHIN, A.Yu. FEDORIN RADICAL POLYMERIZATION OF DIETHYL FUMARATE IN PRESENCE OF IONIC LIQUID

Results of radical polymerisation of diethyl fumarate in the presence of the ionic liquid ethylpyridinium bis(trifluoromethylsulfonyl) imide, with initiators -2.2'-azobisisobutyronitrile (AIBN) and benzoyl peroxide (BP) are presented. The dependence of polymer yield on molar ratio of ionic liquid: diethyl fumarate, type and amount of the initiator as well as a duration of process was shown.

**Key words:** ionic liquids, radical polymerization, diethyl fumarate, ethylpyridinium bis(trifluoromethylsulfonyl) imide, NMR spectra

#### O.A. FEDYAEVA

#### HYDROGENATION OF CARBON OXIDES ON SOLID SOLUTIONS OF CdxHg1.xTe

In given study the results of study of catalytic properties of semi conductor materials CdTe and  $Cd_{0,2}Hg_{0,8}Te$  for hydrogenation reactions of carbon oxides are presented. The main hydrogenation product was shown to be formaldehyde. It was shown by the methods of gas chromatography, chemical analysis, IR spectroscopy, electrophysical ones, pH measurements and non- aqueous conductometric titration. The impact me-

chanism of mutial adsorption of  $CO + H_2$  and  $CO_2 + H_2$  with a participation of intermediate compounds in the form of hydrocarbonyles, formyle ligands and formiate structures was confirmed.

**Key words:** adsorption, active sites, adsorption mechanism, catalytic hydrogenation

#### F.F. CHAUSOV, I.S. KAZANTSEVA, R.G. AKASHKINA, S.P. KUZ'KINA, R.M. ZAKIROVA ANALYSIS OF MOLECULAR STRUCTURE AND OPERATIONAL PROPERTIES OF INHIBITORS OF SCALE AND CORROSION

A comparative study of the molecular structure of inhibitors of scale and corrosion by IR-spectroscopy and X-ray diffraction was carried out. Inhibitors were dsown to differ by levels of protonation of phosphonate groups as well as by content of inorganic impurities, and it leads to the previously identified significant difference in their operational indicators. It was concluded that under coordination of phosphonate group the localized  $\pi$ -bond is retained, whereas the triple axis of symmetry is absent at coordinated phosphonate group.

**Key words:** scale inhibitors, corrosion inhibitors, 1-hydroxyethylidendiphosphonic acid complex with zinc, IR-spectra, X-ray diffraction

## A.A. LIPIN, A.G. LIPIN, D.V. KIRILLOV MODELING PROCESS OF DRYING AND MONOMERS REMOVAL FROM POLYAMIDE IN APPARATUS WITH FLUIDIZED BED

The mathematical description of combine process of drying and monomers removal from polyamide in the apparatus with fluidized bed, which allows predicting moisture and low-molecular-weight compounds content in polymer granules, the temperature condition and process duration is given. The comparison of results of theoretical and experimental studies of the process was carried out.

**Key words:** drying, fluidized bed, mathematical modeling, monomers removal, polyamide

## A.N. BELYAKOV, V.P. ZHUKOV, N.S. ASTASHOV INFLUENCE OF SOLID PHASE CONCENTRATION ON EFFICIENCY OF AERODYNAMIC CLASSIFICATION

The mathematical model of process of powder aerodynamic classification in a gravity apparatus based on Boltzmann equation and taking into account the influence of feed particle size and powder concentration on the efficiency of classification was developed. Some results of process numerical studies are presented.

**Key words:** gravity classification, mathematical model, Boltzmann equation, powder concentration, particles size

# E.A. SKICHKO, K.V. KRUCHININ, E.G. RAKOV, E.M. KOLTSOVA DEVELOPMENT OF PROGRAM COMPLEX FOR MODELING SYNTHESIS KINETICS AND STRUCTURE OF CARBON NANOTUBES, NANOFIBERS

The modeling the synthesis kinetics of carbon nanotubes and nanofibers by means of methane catalytic decomposition process was carried out. Programs were developed which allow obtaining an information on the concentration of every compound taking place in the pyrolysis process in any moment of time in any position in the reactor. Also, programs allow simulating the growth and formation of nanotubes and nanofibers of different structure.

**Key words:** methane catalytic pyrolysis, carbon nanotubes, nanofibers, modeling, structure

# A.S. SUHANOV, A.B. KAPRANOVA, A.P. LUPANOV, A.E. LEBEDEV MECHANICS OF MOVEMENT OF FRIABLE MEDIA ALONG CURVILINEAR BLADES OF CENTRIFUGAL BREAKING

On the heterogeneous systems mechanic the mathematical description of friable medium movement along curvilinear blade of the centrifugal breaking was proposed at the assumption of uniform outflow of the material from the blade. The method of the estimation of percussive velocity of the movement of friable medium was developed. That method allows calculating the angle characteristic of the set-up blade as a function of its constructional and operation parameters.

**Key words:** friable mixture, dispersed phase, porosity, restitution coefficient, centrifugal breaking, curvilinear blade, dry friction law, heterogeneous systems mechanics