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C O N T E N T S

C H E M I S T R Y
(inorganic, organic, analytical, physical, colloid and high-molecular compounds)

C H E M I C A L T E C H N O L O G Y
(inorganic and organic substances. Theoretical fundamentals)

ECOLOGICAL PROBLEMS OF CHEMISTRY AND CHEMICAL TECHNOLOGY

SHORT COMMUNICATIONS

PERSONALS

A B S T R A C T S

A.Sh. SUNAGATULLINA, R.N. SHAKHMAEV, V.V. ZORIN

SYNTHESIS OF *TRANS*- AND *CIS*- ETHYL-5-CHLOROPENT-4-ENOATES

Stereochemically pure *trans*- and *cis*- diethyl (3-chloroprop-2-en-1-yl)propanedioates were obtained using commercially available 1,3-dichloropropene [1] and the possibility of its decarboxylation was investigated. *Trans*- and *cis*- diethyl (3-chloroprop-2-en-1-yl)propanedioates at 180 °C in the presence of LiCl and H_2O in DMSO formed the corresponding ethyl-5-chloropent-4-enoates. Thus, the isomerization of double bond is not practically observed.

Key words: 1,3-dichloropropene, diethyl (3-chloroprop-2-en-1-yl)propanedioate, ethyl-5-chloropent-4-enoate, decarboxylation, vynilchlorides

G.P. KOZLOVSKAYA, E.V. KOZLOVSKIY, V.V. MAKAROV, N.L. OVCHINNIKOV, E.A. LENIVTSEVA

DETERMINATION OF VANADIUM COMPOUNDS IN RAW CLAY MATERIALS AND CERAMIC PRODUCTS

The proposed method allows to determine accurately the vanadium content in the raw clay materials and ceramic samples including soluble vanadium compounds, thus to predict the appearance of green-yellow coatings on the surface of ceramic products.

Key words: raw clay materials, ceramic goods, vanadium compounds, green-yellow coatings, X-ray fluorescence analysis

M.Z. ZARIFYANOVA, I.SH. KHUSNUTDINOV, P.I. GRYAZNOV, I.V. ARISTOV, S.D. VAPHINA, A.V. KONSTANTINOVA

OIL SULFOXIDES. REPORT 2. OPTIMIZATION OF CHOICE OF RAW MATERIALS FOR OIL SULFOXIDES OBTAINING USING QUANTUM-CHEMICAL CALCULATIONS

The calculation of atomic charges in molecules of sulfoxides on the basis of quantum-chemical method B3LYP/6-31 G (d, p) involving data on their molecular weight and boiling point of sulfides that precede them, allowed to determine the optimal intervals of boiling the diesel fraction as a row materials for obtaining oil sulfoxides as extractants of nonferrous metals.

Key words: quantum-chemical calculation, charge on the oxygen atom, extraction ability, sulfides, sulfoxides, molecular weight, boiling point

G.R. GURBANOV

QUAZI-TRIPLE SYSTEM Sb_2S_3-PbS-Bi_2S_3

Quasi-triple system Sb_2S_3-PbS-Bi_2S_3 was studied with the differential-thermal, X-ray and micro structural methods of analysis as well as with the micro hardness measurement. The quadruple compound $PbSbBiS_4$ melting congruently at 870 K was discovered. The compound $PbSbBiS_4$ was established to crystallize in rhombic system with lattice parameters of a=15.72, b=11.36, c=4.41Å.

Key words: physical and chemical analyses, state equilibria, Sb_2S_3-PbS-Bi_2S_3 system, chemical transport reaction

V.V. BIKTAGIROV, V.F. ANUFRIENKO, E.V. BIKTAGIROVA

INTERACTION OF PYRIDINE WITH COMPLEXES OF ALKYLATED Ti(III) IONS IN CATALYST FOR POLYMERIZATION OF DIENE COMPOUNDS ON ESR DATA

The formation of pyridinate of alkylated Ti(III) ions in $TiCl_4$/ oligopiperylene + TIBA catalyst was discovered by ESR spectroscopy method. Interaction of a catalyst with pyridine is accompanied by disordering of associated structure of titan and by detection of ESR spectra of isolated Ti(III) ions.

Key words: alkylated Ti(III) ions, pyridine, ESR

E.I. SHIMANSKAYA, V.Yu. DOLUDA, E.M. SULMAN

STOICHIOMETRIC OXIDATION OF 2-METHYLNAPHTHALENE WITH APPLICATION OF NANOSTRUCTURED CATALYTIC SYSTEMS

The article presents the results of study of 2-methylnaphthalene non-catalytic and catalytic oxidation with use of Au-containing catalyst in acetic acid medium. The selectivity of the oxidation process in the presence of a catalyst was increased on 30% as compared with the non-catalytic process.

Key words: 2-methylnaphthalene oxidation, 2-methyl-1,4-naphthoquinone, catalytic system, selectivity, activation energy

A.O. GRECNINA, O.V. POTYOMKINA, S.A. KUVSHINOVA, D.M. VASILIEV, V.A. BURMISTROV, O.I. KOIFMAN

INFLUENCE OF SOME ANISOTROPIC AZO - AZOXYBENZENES ON TNERMICAL STABILITY AND PHYSICAL- MECHANICAL PROPERTIES OF FILMS FROM PLASTICIZED POLYVINYLCHLORIDE

In given study the plasticized PVC film samples containing anisotropic azo - azoxybenzenes with therminal substituents were obtained. The plasticized PVC film samples modified mesogens were established to possess the thermal stability higher the same parameters for PVC film samples containing industrial stabilizer as well as good physical and mechanical properties.

Key words: anisotropic compound, polyvinylchloride, simultaneous thermal analysis, thermal stability, light-thermo ageing, physical and mechanical properties, abradability

D.B. MURIN, A.M. EFREMOV, V.I. SVETTSOV, S.A. PIVOVARYONOK, OVTSYN A.A., SHABADAROV S.S.

RADIATION INTENSITIES AND CONCENTRATIONS OD ACTIVE SPECIES IN GLOW DISCHARGE PLASMA IN MIXTIRES OF HYDROGEN CHLORIDE WITH ARGON AND HELIUM

The study of influence of argon and helium on radiation intensities of lines and bands and concentrations of active species was carried out in hydrogen chloride plasma at conditions of DC glow discharge. The calculation of excitation rate constants and electron density was carried out by mathematic modeling.

Key words: plasma, radiation, intensity, excitation, concentration, hydrogen chloride

K.B. KOBRAKOV, V.I. RODIONOV, A.G. RUCHKINA, D.N. KUZNETSOV, G.S. STANKEVICH, L.I. ZOLINA, O.V. KOVALCHUKOVA

SYNTHESIS OF HETERO ARYL CONTAINING BIS AZO DYES AND STYDY OF THEIR INTERACTION WITH IONS AND NANO-SCALE PARTICLES OF METALS

Synthesis of new hetero aryl containing azo dyes was described. It was shown that they form in solutions complexes with ions Fe, Ag, Cu, Cr of structure 1:2, as well as polymeric structures with nano-scale particles of silver. Synthesized dyes provide a good stability of painted fabrics (cotton, wool, silk) to physical and chemical actions.

Key words: hetero aryl azo compounds, dyes, chelate groups, metal ions, nano-scale particles, coloring

N.Ch. MOVSUM-ZADE, G.Yu. ALEKSANDROVA

CORRELATION OF STRUCTURE AND PROPERTY OF N-CONTAINING OF HETEROCYCLES BY QUANTUM-CHEMICAL CALCULATIONS

By means of hybrid method of density functional B3LYP with 6-31G(d) basic set, in combination with Gaussian 98 program the calculation of molecular structures of substituted nitriles and fomed from them the s-triazine derivatives was carried out.

Key words: quantum-chemical calculation, molecules structure, DFT B3LYP, nitriles trimerization, heterocyclic compounds

A.N. ZHELEZNOVA, A.A. ILYIN, A.P. ILYIN, N.N. SMIRNOV, Yu.M. KOMAROV

LOW-TEMPERATURE OXIDATION OF COPPER IN PROCESS OF MECHANO-CHEMICAL ACTIVATION IN VAPOR-OXYGEN-AMMONIA ENVIRONMENT

By X-ray, X-ray diffraction, thermogravimetry methods a process of mechano-chemical synthesis of copper oxide from the metal powder was studied. The kinetic aspects of oxidation depending on the time and the method of mechanical activation were investigated.

Key words: copper oxide, mechano-chemical synthesis, oxidation

I.G. TRUNOVA, K.M. ELKIND

STUDY OF POSSIBILITY OF USING AZEOTROPES OF HALIDE ACIDS FOR PRACTICAL AND THEORETICAL PURPOSES

Possibility of use of a rectification method of azeotropic solutions for regeneration of used solutions of hydrochloric acid of 0.5-1.0 concentration containing ions of heavy metals was studied. At the ratio of recycled solution to volume of residual solution of 1: (1÷5) the acid concentration in distillate was shown to correspond to concentration of the added solution. The offered method allows returning not less than 70 % of the used acid to production.

Key words: regeneration, hydration numbers, hydrochloric acid, azeotropic solutions, heavy metals, rectification, closed cycles

N.V. KSANDROV, N.N. KOTOVA

DEPENDENCY OF CONCENTRATION OF SULFURIC ACID SOLUTION OBTAINED AT ACTIVE CARBON REGENERATION ON ACID CONTENT ON CARBON

The dependence of concentration of acid solution obtained at extraction regeneration of active carbon which absorbs preliminary the SO_2 on content of sulfuric acid formed on carbon was studied.

Key words: active carbon, sulfuric acid, sulfur dioxide adsorption, active carbon regeneration

A.G. TKACHEV, A.V. MELEZHIK, T.P. DYACHKOVA, A.N. BLOKHIN, E.A. BURAKOVA, T.V. PASKO

CARBON NANOMATERIALS OF "TAUNIT" SERIES: PRODUCTION AND APPLICATION

Improved technologies for production of carbon nanomaterials of the "Taunit" series based on the principle of catalytic pyrolysis of hydrocarbons, and creating the technology lines for the carbon nanomaterials production were proposed. Investigations of obtaining functionalized nanotubes containing surface carboxyl, hydroxyl, phosphate groups, and analysis of the best methods of introducing functional groups under the action of liquid and gaseous reactants were carried out.

Key words: carbon nanomaterials, catalytic pyrolysis, functionalization, functional groups

V.V. PANTELEEVA, A.B. SHEIN

IMPEDANCE OF CoSi-ELECTRODE IN SODIUM HYDROXIDE SOLUTION

The results of investigation of anodic behaviour of CoSi in NaOH solution at the potentials from corrosion potential up to oxygen evolution potential by polarization and impedance measurements are presented. Impedance spectra in passive field are described taking into consideration the presence of double-layer passivating oxide film on electrode surface. At the potentials from the passive field up to the beginning the O_2 evolution impedance spectra are described in accordance with the process of OH^- penetration into the oxide film. Equivalent electric circuits for the different fields of electrode potential were proposed.

Key words: cobalt, silicide, anodic dissolution, passivation, impedance

V.V. SAYAPOVA

STUDY OF SEDIMENTATION RATE OF SLIME FORMED AFTER ECDM OF HEAT-RESISTING ALLOYS IN VARIOUS ELECTROLYTES

The slime sedimentation rate after ECDM of heat-resisting alloys ЖС-6У and ЖС-6У+TiC was investigated in various electrolytes for development of separation methods and slime recovering. Influence of the electrolyte nature on structure received slimes and sedimentation rate was revealed: received slime is large dispersive in electrolytes on the sodium nitrate basis. It is precipitated easily. Fine (small-dispersed) slime is formed in 15 % NaCl which makes difficult the fast slime separation from a solution. Introduction of high-melting disperse compounds changes properties and structure of heat resisting alloys that influences on properties and precipitation rate of formed slimes.

Key words: electro-chemical dimension treatment, electrolyte, slim, precipitation rate

V.I. PAVLENKO, V.V. PROZOROV, L.L. LEBEDEV, Yu. I. SLEPOKON, N.I. CHERKASHINA

INCREASE IN EFFICIENCY OF ANTICORROSIVE TREATMENT OF NUCLEAR POWER EQUIPMENT BY PASSIVATION IN ALUMINUM-CONTAINING SOLUTIONS

Comparative characteristics of oxide coatings obtained on steel of St20 grade with different ways of passivation used in thermal and nuclear power engineering and proposed ones - treatment with a solution containing aluminum ions of the composition: 25-50 mg / kg of nitric acid +10-50 mg / kg of aluminum nitrate are given. In comparison with treatment with nitrous acid, currently used for the passivation of equipment and pip-

ing of the condensate-feed tract of nuclear power plants with channel reactors of high power (RD EO 0236-00), the technology of preparation of the solution is simplified and the time of solution preparation is decreased.

Key words: passivation, corrosion rate, nuclear power plant

V.D. VORONCHIKHIN

METHODOLOGY OF CREATION OF RUBBER- OLIGOMERIC COMPOSITIONS. PART 1. EXPERIMENTAL APPROACH

In article the primary level of methodology of creation of rubber-oligomeric compositions is presented. The schemes showing interrelation of oligomers with components of polymeric composite materials and nature of influence on the main properties of compounds were offered. The modified scheme of development of the production technology of products of polymeric materials taking into account the influence of oligomers was proposed.

Key words: methodology, olygomers, rubber-olygomeric compositions

Ya.O. MEZHUEV, Yu.V. KORSHAK, M.I. SHTILMAN, A.I. PISKAREVA, I.V. SOLOVYOVA

OXIDATIVE DESTRUCTION OF POLYPYRROLE AS SIDE PROCESS AT CONDITIONS OF OXIDATIVE POLYMERIZATION OF POLYPYRROLE

The dependences of polypyrrole yield on ratio of ammonia peroxidisulfate and pyrrole in the reaction system as well as on temperature were studied. The existence of oxidative destruction of polypyrrole was established in the process of its synthesis. The new mechanism of oxidative destruction of polypyrrole was proposed.

Key words: polypyrrole, destruction, oxidation, polymerization

S.I. NIFTALIEV, R.V. KORABLIN, E.M. GORBUNOVA, E.A. KOVYRYALOVA

LACTOSE MINOR DERIVATES PRODUCTION

Possibilities of biotransformation of lactose to its derivatives were studied. The tagatose and fucose were produced from secondary lactose-containing raw materials. The indentification and analysis of carbohydrates was carried out.

Key words: lactose, derivates, tagatose, fucose

R.M. KUMYKOV, A.K. VOLOGIROV, A.K. MIKITAEV, A.L. RUSANOV

NEW POLYETHERPHLALIMIDS ON BASE OF CHLORALE DERIVATIVES WITH PHTHALIMID O- SUBSTITUTES WITH IMPROVEMENT PROCESSING TO GOODS

For the first time, soluble polyetherphthalimids containing phthalimid o-substitutes were obtained with the interaction of 1,1-dichlor-2,2 bis(3,4-diaminophenyl) ethelene with bis(etherphthal anhydrides). The influence of introduced amount of phthalimide substitutes and dichlorethethylene groups to polymer chains on solubility, thermal and strenght properties of synthesized polymers was studied.

Key words: polyetherphthalimide, polycyclocondensation, solubility, thermal resistance

O.V. KOZLOVA, O.I. ODINTSOVA, E.V. GARASKO

USE OF HUMIC COMPOUNDS AT CREATION OF TEXTILE PRODUCTS OF MEDICAL APPOINTMENT

Perspective directions are designated and efficiency of creation of textile products of medical appointment on the basis of natural biologically active substances was shown. The results of studies of sorpbtion and desorbtion processes of preparation on the base of humic compounds immobilized to textile carrier were presented.

Key words: medicine, textile materials, biologically active substances, humic compounds

A.V. DEDOV, V.P. STOLYAROV, V.G. NAZAROV

MODELLING KINETICS OF PLASTICIZER EXTRACTION FROM POLYVINYLCHLORIDE AT ITS HIGH CONTENT

The model for forecasting the plasticizer extraction kinetic from polyvinylchloride was offered at the high content of a component in polymer. The model is intended for forecasting the extraction kinetic of the process initial step after which there is a reduction of process rate. The reasons of extraction rate change after desorption of certain fraction of plasticizer were considered.

Key words: extraction, plasticizer, polyvinylchloride, model, desorption

A.I. BALUNOV, V.P. MAIYKOV

OPTIMAL SAMPLING OF PRODUCTS DURING RECTIFICATION. ENTROPIC AND INFORMATION ANALYSIS

Entropic and information analysis of rectification was carried out including consideration of task features in design and verifying statements. Selection criteria of optimal product sampling were formulated for each statement, as well as their system consistency was shown. Rectification peculiarities of multicomponent and continuous mixtures were noted. Procedure of inspection and analysis of operating efficiency of active rectification columns was given.

Key works: rectification, product sampling, multicomponent and continuous mixtures, maximum entropic principle, minimum entropic principle

O.O. BABICH, A.Yu. PROSEKOV, L.S. SOLDATOVA

MODELING CONTINUOUS BIOTECHNOLOGICAL PROCESS OF OBTAINING L-PHENYLALANINE-AMMONIA-LYASE

The aspects of mathematical modeling the continuous biotechnological process of obtaining L-phenylalanine-ammonia-lyase – the enzyme used in phenylketonuria therapy were considered. For a basis of studying the obtaining kinetics of L-phenylalanine-ammonia-lyase by pigmental yeast Rhodotorula rubra Y1193 the Lyudekinga-Payri's kinetic ratio was based. As a result of modeling the continuous biotechnological process of obtaining the L-phenylalanine-ammonia-lyase the main regularities of the process allowing optimizing concentration of enzyme under production conditions were characterized.

Key works: L-phenylalanine ammonia-lyase, mathematical model, kinetics of the microorganisms strain, biomass, substrate, Luedeking-Piret equation

N.L. OVCHINNIKOV, L.N. OVCHINNIKOV, V.E. MIZONOV

MODELING ABSORPTION OF LIQUID BY FLOATING ON ITS SURFACE POROUS CYLINDER

A cell mathematical model of forced diffusion of liquid into a floating on its surface porous cylinder through the contact arc was proposed. The evolution of liquid concentration in the cross section of the cylinder and its total absorption kinetics at different Peclet number was described.

Key words: porous cylinder, cell model, transition matrix, concentration distribution, absorption kinetics

V.E. MIZONOV, N.N. YELIN, A.V. POPELYSHKO

CELL MODEL OF HEAT STATE OF CROSS SECTION OF HEAT INSULATED PIPELINE

A cell mathematical model for description of the transient heat process in cross section of heat insulated pipeline at the decrease of outside temperature up to negative value that causes freeze-up of heat insulation was proposed. The specific heat of phase transformation was shown to delay the cooling the transported liquid. Some examples of calculation of temperature distribution in various cross sections were given.

Key words: long pipeline, cross section, heat insulation, freeze-up, temperature distribution

A.M. GORBUNOVA, B.G. SAPOZHNIKOV

EXPERIMENTAL STUDY OF EXTERNAL MASS TRANSFER IN BED OF DISPERSE MATERIAL EXPOSED TO VIBRATION

Using the model method based on process of evaporation of spherical bodies of 12-14.5 mm diameter which were produced from naphthalene and which occupied the fixed position in the layer centre the external mass-exchange was experimentally studied in disperse material exposed to vibration action. For quantitative characteristic of process the mass transfer coefficient divided on difference of naphthalene concentration was used. Data on effect of vibration parameters and dimention of disperse material particles were obtained. These data show the high intensive process of mass transfer in examined system.

Key words: mass-exchange, vibration, dispersive material

R.G. SAFIULLIN

ON LIMITS OF MODE OF MONODISPERSE SPRAYING WITH ROTATING POROUS SPRAYERS

The theoretical dependence for the rate of filtration through the wall of the porous rotating sprayer (PRS) which takes into account the porous structure, geometric characteristics of the PRS and properties of liquid was compared with the known experimental data. The upper limit of applicability of the obtained depend-

ence was studied. The range of the limit angular velocity of PRS's rotation in which inleakage rate onto the surface grains corresponds to the "dripping" (monodisperse) mode of spraying was obtained.

Key words: porous rotating sprayer, filtration rate, monodisperse sprayer

Yu.G. SHIROKOV

PHENOMENOLOGY OF PERIODIC REACTIONS AT DEPOSITION OF INSOLUBLE HYDROXIDES OF Fe(III), Al(III), Pb(II)

The experimental data characterizing the features of formation mechanism of sparingly soluble hydroxides Fe (III), Al (III), Pb (II) were presented. The neutralization process of nitro-acid salts with the ammonia water was carried out in the presense of gelatine-like substances and was fixed on film under microscope. The rate of interface movement was calculated on the base of photography results and periodic character of chemical processes was established. The steps characterising the pecularities of solid phase formation were revealed. The obtained results explaine the appearance of Liesegang's rings and it can be used for development of scientific bases of preparing the precipitated catalysts.

Key words: visual approach, periodic reactions, Liesegang rings, interface, reaction rate

L.N. OLSHANSKAYA, A.S. KHALIEVA, O.V. TITORENKO, N.A. EFREMOVA

INFLUENCE OF COPPER AND LEAD ON DEVELOPMENT OF HIGHER PLANTS AND PHYTOREMEDIATION OF SOIL

Processes of soil purification from heavy metal ions (HMI) were studied with the method of phytoremediation. Calculated values of soil purification efficiency and adsorption capacity of plants showed the dependence of these parameters on HMI concentrations in soil. Plants adsorption capacity on copper ions was found lower than for more toxic lead ions. The following set of HMI sorption ability was established: lettuce> mustard> haricot> pumpkin.

Key words: phytoremediation, soil, heavy metals, higher plants, purification efficiency, adsorption

A.E. PETROV, S.A. SMIRNOV, V.A. TITOV

POPULATIONS OF LOWER VIBRATIONAL LEVELS OF $N_2(X^1\Sigma_g^+)$ AND THEIR EFFECT ON CHARACTERISTICS OF ELECTRON GAS IN ATMOSPHERIC PRESSURE AIR PLASMA

Intensities of $N_2(C^3\Pi_u \rightarrow B^3\Pi_g$, υ=0–4) radiation bands were measured in atmospheric pressure direct current discharge in air. Populations of $N_2(X^1\Sigma_g^+$, V=0–4) vibration levels were calculated using data on these intensities, gas temperature and electric field strength. Effect of the 2-nd kind electron collisions with vibrationally excited $N_2(X^1\Sigma_g^+$, V=0–4) molecules on electron assisted processes rate constants was analyzed.

Key words: plasma, air, nitrogen, vibrational excitation, electron energy distribution function, electron kinetics