

CONTENTS

REVIEWS

Khusnutdinov I.Sh., Safiulina A.G., Zabbarov R.R., Khusnutdinov S.I.
Utilization methods of oil-slimes3

CHEMISTRY

(inorganic, organic, analytical, physical, colloid
and high-molecular compounds)

Chapurkin V.V., Medvedev V.P., Chapurkin S.V.
Peculiarities of primary peroxide derivatives synthesis of reaction of fluorine-containing carbonyl
compounds with hydrogen peroxide.....21

Agatyev P.A., Shlenev R.M., Tarasov A.V.
Synthesis of sulfonyl chloride and sulfonyl amide derivatives of 2,5-diphenyl-1,3,4-oxadiazoles25

Smirnov A.N., Solomonik V.G.
Second-order spin-orbit coupling in heavy element-containing species: non-empirical molecular spectroscopy
and thermochemistry of thallium halides28

Golubev A.E., Larina Yu.N., Kuvshinova S.A., Burmistrov V.A.
Rheological properties of solution of cellulose diacetate – hydrophilic polymer in protonic solvents33

Kuz'mina I.A., Usacheva T.R., Sitnikova K.A., Belova N.V., Sharnin V.A.
Solvation of pyridine, 2,2'-dipyridyl and piperidine in methanol and acetonitrile38

Sagdeev K.A., Khazipov M.R., Sagdeev A.A., Gumerov F.M.
Solubility of polyisoprene in supercritical carbon dioxide43

Tvardovskiy A.V., Nabiulin V.V., Fomkin A.A.
Change in thermodynamic parameters of carbonad sorbent AR-V at benzene adsorption46

CHEMICAL TECHNOLOGY

(inorganic and organic substances.
Theoretical fundamentals)

Kunin A.V., Lapshin D.N.
Determination of hydrophobization mechanism of silicon dioxide of WC-120 trade mark
under mechanical loads50

Popova S.S., Ryabukhova T.O., Okisheva N.A.
Effect of copper electrode modification on its electrochemical behavior in amino acids solution.....55

Razgovorov P.B., Nagornov R.S., Razgovorova M.P., Grechin O.V.
Regulation of aluminosilicate materials acid-base properties for action on purification degree of olive oil58

Cherednichenko A.G., Avetisov R.I., Akkuzina A.A., Avetisov I.Kh.
Application of mass spectrometry with inductively coupled plasma for analysis of inorganic impurities
distribution in synthesis process and purification of aluminum tri-(8-oxyquinolate).....63

Portsel M.N., Novikov V.Yu., Konovalova I.N., Dolgopyatova N.V.
Application of electro-chemical deposition for purification of chondroitin sulphate extracted
from sea hydrocoles.....66

Verloka I.I., Bakin M.N., Kapranova A.B. On experimental distributions of particles of loose components in rarefied flows	70
Natareev S.V., Bykov A.A., Zakharov D.E., Natareev O.S. Dynamics of sorption and desorption of copper ions in cationite ring layer	73
Kotkov A.A., Mizonov V.E., Yelin N.N. Cell model of heat and moisture transfer kinetics at drying sheet material by parallel gas flow	77
Varlamov E.S., Bobkov S.P. Gas environment temperature prediction algorithm under fire in building	82

ECOLOGICAL PROBLEMS
OF CHEMISTRY AND CHEMICAL TECHNOLOGY

Ergozhin E.E., Chalov T.K., Nikitina A.I., Khakimbolatova K.Kh. Study of sorption selectivity of heavy metal cations by new macroporous anionites	85
Kholodnov V.A., Lebedeva M.Yu. Mathematic modeling water-ecological processes at conditions of interval uncertainty of information by example of study of effect of wastewater emission of industrial enterprise to river	89

A B S T R A C T S

I.Sh. KHUSNUTDINOV, A.G. SAFIULINA, R.R. ZABBAROV, S.I. KHUSNUTDINOV
UTILIZATION METHODS OF OIL-SLIMES

In the review the generalized classification of oil-slime forming at oil-refining and oil-producing industries is presented. Comparative analysis of methods of oil-slimes neutralization and utilization is given.

Key words: oil-slime, utilization, neutralization

V.V. CHAPURKIN, V.P. MEDVEDEV, S.V. CHAPURKIN
PECULARITIES OF PRIMARY PEROXIDE DERIVATIVES SYNTHESIS OF REACTION OF FLUORINE-CONTAINING CARBONYL COMPOUNDS WITH HYDROGEN PEROXIDE

At interaction of aliphatic, cyclic and aromatic fluorine-containing carbonyl compounds with hydrogen peroxide 1-hydroxyl-1-hydroperoxides were formed, hydro carbonic analogs of which are not mainly stable. Possibility of their extraction and further chemical transformations are discussed.

Key words: hydrogen peroxide, fluorine-containing carbonyl compounds, hydroxyl hydroperoxides, trifluormethyl, pentafluorophenyl

P.A. AGATYEV, R.M. SHLENEV, A.V. TARASOV
SYNTHESIS OF SULFONYL CHLORIDE AND SULFONYL AMIDE DERIVATIVES OF 2,5-DIPHENYL-1,3,4-OXADIAZOLES

The reaction of benzohydrazide acylation with 2-substituted-5-sulfobenzoic acid dichlorides and subsequent cyclization of the intermediates in thionyl chloride was investigated. A new method of indirectly introducing of the sulfonyl chloride and sulfonamide group in the 2,5-diphenyl-1,3,4-oxadiazoles was developed.

Key words: chlorosulfonation, 1,3,4-oxadiazole, sulfobenzoic acids dichlorides, sulfonul chloride, acylation, sulfonylamides

A.N. SMIRNOV, V.G. SOLOMONIK
SECOND-ORDER SPIN-ORBIT COUPLING IN HEAVY ELEMENT-CONTAINING SPECIES: NON-EMPIRICAL MOLECULAR SPECTROSCOPY AND THERMOCHEMISTRY OF THALLIUM HALIDES

Second-order spin-orbit coupling (SOC) effect on the molecular properties of heavy-atom containing species is studied by the two- and four-component relativistic methods, using TIX molecules ($X = F, Cl, Br, I$) as an example. Calculations are carried out by the coupled cluster methods, both the conventional singles-doubles with a perturbative correction for triple excitations, CCSD(T), and an explicitly correlated, CCSD(T)-F12, each one combined with an extrapolation to the complete basis set limit. Core-valence and higher-order electron correlation effects up to CCSDT(Q) are evaluated. Rather significant second-order SOC effects are revealed: SOC tends to shorten the TI-X bond length, r_e , by 0.005–0.013 Å, to increase vibrational frequency, ω_e , by 1–3 cm^{-1} , and to increase the dissociation energy of the TII molecule, D_0 , by 1.6 $\text{kcal}\cdot\text{mol}^{-1}$. Theoretical molecular properties r_e , ω_e , and D_0 are in excellent agreement with experimental data: mean absolute deviation from experiment amounts to 0.0004 Å, 1.3 cm^{-1} , and 0.4 $\text{kcal}\cdot\text{mol}^{-1}$, respectively.

Key words: molecular structure and spectra, second-order spin-orbit coupling, coupled cluster methods CCSD(T), CCSD(T)-F12, CCSDT(Q), complete basis set, core-valence electron correlation, higher-order correlation corrections, thallium halides

A.E. GOLUBEV, Yu.N. LARINA, S.A. KUVSHINOVA, V.A. BURMISTROV
**RHEOLOGICAL PROPERTIES OF SOLUTION OF CELLULOSE DIACETATE – HYDROPHILIC
POLYMER IN PROTONIC SOLVENTS**

By the method of rotational viscosimetry the rheological properties of cellulose diacetate solutions were studied in the presence of chitosan and oxypropyl cellulose in a binary solvent mixture of acetic acid-water. A closeness of given systems to Newtonian fluids was shown. The activation mechanism of cellulose diacetate solutions flow was established. Cellulose diacetate is a hydrophilic polymer in a mixed solvent of acetic acid and water of various compositions. The thermodynamic parameters of the viscous flow were calculated. The influence of water and polymer additives on the rheology of cellulose diacetate solutions was revealed.

Key words: cellulose diacetate, chitosan, oxypropyl cellulose, rheology, dynamic viscosity, viscous flow activation entropy

I.A. KUZ'MINA, T.R. USACHEVA, K.A. SITNIKOVA, N.V. BELOVA, V.A. SHARNIN
**SOLVATION OF PYRIDINE, 2,2'-DIPYRIDYL AND PIPERIDINE IN METHANOL
AND ACETONITRILE**

The geometrical parameters of pyridine (py), 2,2'-dipyridyl (2,2'-dipy) and piperidine (ppd) were investigated by means of quantum-chemical calculations. The distribution of electron density in the amine molecules in a free state and in a solvated state was studied and the enthalpies of py, 2,2'-dipy and ppd solvation in MeOH and AN were calculated. A comparative analysis of the results with the data on the transfer enthalpies of amines from MeOH to MeOH-AN mixed solvents, obtained by calorimetric method, was carried out. The changes in the energy of amines solvation at changing the composition of the solvent MeOH→AN were found to depend mainly on changes in a solvation state of their reactionary sites.

Key words: methanol, acetonitrile, pyridine, 2,2'-dipyridyl, piperidine, solvation

K.A. SAGDEEV, M.R. KHAZIPOV, A.A. SAGDEEV, F.M. GUMEROV
SOLUBILITY OF POLYISOPRENE IN SUPERCRITICAL CARBON DIOXIDE

Experimental results are presented on the solubility study of pure and modified (polar additive-3.5 wt.% of chloroform) polyisoprene in supercritical carbon dioxide at temperatures of 343 K, 373 K, 393K in a pressure range of 15-34 MPa.

Key words: polyisoprene, supercritical carbon dioxide, solubility, co-solvent, crossover behavior

A.V. TVARDOVSKIY, V.V. NABIULIN, A.A. FOMKIN
**CHANGE IN THERMODYNAMIC PARAMETERS OF CARBONAD SORBENT AR-V
AT BENZENE ADSORPTION**

A thermodynamic analysis of adsorption deformation of adsorbents was carried out. Calculations of changes in entropy and internal energy are presented for the carbon adsorbent AR-V at adsorption of benzene vapors.

Key words: adsorption, adsorbent, adsorbents adsorptive deformation, dilatometric method, adsorbents adsorptive deformation thermodynamics

A.V. KUNIN, D.N. LAPSHIN
**DETERMINATION OF HYDROPHOBIZATION MECHANISM OF SILICON DIOXIDE OF WC-120
TRADE MARK UNDER MECHANICAL LOADS**

In this work, mechanochemical modification of amorphous silicon dioxide (white carbon WC-120) with organosilicon liquid 136-41 was used as a way to make SiO₂ powder hydrophobic. Using IR-Fourier spectroscopy and element analysis it was determined that hydrophobization process includes chemisorption and physical adhesion of organosilicon liquid molecules on the surface of SiO₂. According to the study, amorphous SiO₂ shows the highest water-repellent properties if it is grinded during 10 min. with 8-10 wt.% of organosilicon liquid 136-41 in a vibration mill. The amount of energy inputted to material is equal to 1000-1100 J/g.

Key words: hydrophobization, silicon dioxide, mechanochemical activation, chemical bond, active sites, modification, surface, hydrophobicity

S.S. POPOVA, T.O. RYABUKHOVA, N.A. OKISHEVA

**EFFECT OF COPPER ELECTRODE MODIFICATION ON ITS ELECTROCHEMICAL BEHAVIOR
IN AMINO ACIDS SOLUTION**

Effect of the electrode nature on the electrochemical behavior of amino acids -valine, leucine, methionine and asparaginic acid- was studied. It was established that the surface condition and the electrode surface layer material nature, in particular, considerable effects on the amino acids adsorption process. It allows to suggest their participation in the electrochemical process in a form of complexes in a solution and the surface complexes.

Key words: electrode surface, amino acids, adsorption

P.B. RAZGOVOROV, R.S. NAGORNOV, M.P. RAZGOVOROVA, O.V. GRECHIN

**REGULATION OF ALUMINOSILICATE MATERIALS ACID-BASE PROPERTIES FOR ACTION
ON PURIFICATION DEGREE OF OLIVE OIL**

Activated powder blue and pink clay with using acetic acid and the sodium carbonate changed the number of acidic and basic sites because contact of surface with an activating agent. Predomination appropriate sites in clay depends on the type of activators or the result of the presence of both active sites in these compositions. Such sites presence influences on the sorption ability of given materials in respect to different impure ingredients of olive oil.

Key words: blue clay, pink clay, pK spectra, IR spectra, olive oil, impure ingredients, free fatty acids, peroxides

A.G. CHEREDNICHENKO, R.I. AVETISOV, A.A. AKKUZINA, I.Kh. AVETISOV

**APPLICATION OF MASS SPECTROMETRY WITH INDUCTIVELY COUPLED PLASMA
FOR ANALYSIS OF INORGANIC IMPURITIES DISTRIBUTION IN SYNTHESIS PROCESS
AND PURIFICATION OF ALUMINUM TRI-(8-OXYQUINOLATE)**

The process of inorganic impurities distribution was studied at synthesis and purification of aluminum tri-(8-oxyquinolate) by the method of mass spectrometry with inductively coupled plasma. Sources of contamination of final product were established. The improvement of technological process for enhancement of its quality was carried out.

Key words: mass-spectrometric analysis, organic phosphors, OSID-technology

M.N. PORTSEL, V.Yu NOVIKOV, I.N. KONOVALOVA, N.V. DOLGOPYATOVA

**APPLICATION OF ELECTRO-CHEMICAL DEPOSITION FOR PURIFICATION
OF CHONDROITIN SULPHATE EXTRACTED FROM SEE HYDROCOLES**

The purification method of chondroitin sulphate from salmon cartilaginous tissue and northern scate was proposed. Given method allows obtaining the receipt with mass-fraction of this polysaccharide of 90-95%. The method is based on electro-deposition of chondroitin sulphate, formation of hydro gel, its stabilization, washing and drying. The average molecular weight, optical and surface activity of chondroitin sulphate was determined for substance obtained on known technology and with application of electro-deposition.

Key words: see hydrocoles, chondroitin sulphate, electro-chemical deposition, hydro gel

I.I. VERLOKA, M.N. BAKIN, A.B. KAPRANOVA

**ON EXPERIMENTAL DISTRIBUTIONS OF PARTICLES OF LOOSE COMPONENTS
IN RAREFIED FLOWS**

The experimental results on determination the spraying angle are considered for particles of solid dispersed media at the interaction with brush elements having unidirectional spiral helical winding on cylindrical surface of the mixing drum, which is rotated above moving horizontal belt.

Key words: loose material, mixing, mixing drum, brush elements, spraying angle

S.V. NATAREEV, A.A. BYKOV, D.E. ZAKHAROV, O.S. NATAREEV

DYNAMICS OF SORPTION AND DESORPTION OF COPPER IONS IN CATIONITE RING LAYER

The mathematical description was proposed for the ion exchange adsorption and desorption processes of copper ions in an apparatus with ring layer of sulfonic acid cationite. The adequacy of description to real process was established.

Key words: ion exchange, apparatus with fixed ring layer of cationite

A.A. KOTKOV, V.E. MIZONOV, N.N. YELIN
**CELL MODEL OF HEAT AND MOISTURE TRANSFER KINETICS AT DRYING
SHEET MATERIAL BY PARALLEL GAS FLOW**

A cell mathematical model of heat and moisture content evolution in a material sheet at drying by a gas flow which is parallel to its surface is proposed. The longitudinal section of the material is presented by a two-dimensional net of cell while the gas flow is presented by one-dimensional net. The cells of material contacting with the gas cells can exchange with heat and moisture, which propagate then over the material by means of heat and moisture conduction. Some results of numerical experiments are presented and influence of the reverse of gas flow on the drying process is estimated.

Key words: sheet material, moisture content, drying, heat emission, moisture emission, heat conduction, moisture conduction, cell model, state vector, transition matrix, gas supply reverse

E.S. VARLAMOV, S.P. BOBKOV
GAS ENVIRONMENT TEMPERATURE PREDICTION ALGORITHM UNDER FIRE IN BUILDING

An algorithm was proposed for predicting temperatures of fire in buildings and industrial facilities on the basis of information received from the radio channel monitoring system fire parameters.

Key words: gas environment temperature, industrial plants protection, facility state monitoring, fire elimination

E.E. ERGOZHIN, T.K. CHALOV, A.I. NIKITINA, K.Kh. KHAKIMBOLATOVA
STUDY OF SORPTION SELECTIVITY OF HEAVY METAL CATIONS BY NEW MACROPOROUS ANIONITES

The new complexing anionite with network structure on the bases of glycidyl benzylamine, allyl glycidyl ether and polyethylenimine was obtained. It has static exchange capacity on 0.1 N solution of HCl of 4.8 mg-eq/g, due to this anionite can be used for sorption of various metals in hydrometallurgy for solving environmental problems. The sorption of divalent ions of copper, nickel and cobalt from model sulfate one-, two- and three-component solutions in static conditions was investigated. The effect of solution concentration on the anionite sorption characteristics was studied.

Key words: anionite, copper, nickel and cobalt ions, sorption isotherms, sorption capacity, selectivity

V.A. KHOLODNOV, M.Yu. LEBEDEVA
**MATHEMATIC MODELING WATER-ECOLOGICAL PROCESSES AT CONDITIONS
OF INTERVAL UNCERTAINTY OF INFORMATION BY EXAMPLE OF STUDY OF EFFECT
OF WASTEWATER EMISSION OF INDUSTRIAL ENTERPRISE TO RIVER**

In given article the effect of wastewater emission of industrial enterprise on pollution degree in City River was studied at conditions of interval uncertainty of initial information. On the basis of mathematic model of process under study the stationary non-conservative transfer of pollutants is considered. Also, changes in concentrations of dissolved oxygen, biochemical oxygen demand and nitrates along the river length are estimated at different disturbances in parameters of wastewater emission with industrial enterprises.

Key words: wastewater, interval uncertainty, dissolved oxygen concentration, oxygen deficit, biochemical oxygen demand, nitrates concentration, Mathcad