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A.A. MERKIN, A.A. KOMAROV, O.V. LEFEDOVA

KINETICS FEATURES OF HYDROGENATION OF NITRO- AND NITROSO SUBSTITUTED BENZENES ON SKELETAL NICKEL IN AQUEOUS AND AQUEOUS-ALCOHOLIC MEDIA

In given article reaction kinetics and step order of transformation of some substituted nitro- and nitrosobenzene in aqueous-organic media on nickel skeletal catalyst was considered. Differences and similarities in behavior and step order of transformations of nitro- and nitroso- groups were discussed, as well as the reasons of possible side reactions accompanying the hydrogenation reactions under study.

Key words: liquid-phase hydrogenation, aliphatic alcohols, skeletal nickel, dehydrogenation, oxidation, substituted nitro- and nitrosobenzenes, adsorption, rate, rate constant, macrokinetic area, diffusion inhibition

O.V. MATSEVICH, Z.S. SAMIGULLINA, V.M. YANBORISOV

EFFECT OF SOLVENT ON FORMATION OF ACTIVE SITE OF POLYCONDENSATION REACTION OF PSEUDO CHLOR ANHYDRIDES OF AROMATIC O-KETOCARBOXYLIC ACIDS BY EXAMPLE OF 3-CHLORINE-3-PHENYLPHTHALILIDENE IN ENVIRONMENT OF NITROBENZENE

In the frame of supermolecule theory the theoretical study of solvation of the active site of polycondensation of 3-chlorine-3-phenylphtalilidene with solvent, nitrobenzene, was carried out. The first solvation shell was established to content three solvent molecules. The formation of complexes with the solvent does not change in an electron density on the functional carbon atom of 3-chlorine-3-phenylphtalilidene. The solvent does not complicate the coordination of the active site by next monomer molecule.

Key words: polyarylenephtalides, polycondensation, nitrobenzene, quantum-chemical calculation, heat effect, complexation, solvate shell, supermolecule theory

D.G. KIM, E.V. BERDNIKOVA

HALOGENATION OF 2-ALLYL-6-PHENYL-3(2H)-PYRIDAZINONE

It was shown that 2-allyl-6-phenyl-3(2H)-pyridazinone reacts with iodine to form 2-(iodomethyl)-6-phenyl-2,3-dihydrooxazolo[3,2-b]pyridazinium polyiodide, and with bromine - to form 2-(2,3-dibromopropyl)-6-phenyl-3(2H)-pyridazinone.

Key words: 2-allyl-6-phenyl-3(2H)-pyridazinone, 2-(2,3-dibromopropyl)-6-phenyl-3(2H)-pyridazinone, 2-(iodomethyl)-6-phenyl-2,3-dihydrooxazolo[3,2-b] pyridazinium polyiodide, mass spectrum, halogenation

T.R. PROSOCHKINA, R.G. SHESTAKOVA, K.G. KICHATOV, E.A. KANTOR

COMPUTATIONAL ANALYSIS OF STRUCTURING 3,6-BIS(4-BUTYLPHENYL)PYRIDAZINE

The computer simulation of 3,6-Bis(4-butylphenyl)pyridazine structure was carried out. The probability of each configuration of dimers (stacking, in-plane and terminal) was revealed. The estimation of relative probability of various configurations of investigated dimers was carried out and the value of the translation rigidity of molecules in dimers was calculated. This parameter is compared with the liquid crystal properties.

Key words: mesophase, structuring, computer simulation, intermolecular interactions, dimers, quantum chemistry, translation rigidity

**V.S. GASANOV, A.A. MAKHMUDOVA, G.V. BABAIEVA, K.O. ISKENDEROVA, S.N. KAKHRAMANOVA
SYNTHESIS AND RESEARCH OF L-ETHYLTIOMHETYL-2-ARYLOXYETHYL-N-ARYL-CARBAMATES AND THIOCARBAMATES**

1-Ethylthio-3-aryloxypropane-2-oles were synthesized under the action of 3- chlorine-1-ethylthio- propane-2-ol on substituted phenols as well as by action of 1-chlorine-3-aryloxypropane-2-ol on ethane-1-thiol in alkaline medium. The last are formed 1-(ethylthiomethyl)-2- (aryloxy)-ethyl-N-arylcarbmates and thiocarbmates under condensation with aromatic isocyanates and isothiocyanates which were tested as additive to the lubricating oils.

Key words: 3-chloro-1-ethylthioiopropane-2-ol of carbamic and thiocarbamic acid, sulfur- and nitrogen-containing organic compounds

*G.Z. RASKIL'DINA, L.F. KORZHOVA, N.G. GRIGOR'EVA, B.I. KUTEPOV,
A.N. KAZAKOVA, S.S. ZLOTSKY*

**HETEROGENEOUS CATALYTIC ADDITION OF MONOCARBONIC AND DICARBONIC
ACIDS TO OLEFINS**

The interaction of olefins with monocarbonic and dicarbonic malonic acid was studied in the presence of the H-Beta zeolite catalyst proceeding with the formation of the corresponding ethers and esters.

Key words: olefins, zeolite, ethers and esters

E.M. KOMINA, O.V. MALKOVA, V.G. ANDRIANOV, A.S. SEMEYKIN

**KINETIC OF COMPLEXATION OF PYRIDYLDERIVATIVES OF PORPHYRINS WITH ZINC
ACETATE IN ACETONITRILE**

The complexation kinetic of derivatives of porphyrins in acetonitrile - $Zn(Ac)_2$ solutions at 298-318 K were studied. The apparent constants of complexation of these porphyrins were determined. The kinetic parameters of the process ($k_v, E_a, \Delta S$) for reaction of coordination of porphyrins with $Zn(Ac)_2$ in AN were calculated.

Key words: pyridylporphyrin, complexation, acetonitrile

M.R. KORCHUGANOVA, Z.N. ESINA, V.V. MURASHKIN

**OPPORTUNITIES OF PCEAS MODEL FOR CALCULATION OF PHASE EQUILIBRIA
LIQUID-SOLID AND LIQUID-VAPOR AT CONSTANT PRESSURE**

A mathematical model of phase equilibrium liquid-solid and liquid-vapor for binary and multicomponent mixtures, obtained by minimizing the excess Gibbs energy on solvation parameter was presented. The universal nature of the model PCEAS (Phase Chart Eutectic and Azeotropic Systems) allows to predict the equilibrium liquid-solid and liquid-vapor at constant pressure.

Key words: equilibrium liquid-solid, liquid-vapor, eutectic, azeotrope, solvation parameter, association parameter, excess Gibbs energy

R.S. MIRZOEV, R.M. EL'MESOVA, A.A. KYAROV, R.A. SHETOV, N.I. MASCHUKOV, M.Kh. LIGIDOV
**QUANTITATIVE BUILDING SOLUBILITY DIAGRAM OF $Na^+||Cl, CO_3^{2-}, MoO_4^{2-}-H_2O$ SYSTEM AT
25 °C APPLYING PITZER'S EQUATION**

The prediction of the solubility diagrams for $NaCl - Na_2CO_3 - Na_2MoO_4 - H_2O$ system by Pitzer equations at 25 °C was carried out. The results of calculation of salt solubilities in a system were confirmed by experimental studies of nonvariant and monovariant equilibrium.

Key words: solubility; sodium chloride, sodium carbonate, sodium molybdate, modeling; Pitzer's equation; solubility diagram

V.V. KIRILLOV, A.Yu. KOSTYUKOV

**INFLUENCE OF HYDRATION ON FREEZING TEMPERATURE OF AQUEOUS SOLUTIONS
OF SODIUM AND POTASSIUM CHLORIDES**

For the first time, for calculation of freezing point decrease Δt of aqueous sodium and potassium chloride it was proposed to take into account the ion-dipole interaction. For this purpose, the coefficient K_s was introduced to the well-known formula. This coefficient takes into account the hydration of ions in the first coordination sphere. This coefficient depends on the mole fraction of the non-bonded solvent. Calculations by formula $\Delta t = i \cdot K_{kp} \cdot C_m \cdot K_s$ allowed to obtain values of freezing point decrease of solutions (in particular, for solutions of $CaCl_2$) which are close to experimental ones.

Key words: solutions freezing temperature, electrolyte solutions, hydration, ion-dipole interaction

A.N. LOPANOV, E.A. FANINA, I.V. PRUSHKOVSKIY

**AGGREGATION OF GRAPHITE DISPERSIONS IN HETEROGENEOUS SYSTEMS BASED
ON CARBONATES OF ALKALI EARTH METAL**

The model of the electrical conductivity of a heterogeneous system based on alkaline earth metals and graphite dispersions was presented. Electrical properties of heterogeneous based graphite dispersions in alkaline earth metal carbonate dependent on several key parameters. The most important of them are the degree of aggregation of conductive particles and the electrical conductivity of a single unit. It was shown that the threshold concentration of electrical conductivity for alkaline earth metal carbonate, equal to 0.05, is essentially below of the threshold concentration of the electrical conductivity of the fluid systems dispersions of graphite in electrolytes equal to 0.15 due to the higher value of the Hamaker's constant. The effective activation energy of

the electrical conductivity of the graphite dispersions in carbonates of alkaline earth metals was determined. The activation energy of the electrical conductivity was shown to increase from 3 to 7 kJ / mol with the increasing the mass fraction of graphite dispersions from 0.1 to 0.75.

Key words: electrical conductivity, aggregation, Hamaker's constant, activation energy

N.A. ZHUK, N.V. ROZHKINA

EFFECT OF COMPOSITION NONSTOICHIOMETRY ON FORMATION AND ELECTRICAL PROPERTIES OF Bi_3NbO_7

The deficiency of niobium atoms in the cation sublattice of bismuth niobate was established to result in the increase in a temperature of phase transformations and in a narrowing the temperature range of formation of the tetragonal phase. The conductivity of the solid solutions of cubic modification of $\text{Bi}_3\text{Nb}_{1-x/3}\text{O}_{7-\Delta}$ is two orders of magnitude higher than the conductivity of bismuth niobate solid solution with bismuth deficit.

Key words: bismuth niobate, phase transition, composition non-stoichiometry, dielectric constant, total electrical conductivity

S.E. BUTUZOV, A.S. VOROBYOV, A.E. KOSMATENKO, Yu.V. SOKOLKIN

BORON NITRIDE USING AS SEPARATOR IN SILICONIZING GRAPHITES AND CARBON COMPOSITE MATERIALS

Keeping method of coating, filament and matrix of goods from carbon/silicon carbide composites details obtained with siliconizing the carbon/carbon composite using boron nitride as a separator was described.

Key words: boron nitride, carbon/silicon carbide composites, silicification

O.V. ALEKSEEVA, A.N. RODIONOVA, N.A. BAGROVSKAYA, A.V. AGAFONOV **PROPERTIES OF COMPOSITES BASED ON HYDROXYETHYLCELLULOSE AND ALUMINOSILICATES**

Polymer hydroxyethylcellulose matrix modification using particles of aluminosilicates was carried out by mechanochemical method and polymeric film materials were obtained. The influence of the nature and concentration of the filler on the structure and mechanical properties of polymer composites were studied.

Key words: hydroxyethylcellulose, bentonite, organoclay, composite, mechanical properties

O.G. VOLOKITIN, V.I. VERESHCHAGIN, G.G. VOLOKITIN, N.K. SKRIPNIKOVA, V.V. SHEKHOVTSOV **SILICATE MELTS OBTAINING WITH HIGH SILICATE MODULUS FROM QUARTZ-FELDSPAR RAW MATERIALS BY PLASMA TECHNOLOGY**

This article devotes to study of possibility of obtaining and production of high temperature silicate melt from quartz- feldspar containing wastes of concentration of molybdenum ores of Sorsk ore-dressing and processing enterprise.(Khakassiya) using the energy of low-temperature plasma.

Key words: silica feldspar raw material, silicate melt, electrical-plasma device, waste utilization

I.A. BLAIYDA, T.V. VASYL'EVA, L.I. SLYUSARENKO, V.F. KHITRICH

BEHAVIOR OF GERMANIUM AND GALLIUM AT ASH PROCESSING FROM COAL COMBUSTION BY CHEMICAL AND MICROBIOLOGICAL METHODS

The comparative analysis of behavior of germanium and gallium was carried out at ash processing from coal combustion with the acid leaching and microbiological leaching with thiobacteria. The comparative complex chemical and microbiological assessment of the initial ash and by-products was given. It was found that during the leaching by hydrochloric acid gallium and germanium was extracted in solution on 81.85 and 86.24%; due to the oxidizing activity of own microbiota microorganisms on 89.75 and 86.14%, respectively. The advantages and disadvantages of the proposed alternative processing methods were shown.

Key words: gallium, germanium, leaching, microbiota, thiobacteria

I.M. RYSHCHENKO, A.S. SAVENKOV, I.S. BELOGUR

STUDY OF FERTILIZER TECHNOLOGY ON BASE OF PHOSPHATE- GLAUCONITE CONCENTRATE OF UKRAINE

In given article the results of ammoniation study of nitric acid extraction obtained with decomposition of low-grade stock of Novo-Amvrosiev's deposit. Extraction ammoniation was carried out in a presence of sulphuric acid and ammonium sulphate. The interaction mechanism was established. A number of high-efficiency nitrogen-phosphor-containing fertilizers were obtained.

Key words: low-grade ore, nitric acid, sulphuric acid, decomposition, gypsum, neutralization, fertilizers

E.A. TATARINTSEVA, A.V. KARPENKO, V.A. LEMAEV, I.V. DOLBNYA, L.N. OLSHANSKAYA
**MODIFICATION OF THERMOPLASTICS AS WAY OF SORPTION MATERIALS OBTAINING
FOR WASTEWATER PURIFICATION**

The compositions of polymeric compositions from thermoplastic wastes (polyethylene terephthalate), expanded graphite (TEG) and blowing agent were developed for the creation of adsorption materials. The physical-mechanical properties (attrition, grindability, density, porosity, specific surface area), structure and adsorption properties were studied.

Key words: wastes, thermoplastics, fillers, foaming agents, adsorption

M.D. PLOTNIKOVA, A.B. SHEIN
**STEEL PROTECTION FROM HYDROGEN SULFIDE CORROSION WITH FLEK INHIBITORS
AT HIGHER TEMPERATURES**

In given paper the results of study of influence of inhibitory compositions on the base of imidazoles on corrosion-electrochemical behavior of steel 3 were given for acid solutions containing hydrogen sulfide and free from it for the temperature range of 293-333 K. Studies were carried out with the gravimetric and polarized methods. The activation energy of corrosion process was determined.

Key words: corrosion, inhibitor, protective action, temperature

E.G. FILATOVA, G.N. DUDAREVA, A.A. SOBOLEVA, E.A. ANTSIFEROV
**TECHNOLOGY OF ELECTROCOAGULATION PURIFICATION OF WASTEWATER
OF ELECTROPLATING FROM IONS OF HEAVY METAL**

The processes of electrocoagulation of ions of nickel, copper, zinc and iron with aluminum anodes were studied. The optimal parameters of electrocoagulation process- pH, current density, etc- were established. The efficiency of electrocoagulation method of purification at industrial conditions was not less than 96.5%, the specific electricity consumption was 0.46 kW·h/m³.

Key words: electrocoagulation, galvanic sinks, aluminum anodes, nickel ions, copper ions, zinc ions, iron ions

A.A. KOLESNIKOV, M.O. MESNIK
EFFICIENCY OF USE OF ELECTRON BEAM OF ELECTRON ACCELERATORS FOR VULCANIZATION OF ARTIFICIAL LEATHERS

In given article on the base of data obtained the results for energy calculation of applying accelerator of electrons are given for the process of vulcanization of artificial leathers on the base of elastomers.

Key words: electron irradiation doses, elastomeric artificial leather, film materials

S.P. RUDOBASHTA, G.A. ZUEVA, V.M. DMITRIEV, N.A. ZUEV
MASS CONDUCTIVITY DURING DRYING COLLOIDAL CAPILLARY-POROUS MATERIALS

Results of experimental research of mass conductivity properties of typical colloidal capillary- porous materials - seeds of vegetables are given and analyzed. The comparison of mass-conductivity coefficients of these materials with mass-conductivity coefficients for other colloidal capillary- porous materials-grains-is given.

Key words: mass conductivity, drying, kinetic mode, colloidal capillary-porous materials

R. WÓJTOWICZ, A.A. LIPIN
MODELLING OF LIQUID FLOW IN MIXING DEVICE: INFLUENCE OF TURBULENCE MODEL

The results of mathematical modelling a turbulent liquid flow in a mixing device with a turbine impeller are presented. The influence of a turbulence model on the numerically predicted values of flow parameters was examined. The calculations were carried out using the numerical codes of Computational Fluid Dynamic (CFD) and Reynolds-Averaged Navier-Stokes equations (RANS) approach. For closure of equation system two equations describing turbulence model were added. Three models of turbulence method were applied. These models were the models of k-ε family: the standard k-ε, the renormalization-group (RNG) k-ε and the Realizable k-ε model.

Key words: mathematical modelling, k-ε turbulence model, mixing, turbine impeller

A.G. LIPIN, M.P. BURCHU, A.A. LIPIN
**MASS TRANSFER KINETICS AT ELECTRODIALYSIS SEPARATION OF ORGANIC
COMPOUNDS SOLUTIONS AND ELECTROLYTES**

The results of experimental investigation of ternary solutions separation by electro dialysis technique are presented. The solution is organic compound – inorganic salt – water. The mathematical model allowing predicting the rational technological parameters of separation were developed.

Key words: electro dialysis, mass-transfer, ternary solution, mathematical modelling

M.A. CHESHINSKIY, A.N. LABUTIN
**OPTIMIZATION OF STEP OF ABSORPTION OF GAS-LIQUID STRONGLY EXOTHERMAL
PROCESS OF OXYETHYLATION**

In given paper the method for determining the optimal dimensions of the absorber was proposed. Optimal dimensions provide a given value of the degree of saturation of liquid by absorbed component taking into account polydispersity of the liquid spray and distribution of the particle on exit angle from the nozzle. The method is based on a heat-mass exchange process model for single liquid drop with the gas phase.

Key words: oxyethylation, absorption step, spraying, simulation, optimization

S.N. GRIDCHIN
**STABILITY CONSTANTS OF ZINC, CADMIUM, COBALT(II), AND NICKEL(II)
COMPLEXES OF HEXAMETHYLENEDIAMINE-N,N,N',N'-TETRAACETIC ACID**

Stability constants of Zn^{2+} , Cd^{2+} , Co^{2+} , and Ni^{2+} complexes of hexamethylenediamine-N,N,N',N'-tetraacetic acid were determined potentiometrically at 298.15K and an ionic strength of 0.1 (KNO_3). The results obtained were compared with the corresponding data on related compounds.

Key words: complexones, chelates, stability constants, alkylenediaminetetraacetic acids

S.V. DOBRYDNEV, Yu.A. SOLOMATINA, M.Yu. MOLODTSOVA
**INFLUENCE OF RATIO OF AMMONIA AND AMMONIUM HYDROGEN CARBONATE
ON SYNTHESIS OF BASIC ZINC CARBONATE**

The basic zinc carbonates were synthesized in ammonium-carbonate solutions under heterogeneous conditions at different ratios of ammonia and ammonium hydrogen carbonate. It was shown that at a ratio of $NH_3 \cdot H_2O : NH_4HCO_3 = 3:1$ in the basic zinc carbonates the ultra-dispersed and radiographic-amorphous phases were formed as a result of thermolysis of which the zinc oxide powder with a particle size of 10 - 20 nm was obtained.

Key words: ammonia-carbonate solutions, zinc oxide, basic zinc carbonates, x-ray-phase analysis, thermolysis