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C O N T E N T S

R E V I E W S

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

CHEMICAL TECHNOLOGY
(inorganic and organic substances.
Theoretical fundamentals)

SHORT COMMUNICATIONS

A B S T R A C T S

L.N. MIZEROVSKIY, K.P. SMIRNOVA

ANALYSIS OF TEMPERATURE DEPENDENCES OF ARGON, KRYPTON AND XENON SOLUBILITY IN *n*-ALKANES UNDER ATMOSPHERIC PRESSURE

Within the framework of the conception according of which the solubility of simple gases in liquids depends on the ratio of characteristic parameters of components (the volume of intermolecular space available for diffusion transitions of gas particles, the distribution constant between the own phase and the liquid volume (K_D), the Van der Waals volume of mole of gas particles) the available literature data on the solubility of Ar, Kr and Xe in *n*-alkanes and some isoalkanes C_8 under atmospheric pressure and different temperatures are analyzed. It is shown that K_D of these gases in alkanes does not depend on the size of their molecules and decreases with the temperature increasing. The absolute value of the solubility changes with temperature by complicated way depending on the ratio of temperature coefficients K_D, molar volume of liquid and concentration of the gas in own phase. Taking into account the author's studies published before the conclusion was made that physically clear explanation of temperature influence on inert gases solubility is not possible without usage of new concept.

Key words: argon, krypton, xenon, alkanes, solubility, temperature influence

P.V. FABINSKIY, E.E. SERGEEV, O.A. BAYUKOV, V.A. FEDOROV

PHOTO-CHEMICAL SYNTHESIS OF IRON (II) BIS(FERROCENOYL)ACETONATE

The iron (II)bis(ferrocenoyl)acetonate was obtained by the photolysis of ferrocenoylacetone in coordinating solvent. The compositions and structures of the complex obtained were proved by elemental analysis, IR, electronic, and ^{57}Fe Mössbauer spectroscopy.

Key words: photolysis, complex compound, element composition, IR, electronic spectrum, Mössbauer effect

A.D. BADIKOVA, A.M. MUSINA, F.KH. KUDASHEVA, R.N. KHAIYRULLINA, R.N. GIMAEV

REGULATION OF PHYSICAL-CHEMICAL PROPERTIES OF OLIGO-ESTERS OBTAINED ON BASE OF PRODUCTION WASTE OF TEREPHTHALIC ACID

Optimal conditions and parameters of process of obtaining the oligo-esters with various physical and chemical parameters were determined with IR spectroscopy applying.

Key words: technical terephthalic acid water free, infrared spectroscopy, oligo-esters

E.V. SMIRNOVA, E.A. KURGANOVA, YU.B. RUMYANTSEVA, G.N. KOSHEL

OXIDATION OF ISOPROPYLBENZENE IN PRESENCE OF *N*-HYDROXYPHTHALIMID

The reaction of liquid phase oxidation of isopropylbenzene in the presence of N-hydroxyphthalimid was studied. The use of *N*-hydroxyphthalimid and its 3- and 4-methyl-substituted analogs was found to be a success to raise the oxidation rate of isopropylbenzene in 2,5 – 3 time at selectivity above 90 % (as comparing with industrial indices). That can raise the economic effectiveness of the process. The influence of by-products on oxidation process of isopropylbenzene was studied.

Key words: liquid phase oxidation, isopropylbenzene, hydroperoxide, nitrogen-containing catalyst, *N*-hydroxyphthalimid, oxidation by-products

A.Yu. MEDVEDEVA, Yu.M. ATROSHCHENKO, I.V. SHAKHKEL'DYAN, I.E. YAKUNINA, A.N. SHUMSKIY, K.I. KOBRAKOV

SYNTHESIS AND STRUCTURE OF NEW DERIVATIVES OF 11-*R*-1,9-DINITRO-13-(2-OXO-PROPYL)-6,11-DIAZATRICYCLO[7.3.1.0^{2,7}]TRIDECA-2,4,6-TRIENE-8-ONES

Set of 11-R-1,9-dinitro-13-(2-oxopropyl)-6,11-diaza-tricyclo[7.3.1.0^{2,7}]trideca-2,4,6-triene-8-ones was synthesized by Mannich reaction with Yanovsky adducts of 5,7-dinitro-8-hydroxyquinoline. The structure of the synthesized compounds was proved by 1D and 2D NMR spectroscopy.

Key words: Yanovsky adducts of 5.7-dinitro-8-hydroxyquinoline, Mannich reaction, NMR spectroscopy

V.M. MISIN, N.N. SAZHINA, E.I. KOROTKOVA, E.V. DOROZHKO, O.A. VORONOVA, T.A. KOROTKOVA

COMPARATIVE ANALYSIS OF CONTENT OF ANTIOXIDANTS AND THEIR ACTIVITY IN SAPS OF SOME MEDICINAL PLANTS

A comparative quantitative analysis of the total content of antioxidants and their activity with respect to the process of electro reduction of oxygen in saps of some medicinal plants were determined by two methods: amperometry and voltammetry. The high correlation of results was shown (r=0.96).

Key word: antioxidant activity, amperometry, voltammetry, medicinal plants

F.F. CHAUSOV

EFFECT OF ADSORBED IMPURITIES ON CRYSTAL GROWTH OF LOW-SOLUBLE SALTS FROM STRONG SUPERSATURATED SOLUTIONS

The crystal growth of low-soluble salts from highly supersaturated solutions in presence of absorbable impurities was described using the model of percolation through sites on a square two-dimensional lattice. It allows giving the quantitative estimation of surface critical coverage at which the crystallization rate decreases abruptly.

Key words: crystal growth, impurities influence, surface critical coverage, percolation model, covering critical degree

N.M. KASUMOVA

RESEARCH OF THERMODYNAMIC REGULARITIES OF CATALYTIC PROCESS OF SULFURS DIOXIDE REDUCTION

Thermodynamic calculations of the system SO_2–CH_4–N_2, SO_2–CH_4–O_2– N_2, SO_2–CH_4–H_2O–N_2, and SO_2–H_2–N_2, SO_2–H_2–O_2– N_2, SO_2–H_2–H_2O–N_2 were carried out. The calculations showed that the sulfur maximal equilibrium of 63-70% for CH_4 is reached at the temperature of 700°C and for 97–98% of H_2 at 200°C. The oxygen and water vapor presenting in initial gas phases (SO_2–CH_4 and SO_2–H_2) decrease the equilibrium sulfur yield at all temperature ranges and ratios of initial components under study.

Key words: thermodynamic calculations, pyrometallurgical plants, carbon monoxide and hydrogen, sulfur dioxide, methane

A.E. SOBOLEV, V.I. LUTSIK, O.V. TURKOVSKAYA

KINETICS OF CALCIUM CARBONATE INTERACTION WITH OXYETHYLIDENEDIPHOSPHONIC ACID SOLUTIONS

The kinetics of calcium carbonate interaction with oxyethylidenediphosphonic acid solutions was studied using the rotating disk method. The dependences of the specific rate of $CaCO_3$ dissolution on acid concentration, pH value of solution, temperature, disk rotation frequency, and duration of measurements were determined. According to the obtained kinetic model, the process is diffusion-controlled. The limiting stage is diffusion of hydrogen ions to the mineral surface.

Key words: dissolution kinetics, calcium carbonate, oxyethylidenediphosphonic acid, rotating disk method

I.N. TERSKAYA, A.S. NAUMOV

KINETICS OF Cu (II) REDUCTION BY SODIUM HYPOPHOSPHITE

The reaction of Cu^{2+} ions reduction by sodium hypophosphite was studied. On the base of kinetic and electrochemical data in comparison with the literature data a number of regularities were pointed out, namely, a reaction proceeds according to a dissociative mechanism, electron transfer proceed probably via a metal solid phase. Cu^{2+} ions reduction can be considered as a subsequent reaction and in a reaction system a significant accumulation of Cu intermediate form is observed. The size of metallic copper particles does not depend greatly upon the nature of a reducing agent. Probably, a reducing agent influences to a greater degree upon the step nucleus growth of a metallic phase rather than a stape of crystals growth.

Key words: kinetics, hypophosphite, reduction, copper salts, catalyst, dissociative mechanism, electron transfer through, effect of reducing agent nature, rate constant, activation energy, size of metallic phase particles.

I.V. SMIRNOVA, M.P. NEMTZEVA, O.V. LEFYODOVA, M.K. LUKOVITSINA

ESTIMATION OF DEGREE OF SKELETON NICKEL CATALYST DEACTIVATION AT LIQUID-PHASE HYDROGENATION OF SUBSTITUTED NITROBENZENES

The influence of skeleton nickel catalyst amount on the hydrogenation rate of substituted nitrobenzenes was studied. The main reason of the reaction rate decrease under low catalyst content was established to be the high oxibility ability of the nitrogroup. The estimation methodology of degree of skeleton nickel catalyst deactivation at liquid-phase hydrogenation of substituted nitrobenzenes was proposed.

Key words: deactivation, skeleton nickel catalyst, substituted nitrobenzenes, liquid-phase hydrogenation

L.N. MOROZOV, S.V. MAKHON'KO, P.S. PAVLICHENKO, M.S. POPOV

FORMATION OF CATALYTIC PROPERTIES OF SUPPORTED $CuO/K_2O/SiO_2$ CONTACTS DURING METHANOL DEHYDROGENATION

Catalytic properties of supported copper-containing $CuO/K_2O/SiO_2$ contacts in the reaction of methanol dehydrogenation were examined. The process of achievement of stationary operation condition with the catalyst was shown to be rather long and accompanied by change in its selectivity from methylformiate to formaldehyde.The results obtained were interpreted in terms of the changes in the surface of the catalyst copper component under reduction and the formation of carbon surface species with the participation of potassium oxide.

Key words: methanol, formaldehyde, methylformiate, heterogeneous catalysis

T.P. PETROVA, E.E. STARODUBETS, S.V. BORISEVICH, A.M. SHAPNIK

ELECTRO-REDUCTION OF Bi(III)-IONS IN ETHYLENEDIAMINETETRAACETATE-THIOUREA WATER SOLUTIONS

The electroreduction of bismuth(III) ions in ethylenediaminetetraacetate-thiourea water solutions was investigated by linear voltammetry at stationary bismuth electrode. The conditions of formation of mixed ligand complexes were found. The electrochemically active $[BiEdtaThio]^-$ complex was established to discharge more rapidly as comparing with the $[BiEdta]^-$ complex. The obtained results were discussed in terms of modern quantum mechanical theory of outersphere electron transfer in polar solvents using DFT calculations.

Key words: voltammetry, electro-reduction, bismuth, complexes, thiourea, ethylenediaminetetraacetate-ions, DFT calculations

V.A. BELETSKAYA, E.L. RUMYANTSEVA

FEATURES OF STRUCTURE FORMATION OF COLLOIDAL SILICA IN TECHNOGENIC SALTS SOLUTIONS

The decomposition of highly basic steelmaking slags with acids was shown to accompanied by complex colloid-chemical processes involving colloidal silica isolation, neutralization coagulation cations of technogenic solution to form the corresponding hydrosilicates, their hydrolysis and gel formation. The comparative analysis of the pecularities of structure formation of colloidal silica in the technogenic saline solutions was carried out.

Key words: sol of silicic acid, structure formation, neutralization coagulation, viscosity, gel

O.V. GORNUKHINA, I.A. VERSHININA, O.A. GOLUBCHICOV

RESEARCH OF SURFACE STRUCTURALLY-CHEMICAL MODIFICATION OF POLYPROPYLENE FILMS WITH POLYVINYL ALCOHOL

The experimental data showing the opportunity of structurally-chemical modification of a surface of polypropylene materials with polyvinyl alcohol are presented. The grafting of polyvinyl alcohol on a surface of polypropylene was carried out by polymeranalogous transformations. Optimum conditions of chemical modification of polypropylene by polyvinyl alcohol were established. Also, the superficially grafted polyvinyl alcohol was shown can act as an anchor group for immobilization chemically and biologically active substances.

Key words: polypropylene, structurally-chemical modification, polymer surface, surface modification, polyvinyl alcohol

N.L. PECHNIKOVA, A.V. LYUBIMTSEV, T.A. AGEEVA, S.A. SYRBU

SYNTHESIS AND COPOLYMERIZATION OF MONOMERS BASED ON MONO-*MESO*-OXYPHENYLPORPHYRIN

Tetrapyrrole macroheterocyclic compounds were obtained by an alkylation of allyl bromide and acylation by chlorides of acrylic and pentenoic acids of mono-*meso*-oxyphenylporphyrin. These compounds have the vinyl group in the phenyl ring of macroheterocycle and can serve as monomers for copolymerization with other conventional vinyl monomers.

Key words: porphyrin, alkylation, acylation, copolymerization, monomers

U.G. MAGOMEDBEKOV, U.G. GASANGADZHIEVA, Kh.M. GASANOVA, N.Kh. MAGOMEDBEKOV

DYNAMICS OF PROCESSES OF HOMOGENEOUS OXIDATION OF GLUTATHIONE IN PRESENCE OF OXYGENATED COMPLEXES OF IRON (II) WITH DIMETHYLGLYOXIME AND CYTOSINE

The results of evaluation of dynamic characteristics of process of homogeneous oxidation of glutathione in the presence of oxygenated complexes of iron (II) with dimethylglyoxime and cytosine are represented. On the basis of the analysis of time rows by the methods of discrete Fourier transformation reconstruction of the dynamics on temporal sequences, calculation of characteristic Lyapunov indicators and Kolmogorov-Sinai entropy it was obtained that dissipative structures appear in the form of realization of dynamic chaos of spatiotemporal nature in the system under study. It was pointed out, that considered approaches of the description of dynamics on the basis of the analysis of time series can be applied successfully with respect to the oscillatory processes of any nature.

Key words: glutathione, oxidation, dynamics, dissipative structures, dimension of phase spase and attractor, Lyapunov's indicators, Kolmogorov-Sinai entropy

V.Ya. TOLMACHEVA, V.G. BONDALETOV, L.V. TIMOSHCHENKO, E.I. IONOVA

KINETICS OF INTERACTION BETWEEN 9-HYDROXYMETHYL CARBAZOLE AND ALCOHOLS

Kinetics of the interaction between the 9-hydroxymethyl carbazole (9-HMC) and alcohols was studied. The formation of 9-(alkoxymethyl) carbazole was established to occur only at excess of alcohols in the presence of acid catalyst. The reactivity of 9-HMC with respect to various alcohols was determined by comparing the rate constants of pseudo-first order and equilibrium constants. The influence of relative acidity of alcohols and different substituents in the carbazole nucleus on the rate of interaction of 9-HMC with alcohols was studied.

Key words: alkoxymethylcarbazoles, alcohols, kinetics, reactivity

G.I. EGOROV, D.M. MAKAROV

INFLUENCE OF PRESSURE ON EXCESS THERMODYNAMIC CHARACTERISTICS OF WATER- DIMETHYLSULFOXIDE MIXTURES

Excess molar volumes V_m^E, changes in the excess molar thermodynamic characteristics such as Gibbs energy $\Delta_{P_o \to P} G_m^E$, entropy $\Delta_{P_o \to P} S_m^E$ and enthalpy $\Delta_{P_o \to P} H_m^E$ of water - dimethylsulfoxide mixture were calculated in the temperature range of 298.15-323.15 K and pressure range of 0.1-100 MPa. It was revealed that values of V_m^E are negative for all mixture compositions and for all range of pressure and temperature. Composition dependences of $\Delta_{P_o \to P} G_m^E$, $\Delta_{P_o \to P} S_m^E$ and $\Delta_{P_o \to P} H_m^E$ are characterized by the presence of extremes. The endothermic maximum is observed on the composition dependence of $\Delta_{P_o \to P} H_m^E$ in the range of small amounts of dimethylsulfoxide. Entropy change at these DMSO concentrations shows the lowering pressure effect in the process of system ordering.

Key words: water, dimethylsulfoxide, mixture of nonelectrolytes, influence of pressure, excess thermodynamic characteristics

K.R. RAMAZANOV, A.V. AFONIN, D.A. VERIN

OPTIMIZATION OF TECHNOLOGICAL PROCESS OF CRYSTALLIZATION OF AMMONIUM SULPHATE AT PROCESSING MOTHER LIQUOR OF ACRYLATE PRODUCTIONS

The physicochemical foundations of the crystallization process of ammonium sulphate from aqueous liquids, purified mother liquors of methylmethacrylate production, and organic impurity-contaminated mother liquors were analyzed. The estimation of some controllable technological parameters (pH, temperature, pressure, mother liquor composition, the presence of organic impurities) on the crystallization process of ammonium sulphate was carried out.

Key words: ammonium sulphate, crystallization, mother liquor of methylmethacrylate production

S.V. KOVALEV, K.S. LAZAREV, M.S. SELEZNEVA, I.V. KOTEL'NIKOVA

STUDY OF OSMOTIC PERMEABILITY IN AQUEOUS SOLUTION OF FERROUS SULFATE

In this study developed a method and system for experimental studies of osmotic permeability of the membrane apparatus with a flat channel in the flow mode, depending on the concentration and temperature of the solution.

Key words: membrane, osmos, permeability

G.K. SHURDUMOV, Yu.L. KARDANOVA

SYNTHESIS OF COPPER TUNGSTATE IN MELTS OF SYSTEMS (Li_2WO_4-Na_2WO_4) WITH EUTECTIC OF $CuSO_4$

In the given work the experimental data on development of rational method of copper tungstate production, its synthesis and identification in melt of systems eutectic (Li_2WO_4-Na_2WO_4) -$CuSO_4$ are presented.

Key words: synthesis, copper tungstate, thermal analysis, melting diagram

A.V. KOLYADO, E.V. DOROKHINA, I.K. GARKUSHIN

PHASE EQUILIBRIA IN SYSTEM PERCHLOROMETHANE-N-OCTADECANE

The results of phase equilibria study in a binary system perchloromethane - *n*-octadecane are presented. For this sysntem the parameters of point of non-variant equilibrium were determined. A comparison calculated on Schroder - Le-Shatele's method and experimentally found composition of eutectic has shown, that the relative deviation on a content of perchloromethane doesn't exceed 1.22 percents. It indicates that the system perchloromethane - n-octadecane is close to the ideal one.

Key words: n-octadecane, perchloromethane, eutectic, phase equilibria, refraction index

L.V. KOROLEV, D.O. BYTEV

PROCESSES MODELING RANDOM TRANSFER AT CONDITIONS OF LOCAL NON-EQUILIBRIUM

A continuous random jumps model taking into account the local nonequilibrium is proposed to describe the stochastic tranfer processes. The influence of form of distributions specifying the time and space parameters of single jump on macroscopic behaviour of process was investigated.

Key words: random transfer, nonequilibrium, diffusion

I.A. BOLOTOV, P.V. ZHUKOV, V.E. MIZONOV, S.A. DOBROTIN, V.A. ZAITSEV

MODELING OF HEAT CONDUCTION IN RING DOMAIN AT UNSTEADY BOUNDARY CONDITIONS

A cell mathematical model of temperature evolution in a ring domain at unsteady boundary conditions was proposed. The model can be used to describe unsteady temperature field in a roller with a local heat source running over its periphery. Computational examples demonstrating workability of the model and influence of process parameters on the temperature field are presented.

Key words: cell model, heat conduction, unsteady boundary conditions, state vector, transition matrix

A.N. BELYAKOV, V. P. ZHUKOV

INFLUENCE OF REGIME AND DESIGN PARAMETERS ON EFFICIENCY OF AERODYNAMIC CLASSIFICATION

A mathematical model of aerodynamic classification of powders in a gravity classifier, considering the influence of regime and design parameters on the efficiency of classification was developed on the base of the Boltzmann equation. Some results of numerical research of aerodynamic classification are presented

Key words: gravity classification, mathematical model, Boltzmann equation

L.A. MOSTOV, S.A. ERMAKOV, A.A. ERMAKOV

IDENTIFICATION OF REGIMES OF A SUBSTANCE MASS TRANSFER AT CONDITIONS OF SPONTANEOUS INTERFACIAL CONVECTION IN A LIQUID-LIQUID SYSTEM

Regimes of mass transfer through a plane interface were identified in a liquid-liquid system. The mass transfer is represented as a sum of two processes running simultaneously. The first process proceeds on the diffused-convection mechanism. The second process proceeds on the mechanism of spontaneous interfacial convection. The identification of regimes of mass transfer was shown using experimental data of influence of coercive convection on the mass transfer of butyric acid from benzene to aqueous solution of sodium hydroxide.

Key words: spontaneous interfacial convection, mass transfer, Monte-Carlo method

Z.E. BAIYRAMOVA, A.M. MAGERRAMOV, M.N. MAGERRAMOV, I.A. ALIEV, A.G. LYUTFALIEV, Kh.A. GARAZADE

ON ESTERIFICATION OF CARBOXYLIC ACIDS WITH ALCOHOLS

The opportunity of obtaining ethers with high enough yieds with the esterification of carboxylic acids with alcohols in the presence and absence of the catalyst without a release of formed water was established.

Key words: carboxylic acids, alcohols, esterification, oil acids, sulfuric acid