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## A B S T R A C T S

*O.Yu. POLETAEVA, G.Yu. KOLCHINA, A.Yu. ALEXANDROVA, E.M. MOVSUM-ZADE,  
I.Z. MUKHAMETZYANOV*

**INVESTIGATION OF INFLUENCE OF GEOMETRIC AND ELECTRONIC STRUCTURE  
OF ANTIOXIDANT ADDITIVES MOLECULES ON THEIR EFFICIENCY OF ACTION IN FUEL**

Using non-empirical RHF/6-31G(p) approximation for a gas phase, as well as with the use of quantum-chemical calculations of the high-level by B3LYP/6-31+G(d,p) method for the solvent the geometric and electronic structure and the standard enthalpy of formation of antioxidant additives were investigated. On this basis the estimation of their reactivity was carried out (atomic charges, Fukui coefficients). Atoms which are the most likely points of electrophilic and nucleophilic attack were revealed. The molecules rigidity was determined as well. The parameters mentioned above determine the behavior of the test compounds in the fuel.

**Key words:** antioxidant additives, reactivity, bond lengths, bond and dihedral angles, standard formation enthalpy, dipole moment

*I.A. KUZ'MINA, T.R. USACHEVA, K.I. KUZ'MINA, M.A. VOLKOVA, V.A. SHARNIN*  
**INFLUENCE OF REAGENTS SOLVATION ON GIBBS ENERGY CHANGES OF REACTION  
OF [Ag18K6]<sup>+</sup> COMPLEX FORMATION IN MIXED METHANOL-ACETONITRILE SOLVENTS**

The influence of methanol-acetonitrile solvents composition on the stability of complex Ag<sup>+</sup> with 18-crown-6 was studied. Replacement of MeOH by acetonitrile leads to the decrease in stability of [Ag18K6]<sup>+</sup>. The ratio of the reagents solvation contributions into the Gibbs energy changes of the [Ag18K6]<sup>+</sup> complex formation reaction at the solvation composition change was analyzed. The main role of the Ag<sup>+</sup> ion solvation contribution in the  $\Delta_r G$  changes at transfer from MeOH to its mixtures with AN was revealed. The applicability of the equation proposed by us earlier for predicting the [Ag18K6]<sup>+</sup> stability changes at the replacement of one solvent by another according to changes of the  $\Delta_r G(\text{Ag}^+)$  was confirmed.

**Key words:** thermodynamics, complex formation, solvation, Gibbs energy, silver ions (I), 18-crown-6 ether, methanol-acetonitrile mixed solvents

*S.M. MEDVEDEVA, G.M. MANAKHELOKHE, Kh.S. SHIKHALIEV*  
**SYNTHESIS OF 8-R-5'-R'-4,4,6- TRIMETHYL-3'-ARYL-4H,4'H-SPIRO[PYRROLE[3,2,1-  
IJ]QUINOLINE-1,2'-[1,3]THIAZOLIDINE]-2,4'-DIONES**

8-R-5'-R'-4,4,6-trimethyl-3'-aryl-4H,4'H-spiro[pyrrolo[3,2,1-ij]quinoline-1,2'-[1,3]thiazolidine]-2,4'-diones were synthesized by reacting 8-R-4,4,6-trimethyl-4H-pyrrolo[3,2,1-ij]quinoline-1,2-dione with arylamines and 2-mercaptoacetic acid (2-mercaptoacetic acid) in one and two (with isolation of the intermediate 8-R-4,4,6-trimethyl-1-(arylimino)-4H-pyrrolo[3,2,1-ij]quinolin-2(1H)-ones) steps.

**Key words:** hydroquinoline, spiroheterocycle, thiazolidin-4-one, 2-mercaptoacetic(propionic)acid, three-component cyclocondensation, spiro-pyrroloquinolinethiazolidine

*E.A. GUREEVA, A.V. BORISOV, G.P. SHAPOSHNIKOV*  
**SYNTHESIS OF 3,4-DICARBOXYLIC ACID OF BIPHENYL**

Given article reports on the new methods of synthesis of 3,4-dicarboxylic acid of biphenyl, allowing to increase the yield of target product up to 47 %.

**Key word:** 3,4-dicarboxylic acid of biphenyl, bromobenzene, 4-bromophthalic acid, mass-spectroetry, IR spectroscopy

**A.A. ROMAN, A.A. GOLICHENKO, A.V. SHTEMENKO**  
**CLUSTER COMPOUNDS OF RHENIUM (III) WITH TRYPTOPHAN**

The methods of synthesis of complex compounds of dirhenium (III) with tryptophan were developed. Composition and structure of received complexes were determined by the methods of elemental analysis, EAS, IR-spectroscopy, measuring of the molar conductivity.

**Key words:** rhenium, clusters, tryptophan, quadruple bond

*Yu. L. SUPONITSKY*

**THERMAL PROPERTIES OF RARE EARTH OXOCOMPOUNDS AND ELEMENTS OF VI GROUP**

Thermal properties of rare earths oxosalts containing acid anions formed with elements of VI group and nitrogen were systematized. The anomaly of thermal dissociation for sulphate-sulphite and selenite-selenate vapors was established. Cerium compounds are the least thermo stable in series iso-anion salts of rare earth salts. Peculiarity of thermal dissociation of oxosalts the anion of which is formed with non-metal is formation of intermediate stable compound like  $\text{Ln}_2\text{O}_2\text{CO}_3$ ,  $\text{LnONO}_3$  containing  $\text{LnO}^+$  crystal chemical ion. Similar oxocompounds are formed at the thermal dissociation of halogens and chalcogenides of rare earth metals in air.

**Key words:** thermal analysis, rare earths oxocompounds, sulfates, selenates, chromates, molybdates, tungstates, carbonates, cerium oxosalts

*E.V. EFREMOV, D.V. FILIPPOV, A.V. BARBOV, A.A. MERKIN*

**THERMAL ANALYSIS OF PALLADIUM CATALYSTS WITH DIFFERENT NATURE  
OF SUPPORT AND CONTENT OF ACTIVE METAL**

By the methods of thermal analysis - thermogravimetry, differential scanning calorimetry and the temperature-programmed reduction of catalysts the studies of processes occurring at heating samples of palladium catalysts were carried out. Phase changes in catalysts were shown to be directly associated with the processes of hydrogen adsorption-desorption. The quantity of desorbed hydrogen was established to depend on the concentration of the catalytically active metal and the nature of the support.

**Key words:** palladium catalysts, thermogravimetry, differential scanning calorimetry, temperature-programmed reduction, hydrogen thermal desorption

*A.G. TITOVA, M.A. KRESTYANINOV, A.M. ZAICHIKOV*

**THERMODYNAMIC AND STRUCTURAL CHARACTERISTICS OF AQUEOUS SOLUTIONS  
OF HYDROXYL- AND AMINO- DISUBSTITUTED ETHANES**

Thermodynamic characteristics of aqueous solutions of disubstituted ethanes were calculated. The results obtained allow revealing regularities of changes in the structural properties of the mixtures studied. The correlation of the entropy and enthalpy characteristics of the water-organic solvent systems with the excess packing coefficients suggests that the universal interactions determine the structural and energy properties of aqueous solutions. Structural and thermodynamic properties of aqueous ethylenediamine solutions turn out to be most similar to corresponding dependencies in mixtures of water with aprotic amides.

**Key words:** internal pressure, intermolecular interactions, thermodynamic and structural properties of aqueous non-electrolyte solutions, water, disubstituted ethanes

*L.Ya. TSARIK, A.V. ROKHIN, S.V. KAZAK, A.Yu. FEDORIN*

**NMR  $^{13}\text{C}$  STUDY ON COPOLYMERIZATION OF DIETHYL FUMARATE  
AND *p*-DIVINYLBENZENE**

In order to prevent crosslinking in radical copolymerization of diethyl fumarate and *p*-divinylbenzene, the reaction mixture was brominated. The double bonds of the unreacted monomers and divinylbenzene units in the copolymers react readily with bromine. Reaction mixture and the separated copolymers were studied by  $^{13}\text{C}$  NMR after bromination. The presence of alternating units in the copolymers of both monomers, as well as divinylbenzene block units was proved. Microgels of copolymers are formed by intrachain crosslinking of double bonds in divinylbenzene units of the copolymers.

**Key words:** divinylbenzene, diethyl fumarate, copolymerization, bromination, NMR spectroscopy, micro gels

*V. Yu. VOSKRESENSKY*

### **UNKNOWN PECULIARITY OF COMPLEX THERMODYNAMIC SYSTEMS**

Experiments with complex thermodynamic system with polyvariant equations of state (nickel) have demonstrated a disturbance of equilibrium in unified equation of I and II principles of thermodynamics for  $\delta Q$ . The reason for  $\delta Q$  non-holonomy may be associated with thermal nonuniformity of  $\delta Q$  addends, which is confirmed by disclosing non-thermal equations of state of nickel. They point to the existence of non-thermal subsystems for nickel. No polyvariant addends  $\delta Q$  of Pfaffian form have been detected. No necessity in the second principle of thermodynamics within the framework of equilibrium thermodynamics has been established. Macroscopic and microscopic aspects of thermodynamics are congruent.

**Key words:** bi- and polyvariantness, fluctuations, holonomy, homogeneity, Pfaffian form, principles of thermodynamics, thermal subsystem, unthermal subsystem, entropy

*A.A. REDOZUBOV, A.S. KRAEV, A.V. AGAFONOV*

### **INFLUENCE OF CONDITIONS OF SOL-GEL SYNTHESIS ON PHYSICO-CHEMICAL PROPERTIES OF TITANIUM DIOXIDE NANOPOWDERS AND THEIR EFFECTIVENESS AS FILLERS OF ELECTORRHEOLOGICAL FLUIDS**

New experimental data on the effect of conditions of sol-gel synthesis on the physico-chemical properties of nano titanium dioxide are given. The author's interpretation is given on the features of the influence of the structure and hydration of titanium dioxide nanoparticles prepared by sol-gel method as a filler of electrorheological fluids on the value of the electrorheological effect.

**Key words:** sol-gel synthesis, pH influence, electrorheology, titanium dioxide

*M.A. LUCHININA, A.V. AGAFONOV*

### **SYNTHESIS OF NANOROD STRUCTURES OF TITANIUM DIOXIDE MODIFIED WITH GOLD AND SILVER NANOPARTICLES AND THEIR PHOTOCATALYTIC PROPERTIES**

The method for obtaining nanorod structures of titanium dioxide modified with nanoparticles of gold and silver, based on the polyol synthesis of nanorods in the presence of titanium glycolate polyvinylpyrrolidone, precursor of nanoparticles of gold and silver, was proposed. The reduction process of gold nanoparticles on the surface of the nanorods of titanium glycolate was carried out. The comparison of the photocatalytic activity of titanium dioxide nanocomposites of rod-like structure, and nanoparticles modified with gold and silver with unmodified nanorod structures of  $\text{TiO}_2$  was carried out.

**Key words:** titanium dioxide, titanium glycolate, nanorods, polyvinylpyrrolidone, gold nanoparticles, silver nanoparticles, nanocomposite

*D.V. KADNIKOV, S.A. SMIRNOV, V.V. RYBKIN*

### **STUDY OF INFLUENCE OF ETCHING PRODUCTS OF POLYETHYLENE FILM ON PARAMETERS OF NON-EQUILIBRIUM AIR PLASMA**

The aim of this work is to study the impact of the loading effect of the plasma-chemical reactor on kinetics of etching of the polyethylene film and on the parameters of DC glow discharge in air. The etching rate is increased in the increasing the discharge current, the linear velocity of the gas flow and depends slightly on the gas pressure at constant any external parameters.

**Key words:** plasma air, loading effect, etching rate, non-equilibrium plasma, electric field strength

*E.M. MOVSUM-ZADE, G.A. KHABIBULLINA, A.S. BELYAEVA, A.A. NIKITINA*

### **RESEARCH OF COMPONENT COMPOSITION OF VAT RESIDUE OF 2,6-DI-TERT-BUTYL-4-METHYL-BUTYLPHENOL PRODUCTION**

By the methods of quantum-chemical modeling, high performance flash chromatography, NMR - spectroscopy the comprehensive study of the component composition of vat residue of 2,6-ditertbutyl-4-methylbutylphenol was carried out. The most likely mechanism of the reaction was shown to involve a cleavage of the C-N bond in quaternary ammonium salt of Mannich base. This leads to the synthesis of 2,6-ditertbutyl-4-methylphenol and 4,4'-ethylenebis (2,6-di-tert-butylphenol) which is the basic stable side compound.

**Key words:** 2,6-di-tert-butyl-4-methyl-butylphenol, vat residue, 4,4'-ethylenebis (2,6-di-tert-butylphenol), quantum chemical calculations

***Yu.V. POLENOV, E.V. EGOROVA, O.I. ODINTSOVA, A.A. PROKHOROVA***  
**ADSORPTION OF GLUCOPONES, UKANILS AND THEIR BINARY MIXTURES  
ON LIQUID-GAS INTERFACES**

The adsorption on the liquid-gas interfaces of a number of polyoxyethylenated alcohols, alkylpolyglucosides and their binary mixtures was investigated. The interaction parameters and the composition of the adsorption layers were determined using the pseudo-phase model of micelle formation of Rubingh and Rosen. The binary mixtures compositions having the most ability to micelle formation were established. Their efficiency was shown as components washing cotton textile.

**Key words:** adsorption, surfactant, glucopon, ukanil, Traube's constant, surface tension

***I.M. BORISOV, S.T. RASHIDOVA, R.S. LUKSHA***  
**WATER-ABSORBING CAPACITY OF COPOLYMERS OF DIALLYLDIMETHYLAMMONIUM  
CHLORIDE AND ACRYLAMIDE**

The new hydrogel - copolymer of diallyldimethylammonium chloride and acrylamide was synthesized. It was shown that the high efficiency of water absorption is achieved at the synthesis of the hydrogel under the molar ratio of 3:1 or 5:1, and high initiation and formation rate of particle with the size of 107 microns or 198 microns.

**Key words:** hydrogel, diallyldimethylammonium chloride, acrylamide, macromolecules sizes, swelling

***V.I. PAVLENKO, I.V. SOKOLENKO, A.V. NOSKOV***  
**COMPOSITE MATERIAL OF NEW TYPE FOR COMPLEX RADIATION SHIELDING**

The work presents the results of the development of a new highly effective radiation-shielding material for complex protection against gamma- and neutron radiation. Composition and production technology of an absolutely new composite material was developed. It is a leadborosilicate glass matrix reinforced by modified nanotubular chryzotile. Produced composite has a range of considerable advantages over its analogs and it can be used to solve various problems connected with protection against ionizing radiation.

**Key words:** composite material, complex radiation shielding, glass matrix, efficiency

***N.A. ZHUK, L.A. KOKSHAROVA***  
**ELECTRICAL AND MAGNETIC PROPERTIES OF NICKEL-CONTAINING SOLID SOLUTIONS  
OF BISMUTH NIOBATE  $\text{Bi}_3\text{NbO}_7$**

Solid solutions of  $\text{Bi}_3\text{Nb}_{1-x}\text{Ni}_x\text{O}_{7-0}$  are formed in a narrow concentration range of  $x < 0.065$ . By ESR and magnetic susceptibility methods the state of nickel atoms in solid solutions of bismuth niobate of cubic modification was determined. The results of measurement of the capacitance and the dielectric loss tangent of samples of solid solutions are presented in the temperature range from 313 K to 1053 K and in an alternating field at frequencies of 1 kHz - 100 kHz.

**Key words:** bismuth niobate, fluorite structure, heterovalent substitution, magnetic susceptibility, dielectric permeability, total electrical conductivity

***V.S. BAIYKOVA, I.I. OSOVSKAYA, G.V. RAKITINA***  
**SORPTION PROPERTIES OF NON-GRINDING CELLULOSE FIBERS**

The problems of applied and fundamental nature of paper manufacturing using the alternative technology (airformation) with a help of physical-chemical methods complex are considered. Reological and sorption properties, interactions of cellulose and water and bonds formation in a paper sheet are investigated.

**Key words:** cellulose, paper formation, surface properties, bond formation, calorimetry, sorption

***I.V. PANOV, S.P. SHAVKUNOV***  
**INVESTIGATION OF INFLUENCE OF SODIUM POLYACRYLATE ADDITION ON PROCESS  
OF WIDENING OF TUNNELS OF ETCHED ALUMINIUM FOIL**

The effect of addition of sodium polyacrylate (PAAS) on widening of etched tunnels of aluminium foil in 3%  $\text{HNO}_3$  solution was studied by polarization curves (PC) and electrochemical impedance spectroscopy (EIS). The PAAS addition was shown to be a polymeric mixed-type inhibitor. PAAS addition results in the decrease in the dissolution of exterior surface of the foil and in the increase in the dissolution of interior surface of etched tunnels of aluminium foil.

**Key words:** polymer corrosion inhibitors, sodium polyacrylate, widening etched tunnels, polarization curves, EIS

*R.K. GIMRANOV, R.A. KANTYUKOV, O.B. BUTUSOV, V.P. MESHALKIN, A.G. POPOV, R.R. KANTYUKOV*

**COMPUTER-AIDED ANALYSIS OF INTEGRAL PARAMETERS AND INDEXES FOR COMPLEX ASSESSMENT OF GAS FLOW PULSATION IMPACT ON PIPELINE WALLS**

Mathematical model of unsteady gas flow in two-dimensional pipe was developed. New integral parameters for assessment of gas flow pulsation impact on pipe walls were proposed. Gas flow parameters were calculated in ethylene production pipe using developed model.

**Key words:** unsteady gas flow, pipeline, mathematical modeling, integral indexes

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

**LOCALIZATION OF HEAVY METALS (Pb, Ni) IN TISSUES AND ORGANS OF BEANS AND SOYBEANS DURING ITS EXTRACTION FROM SOIL BY PLANTS WITH AND WITHOUT EFFECT OF MAGNETIC FIELD AND UV IRRADIATION ON SEEDS OF PLANTS**

Histochemical studies on accumulation and distribution of lead and nickel in phytomass of bean and soybean with and without pretreatment with the constant magnetic field and UV-radiation on the seeds of plants were carried out. It is shown that the metals mostly locate into the roots which protect the stems and leaves from pollutants. The physical fields impacted a beneficial effect on the plants increasing its viability.

**Key words:** localization, heavy metals (Pb, Ni), bean, soybean, magnetic field, UV-radiation