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D.V. CHACHKOV, O.V. MIKHAIYLOV

QUANTUM-CHEMICAL CALCULATION OF MOLECULAR STRUCTURE OF TRANS-ISOMER CHELATE COMPLEX FORMING IN Ni(II)–AMINOMETHANETHIOHYDRAZIDE SYSTEM

By means of hybrid method of density functional B3LYP/6-31G(d) the calculation of geometrical parameters of trans-isomer of NiL₂ chelate complex with singly deprotonated form of aminomethanethiohydrazide H₂N-C(=S)-NH-NH₂ (HL) formed as a result of complexing between nickel(II) trioxonitrate(V) of Ni(NO₃)₂ and HL at pH 7-9 has been carried out. The calculation results have been compared with structural data for that complex which appear recently in literature. The good agreement between calculated and literature structural data for this complex has been marked. It confirms an applicability of given method for calculation of chelate complexes with cycles of small number of atoms.

Key words: B3LYP chelate complex, aminomethanethiohydrazide, nickel (II)

M.T. MUNKUEVA, L.M. DIMOVA, G.I. SMIRNOV, G.V. RATOVSKIY

STUDIES OF POLYPHOSPHORIC ACID AND SORBENTS ON ITS BASE

The polyphosphoric acids obtained by oxide phosphor (V) or pyrophosphoric acid addition to orthophosphoric acid have been studied. On its base the inorganic sorbents of tin (IV) polyphosphate have been synthesized. Specific features and ion-exchange properties of the synthesized sorbents have been studied.

Key words: polyphosphoric acids, tin (IV) polyphosphate, ion-exchanger, ion-exchange properties, structure

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

CARBOXAMIDES DERIVATIVES OF 1-R-2-(2-PHENYLETHYL)-1-H-BENZO[D]IMIDAZOLE-5-AMINES

A series of 1-R-2-(2-phenylethyl)-1-H-benzo[d]imidazole-5-amines has been synthesized by condensation of 1,2,4-triaminobenzenes with 3-phenylpropionic acid. The combinatorial library of carboxamides derivatives for preclinical stage of developing new drugs has been obtained by liquid-phase parallel synthesis.

Key words: benzimidazoles, combinatorial synthesis

T.G. VOLKOVA, K.V. BALAKIN, Ya.A. IVANENKOV, N.A. MAGDALINOVA, M.V. KLYUEV

PREDICTION OF TARGET - SPECIFIC ACTIVITY OF ALKYLIDENANILINES AND SECONDARY AMINES OBTAINED ON THEIR BASE: COMPUTER MODEL

The classification model which allows predicting the efficiency of non-covalent complexes formation between low-molecular organic compounds (alkylidenanilines and its derivatives) and protein macromolecules (biotargets) has been constructed. The presence of a target specific activity of tested compounds has been shown by virtual screening.

Key words: biological activity, aliphatic-aromatic azomethines, secondary amines, "structure - property" ratio

L.G. EVSEVLEEVA, M.S. KIRIK

DATABASE FOR DISPLACEMENT REACTION REALIZING IN FLOW FOLLOWED BY ION-METRIC DETECTION

The data base has been created using of which it is possible to choose a chemical configuration of the system for displacement reaction at steady-flow condition.

Key words: displacement reaction, conventional equilibrium constant, potential forming ion

S.A. SHAPOVALOV, Ya.S. KISELEVA

INTERACTION OF CRESOL RED, THYMOL BLUE AND PHENOL RED ANIONS WITH CATIONIC DYES IN AQUEOUS SOLUTION

The formation of associates between one or two charged anions of o-cresol red or thymol blue as sulphonaphthalen dyes and cations of pinacyanol or quinaldine red as cyanine dyes has been considered in aqueous solutions. The values of equilibrium constants of association have been determined on the basis of spectrophotometric data. The geometric and energetic characteristics (enthalpy of formation) of ions and associates have been calculated by the AM1 semiempirical method, and the probable structure of associates has been proposed.

Key words: association, solution, cresol red, thymol blue, phenol red, absorption spectra, sulphonaphthalenins, formation enthalpy

N.V. BELOVA, G.V. GIRICHEV, N.I. GIRICHEVA, T.A. ZHUKOVA, N.P. KUZMINA

MOLECULAR STRUCTURE OF TRIS-DIPIVALOYLMETHANATE GALLIUM ON DATA OF ELECTRON DIFFRACTION AND QUANTUM CHEMICAL CALCULATIONS

Based on quantum chemical calculations (DFT/B3LYP) and reinterpretation of gas electron diffraction data the D₃ molecular structure of gallium tris-divaloylmethanate, Ga(thd)₃, has been established. The molecule Ga(thd)₃ has

plane chelate rings and GaO₆ antiprismatic polyhedron (the rotation of O-O-O triangles from their position in regular trigonal prism is $\theta=28.2(1.2)^{\circ}$). Main molecular parameters are: $r_{\text{hl}}(\text{Ga-O}) = 1.947(4)\text{\AA}$, $r_{\text{hl}}(\text{C-O}) = 1.271(3)\text{\AA}$, $r_{\text{hl}}(\text{C-C}_r) = 1.409(4)\text{\AA}$, $r_{\text{hl}}(\text{C-C}_l) = 1.548(4)\text{\AA}$, $r_{\text{hl}}(\text{C}_r\text{-C}_m) = 1.538(4)\text{\AA}$, $r_{\text{hl}}(\text{C}_m\text{-H}) = 1.091(3)\text{\AA}$, $\angle(\text{O-Ga-O}) = 89.8(0.6)^{\circ}$, $\angle(\text{Ga-O-C}) = 128.8(0.7)^{\circ}$, $\angle(\text{C-C}_r\text{-C}) = 122.4(1.4)^{\circ}$.

Key words: gas electron diffraction, β -diketones, gallium tris-dipivaloylmethanate, molecular structure

T.N. BOKOVIKOVA, O.N. BUGAETS, K.Z. NOVITSKAYA

LUMINESCENT PROPERTIES OF SYSTEMS OF JOINTLY PRECIPITATED HYDROXIDES OF EUROPIUM AND IRON

Luminescent properties of systems obtained by continuous co-precipitation of Europium and Iron hydroxides have been studied at stage of crystallization of amorphous products. Their complex investigation with help of physico-chemical methods has been carried out. The following methods have been used: differential and thermal analysis, IR spectroscopy, roentgenoluminescence, energy dispersion. The Eu³⁺ absorption spectra in system in the range of 741.4-746.9 nm has been studied. The dependence of systems luminescent intensity on synthesis conditions, components, concentration, structure, temperature and time has been established.

Key words: luminophors, Europium, metals, synthesis, structure, spectra, aging

V.G. SOLOMONIK, A.N. SMIRNOV, O.A. VASILIEV

THE LaF₃ NON-RIGID MOLECULAR STRUCTURE AND ITS EFFECT ON THE LANTHANUM TRIFLUORIDE VIBRATIONAL SPECTRUM AND THERMODYNAMIC PROPERTIES

The LaF₃, LaF, and LuF molecular properties have been calculated at the coupled cluster CCSD(T) level of theory with various basis sets ranging from triple-zeta to multiple-zeta quality. Scalar relativistic effects have been taken into account by means of the relativistic effective core potential and, in all-electron calculations, using the Douglas-Kroll-Hess Hamiltonian. Basis set incompleteness error has been removed by a counterpoise correction of the basis set superposition error, or by means of an extrapolation to the complete basis set (CBS) limit. The LaF₃ inversion potential has been studied in detail. High structural non-rigidity of the molecule has been revealed: the inversion barrier height is 120 cm⁻¹ at the CCSD(T)/CBS level of theory. The LaF₃ inversion vibrational spectrum has been calculated variationally. The band at 81 cm⁻¹ observed in the IR absorption spectrum of the neon matrix-isolated LaF₃ molecule (J.W. Hastie, R.H. Hauge, J.L. Margrave. *J. Less-Common Metals*. 1975, v.39, p.309) has been assigned to the inversion mode overtone $\nu_{\text{inv}} = 4 \leftarrow 1$ ($\nu_2 = 2^+ \leftarrow 0^-$) rather than to the fundamental transition $\nu_2 = 1 \leftarrow 0$ as it was assumed before. The LaF₃ partition function has been found using a direct summation of vibrational states calculated ab initio at the CCSD(T)/CBS level, and the LaF₃ gas phase thermodynamic functions have been calculated

Key words: lanthanum and lutetium monofluorides, lanthanum trifluoride, molecular structure and spectra, non-rigid structure, thermodynamic functions, quantum-chemical calculations, coupled-cluster method, basis set superposition error, complete basis set limit

S.V. LANOVETSKIY, V.Z. POIYLOV, A.M. SIZYAKINA, O.K. KOSVINTSEV, A.V. STEPANOV

STUDY OF KINETIC PARAMETERS OF CRYSTAL GROWTH PROCESS OF MANGANESE ACETATE TETRAHYDRATE

Results of study of growth rate of manganese acetate tetrahydrate crystal are given. Data on influence of various factors on crystal growth rate in over saturated solutions of manganese acetate solution have been obtained. The solution temperature influence on crystal growth mechanism has been determined.

Key words: manganese acetate tetrahydrate, crystal growth rate, crystallization, growth mechanism

E.L. TIKHOMIROVA, S.M. MASLOBOEVA, D.V. MAKAROV

STUDY OF KINETICS OF DEHYDRATION AND DECOMPOSITION OF POTASSIUM PEROXPENTAFLUOROTANTALATE MONOHYDRATE

The kinetics of potassium peroxy-pentafluorotantalate dehydration and decomposition has been investigated in the temperature range of 140-370 °C. The processes have been shown to proceed in the diffusion-kinetic region. Apparent rate constants and apparent activation energies have been calculated.

Key words: potassium peroxy-pentafluorotantalate, processes of dehydration and decomposition, thermal effects, kinetics, apparent rate constants, activation energy

L.E. OPARINA, N.R. ISHKULOVA, L.B. KOCHETOVA, N.V. KALININA, L.V. KURITSYN, T.P. KUSTOVA

SOLVENT INFLUENCE ON KINETICS OF AMINOACIDS REACTIONS WITH ACTIVATED NITROGROUP OF PHENYL ESTERS OF BENZOIC ACID

Kinetics of the reactions of glycine, L-proline and L-valine with substituted phenyl esters of benzoic acid in the water-1,4-dioxane solvent (water – 30-80 mass. %) has been studied. The rate constants for all investigated reactions have been established to increase in water mole fraction in 1,4-dioxane. Activation energies and entropies of the reaction of glycine with the 4-nitrophenyl ester of benzoic acid have been determined. The compensation effect has been discovered. It was show, that the mechanism of α -aminoacids interaction with complex esters didn't change at transition from isopropanol aqueous solutions to aqueous 1,4-dioxane.

Key words: reactivity, N-acylation, α -aminoacids, esters, water-1,4-dioxane

**D.V. FILIPPOV, M.V. ULITIN, A.A. MERKIN, M.A. RYAZANOV, A.V. KRAVCHENKO,
INVESTIGATION OF SURFACE ACID-BASE PROPERTIES OF DEPOSITED PALLADIUM CATALYST**

The acid-base and adsorption properties of active sites of the palladium catalyst surface have been studied with the combination of potentiometric and pK-spectroscopy methods in aqueous solutions.

Key words: deposited palladium catalyst, pK-spectrum, adsorption

**N.N. VERDIEV, Z.N. VERDIEVA, V.R. KAZANBEKOV, M.Sh. ZEYINALOV
PHASE COMPLEX OF SYSTEM $K_2F_2 - MgF_2 - CaF_2$**

The phase complex of $K_2F_2 - MgF_2 - CaF_2$ system has been studied with the differential thermal (DTA) and visual-polythermal (VPM) methods of physico-chemical analysis. The thermal-physical parameters of double components and three-components non-variant compositions have been revealed.

Key words: physical-chemical analysis, differential - thermal analysis, system liquidus, non-variant compositions, eutektik

**S.V. KOVALEV, S.I. LAZAREV, A.V. ERLIKH, V.V. MAMONTOV
STUDY OF COEFFICIENT OF DIFFUSION PERMEABILITY OF TIN SULFATE ON FLOW MEMBRANE
SET UP OF PLANE-CHAMBER TYPE**

In the work the experimental studies of diffusion permeability of OPM-K, ESPA, MGA-80P back osmotic membranes are given as a function of concentration and temperature for water solution of tin sulfate. The data were obtained on flow set up of plane-chamber type.

Key words: back-osmotic membrane, solution, diffusion coefficient of permeability

**E.Yu. MOSHCHENSKAYA, A.I. GARKUSHIN, I.K. GARKUSHIN
CALCULATION OF TOP AND LOWER CRITICAL POINTS IN SYSTEMS WITH LIMITED SOLUBILITY
IN LIQUID STATE**

In the work the calculation method of top and lower critical points of solubility diagrams on the limited experimental data is given. This method has been shown to allow reducing the number of experimental compositions for revealing critical points characteristics.

Key words: separation, top and lower critical points, calculation

**A.V. BALMASOV, E.N. CHASHINA
ELECTROCHEMICAL BEHAVIOUR OF COPPER IN AQUEOUS-AMINOALKOHOL KSCN SOLUTIONS
AT CONDITIONS OF CYCLIC POLARIZATION**

The electrochemical behaviour of copper has been studied in aqueous and aqueous-triethanolamine solutions of potassium thiocyanate by cyclic voltammetry. In potassium thiocyanate solutions the oxidation of metal copper occurred in two stages leading to Cu (I) and Cu (II) formation, respectively. Products of copper oxidation are reduced stepwise firstly to Cu (I) then to Cu (0). TEA addition in the composition of the solution leads to simplification of dissolution process of bivalent copper compounds. It is connected with formation of Cu (II) complex compounds.

Key words: copper, electrochemical behaviour, amino-alcohol, complexation

**O.V. PONOMAREVA, I.V. KOMLEV, V.A. PETUKHOV, O.R. KHROLOV, S.P. BELOV, E.E. NIFANT'EV
SPECTRAL-LUMINESCENT PROPERTIES OF DCM-FAMILY DYES IN ACRYLATE MONOMERS
AND POLYMERS AND THEIR COMPOSITIONS**

The spectral-luminescent characteristics of dyes for the red spectral range-DCM and parent substances have been studied in MMA, BMA, homo- and copolymers on their base. Dependencies of spectral properties both on the structure of synthesized dyes and rigidity and polarity of obtained acrylate matrixes caused their composition have been discussed.

Key words: DCM- family dyes, spectral-luminescent properties, acrylate polymers, inner plastification

**E.A. MEZINA, I.M. LIPATOVA, N.V. LOSEV
INFLUENCE OF HYDROACOUSTIC ACTION ON COMPATIBILITY OF CHITOSANE
WITH CELLULOSE TRIACETATE**

Possibility and efficiency of the application of hydroacoustic effects realized in the rotor-pulse device for production of high homogeneous compositions from mixtures of chitosan with cellulose triacetate has been studied.

Key words: chitosane, cellulose triacetate, polymer mixture, hydroacoustic action, rotor-pulse device

**Ya.O. MEZHUEV, Yu.V. KORSHAK, M.I. SHTILMAN, A.A. KOLEDENKOV, M.S. USTINOVA
KINETICS OF OXIDATION OF AMINO BENZOIC FRAGMENTS AT ANILINE POLYMERIZATION**

In the given work a novel mechanism has been proposed for oxidative polymerization of aniline. Methods of experimental determination of these model parameters have been considered. The new explanation of autoacceleration effect has been proposed.

Key words: aniline, polymerization, kinetic, mechanism

**V.A. ROZENTSVET, V.G. KOZLOV, E.F. ZIGANSHINA, N.P. BOREIYKO, Yu.B. MONAKOV
CATIONIC POLYMERIZATION OF ISOPRENE UNDER ACTION OF VANADIUM OXYTRICHLORIDE**

The cationic polymerization of isoprene under the action of vanadium oxytrichloride proceeds with a high rate up to deep monomer conversions without additions of protonodonor compounds to catalytic system. The characteristic feature

of the process is the presence of an induction period the duration of which increase at the polymerization temperature decrease. Regularities of the formation of the polyisoprene molecular parameters are principally the same as described previously for titanium and boron haloids based catalysts. However, the formation of branched and insoluble fractions in polyisoprene takes place at significantly lower concentration of the polymer in the reaction media.

Key words: cationic polymerization, isoprene, vanadium oxytrichloride, molecular parameters, microstructure

O.F. SHISHLOV, A.A. KOVALEV, V.V. GLUKHIKH

IN-SITU STUDY OF RESOLE PHENOL-CARDANOL-FORMALDEHYDE RESIN SYNTHESIS

The synthesis of resole type phenol-cardanol-formaldehyde resin (PCFR) by means of simultaneous condensation of phenol, cardanol (phenol of natural origin) and formaldehyde in aqueous media in the presence of sodium hydroxide as a catalyst and a molar ratio between components 1 : 0.035 : 2.263 : 0.875, respectively, has been studied. Sodium hydroxide has been added with two portions. The process has been controlled with the calorimetric and infrared spectroscopy methods. Experimental results allowed estimating the influence of two step sodium hydroxide addition on heat formation and change dynamic in monomer, semi-products and final product concentrations during PCFR synthesis.

Key words: synthesis, resole type phenol-cardanol-formaldehyde resin, IR spectroscopy, calorimetric measurements

L.A. KOCHERGINA, O.N. KRUTOVA, A.V. EMELIANOV

THERMODYNAMIC OF STEPWISE DISSOCIATION OF L-PHENYLALANINE AND D,L-β-PHENYL-α-ALANINE IN AQUEOUS SOLUTION

The heat effects of interaction of two optical isomers of L-phenylalanine and KOH and HNO₃ solutions have been measured by direct calorimetry at 288.15; 298.15K and 308.15K and at several ionic strengths in the presence of KNO₃ and LiNO₃. The standard thermodynamic characteristics of acid-base interaction reactions have been calculated in aqueous solutions of L-phenylalanine and D,L-β-phenyl-α-alanine.

Key words: thermodynamics, isomers, solutions, L-phenylalanin, D, L – β-phenyl – α-alanin

O.A. GOLUBCHIKOV

ENERGY-SAVING MATERIALS

Methods of production of new heat-insulating materials “Penlyt” and “Techfoam” and their properties are described. The materials are intended for heat insulation of buildings, industrial and energetic objects. The characteristics of traditional and new heat saving materials are compared.

Key words: heat-insulating materials, production methods, properties

I.V. TURCHANINOVA, D.A. FILIMONOV, M.I. BAZANOV, V.E. MAIYZLISH

STUDY OF ELECTROCHEMICAL AND ELECTROCATALYTICAL PROPERTIES OF SERIES OF DERIVATIVES OF COPPER PHTHALOCYANINE

The redox behavior of series of derivatives of copper phthalocyanines has been studied with cyclic voltammetry method in alkaline solution. The estimation of electro-catalytic activity of compounds has been given in the reaction of electro-reduction of molecular oxygen.

Key words: phthalocyanine and its derivatives, electrochemical conversion, macroheterocyclic complex, cyclic voltammetry, copper, molecular oxygen

M.V. TESAKOVA, V.I. PARFENYUK, V.A. GODLEVSKIY

TRIBOTECHNICAL PROPERTIES OF COMMERCIAL LUBRICANTS WITH ADDITIONS OF ULTRA DISPERSED COPPER CONTAINING POWDERS

The possibility of improvement of tribotechnical properties of commercial lubricants by introduction into this composition ultra dispersed copper containing powders obtained by electrochemical method has been shown. The efficiency of additives reaches a ultimate value at ultra dispersed copper containing powders concentration into lubricant of 20 mass.%. Maximal efficiency of copper containing powders additions manifests at large loads nearby of dry friction conditions.

Key words: lubricating compositions, ultra dispersed copper containing powders, tribotechnical characteristics

V.Yu. PROKOF'EV

INTERRELATION BETWEEN PASTE EXTRUSION CONDITIONS AND MECHANICAL STRENGTH OF GRANULES

The influence of extrusion rate and extrusion nozzle size on mechanical strength has been studied for granules obtained from pastes with various structural-mechanical and rheological properties. The extremal dependence of mechanical strength on rheological parameters has been revealed. The correlation between paste flow mode into extrusion nozzle channel and granule strength has been established.

Key words: paste, extrusion, rheology, structure-mechanical properties, mechanical strength

N.S. MAMEDOVA

RESULTS OF DEVELOPMENT AND STUDY OF CONTINUOUS ADSORPTION-ISOMERIZATION PROCESS OF MOTOR PETROL OBTAINING

In the article the results of development and study of the process of obtaining the environmentally safe benzine with continuous absorption combined with isomerization are shown. The technological scheme and process material balance is given. The micro-spherical zeoliteCaA has been used as adsorbent whereas a hydrogen form of modified high-

siliceous mordenite-containing natural zeolite has been used as a catalyst. The dynamics of the zeolite adsorption capacity decrease on normal paraffins has been studied as well as a loss with transporting agent of zeolite dust.

Key words: internal combustion engine, zeolite adsorption capacity, motor fuels, additives, antiknock compound

Z.K. MUHIDINOV, R.M. GORSHKOVA, A.S. DZHONMURODOV, D.Kh. KHALIKOV, Kh.I. TESHAEV, L.S. LIU, M.L. FISHMAN

ULTRA-FILTRATION CONCENTRATION AND PURIFICATION OF PECTIN POLYSACCHARIDES

In given work the processes of dia-ultra-filtration concentration and purification have been studied for pectin solutions obtained from various vegetable row using plane and hollow fiber membranes of different type. The influence of type and material of membranes and hollow fiber structure on main parameters of concentration process has been studied. Hollow fibre membranes have been shown to have a set of advantages as comparing with the plane ones. A membrane permeability depends on pectin etherification degree.

Key words: dia-ultrafiltration, membrane, pectin substances, etherification degree

Yu. E. TOKACH, Yu. K. RUBANOV

TECHNOLOGY OF PROCESSING WASTE PRODUCTS OF GALVANIC PRODUCTION

The technology of processing galvanic slimes and sewage has been proposed. The influence of mechanical and chemical activation at retreatment of galvanic production slimes on efficiency of heavy metals extraction has been studied. Results of metal extraction with electro-flotation method have been presented.

Key words: galvanic slime, sewage, heavy metals, chloride ions, mechanical activation, heat treatment, leaching, electroflotation

L.G. EVSEVLEEVA

GRAPH -THEORY APPROACH TO STUDYING DYNAMICS OF REACTION SYSTEMS IN STEADY-STATE FLOW CONDITIONS

The article describes possible steady-state conditions of reaction systems in a flow with the use of the graph theory language. Using reactions of potential formation of ion-selective membrane as an example, the possibility of linear relation existence between flows and forces has been discussed in flow system corresponding to Onsager reciprocal relation.

Key words: graf method, stationary stream

E.S. PATMAR, N.I. KOLTSOV

DETERMINATION OF STATIONARY STATES NUMBER OF CATALYTIC REACTIONS. MESSAGE 2

The method allowing to determine the number of internal stationary states of catalytic reactions proceeding on multistage nonlinear mechanisms is given. The examples illustrating the given approach for various mechanisms of reaction of catalytic oxidation of monoxide carbon are presented.

Key words: method, steady and unsteady internal stationary states, catalytic reactions, intermediate substances, stoichiometry, stage, mechanism

O.I. NIKOLAEVA, T.A. AGEEVA, M.E. GLAZKOVA, O.I. KOIFMAN

RESEARCH OF SOLUBILITY METHYLPHAEOPHORBIDE «A» AND HIS COPPER COMPLEX IN ORGANIC SOLVENTS

Solubility of methylphaeophorbide «a» and his of copper complex was determined in methyl methacrylate, tetrahydrofuran and in their mix (1:1) at 25 °C and 6 °C of the method of isothermal saturation of a solution with spectrophotometric the control of concentration of porphyrin.

Key words: solubility, methylphaeophorbide «a», copper complex of methylphaeophorbide «a», tetrahydrofuran