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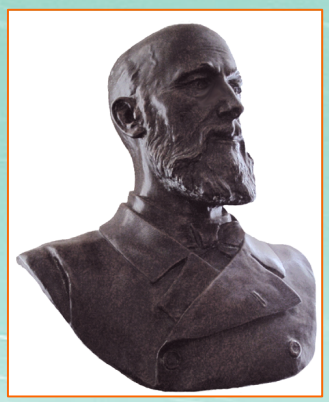

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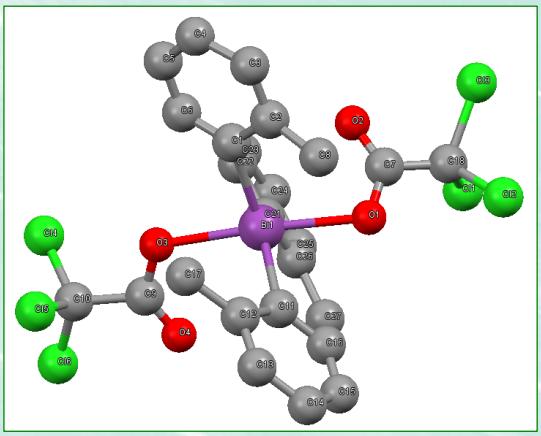

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*Subsection:* Chemistry of Fullerenes. *Registration Code of Publication:* 14-37-1-1
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http://butlerov.com/readings/
Contributed: January 21, 2014.

# Electronic and geometric structure of a number of fullerene isomers $C_{90}$ and structure of their chlorine and perfluoroalkyl polyadducts

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***Keywords:*** *fullerene $C_{90}$, IPR isomers, electronic structure, pyramidality, radical addition, chlorine and perfluoroalkyl derivatives, method of density functional theory.*

**Abstract**

For the first time we have shown the distribution of electron density and presented it as a traditional valence scheme, i.e. as simple, double and delocalized PI-bonds in molecules of IPR isomers of fullerene $C_{90}$: $46(C_{2v})$, $35(C_s)$, $30(C_1)$, $28(C_2)$, $32(C_1)$, $34(C_s)$, which are the predecessors of polyadducts $46(C_s)Cl_{32}$, $35(C_s)Cl_{24}$, $35(C_s)Cl_{28}$, $30(C_1)Cl_{22}$, $28(C_2)Cl_{26}$, $32(C_1)Cl_{24}$, $34(C_s)Cl_{32}$ and $32(C_1)(CF_3)_{12}$, $35(C_1)(CF_3)_{14}$, $30(C_1)(CF_3)_{18}$. The hexagons with delocalized π-bonds have been shown to be the most likely positions for addition of Cl and $CF_3$ radicals that reflects the important role the fullerene molecular electronic structure plays in the radical addition reaction.

*Thematic Section:* Preparative Research. **Full Paper**
*Subsection:* Organic Chemistry. *Registration Code of Publication:* 14-37-1-13
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: January 29, 2014.

# Synthesis of novel bifunctional thiophene and furan-containing isoxazole carboxamides

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***Keywords:*** *isoxazoles, sulfonylchlorination, electrophilic substitution, sulfonamides, carboxamides, isoxazole carboxylic acids.*

**Abstract**

Multistep method for synthesis of new bicyclic thiophene and furan containing isoxazolcarboxamides has been developed. The reaction of sulfochlorination of these molecular systems in their interaction with chlorosulfonic acid was investigated. The position of substitution in the process of electrophilic attack was determined by the method of two-dimensional correlation $^{1}H$-$^{1}H$ nuclear magnetic spectroscopy using the nuclear Overhauser effect.

*Thematic Section:* Preparative Research. **Full Paper**
*Subsection:* Coordination Chemistry. *Registration Code of Publication:* 14-37-1-21
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: January 15, 2014.

# Synthesis and adsorption on the gold surface di(4-(2-hydroxy-benzalimino)phenyl)-disulfide and its complexes with Co(II) and Cu(II)

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***Keywords****: disulfide, iminophenol complexes, cobalt(II), copper(II), coordination compounds, cyclic voltammetry, contact angles.*

## Abstract

Di(4-(2-hydroxy-benzalimino)phenyl) disulfide (**1**) has been synthesized by the reaction of salicyl-aldehyde and 4,4'-diaminodiphenyl disulfide with a yield of 98%. The complexation of the compound **1** with cobalt(II) and copper(II) chlorides and acetates has been investigated. Electrochemical studies of the prepared ligand and its chlorinated complexes by cyclic voltammetry have been made. The possibility of adsorption of the compound **1** on the gold surface and the formation of Co(II) and Cu(II)complexes with adsorbed ligand has been demonstrated by the contact angle of water droplets measurement.

*Thematic Section:* Preparative Research. **Full Paper**
*Subsection:* Organometallic Chemistry. *Registration Code of Publication:* 14-37-1-29
Publication is available for discussion within the functioning of the permanent internet-Conference "New methods of synthesis, structure and application of organoelemental compounds"
http://butlerov.com/synthesys/
Contributed: February 15, 2014.

# Synthesis and structure of *bis*(trichloroacetate) tri-*ortho*-tolylbismuth

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***Keywords:*** *tri-ortho-tolylbismuth, bis(trichloroacetate), dibenzoate, synthesis, structure.*

**Abstract**

Reaction of tri-*ortho*-tolylbismuth, carboxylic acid and hydrogen peroxide was conducted to obtain bis-(trichloroacetate) tri-*ortho*-tolylbismuth (**I**) (92%) and dibenzoate of tri-*ortho*-tolylbismuth (96%). According to the X-ray data, bismuth atoms in **I** have a distorted trigonal-bipyramidal environment (excluding additional coordination of carbonyl oxygen atoms) with *ortho*-tolyl ligands in equatorial positions. Lengths of Bi-C bonds in I constitute 2.20(2), 2.23(2), 2.25(2) Å, and distances Bi-O and Bi···O(=C) are equal to 2.33(1), 2.31 (3) and 3.12(3), 3.18(3) Å. Equatorial angle CBiC on the side of one contact Bi···O(=C) is increased (132.0 (9)°); the value of the similar angle on the side of other contact Bi···O(=C) (114.8(9)°) approaches the value of the third equatorial angle (113.2(9)°).

*Thematic Section:* Kinetic Research. **Full Paper**
*Subsection:* Organic Chemistry. *Registration Code of Publication:* 14-37-1-33
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: January 30, 2014.

*Topic:* Kinetics and mechanism of acyl transfer reactions. Part 7.

# Influence of pH medium on the reactivity of amines in *N*-acylation

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***Keywords:*** *acylation, aliphatic and aromatic amines, benzoyl chloride, medium effects.*

**Abstract**

The calculation of effective rate constants of reactions of mono substituted anilines with benzoyl chloride is carried out taking into account the contribution of kinetic and thermodynamic factors to the reaction rate. It is shown that a type of Brensted dependence can be change with the variation of ratio of amine pH and $pK_a$ values which determines the free amine part in the solution. It has been established that when studying the kinetics of the reactions with participation of aliphatic amines it is necessary to create pH medium, exceeding $pK_a$ amine, not less than 2 log. units. The conclusion is made that on carrying out kinetic investigations it is necessary to take into account accurately the parts of any compounds of reactive forms, able to protonation and deprotonation, since in water-containing media the protic acids can inhibit acylation of amines.

*Thematic Section:* Biochemical Research. **Full Paper**
*Subsection:* Analytical Chemistry. *Registration Code of Publication:* 14-37-1-39
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: January 9, 2014.

*Thematic course:* DNA sensor based on glassy carbon electrode modified with poly (neutral red). Part 2.

# Determination of daunorubicin and damaging action of Fenton's reagent

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***Keywords****: DNA sensor, biosensor, electro polymerization, electrochemical impedance measurement, quartz crystal microbalance.*

**Abstract**

DNA-based sensors have been developed using electropolymerized phenazine dye of neutral red and electrostatically adsorbed DNA to detect reactive oxygen species and intercalators. The action of these compounds determines the characteristics of the charge distribution and stabilization of the oxidized form of the dye, which reduces the peak current recovery of phenazine in voltammetric measurements and changes the parameters of electrochemical impedance sensor for impedimetric sensor. The possibility of impact sharing between intercalators and DNA oxidation in the direction of the resistance change and capacitance of charge transfer layer has been shown. Changes in the composition of the surface layer of the biosensor in the accumulation of DNA from oxidising agents and daunorubicin were confirmed by quartz crystal microbalance. The developed DNA sensors can be used in ecological and analytical control and biomedical research for detecting of DNA-damaging factors and the qualitative and semiquantitative determination of pharmaceuticals – DNA intercalators.

**Full Paper** _____ *Thematic Section:* Biochemical Research.
*Registration Code of Publication:* 14-37-1-48 *Subsection:* Inorganic Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: January 20, 2014.

# Synthesis and research of bioresorbability of silicon-substituted hydroxyapatite

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***Keywords:*** *hydroxylapatite, silicate ions, silicon-hydroxyapatite, extracellular fluid, structure, dissolution, bioresorbability.*

**Abstract**

By precipitation from a model solution of extracellular fluid samples we have synthesized hydroxyapatite and silicon-substituted hydroxyapatite. X-ray and IR spectroscopy analyses have been used to identify the structure and phase composition of the compounds obtained. It is established that during the deposition of the solid phase, a partial substitution of the phosphate ions took place in the hydroxyapatite structure of silicate ions. Studied bioresorbable calcium phosphate was modified in various environments: hydrochloric acid, isotonic solution. It has been found that with the increase of the proportion of silicate ions in the apatite structure, bioresorbability of silicon increases.

*Thematic Section:* Physicochemical Research. **Full Paper**
*Subsection:* Biochemistry. *Registration Code of Publication:* 14-37-1-55
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: February 6, 2014.

# Influence of the dispersion medium composition on the stability and electrokinetic properties of bilirubin

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***Keywords****: bilirubin, stability of dispersions, electrokinetic properties, zeta potential, microelectrophoresis, isoelectric point.*

**Abstract**

The electrokinetic properties and stability of aqueous dispersions with bilirubin have been investigated by the method of microelectrophoresis and photometry according to the composition of the dispersion medium (pH, concentration of singly-, doubly- and triple-charged electrolytes, amino acids). The acid-base equilibrium for the aqueous dispersions of bilirubin takes several hours to be established. The pH of the isoelectric point of bilirubin measured by microelectrophoresis in potassium chloride solution makes up 3.9 ± 0.1. It has been shown that the interaction of bilirubin with the simplest amino acids, iron cations II,III has a specific character.

**Full Paper** _____ *Thematic Section:* Technological Research.
*Registration Code of Publication:* 14-37-1-62 *Subsection:* Electrochemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: December 20, 2014.

# Influence of parameters of the electro-chemical process on the granulometric composition and morphology of titanium powder

© **Alexander V. Varaksin**,[1] **Viacheslav L. Lisin**,[2]* **Victor A. Kostilev**,[1]* **Leopold I. Leontiev**,[2]* **Robert G. Zakharov**,[2] and **Sophia A. Petrova**[2+]

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***Keywords****: nanopowder, titanium, electrochemical reduction, salt melt.*

**Abstract**

The influence of the parameters of electrochemical process (temperature and current density) on morphology and granulometric composition of superdispersed titanium powder was studied. It was established that particle size is increased with increasing the current density and temperature of the process. At the same time, the influence of the current density on the particle size is indirect, because an increase of current density leads to the appearance of the local heating centers and, as a consequence, to the particle growth in the producing metal.

**Full Paper** _____ *Thematic Section:* Technological Research.
*Registration Code of Publication:* 14-37-1-68 *Subsection:* Electrochemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: December 30, 2014.

# Electrochemical metal plating on superdispersed and nanosized carbides of tantalum and tungsten

© **Alexander V. Varaksin**,[1] **Viacheslav L. Lisin**,[2]* **Victor A. Kostilev**,[1]* **Leopold I. Leontiev**,[2]* **Robert G. Zakharov**,[2] and **Sophia A. Petrova**[2+]

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***Keywords****: titanium carbide, tungsten carbide, plating, nanopowder, superdispersed powder, chemical transport reactions.*

**Abstract**

In the work, investigations of metal plating (by iron, chromium, nickel, and titanium) on the nanosized and superdispersed powders of titanium and tungsten carbides obtained by electro-chemical reduction were carried out. Plating was made by the method of chemical transport reactions in the salt melt. It is shown that the surface of the conglomerates, composed of 2-3 tungsten carbide particles, is covered by impacted continuous Ni and Cr layers. The surface of titanium carbide particles is covered by $Fe_2Ti$-FeTi intermetallic layers, 100 nm in thickness.

**Full Paper** _____ *Thematic Section:* Electrochemical Research.
*Registration Code of Publication:* 14-37-1-76 *Subsection:* Electrochemistry.
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http://butlerov.com/readings/
Contributed: December 30, 2014.

# Electrochemical production of superdispersed and nanosized powders of metal and their carbides

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***Keywords****: superdispersed powder, electrochemical reduction, tantalum carbide, tungsten carbide.*

**Abstract**

In the work superdispersed and nanosized powders of metallic Ni, Cr, Mo, Co, Ta, W, Fe, as well as a mixture of specified composition powders, equal to the 12X18H10T alloy, were obtained by electrochemical process in the salt melt. To produce nanopowders of tantalum carbide TaC and tungsten carbide WC the electrochemical process of volumetric crystallization and the method of chemical transport reactions were used in combination. It is possible to obtain stoichiometric non-defect nanocrystalline powders of refractory metal carbides under moderate temperatures (600-1100 °C). The initial steel was decomposed into a number of stable compounds during electrochemical reduction.

**Full Paper** _____ *Thematic Section:* Physicochemical Research.
*Registration Code of Publication:* 14-37-1-84 *Subsection:* Physical Chemistry of Explosives.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
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# Co-crystallisates of some cyclic nitramines with polar solvents

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***Keywords:*** *cyclic nitramines, polar solvents, co-crystallisates, thermal decomposition, microscopy.*

**Abstract**

The article presents the results of research on the production co-crystallisates of cyclic nitramines (RDX, HMX, BCHMX, HNIW) with polar solvents containing different complexing groups, including the solvents of the class of linear nitramines. We identified some characteristics of co-crystallisates obtained by different methods.

**Full Paper** _____ *Thematic Section:* Theoretical Research.
*Registration Code of Publication:* 14-37-1-102 *Subsection:* Colloidal Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: January 29, 2014.

# Cluster electric aura of colloid-chemical oxyhydrate systems

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***Keywords:*** *Lagrangian maps, oxyhydrate gel systems, colloid clusters, spontaneous pulsation current, spike surge, diffuse double electric layer, bi-particle interactions, topological continuum, dissociation-disproportion destruction of macromolecules, Whitney's theory, geometry of caustics.*

**Abstract**

The research that we conducted into nonlinear properties of gel oxyhydrate systems revealed the following oscillatory dilatancy, oscillatory (pulsation) electrical conductivity, spontaneous electrical current of the gel self-organization accompanied by polarization phenomena, tinting of gel systems, oscillatory optical and sorptive properties, and many more. Those properties are attributed to wide occurrence of periodical processes in colloid chemistry of gel oxyhydrate systems of rare-earth elements, as well oxides-hydroxides of some of the *d*-elements, such as zirconium, niobium, titanium, etc. It is coherent chemistry that conducts researches into the subject, that is to say, chemistry of oscillatory periodical processes. The problem is that both classical inorganic chemistry and colloid chemistry remain far from understanding and elaborating an oscillatory development paradigm of the phenomena. However, even now the phenomena in question make it possible to see colloid systems crystallography in a new light, and to study changes in the shapes of colloid clusters in time. Our other approaches to the research into structures of gel colloid systems in time are rather of speculative nature.

**Full Paper** _____ *Thematic Section:* Theoretical Research.
*Registration Code of Publication:* 14-37-1-112 *Subsection:* Colloidal Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: March 7, 2014.

# Electroglobules, fulleroids and multipoles. Electric oscillations in oxyhydrate gels of *d*- and *f*-elements.

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***Keywords:*** *Lagrangian maps, electroglobules, fulleroids, multipoles, oxyhydrate gel systems, colloid clusters, spontaneous pulsation flow, diffuse double electric layer, topological continuum, dissociation disproportion mechanism, Whitney theory, geometry of caustics.*

## Abstract

We have obtained an equation for the electric structure of gel, conducted the self-consistency procedure for the distribution of dipoles in oxyhydrate gels, and introduced the terms macromolecular quadrupoles, octupoles, etc. Gel electric moments of higher even orders are the higher powers of the Laplace operators of orders six, eight, ten, etc. A new general ratio $j = \sum_{i=1}^{2k} \tilde{C}_i \sin\left(\omega_i x + \tilde{\varphi}_1\right)$ has been obtained, where new amplitudes and phases are obtained by adding oscillations with various phases, put down by formulas: $\tilde{C}_i \sin\left(\omega_i x + \tilde{\varphi}_i\right) = -4\pi\lambda q_0 C_i \left\{\left(\alpha_3\omega_i^2 - \alpha_5\omega_i^4 + ...\right)\sin\left(\omega_i x + \varphi_i\right) + \left(\tilde{\alpha}_2\omega_i^1 - \alpha_4\omega_i^3 + ...\right)\cos\left(\omega_i x + \varphi_i\right)\right\}$ that are described by the values of currents that in turn depend on the spatial periodic structures. In other words, we have experimentally established a relation between current $j$ and the nanoclusters of system $n$.

The analysis of the experimental data suggests that, lightweight clusters the quadrupoles of which provide a relatively weak current surge with a narrow amplitude determine the principal portion of time oscillations. Alongside with those clusters, there are elements of order three, four, five, and probably six.

Nanoclusters are formed according to the "magic numbers" rule, which we established in the course of experiments.

Discontinuities in the structure of the core networks and the partial chaotization of that structure form gel defects, to which small-size mobile clusters are attracted by electrostatic or electromagnetic forces, which subsequently become absorbed and arrange on the defects in accordance with their dipole moments. This fact is determined by the values of "magic numbers."

Cluster magic structures are stratified. The internal regions of such fulleroids are formed by, e.g., medium-structured clusters and their multipoles and octupoles. If the multipoles are the like multipoles at that, this generates oscillations in the cluster flows.

The regions inside fulleroids will never be filled tightly, which will also lead to constant cluster "filling-related" oscillations, that is, oscillations related to the filling of the cluster medium with oscillations. Knowing the filling parameters of a fulleroid (that is, the oscillations), one can determine its physicochemical parameters.

**Discussion Column** _____ *Thematic Section:* Theoretical Research.
*Registration Code of Publication:* 14-37-1-124 *Subsection:* Theory of the Structure of Matter.
*Editorial comment:* The article to be published because of its debatable, namely classical approach to the description of the nature of the electronic structure of matter, in particular ionic crystals. Queerness of representations of a new theory of nature of the covalent and ionic bonding, based on the model of the electron ring on the axis of the molecule, is, at first sight, puzzling. Nevertheless, in-depth reading of the material leads to the conclusion that the interpretation may be, at least convenient approximation, which allows, oddly enough, the correct description of the properties, in particular, the dielectric permittivity of ionic crystals. Reviewers of the article believe that a new perspective on the seemingly unshakable foundations of academic theory of the structure of matter allows to initiate a scientific discussion on this topic, which can lead to unexpected results in the fundamental outlook.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: March 12, 2014.

# Molecular structure of ionic crystals

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***Keywords:*** ionic crystals, dielectric polarization, molecular model.

**Abstract**

The problem of describing the so-called ionic crystals on the basis of new ideas about the nature of the covalent bond in accordance with the model of the ring on the molecular axis. The substantiation of the molecular structure of "ionic" crystals is presented. Equations are obtained of dielectric polarization, establishing a connection with the elastic the dielectric permittivity orientation and intramolecular ionic polarizabilities, which are actually responsible for the mechanism of polarization of crystals.

*Thematic Section:* Theoretical Research. _____ **Discussion Column**
*Subsection:* Theory of Materials Structure. *Registration Code of Publication:* 14-37-1-131
Editorial comment: The published material continues the discussion series of the author's articles on studying the applicability of the paradigm of classical physics to the description of the nature of the electronic structure of matter, in this case the metal crystals. The article reviewers believe this approach to be in many respects unconventional and controversial, requiring still deeper comprehension but the author system extension of its applicability to the concept of different types of chemical bonds, gives the right to "life" of the new views, at least in the discussion section. But the author's systematic extension of his concept's applicability to different types of chemical bonds, gives the new views right "to live", at least in the discussion section.

Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
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# The molecular structure of metals

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***Keywords:*** *metal crystals, molecular model, covalent bond, intermolecular interactions.*

**Abstract**

The problem described is the description of metallic crystals, based on the new concepts of the molecular structure of matter, according to which the structural constituents are not the acting ions, as it is customary in certain models, but diatomic molecules in the at the nodes of crystalline lattice. The substantiation of the molecular structure of metals and explanation of the properties and effects observed in the experiment have been given.

**Full Paper** _____ *Thematic Section:* Biochemical Research.
*Registration Code of Publication:* 14-37-1-138 *Subsection:* Biosynthesis.
Publication is available for discussion in the framework of the on-line Internet conference "*Chemical basis for the rational use of renewable natural resources*".
http://butlerov.com/natural_resources/
Contributed: February 27, 2014.

# The influence of the permanent magnetic field on growth and biological activity of callus culture of *Polyscias filicifolia (Moore ex Fournier) Bailey*

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***Keywords:*** *permanent magnetic field (PMP), medical plant tissue culture, antioxidant enzymes, biosynthesis of biologically active agents.*

**Abstract**

The article is devoted to the analysis of the influence of permanent magnetic field (PMP) on growth indicators, the ability to biosynthesis of the biologically active agents (BAA), as well as the level of activity of antioxidant enzymes: superoxide dismutase (SOD), catalase and peroxidase of a strain cells of Polyscias filicifolia (Moore ex Fournier) of Bailey, which were cultivated by biotechnological way. The obtained data have shown that the earlier the plant cells were influenced by PMP, the greater were the changes in the studied indicators.

**Full Paper** _____ *Thematic Section:* Biochemical Research.
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http://butlerov.com/natural_resources/
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# Spectrophotometric analysis of phenolic compounds medicinal calendulas (*Calendula officinalis* L.). Revision study of existing methods.

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***Keywords:*** *Calendula officinalis, Asteraceae, flavonoids, phenylpropanoids, spectrophotometry, solid-phase extraction.*

**Abstract**

Revision study of spectrophotometric methods of analysis of phenolic compounds in *Calendula officinalis* L., including pharmacopoeia, regulatory and others, previously proposed for the study of this plant species has been conducted. It was revealed that none of the existing methods will allow for proper and quantitative analysis of phenolic compounds in *C. officinalis*. A new method for the quantitative analysis of flavonoids and phenylpropanoids using solid phase extraction and spectrophotometry has been developed. Validation studies have shown that the method has satisfactory performance correctness, accuracy, linearity and repeatability.

**Full Paper** _____ *Thematic Section:* Physicochemical Research.
*Registration Code of Publication:* 14-37-1-156 *Subsection:* Toxicological Chemistry.
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# 3-Naphtoylindazoles and 2-naphtoylbenzoimidazoles as novel groups of synthetic cannabinoids: structure, analytical properties and identification of the first representative of this classes in the smoking mixtures, and the same metabolites in urea

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***Keywords****: synthetic cannabinoids, derivatives of 3-naphthoylindazoyle, 2-naphthoylbenzoimidazoles, identification, metabolites, chromatography-mass spectrometry, highly effective liquid chromatography, tandem mass spectrometry high resolution, NVR spectroscopy, IR-spectroscopy.*

## Abstract

Structures of novel synthetic cannabinoids were detected by the methods of LC/MC, including high resolution, high-performance liquid chromatography with tandem spectrometry of high resolution, NMR and IR spectroscopy. The obtained analytic characteristics of (naphtoyl-1)[1-(5-flouropentyl)-1H-indazol-3-yl]methanone, (naptoyl-1)(1-pentyl-1H-benzoimidazol-2-yl)methanone and (naphtoyl-1)[1-(5-flouropentyl)-1H-benzoimidazol-2]methanone allow to identify these compounds in the qualitative analysis of objects of examination of drugs, including smoking blends.

The metabolites of (naphtoyl-1)[1-(5-flouropentyl)-1H-indazol-3-yl]methanone were found and identified by the chemical and toxicological analysis of tests of urine of consumers of smoking blends. The spectrometric data of these metabolites are presented.

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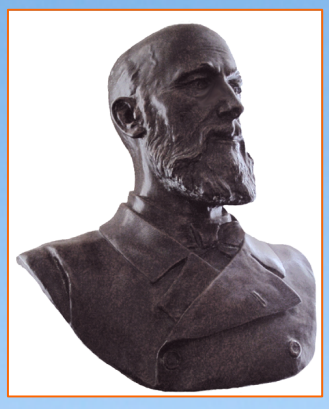

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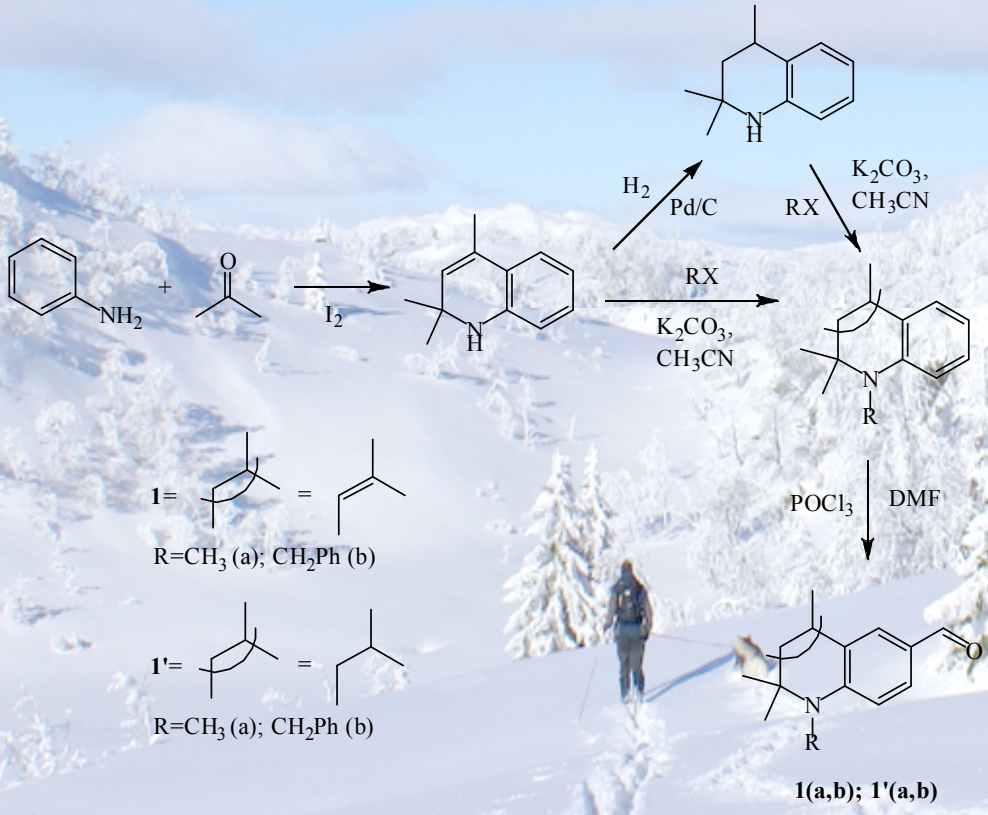


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*Thematic course*: Hydrochemical synthesis of chalcogenide films of metals. Part 18.

# Kinetic-thermodynamic analysis of the colloid-chemical deposition conditions and AFM-investigation of SnS films

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***Keywords:*** *ionic equilibriums, boundary conditions of formation, kinetic studies, colloid-chemical deposition, tin(II) sulfide, tin hydroxide, fractal dimension.*

## Abstract

The boundary conditions of formation of tin (II) selenide and its hydroxide have been defined by means of calculation of ionic equilibriums with the use of thermodynamic constants for "tin chloride − sodium citrate − sodium hydroxide − thiocarbamide" system, taking into account the crystallization factor. The induction period was detected on the kinetic curves deposition of tin(II) sulfide by thiocarbamide. It demonstrates an active role of colloidal hydroxide component of tin(II) during the formation of a solid phase SnS. AFM-investigation of SnS layers at different stages of growth was carried out using fractal formalism. It has been shown that the nucleation and growth of the SnS films occur by the mechanism of cluster-cluster aggregation.

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Contributed: April 11, 2014.

*Thematic Course:* Disposal of waste chromium. Part 1.

# The structure and composition of precipitation during recovery of chromium(VI) iron shavings in sulfuric acid solutions

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***Keywords****: chromium anhydride, chromium contaminated waste waters utilization, wastes of galvanic shops, hydroniumjarosite.*

**Abstract**

The range of $CrO_3$ and $H_2SO_4$ for sulfuric acid aqueous solutions of chromium anhydride, within which formation of soluble crystalline powder sediment complex composition occurred due to oxidation-reduction reactions with participation of metallic iron, was obtained. Held X-ray analysis of sediment has allowed to carry him on the structure of the phase of hydroniumjarosite $(H_3O)Fe_3(SO_4)_2(OH)_6$. Given the high chromium content in the sediments, concluded its phase composition as chromiferous hydroniumjarosite due to the inclusion of $Cr^{3+}$ in the structure by ion-exchange replacement. According to the results of the microscopic studies and elemental analysis the heterogeneity of the microstructure and chemical composition of the sediment for iron, chromium, sulfur and oxygen was revealed. Thus by the end of the deposition process the concentration ratio of iron and chromium in microcrystalline formations is in rather narrow range of values 1.53-1.73.

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# Regularities of benzotriazole derivatives sorption on hypercrosslinked polystyrene and octadecylsilica

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***Keywords:*** *benzotriazole, high performance liquid chromatography, octadecylsilica, hypercrosslinked polystyrene, acetonitrile.*

**Abstract**

The results of the chromatographic study of some benzotriazole derivatives sorption on hypercrosslinked polystyrene and ocktadecylsilica are presented. Physicochemical and electronic parameters of benzotriazole derivatives were calculated. The influence of the molecular structure of the analyte, the nature and composition of the eluent and sorbent for the chromatographic retention of these substances were analyzed.

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# Prediction and experimental studies of phase equilibria in the system cyclododecane – docosane

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***Keywords:*** *cyclododecane, docosane, n-alkanes, heat transfer agent.*

**Abstract**

By differential thermal analysis we have researched the system *n*-docosane – cyclododocane. The studied system is related to the systems of eutectic type (melting point of the eutectic composition of alloy equals 31.9 °C, the content of *n*-docosane 55.0wt %), in which the liquidus complicated by the presence of the polymorphic transition at *n*-docosane. By the DSC method we determined temperature and melting enthalpy of cyclododocane. According to DSC data it has been ascertained that in the temperature range from -60 to +62.8 °C of cyclododocanes no transformations occur in the solid phase.

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*Thematic course:* Aggregate stability of disperse systems. Part 1.

# Investigation of surface electrical properties and coagulation kinetic of monodisperse polystyrene latexe particles with surface carboxyl groups

© **Irina Yu. Shirokova**,[1+] **Vera I. Kuchuk**,[1] **Alexey P. Belyaev**,[1]
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***Keywords:*** *collidal stability, sols coagulation, electrokinetic potential,electrophoretic mobility, polystyrene latex.*

**Abstract**

In this work the electrokinetic behavior of monodisperse polystyrene particles with diameter 0.55 μm and 1.02 μm in the presence of indifferent electrolyte NaCl ($10^{-3}$, $10^{-2}$ and $10^{-1}$ mol/l) and varying pH (3-9) was observed. Using the direct method of flow ultramicroscopy the kinetics of latex coagulation in the solutions of NaCl in the range of pH 3-9 have been studied. Coagulation rate depends on the dispersion medium (pH and electrolyte concentration) and the size of polystyrene particles. Experimental coagulation rate was compared with theoretical rate (calculated in according with Smoluchowsky theory).

*Thematic Section:* Physicochemical Research. **Full Paper**
*Subsection:* Physical Chemistry of Explosives. *Registration Code of Publication:* 14-37-2-39
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# Properties thermoreversible cocrystals with a low temperature of melting on a basis hexanitrohexaazaisowurtzitane

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***Keywords:*** *co-crystals, thermoreversibility, burning, thermal decomposition, combustible binding.*

**Abstract**

Results of researches on producing co-crystals are presented in the article on the basis of hexanitrohexaazaisowurtzitane and on defining their properties. Parameters of thermal decomposition, burning, microstructure, as well as explosive characteristics and features of products of combustion of co-crystals depending on component structure, surplus of one of components and repeated melting of co-crystals with the subsequent cooling are determined. It has been shown that a series of the investigated co-crystals are thermoreversible, have low melting temperature and can be used as a binding basis of energy materials.

*Thematic Section:* Research Into New Technologies. **Full Paper**
*Subsection:* Chemistry of Dyes. *Registration Code of Publication:* 14-37-2-53
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http://butlerov.com/readings/
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# Obtaining nanomodified biocide woolen materials and research into sustainability of their fungicidal properties to wet treatments

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***Keywords:*** *azo dyes, dyeing, modifying drug, nanomodification, silver nanoparticles, fungicidal activity, wet processing.*

**Abstract**

In this paper, we present data on the fungicidal activity of wool fabrics dyed with acid colorant, and on simultaneous treatment by the modifying agent containing silver nanoparticles. The optimal concentration has been found for the working modifier in the dyeing bath which would provide the necessary degree of protection of the colored woolen fabric against fungi causing both mechanical and chemical destruction of fibers. The influence of wet treatment on the exhibited fungicidal activity is discussed.

**Full Paper** _____ *Thematic Section:* Research of New Technologies.
*Registration Code of Publication:* 14-37-2-60 *Subsection:* Petrochemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
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# A way for thermooxidizing cracking of heavy oil residues

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***Keywords:*** *fuel oil, thermal cracking, initiation with oxygen, sulfur compounds.*

**Abstract**

It has been shown that initiation of thermal cracking of fuel oil by the oxygen of the air can be used in industry as as an effective way to produce additional light fractions. The thermal cracking in conditions described in the work (T = 430-440 $^{o}$C, P = 3-7 atm.) via homolytic cleavage of the C–C, as is customary in the literature, hardly occurs. Cracking is a catalytic process and the compounds of both oxygen and sulfur cfn be used as catalysts. Analysis of the modernization cost of the existing plants suggests that material expenditures on upgrading by this method will be a fraction of the cost of construction of new plants by the existing technologies, and their payback period is about 2 years.

**Full Paper** _____ *Thematic Section:* Research Into New Technologies.
*Registration Code of Publication:* 14-37-2-66 *Subsection:* Physical Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
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# Sorbents in wastewater treatment of dyeing and finishing production

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***Keywords****: adsorption, activated carbon, shungite, synthetic dyes, wastewater.*

**Abstract**

Natural shungite sorbent has been researched in comparison with activated carbon for treatment of wastewater containing water-soluble dyes. Physical and chemical characteristics of sorbents, sorption capacity of sorbents and equilibrium adsorption isotherms were studied. It has been shown that shungite is capable to remove efficiently the colorants from aqueous solutions.

*Thematic Section:* Research Into New Technologies._____ **Letter to the Editor**
*Subsection:* Physical Chemistry. *Registration Code of Publication:* 14-37-2-71
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http://butlerov.com/readings/
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# Drying of inert gas with zeolite clinoptilolite

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***Keywords****: drying, zeolite, silica gel, adsorbent, clinoptilolite, inert gas, dew-point.*

## Abstract

Aluminosilicate molecular sieves (zeolite), thanks to the features of the porous structure and the chemical nature, are the best adsorbents applied in technological processes of division, cleaning and a deep drying of gas and liquid mixes. However widespread introduction of synthetic zeolites in the industry is slowed down due to their relative high cost. In this regard, the use of the natural zeolites considerable deposits of which are found both in Russia, and abroad is of special interest.

The paper presents a study on the use of natural zeolite clinoptilolite to dry the inert gas.

*Thematic Section:* Research Into New Technologies. **Full Paper**
*Subsection:* Inorganic Chemistry. *Registration Code of Publication:* 14-37-2-73
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Contributed: March 18, 2014.

# The effect of the chemical nature of initial alkoxides taken for hydrolysis and calcination conditions of obtained precipitates on morphology and a specific surface area of titanium dioxide powders

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***Keywords:*** *titanium alkoxides, hydrolysis, titanium oxohydroxide, titanium dioxide, synthesis, properties.*

## Abstract

The effect of chemical nature of initial alkoxides taken for hydrolysis and calcination temperature of obtained precipitates on morphological characteristics of the final products – titanium dioxide (TD) powders are discussed in the paper.

It has been shown that nature of initial titanium alkoxide influenced on the particles size of the obtained TD powders. The amount of fine particles (less than 0.5 microns) in TD powders is increased from 40.32 to 97.85% in order: titanium tetratertbutoxide → titanium tetraisopropoxide → titanium tetrapropoxide → titanium tetrabutoxide.

Increasing the calcination temperature of oxohydroxide precipitates leads to the growth of average particle size and decreasing of specific surface area (*S*) of the obtained TD powders. Simultaneously, the increase in percentage of narrow pores and decrease in percentage of wide pores in the particles of the material are observed. However, even in TD powders heated above 600 °C approximately 40% of the particles are smaller than 0.5 microns. The value of *S* for samples calcined at 600 and 900 °C remained 50-55 and 8 $m^2/g$ respectively.

*Thematic Section:* Preparative Research. **Full Paper**
*Subsection:* Organic Chemistry. *Registration Code of Publication:* 14-37-2-77
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http://butlerov.com/readings/
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# One-pot, three-component synthesis of 12-(1-alkylhydroquinolin-6-yl)benzimidazoquinazolinones

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***Keywords**: Three-component reaction, fused quinazolinones, benzimidazoquinazolinones, hydroquinoline-6-carbaldehyde.*

**Abstract**

New benzimidazoquinazolinone derivatives are synthesized via a one-pot, three-component reaction of 1-alkylhydroquinoline-6-carbaldehyde, 2-aminobenzimidazole, and cyclohexane-1,3-dione compound. The products were obtained in high yields within 5-10 minutes in refluxing *N,N*-dimethylformamide. The newly synthesized compounds were characterized by $^{1}$H-NMR, and elemental analysis techniques.

*Thematic Section:* Preparative Research. **Full Paper**
*Subsection:* Organic Chemistry. *Registration Code of Publication:* 14-37-2-83
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# Synthesis, structure and photoluminescence of Zn(II) 2-methyl-6,7-difluoro-8-oxyquiolate

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**Pavel A. Slepukhin**,[2] and **Valery N. Charushin**[1,2]*
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***Keywords:*** *2-methyl-6,7-difluoro-8-hydroxyquinoline, Zn(II) complex, X-ray, photoluminescence.*

## Abstract

Synthesis of 2-methyl-6,7-difluoroquinoline Zn(II) complex of structure $[Zn(L\text{-}H)_2]\cdot 2HC(O)NMe_2$ was realized. Structure of the complex has been proved by NMR $^1H$, $^{19}F$ NMR, mass-spectra as well as X-ray data. Atom of Zn was shown to be pentacoordinated, type of coordination of the central atom is the distorted trigonal bipyramid. Complex demonstrates green fluorescence in acetonitrile solution.

*Thematic Section:* Preparative Research. **Short Communication**
*Subsection:* Organic Chemistry. *Registration Code of Publication:* 14-37-2-87
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http://butlerov.com/readings/
Contributed: March 18, 2014.

*Thematic course:* Maleimides and their derivatives. Part 4.

# *Bis*-maleimide, based on butyl ester of 3,5-diaminobenzoic acid

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***Keywords:*** *monoamides of maleic acid, maleimides, cyclization, IR and $^1$H NMR spectra.*

Abstract

Interaction of maleic anhydride with butyl ether of 3,5-diaminobenzoic acid resulted in the synthesis of *bis*-monoamide of maleic acid, by cyclization of which under the action of acetic anhydride the corresponding *bis*-maleimide has been obtained. The synthesized compounds were characterized by IR and $^1$H NMR spectroscopy, their properties are studied.

**Full Paper** _____ *Thematic Section:* Preparative Research.
*Registration Code of Publication:* 14-37-2-90 *Subsection:* Organoelemental Chemistry.
Publication is available for discussion within the functioning of the permanent internet-
Conference "New methods of synthesis, structure and application of organoelemental compounds"
http://butlerov.com/synthesys/
Contributed: February 14, 2014.

# *Bis*(pentafluorobenzoate) and *bis*(1- adamantane carboxylate)-*tris*(5-bromine-2-methoxyphenyl)antimony. Synthesis and structure.

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***Keywords:*** *bis(pentafluorobenzoate), bis(1-adamantanecarboxylate), tris(5-bromine-2-methoxyphenyl)antimony, synthesis, structure.*

**Abstract**

By interaction of *tris*(5-bromine-2-methoxyphenyl)antimony with pentafluorobenzoic and 1-adamantanecarboxylic acids in the presence of hydrogen peroxide we have synthesized *bis*(penta fluorobenzoate) and *bis*(1-adamantanecarboxylate) *tris*(5-bromine-2-methoxyphenyl) antimony $[(5\text{-Br})(2\text{-MeO})C_6H_3]_3Sb[OC(O)R]_2$, where R = $C_6F_5$ (**I**), $C_{10}H_{15}$ (**II**). According to the data of X-ray diffraction analysis, antimony atoms in **I**, **II** have distorted trigonal-bipyramidal coordination. Axial angles OSbO and angles in the equatorial plane CSbC are equal to 177.54(13)°, 171.7(4)° и 110.65(19)°–124.57(19)°, 113.3(12)–127.3(10)° respectively. Bond lengths Sb–O и Sb–C make up 2.086(3), 2.117(3), 2.100(5)–2.106(5) Å (**I**); 2.072(11), 2.074(11), 2.040(19)–2.16(2) Å (**II**). The intermolecular distance Sb···$OCH_3$ и Sb···O=C equals 3.088(5)–3.181(4) Å and 3.213(4), 3.330(5) Å (**I**), 3.100(5)–3.188(5) Å and2.983(5), 3.094(5) Å (**II**).

*Thematic Section:* Preparative Research. **Full Paper**
*Subsection:* Organoelemental Chemistry. *Registration Code of Publication:* 14-37-2-95
Publication is available for discussion within the functioning of the permanent internet-Conference "New methods of synthesis, structure and application of organoelemental compounds"
http://butlerov.com/synthesys/
Contributed: February 14, 2014.

# Features of the structure of 4-nitro phenoxide tetraphenylantimony

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***Keywords:*** *4- nitrophenoxide tetraphenylantimony, features of structure.*

**Abstract**

By interaction of *bis*(4-nitrophenoxy)triphenylantimony with pentaphenylantimony there was synthesized 4-nitrophenoxide tetraphenylantimony with the yield 98%. According to the data of X-ray diffraction analysis, antimony atoms in two crystallographically independent molecules **Ia,b** have distorted trigonal-bipyramidal coordination. Axial angle CSbO and sums of angles CSbC in the equatorial plane are equal to 177.97(7)° and 357.16° (**Ia**), 176.95(7)° and 357.07(7)° (**Ib**). Bond lengths Sb–O and Sb–C make up 2.208(1) and 2.116(2), 2.117(2), 2.118(2), 2.171(2) Å (**Ia**), 2.224(1) and 2.108(2), 2.114(2), 2.129(2), 2.165(2) Å (**Ib**). Features of the structure of tetraphenylantimony aroxide were discussed.

*Thematic Section:* Preparative Research. **Full Paper**
*Subsection:* Organometallic Chemistry. *Registration Code of Publication:* 14-37-2-99
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http://butlerov.com/synthesys/
Contributed: April 16, 2014.

# The preparation of polytungstenphenylsiloxanes by interaction of polyphenylsiloxane with the tungsten oxide(IV) in the conditions of mechanochemicfl activation

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***Keywords:*** *polytungstenphenylsiloxane, polyphenylsiloxane, mechanochemical activation.*

**Abstract**

The interaction of polyphenylsiloxane with tungsten oxide(VI) in conditions of mechanochemical activation has been studied. The polytungstenphenylsiloxanes have been prepared with the yields from 43.3 to 44.8% with the activation time of five or three minutes, respectively. The relation Si/W (9.2-9.3) has been prepared. The relation differed from initial relation (1.0) and did not depend on time of interaction. The composition of the products of interactions has been studied by methods of elemental analysis, IR-spectroscopy, gel-chromatography, X-ray diffractometry.

*Thematic Section:* Preparative Research. **Review**
*Subsection:* Nanochemistry. *Registration Code of Publication:* 14-37-2-103
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: April 15, 2014.

# Chemical methods for producing copper nanoparticles

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***Keywords****: nanoparticles, copper, synthesis, morphology.*

**Abstract**

Chemical methods for producing copper nanoparticles are summarized and analyzed. The main types of processes leading to the production of copper nanoparticles were studied: thermal decomposition of copper compounds; directed selection of ligands to reduce the redox potentials of copper complexes; use of different spatially restricted systems as nanoreactors. The major factors have been shown (redox-potential of complex copper compounds, reducing agent, stabilizers, pH etc.), affecting the morphology and stability of the resulting copper nanoparticles.

**Full Paper** _____ *Thematic Section:* Biochemical Research.
*Registration Code of Publication:* 14-37-2-114 *Subsection:* Analytical Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
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# Identification of PB-22F cannabimimetics' metabolites in urine

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***Keywords:*** *cannabimimetics, metabolism, enzymic hydrolysis, solid-phase extraction, gas chromatography – mass spectrometry.*

## Abstract

Metabolism of quinolin-8-yl-1-(5-fluoropentyl)-1H-indole-3-carboxylate (PB-22F) cannabimimetics is discussed. Identification of PB-22F metabolites in urine of users' smoking mixtures was performed. Gas chromatographic and mass spectrometric characteristics of some PB-22F metabolites derivatives were described. The conclusion of the analytical importance of the main PB-22F metabolites, having a value in the expert practice is given.

**Full Paper** _____ *Thematic Section:* Biochemical Research.
*Registration Code of Publication:* 14-37-2-122 *Subsection:* Analytical Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Chemical basis for the rational use of renewable natural resources*".
http://butlerov.com/natural_resources/
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# *Dreissena polymorpha pall.* (*mollusca*) as a part of mobile bioplato hydrobicenosis as batteries of contaminats

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***Keywords****: environmental pollution, heavy metals, aquatic life, X-ray fluorescence analysis, concentration of pollutants, mobile bioplato.*

**Abstract**

The features of the accumulation of contaminants in Dreissena-fouling organism of mobile bioplato that functioned in the lake Middle Kaban in Kazan were studied. In a comparative aspect, we have shown the perspective of the contribution of heavy metals removal by various aquatic organisms. The role of Dreissena in the accumulation of pollutants have been assessed.

*Thematic Section:* Biochemical Research. **Full Paper**
*Subsection:* Chemical Specificity of Biocenoses. *Registration Code of Publication:* 14-37-2-127
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http://butlerov.com/natural_resources/
Contributed: February 15, 2014.

# *Plumatella fungosa* (*bryozoa*) in the composition of hydrobiocenosis of mobile bioplato as an accumulator of contaminants

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***Keywords:*** *pollution, heavy metals, aquatic organisms, roentgen-fluorescent analysis, contaminants concentration, mobile bioplato.*

## Abstract

Characteristics of contaminants accumulation in hydrobionates in the composition of bryozoa of mobile bioplato, functioning in the biocenose existing in the lake Middle Kaban in Kazan are presented. We have shown the input of different hydrobionates as compared to aquatic organisms in disposing from heavy metals. The role of *Plumatella fungosa* which are able additionally to raise productivity of bioplato functioning have been determined.

*Thematic Section:* Chemical and Technological Research. **Full Paper**
*Subsection:* Organic Chemistry. *Registration Code of Publication:* 14-37-2-131
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http://butlerov.com/readings/
Contributed: March 12, 2014.

# Competition of tautomeric transformations of α-acyl aminoanthraquinones

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***Keywords****: tautomerism, rotational isomerism, electronic absorption spectra, quantum-chemical calculations, correlation analysis, antraquinones, α-acylaminoantraquinones.*

**Abstract**

α-Acylaminoantraquinones have not 9,10-, but 1,10-quinoid structure. Their characteristic feature is competition of two types of tautomerism – acylamino-acylimino and keto-enol, connected with the migration of hydrogen atom in acylamino group. For benzoylaminogroups the most characteristic structure is NHCOPh, and for acetylamino groups − N=C(OH)Me. Both basic and excited states are responsible for tautomeric transformations. Excitation of molecules is accompanied by a shift of tautomeric equilibria.

*Thematic Section:* Chemical and Technological Research. **Full Paper**
*Subsection:* Organic Chemistry. *Registration Code of Publication:* 14-37-2-139
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: March 12, 2014.

# Tautomeric equilibria as a form of existence of matter. Structure and tautomerism of ametantrone – a medicinal substance of anthraquinone series.

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***Keywords****: tautomerism, rotational isomerism, electronic absorption spectra, quantum-chemical calculations, correlation analysis, anthraquinones, ametantrone.*

**Abstract**

Ametantrone is not a derivative of 9,10-antraquinone, it exists as a dynamic equilibrium mixture of hydrochlorides 4,9-bis(alkylamino)-1,10-antraquinone, 9-hydroxy-10-alkylamino-1,4-antraquinone-1-alkyl-imine and 4,9-dihydroxy-1,10-antraquinone-1,10-bis(alkylimine). Properties of ametantrone depend on the ratio of tautomers, changing under the influence of external factors.

**Full Paper** _____ *Thematic Section:* Chemical and Technological Research.
*Registration Code of Publication:* 14-37-2-146 *Subsection:* Chemistry of Fullerenes.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: March 18, 2014.

# Quantum-chemical modeling of the reaction of $C_2H_2$ molecule intercalated with $C_{60}$

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***Keywords****: reactivity, C60, acetylene, octahedral pore.*

**Abstract**

Reactivity of $C_{60}$ was investigated by DFT/PBE/SBK with respect to acetylene intercalated into fullerite Formation of new chemical compounds between $C_{60}$ and $C_2H_2$ in the octahedral pore fullerite was predicted. Spectral properties (IR-spectrum and the NMR chemical shifts) of the compounds were calculated.

**Full Paper** _____ *Thematic Section:* Theoretical Research.
*Registration Code of Publication:* 14-37-2-152 *Subsection:* Physical Organic Chemistry.
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# Stabilization energy of the aromatic aminyl radicals

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***Keywords:*** *aminyl radicals, benzyl radical, diphenylamine radical, correlation equation, phenoxyl radical,bond dissociation energy, stabilization energy of radical.*

**Abstract**

By the dissociation energies of N–H-bonds we calculated stabilization energy of aromatic aminyl radicals of different structure. We have established the rules of additivity for the influence of substituents on the energy of stabilization of mono and bis-substituted diphenylamines and linear correlation between stabilization energies of phenylaminyl and diphenylaminyl radicals. Comparison has been carried out of stabilization for aminyl, benzyl and phenoxyl radicals of similar structure. Linear correlation has been established between stabilization energies of aminyl ($XC_6H_4N^{\bullet}H$) and phenoxyl ($XC_6H_4O^{\bullet}$) radicals. Bibliography – 17 references.

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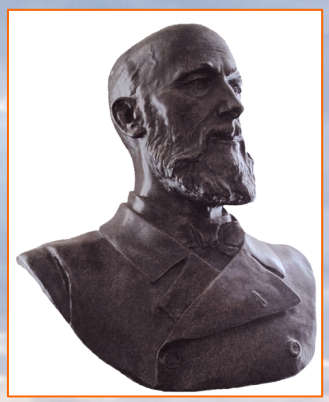

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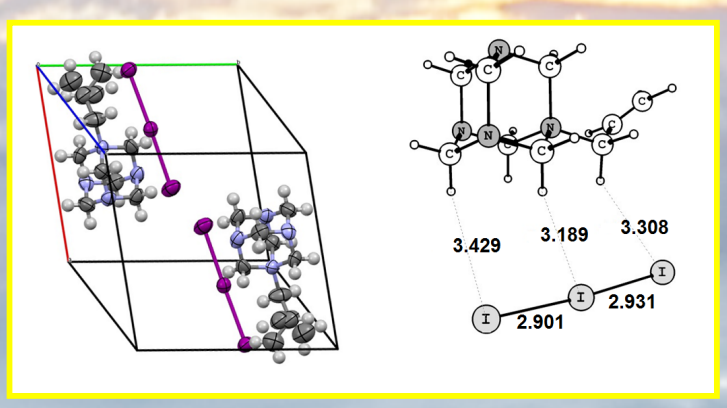


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http://butlerov.com/readings/
Contributed: May 6, 2014.

# Triiodide-anion in allilurotropiniya crystal: noncovalent interaction and spectral characteristics

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***Keywords:*** *triiodide-anion poyiodides, Paman spectroscopy, non-covalent interactions, QTAIM, periodic boundary conditions.*

**Abstract**

A new crystalline structure of allilurotropiniya triiodide $C_9H_{17}N_4^+I_3^-$. Was synthesized and verified by X-ray analysis. Raman spectral characteristics of mono-crystal were investigated both in unpolarized light, and with different relative orientation of the axes of the crystal polarization vector of the incident and scattered light. There have been calculated vibrational modes, active in Raman spectra using the crystalline approximation, periodic boundary conditions and localized atomic basis sets. According to quantum-topological analysis of the electron density (QTAIM) non-covalent interactions involving iodine atoms in the crystal structure are characterized in the studied crystalline structure.

**Full Paper** _____ *Thematic Section:* Preparative Research.
*Registration Code of Publication:* 14-37-3-8 *Subsection:* Organic Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
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# Synthesis of sulfonamides based on thiophenyl-5-oxazole-2-carboxamides

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***Keywords****: sulfochlorination, sulfoamidirovanie, sulfonamides, oxazole derivatives.*

**Abstract**

We developed a method for producing sulfochlorides based on thiophenyl-5-oxazol-2-carboxamides, by reacting with chlorosulfonic acid and thionylchloride. Substitution position was established in sulphochlorination reaction was determined by NMR methods. Interaction of aliphatic and aromatic amines with sulfochlorides has been studied. The structure and purity of these compounds were checked by a set of physicochemical methods of analysis.

*Thematic Section:* Preparative Research. **Full Paper**
*Subsection:* Organic Chemistry. *Registration Code of Publication:* 14-37-3-13
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*Thematic direction:* Hydroxyalkyl of urea and the polymers on their base. Part 1.

# *bis*-*N*,*N*-di-(2-hydroxyethyl)urea on a base of the aliphatic diisocyanate

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***Keywords***: Kurtsius rearrangement, dicarbonic acid, dichloroanhydride, diisocyanate, diethanolamine, hydroxyethyl substituted urea, IR spectra.

**Abstract**

The hydroxyethyl substituted urea *via* interaction of aliphatic diisocyanate with diethanol amide were received. The synthesized compounds are characterized by data of TLC, the element analysis and IR-spectroscopy.

**Full Paper** _____ *Thematic Section:* Physicochemical Research.
*Registration Code of Publication:* 14-37-3-18 *Subsection:* Inorganic Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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# Theoretical confirmation and experimental investigation of the process of the thermozone crystallization-synthesis in the obtaining high-purity silver and thallium(I) halides

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***Keywords****:* silver halides, thallium(I) halides, solubility in HCl and HBr, thermozone crystallization-synthesis (TZCS).

**Abstract**

The solubility of silver halides and monovalent thallium in water and water solutions of halogen acids was explored, as well as theoretical calculations of these processes were carried out on the basis of published data. It has been established that the theoretical solubility differs significantly from the experimental area at higher temperatures. It has been revealed that the calculation of solubility only on the basis of complexation significantly overstates the results of experimental data, as the activity coefficient was not taken into account. A basic method for the synthesis and purification of high-purity sparingly soluble metal halides from water environments was developed during the carried out investigations.

*Thematic Section:* Physicochemical Research. **Full Paper**
*Subsection:* Inorganic Chemistry. *Registration Code of Publication:* 14-37-3-27
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# The thermodynamic functions of monovalent thallium and silver halides dissolution processes in water and hydrohalic acids

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***Keywords:*** *thallium(I) and silver halides, solubility, solubility product, solubility constant, thermodynamics and kinetics of the dissolution process, Gibbs free energy, enthalpy and entropy change, activation energy and dissolution rate constant.*

**Abstract**

The dissolution process of TlHal, AgHal and their solid solutions are discussed in terms of thermodynamic. The individual metal halides solubility products and binary solid solutions dissolution constants are calculated using experimental solubility data. The basic thermodynamic and kinetic parameters of TlHal and AgHal dissolution process in water and hydrobromic acid of different molality are determined at temperatures varying from 298 to 368 K. A method has been proposed for calculating the component solubility of solid solutions on the basis of poorly soluble metal halides.

*Thematic Section:* Geochemical Research. **Full Paper**
*Subsection:* Petrochemistry. *Registration Code of Publication:* 14-37-3-37
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http://butlerov.com/readings/
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# The nature of bitumens of "anomalous" zone of abdrahmanovskaya area of Romashkinskoe oil field

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***Keywords:*** bitumems, biomarkers, "anomalous" zone, Devon, basement rocks, Abdrahmanovskaya area, Romashkinskoe oil field.

**Abstract**

Comparative analysis of geochemical data bitumens of "abnormal" and normal zone of Devonian sediment and weathering crust basement rock of Abdrahmanovskoy area Romashkinsko oil field indicate one producer - Sapropelic substance. By gas chromatography and chromatography-mass spectrometry identified biomarker values of parameters (hopanes, steranes). They indicate that the degree of maturity in catagenetic bitumen "anomalous" zone is greater than normal, but less than the basement rocks. Hydrocarbon composition of the latter differs offset high content of *n*-alkanes in the direction of the lower molecular weight compared with their distribution in bitumens of "anomalous" zone.

**Full Paper** _____ *Thematic Section:* Research into New Technologies.
*Registration Code of Publication:* 14-37-3-46 *Subsection:* Physical Chemistry of Polymers.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: May 31, 2014.

# Structure formation and physicochemical properties of the polymer system based on polyamide – imide and polyethersulphone

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*Supervising author; [+]Corresponding author
***Keywords:*** *polyamide-imide, polyethersulphone, mechanical properties, non-covalent interaction, quantum chemical calculation.*

## Abstract

Solutions of polyamide-imide with small additives of polyethersulphone were an object of research of this work. It is shown that the introduction of small amounts of a solution of polyamideimide polyethersulfone in *N*-methylpyrrolidone significantly modifies the rheological characteristics of the solution. It could cause a positive influence on the hollow fiber preparation on its basis.

By high-temperature Fourier transform infrared spectroscopy there was found non-covalent interactions in the system based on polyamide-imide and polysulfone either with the solvent or without him. Quantum-chemical modeling confirmed the probability of the existence of intermolecular complexes with the solvent and interchain interactions of macromolecules by functional groups. Changes in the dielectric characteristics of polymer blends confirm the formation of intermolecular complexes.

*Thematic Section:* Research into New Technologies._____ **Full Paper**
*Subsection:* Physical Chemistry of Explosives. *Registration Code of Publication:* 14-37-3-57
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: May 24, 2014.

# Influence of additives on the burning rate of nitrate high-energy compositions under atmospheric pressure

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***Keywords:*** ammonium nitrate, high-energy compositions, additives, burning rate.

**Abstract**

In the paper, the results of researches on the influence of additives of various classes of substances on the burning rate of two types of nitrate high-energy compositions are presented at the atmospheric pressure. It is shown that the most effective additives increasing the rate of burning of the considered compositions, are dicarbollyl complexes of metals and ortho carborane which allow 20 times increase of burning rate.

*Thematic Section:* Research into New Technologies. **Full Paper**
*Subsection:* Analytical Chemistry. *Registration Code of Publication:* 14-37-3-63
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: April 21, 2014.

# New approaches to the analysis of drugs based on bioaffinity of interactions and biosensors

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***Keywords:*** *medicines analysis, bioaffinity methods, DNA-sensors, vincristine, amperometric sensors.*

**Abstract**

Bioaffine methods are very actual in being utilized for high sensitivity and selectivity of bioaffinity interactions. The interaction of immobilized DNA with vincristine – antitumor alkaloid was studied. Bioaffinity method using amperometric DNA-sensor was developed. The method has LOD of $2.0 \cdot 10^{-9}$ mol/l.

*Thematic Section:* Biochemical Research. **Full Paper**
*Subsection:* Regularities of Metabolism. *Registration Code of Publication:* 14-37-3-67
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: May 22, 2014.

# Metabolites and tolerant microflora in substrates with the content of white phosphorus 0.1%

© **Anton Z. Mindubaev**,[1]*+ **Farida K. Alimova**,[2] **Sergey C. Ahossiyenagbe**,[2] **Alexandra D. Voloshina**,[1] **ElenaV. Gorbachuk**,[1] **Natalia V. Kulik**,[1] **Salima T. Minzanova**,[1] **Lubov G. Mironova**,[1] and **Dmitry G. Yahvarov**[1]*

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***Keywords:*** detoxication, white phosphorus, sewage sludge, anaerobic conditions, metabolic pathway, metabolites, nuclear magnetic resonance, sulfate reducers, *Bacillus*.

## Abstract

White phosphorus undergoes metabolic oxidation to water-soluble products – hypophosphite and phosphate, as is established by $^{31}$P NMR method. Further metabolism of these compounds should result in harmless phosphate formation, what opens perspectives for practical application of this method. In our previous works we have for the first time obtained the cultures of microorganisms, developing resistance to white phosphorus. At that the attention was mainly paid to $P_4$ mass concentration 0.01%, since just at that concentration white phosphorus undergoes biodegradation. We have also observed microorganisms in substrata with even higher concentration of white phosphorus, however they have not been characterized. In the present work we isolated and characterized bacteria from wastewater with white phosphorus mass content 0.1%. Sulfate reducers, being pure anaerobics, were shown to be strongly suppressed by white phosphorus compared to less specialized microorganisms.

*Thematic Section:* Biochemical Research. **Full Paper**
*Subsection:* Chemical Composition of Plants. *Registration Code of Publication:* 14-37-3-79
Publication is available for discussion in the framework of the on-line Internet conference "*Chemical basis for the rational use of renewable natural resources*".
http://butlerov.com/natural_resources/
Contributed: May 16, 2014.

# Bioelemental composition in the leafs of same medicinal plants and dietary supplements

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***Keywords***: macro-microelements of leaves *Polyscias filicifolia (Moore ex Fournier) (Araliaceae)* и *Ginkgo biloba L. (Ginkgoaceae)* and dietary supplements.

## Abstract

Macro-and microelements composition in the leafs of plants *Polysciasa filicifolia Bailey (Araliaceae)* and *Ginkgo biloba L. (Ginkgoaceae)* have been defined by means of mass spectrometry with inductively – coupled plasma (ICP-MS) method.

The Shii-taki fungi (Lentinula spp.) and some dietary supplements – as the biologically active additives were investigated: "American Ginseng" 100% Euro Ginseng, NPH b.v. (Euro Ginseng / Netherlands. U.K. Grover & Distributor). – "Wild Siberian Ginseng" Root Eleutherococcus senticosus, (U.K. Grover & Distributer, Nature's way products Inc. America's Botanical Expert.). – "Herba Echinacea purpurea" (Nature's way products Inc. America's Botanical Expert). – "Cat's claw" Bark Uncaria Tomentosa (Laif. sertification of ИСО9001:2000). – "The Powders of Garic's" (Il'ya Rogov's[R], A. Nattermann & Cie.Gm). All the vital elements were defined in these experimental objects. The analysis of the obtained data has shown the considerable difference in the content of macro- and microelements.

*Thematic Section:* Biochemical Research. **Full Paper**
*Subsection:* Chemical Composition of Plants. *Registration Code of Publication:* 14-37-3-85
Publication is available for discussion in the framework of the on-line Internet conference "*Chemical basis for the rational use of renewable natural resources*".
http://butlerov.com/natural_resources/
Contributed: May 14, 2014.

# Analysis of carbohydrate composition of *Geranium pratense* L., *Geranium sylvaticum* L., *Geranium palustre* L.

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***Keywords:*** carbohydrates, monosaccharides, polysaccharides, gas-liquid chromatography*, Geranium pratense, Geranium sylvaticum, Geranium palustre.*

**Abstract**

Quantity contents of free monosaccharides and water-soluble polysaccharides in the aerial part and the root part of *Geranium pratense, Geranium sylvaticum, Geranium palustre* were determined using spectrophotometric method in different phenological stages (flower bud emergence, flowering, fruit development, fruit maturity).

Free monosaccharides and water-soluble polysaccharides were isolated from herb material. Monosaccharide composition of these carbohydrate complexes was investigated by gas-liquid chromatography.

**Full Paper** _____ *Thematic Section:* Biochemical Research.
*Registration Code of Publication:* 14-37-3-90 *Subsection:* Chemical Specificity of Biocenoses.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: May 15, 2014.

# Chemical characteristics of juvenile fish in the composition of hydrobiocenosis of a mobile bio Mesa

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***Keywords****:* mobile bio Mesa, environmental pollution, heavy metals, juvenile fish, a perch, X-ray fluorescent analysis, concentration of the polluting substances.

**Abstract**

Features of a chemical composition of fishes from a mobile bio Mesa functioning in the lake the Average Boar of Kazan are studied. In comparative aspect the accumulation of heavy metals is shown by different types of fishes.

*Thematic Section:* Pharmacological Research. **Full Paper**
*Subsection:* Biochemistry. *Registration Code of Publication:* 14-37-3-97
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: June 9, 2014.

*Thematic course*: Physical and chemical methods for activation of pectinolytic enzymes. Part 4.

# Preparation of highly active polygalacturonases

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***Keywords:*** polygalacturonases, activation, methods for purification of enzymes.

**Abstract**

The different approaches to developing methods for preparing of highly active enzyme preparations of polygalacturonases are discussed in this paper. The first approach involves the sequential removal of the individual groups of inactive impurities and obtaining on the last step the purified enzyme solution with high specific activity. It is shown that in this case the yield of total activity may be reduced to 40-50% of the initial value due to losses at each stage of processing. The second approach involves the selective isolation of the desired enzymes from the solution after activating them. Thus it is possible to achieve considerably high values of the specific activity of the enzymes and obtain a yield of total activity above its initial value by 20-30%.

*Thematic Section:* Pharmacological Research. **Full Paper**
*Subsection:* Analytical Chemistry. *Registration Code of Publication:* 14-37-3-105
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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# Determination of drugs of strict account by amperometric monoamine oxidase biosensors

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***Keywords****:* biosensor, monoamine oxidase, carbon nanotubes, golden nanoparticles, drugs compounds.

**Abstract**

Amperometric monoamine oxidase biosensors on the basis of printed graphite electrodes, which are modified by multiwall carbon nanotubes and golden nanoparticles, were developed for the determination of tianeptine and naltrexone. The drugs compounds are related to the strict account medications. An opportunity of using biosensors for controlling residual quantity of drug compounds in biological fluids (urine) while drug monitoring and controlling the basal drug substance in dosage form was presented. The lower limit of detectability while using adrenaline as a substrate is $4.5\times10^{-10}$ M for coaxil and $3.7\times10^{-10}$ M for naltrexone.

*Thematic Section:* Pharmacological Research. **Full Paper**
*Subsection:* Physical Organic Chemistry. *Registration Code of Publication:* 14-37-3-113
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
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# Crystallization of paracetamol of rhombic form

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***Keywords:*** phase transitions, synthesis from the vapor phase, structural studies, thermal research.

**Abstract**

Production of rhombic shape paracetamol has been reported.The method of vacuum evaporation of powder from crystals of monoclinic modification with subsequent condensation of vapor on the copper substrate is used for synthesis.

It has been found that the process is complex and done in the form of superposition of two phase transitions: phase transition of the first order with changing the density and the second order – the one with changing structural order. Second order phase transition occurred in the form of smeared phase transition with the formation of intermediate phase, irreversibly consumed in the process of phase transformation. The data of differential scanning calorimetry, X-ray phase analysis and microphotography is given.

**Full Paper** _____ *Thematic Section:* Pharmacological Research.
*Registration Code of Publication:* 14-37-3-120 *Subsection:* Biochemistry of New Drugs.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: June 10, 2014.

# New organic drug for spleen, Splenactive – a source of natural cytokines, regulators of immune homeostasis

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***Kewwords:*** cytokines, immune modulators, enzymoimmunoassay, pig spleen, the spleen of cattle.

**Abstract**

The spectrum of the main cytokines and their quantitative content in preparations Splenactive and Prosplenactive which are freeze-dried aqueous extracts from the spleen of pigs or cattle have been studied. Organopreparations were prepared without (Prosplenactive) and with the addition of dihydroquercetin as an antioxidant preservative (Splenactive). Identification of cytokines in the preparations was performed using sets of monoclonal antibodies specific for the respective human cytokines by "sandwich" – variant solid phase enzyme immunoassay. It was found that the content of pro- and anti-inflammatory cytokines and interferons injectable solutions Splenactive and Prosplenactive exceed serum levels in the blood of healthy donors or correspond to them. Thus, as a result of studies, the spectrum of the main classes of cytokines and their concentration in preparations Splenactive and Prosplenactive have been defined.

*Thematic Section:* Pharmacological Research. **Full Paper**
*Subsection:* Optimisation of Preparation Formula. *Registration Code of Publication:* 14-37-3-125
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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# Selection an optimal basis for medical pencils with yodopiron

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***Keywords:*** medical pencils, yodopiron, spreadability, relative number of hardness, low molecular weight polyethylene, paraffin, vaseline oil, pentol.

**Abstract**

The article presents the results of the research in developing the optimal composition and technology of medical pencils containing yodopiron, as an antiseptic. The dependence of spreadability and the relative number of hardness on the ratio of base components has been determined. The composition of medical pencil comprising 65% low molecular weight polyethylene, 12% vaseline oil, 8% paraffin, 5% pentols, 5% purified water and 5% yodopiron is recommended. This combination of base components in combination with a pharmacologically active yodopiron has a neutral reaction, provides good adhesion to the skin and mucous membranes with optimum hardness of a pencil.

*Thematic Section:* Chemical and Technological Research. **Full Paper**
*Subsection:* Calculation of the NMR Spectra. *Registration Code of Publication:* 14-37-3-129
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: May 06, 2014.

# Spatial structure and parameters of the NMR spectra of polybutadiene fragments on the basis of quantum-chemical calculations

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***Keywords:*** DFT, magnetic shielding, chemical shift, NMR, polybutadiene, microstructure.

**Abstract**

In the work there were carried out calculations of spatial, electronic structure and parameters of the NMR spectra of model fragments polybutadienes *ab initio* quantum chemistry methods within density functional theory (DFT). It has been established that the calculated values of chemical shifts of protons of $^{1}H$ series model structures are in agreement with experimental data.

**Discussion Column** _____ *Thematic Section:* Theoretical Research.
*Registration Code of Publication:* 14-37-3-134 *Subsection:* Theory of the Structure of Matter.
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# Electronic structure of water

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***Keywords***: water, hydrogen bonds, proton mobility, physical properties.

**Abstract**

Analysis of the electronic structure of water in the chain of causality: atoms of hydrogen and oxygen → water molecules → ice, water has been given. A new approach to the description of the electronic structure of water, based on a new understanding of the nature of the covalent bond between the hydrogen and oxygen atoms has been presented. A model of the "oxygen-hydrogen" bonding as a basis for constructing the supramolecular structure of water has been analyzed. The substantiation of the activation mechanism of intra- and intermolecular electron transfer has been given. The basic physical properties of water in the light of new ideas about the electronic structure of water have been discussed.

*Thematic Section:* Theoretical Research. **Full Paper**
*Subsection:* Physical Organic Chemistry. *Registration Code of Publication:* 14-37-3-149
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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*Thematic course:* Numerical characteristics of the structure of organic molecules. Part 15.

# Relationship of melting points of normal structure alkanes with the energy characteristics of molecules

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***Keywords:*** moment of inertia of the rotational movement, the topological index.

**Abstract**

For a number of normal structure alkanes, the relationship of melting and boiling points with characteristics of structures have been investigated, namely, the components of inertia moment of rotational motion as well as the HOMO energy. For a description of the melting point and the boiling point of the substances in question, we propose a new parameter, equal to the ratio of the total electron energy of alkanes to the value of Wiener topological index to the 2/3 power.

*Thematic Section:* Theoretical Research. **Full Paper**
*Subsection:* Physical Organic Chemistry. *Registration Code of Publication:* 14-37-3-157
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http://butlerov.com/readings/
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*Thematic course:* Numerical characteristics of the structure of organic molecules. Part 16.

# Relationship of melting points of fluoro-, chloro-, and bromoderivatives of normal structure alkanes with moments of inertia of rotational motion

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***Keywords:*** moment of inertia of the rotational movement, the topological index, melting and boiling points, halogenated alkanes.

**Abstract**

For the series of bromium-, fluoro- and chloro-derivatives of normal structure alkanes, the research has been carried out with correlation analysis of relationship of melting and boiling temperatures of the studied substances with characteristics of structures and components of inertia moment of rotational motion of molecules, as well as the new energy and structural parameter $E_W$ (the ratio of the total electron energy (E) to the value of Wiener topological index to the 2/3 power).

The dependences of melting temperature and the boiling point of the substances in question on the characteristics of the structure and components of inertia moment of rotational motion of molecules, as well as on the energy and structural parameters indicate different forms of molecules at the phase transitions.

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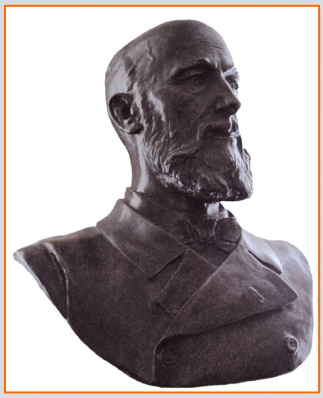

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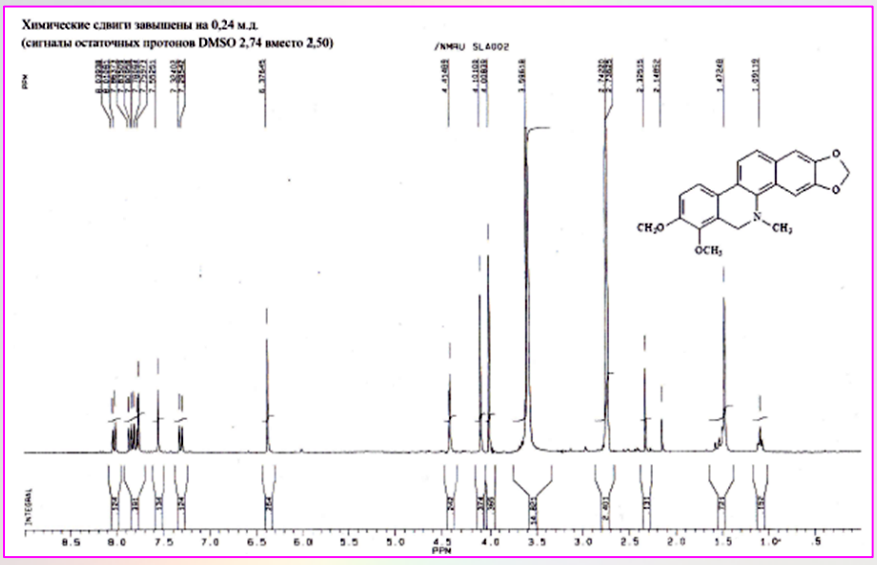


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# Synthesis of 6-substituted 1,2,3-triazolyl derivatives of benzo[*c*]phenanthridine alkaloids and study of their effects on lysosomal proteases activity

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***Keywords:*** alkaloids, benzo[c]phenanthridine, 1,2,3-triazole derivatives, biological activity, lysosomes, cysteine proteases, cathepsins.

**Abstract**

A brief overview on the studies of the biological activity of semi-synthetic derivatives of natural benzo[*c*]phenanthridine alkaloids is presented. According to methods described in literature 6-substituted derivatives of the natural alkaloids sanguinarine and chelerythrine with 1,2,3-triazolyl group at 6-C atom were synthesized and their effects on the lysosomal proteases activity were studied. It is shown that *in vitro* action of the synthesized derivatives on hepatocyte lysosomes leads to an increase of lysosomal cysteine proteases activity accompanied with significant labialization of the lysosomal membrane.

**Full Paper** _____ *Thematic Section:* Biochemical Research.
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# Investigation of antiradical activity of coumarin and Melilotus officinalis extract

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***Keywords:*** coumarin, Melilotus officinalis, γ-radiolysis, antiradical activity, α-carbon-centered radical hydroxyl.

**Abstract**

An assessment of the impact of the extractant on the extraction of coumarin from Melilotus officinalis herbs is provided. It is shown that coumarin extracts is capable of reacting with the carbon-centered radicals. Products of interaction with coumarin carbon-centered radicals investigated by chromate-mass spectrometry.

**Full Paper** _____ *Thematic Section:* Biochemical Research.
*Registration Code of Publication:* 14-38-4-16 *Subsection:* Chemistry of Peptides.
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*Thematic course:* Peptide Inhibitors of Platelet Aggregations. Part 1.

# Development of new peptide antiagregatsionnyh heteromeric with imidazo[4,5-e]benzo[1,2-c;3,4-c']difuroxan moiety

© **Alexey A. Alexeev**,[1]*+ **Maxim I. Brylev**,[1]*+ **Vyacheslav L. Korolev**,[1] **Dmitriy S. Lotorev**,[1] **Anton Yu. Lizunov**,[2] **Natalia I. Zaitseva**,[1] **Lyudmila A. Pavlova**,[1]* **Victor P. Ivshin**,[3] and **Olga Yu. Domasheva**[4]

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***Keywords:*** GPIIb/IIIa receptors of platelets, Inhibition of platelet aggregation, computer simulation, imidazo[4,5-e]benzo[1,2-c;3,4-c']difuroxans, heteromeric peptides.

**Abstract**

With the application of program Algokomb, mathematical simulation of heteromeric peptides comprising imidazo[4,5-e]benzo[1,2-c;3,4-c']difuroxan moiety. Effectiveness of their binding with GP IIb/IIIa-receptors of platelets is confirmed. The generated compounds were synthesized in the conditions of automatic peptide synthesizer Applied Biosys-tems 433A with the use of Fmoc-strategy. Evaluation of antiplatelet activity modeled heteromeric peptides showed the presence of dose-dependent inhibition of ADF-induced platelet aggregations.

**Full Paper** _____ *Thematic Section:* Pharmacological Research.
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# Hepatoprotective component in the protective effect of Rhodiola rosea preparations in chronic intoxication POC

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***Keywords:*** Rhodiola rosea, organophosphorus compounds, liver, toxicity, biomass, tissue culture.

## Abstract

The article highlights the study of hepatoprotective component in the protective action of the drug Rhodiola rosea (*Rhodiola rosea L.*), both of natural and biotechnological origin in chronic intoxication by organophosphorus compounds. The experiment was conducted in two phases on the nonlinear white male rats, for eleven weeks. Preparations were administered in intra-gastric way, as dealcoholized solutions, diluted with distilled water. Damage assessment was carried out on liver histology and morphology, biochemical and enzymological parameters. The obtained results showed a high protective efficacy of therapeutic and prophylactic use of drugs of Rhodiola rosea with respect to induced organophosphate hepatic lesions. The article presents statistically processed data. At its hepatoprotective effect of the drug from the tissue culture was not inferior to officinal liquid extract of Rhodiola.

*Thematic Section:* Pharmacological Research. **Full Paper**
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# Microencapsulation of steroid hormones in the gelatin shell

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***Keywords**:* brassinosteroids, microencapsulation, cholesterol, Solvent Blue 104.

**Abstract**

The article is devoted to microencapsulation brassinosteroids in gelatin shell. Based on the method Zlatkis-Zack developed a technique that allows to control the degree of involvement of the active substance – cholesterol in microcapsules. The highest degree of microencapsulation is achieved using 3% gelatin solution. The kinetics of the release of model compounds, cholesterol and Solvent Blue 104 dyes from microcapsules, was investigated. It was found that microencapsulation allows for a gradual release of the active substance on the whole time interval of soaking seeds.

*Thematic Section:* Pharmacological Research. **Full Paper**
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# Chemical composition of *Pteridium pinetorum*

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***Keywords****:* biologically active substances, sesquiterpenes, carotenoids, flavonoids, phenol carboxylic acid, Pteridium pinetorum, Hypolepidaceae.

**Abstract**

The review of data on the chemical composition of fronds and rhizomes of bracken fern *Pteridium pinetorum* (*Hypolepidaceae*) is presented. The main biologically active substances of *Pteridium pinetorum* are sesquiterpenes, carotenoids, flavonoids and phenol carbonic acids.

**Full Paper** _____ *Thematic Section:* Pharmacological Research.
*Registration Code of Publication:* 14-38-4-42 *Subsection:* Biochemistry.
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# Medical materials based on modified cellulose, chitosan and multienzyme complex

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***Keywords:*** immobilized proteases, inactivation, bandages, chitosan, dialdehydecellulose.

## Abstract

There were investigated the properties of proteinases of proteolytic complex from hepatopankrease crab (PC) immobilized on dialdehydecellulose contains chitosan (Ch). Stabilization of PC proteases was established in the presence of Ch. And during addition of glycerol (Gl) to Ch it is destabilized, when immobilization, drying and storing in the air takes place. The data obtained can be explained by the formation of polyelectrolyte complexes between proteins and Ch, as well as the formation of adducts Ch-Gl.

**Full Paper** _____ *Thematic Section:* Pharmacological Research.
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# The research of biological activity of potential antagonists of $NR_3C_4$ receptor

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***Keywords:*** $NR_3C_4$ receptor, antagonists of $NR_3C_4$, prostate cancer, antagonistic activity.

**Abstract**

The research of antagonists of $NR_3C_4$ receptor was conducted. By means of molecular modeling the preliminary sampling being capable of potential blocker of $NR_3C_4$ receptor was realized. There were synthesized 31 compounds, which are the most perspective in terms of presumptive assessments. By means of test-system PolarScreen Green (Invitrogen P3018) the affinity of the researched compounds were evaluated. The cytotoxicity and antagonistic activity of the research samples on the $NR_3C_4$ receptor in the AR-UAS-bla GripTite™ 293 cells was defined. The most perspective antagonists of the $NR_3C_4$ receptor are samples of 2-(1-naphthyl)-ethyl ester-1-[(3-fluorophenyl)acetyl]-L-proline, 2-(1-naphthyl)-ethyl ester-1-[(4-methylphenyl)-acetyl]-L-proline and 2-(1-naphthyl)-ethyl ester-1-[(4-chlorophenyl)acetyl]-L-proline. They have high affinity and low cytotoxicity.

*Thematic Section:* Pharmacological Research. **Full Paper**
*Subsection:* Biochemistry. *Registration Code of Publication:* 14-38-4-53
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# Development and validation of the method to control eye drops based on "branched oligohexamethyleneguanidine hydrochloride"

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***Keywords:*** oligohexamethyleneguanidine hydrochloride, eye drops, the quantitative determination of the basic substance.

## Abstract

Eye drops based on "branched oligohexamethyleneguanidine hydrochloride" have been offered as an effective medical preparation for treating viral ophthalmic diseases. The possibility of using the Kjeldahl method for the quantitative determination of branched oligohexamethyleneguanidine hydrochloride was evaluated.

**Full Paper** _____ *Thematic Section:* Pharmacological Research.
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# The influence of the collection of plant material on the physical endurance and recovery processes in mice in the experiment re-diving

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***Keywords:*** *physical activity, combination herbal medicinal product, polyphenolic compounds, actoprotective action.*

**Abstract**

The influence of natural polyphenolic compounds included in a new combination of herbal medical product on the physical endurance of mice in the test of the re-swim was studied. It has been found that the course application of aqueous extract of herbal medical product combination in the experimental group of mice did not affect on the duration of the primary swim, but increased to 1.7 times the length of re-swimming compared with the same parameter in the control group ($p<0.001$). This result demonstrates the positive effect of proposed combination herbal medical product on recover processes after physical activity (actoprotective action). It is assumed that actoprotective action of combination herbal medical product due to antioxidant properties of biologically active substances in its composition.

*Thematic Section:* Pharmacological Research. **Full Paper**
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# Hepatoprotective effect of the new combination of herbal medicinal products in comparison with the drug «carsil» (experimental study)

© **Nino R. Chekhani**,[1]*+ **Lyudmila A. Pavlova**,[1] **Sergey V Kosin**,[1] **Yuriy O. Teselkin**,[2] and **Magomed D. Guseinov**[1]

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***Keywords:*** *carbon tetrachloride, toxic hepatitis, combination of herbal medicinal product, hepatoprotective action.*

**Abstract**

In this study hepatoprotective effect of new plants gathering on the model of acute toxic hepatitis in rats induced by carbon tetrachloride was investigated. Hepatoprotective effect has been proved by using thiopental test as well as biochemical and enzymological studies of blood serum of rats. By its influence on the duration of anesthesia using thiopental, liver enzymes activity and some hepato-depended biochemical parameters of blood serum the claimed collection does not differ from the reference drug karsil. It is assumed that the hepatoprotective action of plant collection is due to the presence of phenolic and polyphenolic compounds with antioxidant activity.

*Thematic Section:* Pharmacological Research. **Analytical Review**
*Subsection:* Impact of Drugs on the Microflora. *Registration Code of Publication:* 14-38-4-67
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# Activity spectrum, pharmacodynamics, pharmacokinetics, and acute toxicity of polypeptide antibiotics

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***Keywords:*** polymyxin, cyclic polypeptide, gram-negative bacteria, antimicrobial activity, pharmacodynamics, acute toxicity.

## Abstract

A mixture of cyclic polypeptides – polymyxins – was originally isolated from sporogenous *Bacillus polymyxa* bacterial culture in 1947. Polypeptides are justifiably considered as one of the first classes of natural antibiotics. In Russia the following polymyxins are registered: polymyxin B (for parenteral administration), polymyxin M (oral tablets for the treatment of intestinal infections, liniment, and powder for topical solution), and colistin (derivative of natural polymyxin E). Polymyxins are among the very first classes of natural antimicrobial drugs; they were developed in the early 1940s. This class includes antibiotics (polymyxin B, polymyxin M, polymyxin E – colistin), produced by sporogenous bacteria *Bacillus polymyxa.*

*Thematic Section:* Pharmacological Research. **Full Paper**
*Subsection:* Technology for producing medical materials. *Registration Code of Publication:* 14-38-4-73
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# Development of sterilization technology of hydrogel medical materials based on sodium alginate

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***Keywords:*** Sodium alginate, hydrogel materials, preservatives, sterilization of therapeutic materials.

## Abstract

The article is devoted to the development of sterile medical materials from polymers-polysaccharides with impregnated drugs which are used for the targeted delivery of drugs into the damaged tissue. We have studied the effect of the polysaccharide – sodium alginate on the rheological characteristics of the materials after sterilization. The influence of additives of potassium sorbate and pectin and different kinds of medical materials sterilization on the rheological properties of the material has been revealed.

*Thematic Section:* Pharmacological Research _____ **Full Paper**
*Subsection:* Gas Chromatography. *Registration Code of Publication:* 14-38-4-79
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# Development of gas chromatographic method for the determination of tri-*n*-butyl phosphate in antihemophilic preparations

© **Alexei E. Kovalenko**,[1,2]* **Dmitry A. Kardonsky**,[1,2] **Alexander A. Eganov**,[1,2] **Olga G. Stepanova**,[2] **Svetlana V. Shestakova**,[2] and **Irina I. Pleshakova**[2+]
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***Keywords:*** antihemophilic drugs, tri-n-butyl phosphate, solid phase extraction, gas chromatgraphy.

## Abstract

A simple and reliable method for the quantitative determination of tri-*n*-butyl phosphate in finished dosage forms of medicines derived from human plasma was developed. Tri-*n*-butyl phosphate is isolated from FDF by solid phase extraction and analyzed by gas chromatography with flame ionization detection (GC/FID). Quantitative determination of tri-*n*-butyl phosphate is carried out using tri-*n*-pentilfosfat as internal standard.

*Thematic Section:* Pharmacological Research. **Full Paper**
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# Gas chromatographic determination of tween 80 in the finished dosage forms of medicines derived from human blood plasma

© **Alexey E. Kovalenko**,[1,2]* **Dmitry A. Kardonsky**,[1,2] **Alexander A. Eganov**,[1,2] **Olga G. Stepanova**,[2] **Svetlana V. Shestakova**,[2] and **Irina I. Pleshakova**[2+]

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***Keywords:*** *Tween 80, the liquid-liquid extraction, gas chromatography.*

**Abstract**

A simple and reliable method for the quantitative determination of Tween 80 in finished dosage forms of medicines derived from human plasma was developed. Tween 80 is isolated from FDF by liquid-liquid extraction and analyzed by gas chromatography with flame ionization detection (GC/FID). Quantitative determination of tri-*n*-butyl phosphate is carried out using stearic acid as internal standard.

*Thematic Section:* Pharmacological Research. **Full Paper**
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# Antiulcer preparation on the basis of substance bismuth(III) potassium dicitrate

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***Keywords:*** bismuth tridicitratobismuthate, peptic ulcer disease, Helicobacter pylori, preclinical studies.

## Abstract

X-ray diffraction and chemical analysis were used to investigate the interaction of bismuth citrate(III) of $BiC_6H_5O_7$ with aqueous potassium hydroxide and ammonium of different concentrations. It has been established that the colloidal bismuth subcitrate used as antiulcer medicinal substance in the preparations is a bismuth potassium ammonium citrate. The expediency of producing potassium-bismuth ammonium citrate for anti-ulcer agents such as "De-Nol" (Netherlands) by preparing high purity bismuth citrate in the reaction of nitrate trihydrate oxohydroxobismuth interaction with solutions of citric acid, by dissolving the obtained citrate in an aqueous solution of potassium hydroxide in the presence of ammonium hydroxide followed by crystallization of the product by evaporation or by spray drying. Preclinical studies of general toxicity and local irritant action of bismuth tri dicitrate at the course intragastric inhjection were conducted. A conclusion has been made on the safety of the studied preparation.

**Full Paper** _____ *Thematic Section:* Physicochemical Research.
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# Identification of metabolites of cannabimimetics AM(N)-2201 by the method of gas chromatography with mass spectrometric detection

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***Keywords:*** AM(N)-2201, THJ-2201, synthetic cannabimimetics, metabolites, biotransformation, gas chromatography, tandem mass spectrometry, forensic chemical research, chemical-toxicological studies.

**Abstract**

Metabolites are described to determine the use of cannabimimetics AM(N)-2201 during urine screening procedure for narcotic drugs and with application of methods of liquid-liquid extraction and gas chromatography with mass spectrometry. Search algorithm is characterized for new synthetic cannabimimetic metabolites using gas chromatography with tandem mass spectrometric detection. 17 metabolites are authenticated AM(N)-2201, detected in the urine of consumers of smoking mixtures. It has been established that the major metabolite of AM(N)-2201 is 3-[3-(naphthalen-1-ylcarbonyl)-1*H*-indazol-1-yl]propanoic acid. There were obtained gas chromatographic and mass spectrometric characteristics of trimethylsilyl derivatives of major metabolites, which can be used in the practice of forensic chemical and chemical-toxicological studies.

*Thematic Section:* Physicochemical Research. **Full Paper**
*Subsection:* Colloidal Chemistry. *Registration Code of Publication:* 14-38-4-109
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# Preparation and analysis of the properties of nanoparticles based on amphiphilic poly-*N*-vinyl-2-pyrrolidone

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***Keywords:*** nanoparticles, poly-*N*-vinyl-2-pyrrolydone, indomethacin, rifabutin, amphiphilic polymers.

## Abstract

To produce nanosized particles in an aqueous solution amphiphilic derivatives of poly-*N*-vinyl-2-pyrrolidone (Amf-PVP) were synthesized with different molecular weight of hydrophilic PVP-moiety and one terminal linear alkyl hydrophobic moiety. To explore the possibility of using Amf-PVP as carriers for pharmaceuticals there were obtained micelle particles based on model substances. As model preparations there were selected non-steroidal antiinflammatory agents – indomethacin and broad-spectrum antibiotic – rifabutin. The micellar particles were prepared using the ultrasonic method, followed by evaporation of the organic solvent (emulsion method). Medium size, size distribution and ζ-potencial of particles were determined by dynamic light scattering. For micellar particles of indomethacin the average size was not greater than 200 nm, while for particles of rifabutin it did not exceed 300 nm. ζ-potential of particles was in the range from -4 to -6 mV. The critical micelle concentration (CCM) of the synthesized polymers was in the micromolar range and was determined by fluorescence spectroscopy using diphenylhexatriene (DFHT). It has been shown that with increasing the length of the hydrophobic aliphatic moiety, CCM of polymers decreases, while increasing the molecular weight of the hydrophilic PVP-moiety formed by larger particles.

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*Subsection:* Colloidal Chemistry. *Registration Code of Publication:* 14-38-4-119
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# Oil-in-water nanoemulsions stabilized by vixtures of nonionic surfactant

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***Keywords:*** nanoemulsions, phase inversion temperature method, Span 60, Span 80, Tween 60, Tween 80, Cremophor EL, Solutol HS15.

## Abstract

The phase inversion temperature method was used for nanoemulsion preparation. Nanoemulsions were stabilized by the mixtures of nonionic surfactants: Tween 60, Tween 80, Span 60, Span 80, Cremophor EL, and Solutol HS15. At volume ratios of Tween/Span 2.0-2.4 nanoemulsions with droplet sizes of the dispersed phase equal to 15-30 nm were formed. In the case of stabilization by mixtures of Solutol HS15/Span 60 or Cremophor EL/Span 60 the formulation of nanoemulsions with 20-35 nm droplets occurred in a wider range of volume ratios of surfactants – 0.5-2.5.

Nanoemulsions with surfactants solid at the storage temperature were the most stable. Droplet sizes remained almost unchanged for 20-25 days. This can be explained by the formulation of the solid adsorption layer on droplet surface which prevented coalescence and retarded Ostwald ripening in such colloidal systems.

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# Defining sexual stimulants tadalafil and sildenafil in counterfeit biologically active additives to food

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***Keywords:*** sildenafil, tadalafil, dietary supplement, falsification.

## Abstract

The typical reactions of staining reagents used in forensic investigations of physical evidence – synthetic drugs sildenafil and tadalafil were conducted and described. There were defined the values of the chromatographic mobility in different solvent systems of these substances. The data on heir mass spectra, UV spectra and IR spectra were obtained. Quantitative determination of these substances in the sample batches of adulterated dietary supplements was conducted.

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# Physical Organic Chemistry. Destruction of drugs during radiation induced sterilization.

© **Anastasia V. Fedorova**,[1] **Alexandra V. Satalina**,[1] **Anatoly A. Fenin**,[1]*+ **Irina G. Antropova**,[1] **Natalia D. Oltarzhevskaya**,*[2] **Maria I. Valueva**,[2] and **Alexandra V. Kolaeva**[2,3]

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***Keywords:*** radiation induced sterilization, lidocaine, dioxidine, 5-fluorouracil.

**Abstract**

Process of destruction of dioxidine, lidocaine and 5-fluorouracil in model systems during radiation induced sterilization was studied. An assessment of changes in drug concentration during radiation sterilization of the alginate hydrogel was conducted: the expected change in the concentration is less than 0.1% by weight of the drug composition. The method of gas chromatography-mass spectrometry allowed to determine the structure of products of radiation-chemical reactions.

**Full Paper** _____ *Thematic Section:* Physicochemical Research.
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# Selection of stabilizing system for model cosmetic emulsion

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***Keywords:*** alkyl polyglucosides (APG), model cosmetic emulsions, surfactants mixtures, emulsion stabilization.

**Abstract**

Adsorption and micellization in mixed solutions of nonionic (APG type) and anionic surfactants have been investigated. The interaction parameters in surfactant mixtures have been calculated, the compositions of mixed micelles and adsorption layers have been determined. The synergistic behavior during adsorption and micellization in involved surfactant mixtures was observed. The composition of mixed stabilizing system for model emulsion was selected.

**Full Paper** _____ *Thematic Section:* Physicochemical Research.
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# Biosimular to lowmolecular heparin of sodium enoxaparin

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***Keywords:*** anticoagulants, unfractionated heparin, low molecular weight heparin, biosimilars, sodium enoxaparin.

**Abstract**

By UV spectrophotometry, atomic absorption spectrometry, infrared spectrometry, and viscometry we investigated the interaction of heparin with aqueous solutions of benzethonium chloride. Using the method of reversed-phase HPLC the parameters are set for carrying out the process of benzylation of the complex of heparin with quaternary ammonium salt and the content of benzyl alcohol is determined in the ester of heparin. By alkaline depolymerization of benzyl ester of sodium heparin, biosimilar of low molecular heparin of sodium enoxaparin was obtained. Physicochemical properties of molecular weight distribution and biological activity of the compound were defined. We conducted a study on the anticoagulant activity of anti Xa and IIa clotting factors.

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# Chemical analysis of indazole-3-carboxamide synthetic cannabinoids (AB-PINACA and its derivatives)

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***Keywords:*** AB-PINACA, AB-INACA-F, AB-CHMINACA, synthetic cannabinoids, thin layer chromatography, gas chromatography, mass spectrometry, IR spectroscopy, ultraviolet spectroscopy.

**Abstract**

Analytical characteristics of AB-PINACA and its two derivatives (AB-PINACA-F and AB-CHMINACA), representing the new class of indazole-3-carboxamide synthetic cannabinoids, are reported. To develop these substances different solvents and visualizing reagents for thin layer chromatography were used. Analytical characteristics determined by the mass spectrometry are given. Obtained results can be used for identification of new compounds of this class.

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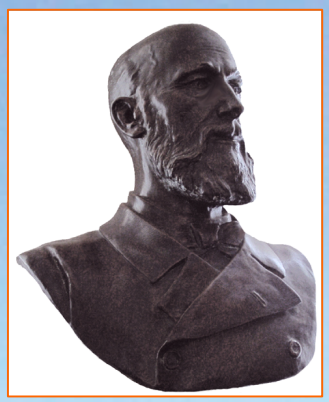

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# Co-crystallizates of benzo-tris-(1,2,5-oxadiazol-2-oxide)

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***Keywords:*** co-crystallizates, benzotrifuroxane, thermal decomposition, solution, melt, mechanical activation.

**Abstract**

The paper presents the results of the research into the stability and properties with benzotrifuroxane okristallizates with hexanitrohexaazaisowurtzitane and anthracene, and new benzotrifuroxane co-crystallizates with benzotriazole and dinitrazapentane, obtained from the solutions, melts and mechanical activation. Thermal behavior of co-crystallizates was studied andidentified by their infrared spectra and density, sensitivity parameters to mechanical impacts.

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# Effect of structure and physico-chemical characteristics of veterinary medicines Vetameks and Melapol plus containing synthetic melatonin on their ability to prolonged action

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***Keywords****:* melatonin, xymedon, phenazepamum, veterinary medicines, viscosity of solutions, prolonged action.

**Abstract**

We revealed the influence of the structure and physicochemical properties of melatonin-based new veterinary medicinal products on their prolonged action. It has been shown that polymer matrix based on Ethyl cyanoacrylate having a molecular weight in the range 2000-25000, modulus of elasticity of 8000-20500 kgf/cm$^2$, containing 5-10 mass % of plasticizer, and active substance up to 30 mass %, provides the prolonged action of melatonin-based new veterinary medicinal products within 90 days.

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# Defining the viscosity of solutions of the veterinary Vetamex drug as a method of forecasting and control of its prolonged action

© **Ludmila N. Punegova**,[1,2]* **Irina I. Kurbanova**,[1,2] **Tamara S. Shitova**,[2] **Dmitry A. Pudovik**,[2] **Oleg G. Sinyashin**,[1] and **Vladimir A. Alfonsov**[1+]

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***Keywords****:* melatonin, xymedon, veterinary medicines, viscosity of solutions, prolonged action.

**Abstract**

The dependence of the prolonging capacity of the veterinary drug Vetamex on viscosity of its solution in chloroform has been established. It is shown that an increase in the mass fraction of volatile matter content of the samples of studied drugs leads to decreased viscosity and reduction in the period of prolonged action, the average molecular weight of the polymer base in the range of 3000-7000 provides the prolonged action of preparations for 90 days or more. The possibility of using the indicator of Vetamex solution viscosity for prediction and control of its prolonged action has been shown. After the accumulation of statistical data and the formation of the appropriate methodology, the index of solution viscosity can be recommended as one of the most important quality indicators of the prolonged action preparation Vetamex.

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*Subsection:* Physical Chemistry. *Registration Code of Publication:* 14-38-5-23
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# Supramolecular reorganization in biopolymers during the adsorptive process

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***Keywords****:* biosynthesis, cellulose, microfibrila, hydrogen bond, nuclear magnetic resonance, adsorption of water vapor.

**Abstract**

The analysis of modern ideas on the structural organization of the cellulose microfibrils is carried out. Based on experimental studies of sorption processes with application of a proton magnetic relaxation the scheme of formation of additional capillary and porous system of cellulose is offered. It is established that at moisture content of cellulose of 8-10% there is a filling of its micropores, being accompanied with the increase of their cross sizes, increase in a specific surface and reduction of crystallinity degree of samples.

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*Thematic course:* Kinetics and mechanism of acyl transfer reactions. Part 8.

# Influence of the solvent water-2 propanol composition on the kinetics of alyphatic amines reactions with 4-nitro phenylbenzoate

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***Keywords:*** acylation, diethyl amine, dibutyl amine, 4-nitro phenylbenzoate, water – 2-propanol, specific solvation, quantum chemical simulation.

**Abstract**

Influence of the composition of the binary system water-2-propanol on the kinetics of diethyl amine and dibutyl amine reactions with 4-nitro phenylbenzoate is investigated. The equations are obtained that connect rate constants of the reactions with the binary solvent composition. A compensation effect is detected. Quantum chemical simulation of diethyl amine and dibutyl amine *H*-complexes with the solvent components is carried out. The kinetic data are compared with orbital characteristics of the solvate complexes.

**Full Paper** _____ *Thematic Section:* Physicochemical Research.
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# Studying the crystallization processes of thallium halides and KRS-6, KRS-5 solid solutions in water and non-aqueous solvents

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***Keywords:*** solid solutions, monadic thallium halides, crystallization in water and non-aqueous solvents, induction period of crystallization, crystallization supersaturation coefficients.

## Abstract

We explored the crystallization processes of monadic thallium halides and $TlCl_{0.74}Br_{0.26}$ (KRS-6) and $TlBr_{0.46}I_{0.54}$ (KRS-5) solid solutions based on them, both in water and non-aqueous solvents within the temperature range of 303 to 353 K. The crystallization induction periods ($\tau_{ind}$), solution cooling velocities (V), supersaturation coefficients for individual monadic thallium halide ($\gamma = C_n/C_{eq}$) and their solid solution ($\gamma = K_{\alpha,Tn}/C_{\alpha,Teq}$) crystallization in water and non-aqueous solvents were defined experimentally. For thallium halides in the latter, the linear dependence of $lg(\tau_{ind})$ on supersaturation coefficients ($\gamma$) were established. We then derived the equations for induction period time ($\tau_{ind}$) in water, formamide, formic acid, ethylene glycol, and ethanol. The scientific approach to the regime development of thallium(I) halide synthesis and purification from the liquid media was also justified.

**Full Paper** _____ *Thematic Section:* Physicochemical Research.
*Registration Code of Publication:* 14-38-5-56 *Subsection:* Physical Chemistry.
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# Effect of activation conditions and a contact time on the *n*-hexane conversion over Ga-modified surface of high-silicon zeolite systems type ZSM-5

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***Keywords****: n*-hexane, zeolite, ZSM-5, air, hydrogen, cracking, isomerization, aromatization.

**Abstract**

Modifying high-silicon zeolite system ZSM-5 by Ga and study of chemical conversion directions of *n*-hexane over surface of this system depending on activation conditions and feed rated were carried out. Comparative analysis of modified and unmodified system showed that the catalyst modifying by Ga make it possible to increase the yield of aromatic hydrocarbons, to reduce intensity of cracking reactions. Based on the experimental data for the conversion products and depending on the process conditions, and the obtained data about a structure and a surface of the studied system. A scheme of conversion of hydrocarbons over surface of this catalytic system was suggested.

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# Influence of sorbent nature on benzotriazole derivatives retention under condition of RP HPLC

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***Keywords:*** benzotriazole derivatives, high performance liquid chromatography, supercrosslinked polystyrene, hypercarb, thermodynamic characteristics of sorption.

**Abstract**

The results of chromatographic research of some benzotriazole derivatives sorption on the octadecylesilicagel, supercrosslinked polystyrene and hypercarb were given. Physicochemical and electronic characteristics of benzotriazole derivatives were calculated. The influence of sorbent nature on the chromatographic retention of these substances was analyzed.

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# Liquid compound stratification details in quasi-ternary system LiF–RbI–$Li_2CrO_4$

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***Keywords:*** phase transition, differential thermal analysis, liquid compound stratification, quasi-ternary system, stable triangle, nonvariant monotectic equilibrium, geometric modeling of phase complex.

**Abstract**

Phase complex of quasi-ternary system LiF–RbI–$Li_2CrO_4$ was studied. This system is a stable triangle of quaternary reciprocal system Li,Rb||F,I,$CrO_4$. System geometric model was designed based on experimental data of polythermal sections. Analysis of model demonstrates that two fields exist in this system. First field is characterized as nonvariant monotectic equilibrium: L2⇄L1+LiF+RbI and second field is characterized as monovariant monotectic equilibrium: L2⇄L1+LiF. In this work phase reactions are presented for non-, mono- and divariant phase equilibria. Eutectic point characteristics were found.

**Full Paper** _____ *Thematic Section:* Physicochemical Research.
*Registration Code of Publication:* 14-38-5-78 *Subsection:* Physical Chemistry.
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http://butlerov.com/readings/
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# Electrosurface properties of silicon oxide(IV) in aqueous solutions of azoles

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*Keywords:* silicon oxide(IV), azoles, electrosuperficial properties.

**Abstract**

The paper is devoted to the study of electrosuperficial properties of quartz (silicon oxide(IV)) in aqueous solutions of simple azoles. To determine the electrokinetic properties of silicon oxide ($SiO_2$) we used the method of micro-electrophoresis. Study of electrokinetic properties of $SiO_2$ surface was held over the function of pH and contact time with the phases of quartz test solutions. It has been found that in solutions of the isoelectric point value of imidazole ($pH_{IET}$) of quartz shift to alkaline region. In solutions of *n*-tetrazole the value $pH_{IET}$ of quartz shifts in acidic region. This paper describes a model of adsorption of cationic and anionic forms of azoles on the surface of $SiO_2$.

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*Registration Code of Publication:* 14-38-5-84 *Subsection:* Physical Organic Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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# Kinetics of gelatin swelling in aqueous solutions of azoles

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***Keywords:*** kinetics of the swelling process, gelatin, cationic form of azoles.

**Abstract**

The present work is a continuation of a series of studies on the sorption of heterocyclic compounds on the surface of the protein. The paper is devoted to the kinetic regularities of interaction of macromolecular compound (in this case, gelatin) with a nitrogen compound. The dependence of the swelling rate structure interacting substance, and the pH of the solution was studied. The azol influence on the swelling of proteins was investigated depending on the time of swelling and the pH of the solution. The results indicated that azoles affect the swelling of gelatine. The swelling rate of gelatin in the same media in the presence of acidic azole of different substituents was markedly different. It can be judged that the presence of electron-donating and electron-withdrawing groups is responsible for the change in the rate of swelling.

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http://butlerov.com/readings/
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# Functional properties of composite sorbents "cation exchanger KU-2×8-metal sulfide"

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***Keywords:*** cation exchanger KU-2×8, composite sorbents, zinc sulfide, copper sulfide (II), lead sulfide, sorption of copper(II), sorption of heavy non-ferrous metals.

## Abstract

The sorption properties of composite sorbents based on strong-acid cation resin KU-2×8 and immobilized in its matrix copper(II), zinc, lead sulfides: KU-2×8–CuS, KU-2×8–ZnS and KU-2×8–PbS was studied. Potentiometric titration of composite sorbents revealed their bifunctional nature, determined dissociation constants values and total capacity of ionic groups. It is shown that full dynamic adsorption capacity of the studied compositions is 1.5-2.0 times higher as compared to a universal cation exchanger KU-2×8 for copper(II), zinc, cadmium at more intensive process kinetics. Synthesized sorbents demonstrated explict selectivity for copper(II) in presence of trace electrolyte, its uptake under these conditions is 1.3-4.5 times higher than that of cation exchanger KU-2×8.

**Full Paper** _____ *Thematic Section:* Physicochemical Research.
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http://butlerov.com/readings/
Contributed: July 31, 2014.

# Produce new solid electrolytes based on the $Li_{8-x}Zr_{1-x}V_xO_6$ system

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***Keywords:*** chemical power source, lithium-ionic conductors**,** solid electrolytes**,** cathode materials.

**Abstract**

The region of existence of solid solutions in the $Li_{8-x}Zr_{1-x}V_xO_6$ system, where $0 \le x \le 0.01$, was determined. The heterovalent doping of the $Li_8ZrO_6$ phase into the zirconium sublattice by the $Li_7VO_6$ phase results in significant increase in the solid solutions conductivity. The $Li_{7.99}Zr_{0.99}V_{0.01}O_6$ solution has the highest value of conductivity ($4.1 \cdot 10^{-1}$ S/cm) at 873 K. The fraction of electronic conductivity in the $Li_{7.99}Zr_{0.99}V_{0.01}O_6$ sample does not exceed 0.1% of the total conductivity value at 873-673 K. The solid solutions of the $Li_{7.99}Zr_{0.99}V_{0.01}O_6$ composition were found to be stable in contact with lithium at temperatures above 533 K. Thus, they may be used as solid electrolytes for lithium chemical power sources.

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# Kinetic analysis of glycathione inhibition of the process of nonenzymatic glycosylation *in vitro* of genetically engineered human insulin

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***Keywords:*** kinetics, non-enzymatic glycosylation of proteins, insulin, glutathione.

**Abstract**

The kinetic characteristics of inhibition by reduced glutathione of the process of nonenzymatic glycosylation of insulin *in vitro* at its initial stage, wherein it consists of two consecutive steps $s$ = 1, 2 and proceeds in quasi-equilibrium regime by the stage1 have been discussed. It has been established that glutathione supplements do not disturb the mechanism of this two-stage process, but reduce its rate and the yield of the final product – fructosamine – at stage 2 by binding glutathione (Y) of insulin (I) as a reagent of stage 1 in the chemical compound of type $I_\alpha Y$ the routing reaction p = 3: $\alpha I + Y = I_\alpha Y$, where α – module of stoichiometric factor of insulin. Thermodynamic calculations of equilibrium concentrations of all components in working solutions by their initial concentrations using the previously found equilibrium constants in steps 1 and 2 show that the routing reaction 3 is implemented at α = 4 has the equilibrium constant $K_3^c(T,[c_k]) = 733$ (T = 277K, $[c_k]$ = 1 mol/m$^3$).

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# The application of NIR-spectroscopy analysis for the study of the chemical composition and metabolic energy of flax shives

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***Keywords***: near infrared spectroscopy, chemical composition, fiber flax, flax shive, crude protein, crude fiber, crude fat.

## Abstract

The chemical composition of flax shives (which is a large-capacity waste of flax processing industry) were studied by NIR-spectroscopy method. Flax shives were obtained from processing flax varieties TOAST 5 and Antaeus. It was shown that the use of bioregulators Biopag-D and Protective-stimulating complex (PSC) on flax fiber in the herringbone phase increased the yield of flax straw by 9-12%, flax – by 1.5-8%, the fibers on the background of the Legislative Assembly – by 6-7%, the yield of flax shivers by more than 2 t/ha as compared to the control. It was revealed with the use of NIR-spectroscopy that the chemical composition of flax shivers meets the requirements on the quality of fodders and mixed fodders. The content of crude protein, depending on the processing of bioregulators in linen stake was 1.7-5.1%, crude fat – 1.0-4.2%, crude ash – 1.7-4.0%, crude fiber – 51st 65% at the optimal concentrations of calcium and phosphorus 0.67-1.02% and 0.15-0.27%, respectively. Metabolic energy of flax shivers based on air-dry matter was on average 7.3 MJ/kg and corresponded to the average value of this indicator for straw cereals. The content of fodder units per 1 kg of dry matter for flax shivers was 0.11-0.23 kg. The maximum value of fodder units were observed for shivers of varieties Antaeus Biopag in processing, and the minimum – for grades TOAST 5 treated with PSC. Data on the chemical composition and metabolic energy value of flax shivers confirmed the possibility of its use as fodders for productive animals.

**Full Paper** _____ *Thematic Section:* Preparative Research.
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# Crystal and molecular structure of tetraphenylantimony acetylacetonate

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*Supervising author; [+]Corresponding author
***Keywords:*** acetylacetonate tetraphenylantimony, structure.

**Abstract**

X-ray analysis was carried out over the crystal acetylacetonate tetraphenylantimony, which is composed of two types of crystallographically independent molecules. Antimony atoms have a distorted octahedral coordination, Sb-C bond lengths vary in the range 2.111(13)-2.173(12) Å, and in heterocycles ($SbO_2C_3$) the distances Sb-O and O-C are equal to 2.225(10)-2.274(10) and 1.22(2)-1.28(2) Å respectively.

**Full Paper** _____ *Thematic Section:* Preparative Research.
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# Reaction of the sodium salt of octantetraone-2,4,5,7 with chloride tetraphenylantimony

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***Keywords:*** reaction, the sodium salt of octantetraone-2,4,5,7, chloride tetraphenylantimony.

**Abstract**

Tetraphenylantimony chloride, reacting with the sodium salt of octantetraone-2,4,5,7 (2:1 mol.) in tetrahydrofuran synthesized organoantimony complex, which structure after recrystallization from chloroform identified by X-ray. It is shown that the coordination of the antimony atoms in the two crystallographically independent centrosymmetric molecules of the binuclear chelate-foot complex is distorted octahedral, *trans*-angles CSbC and CSbO vary in the range 158.2(5)-169.4(4)°, bond lengths are Sb-C 2.133(11)-2.175(17) Å. In the six-membered metallacycles [$SbO_2C_3$] distance Sb-O are 2.209(10)-2.344(8) Å, O-C 1.258(17)-1.300(17) Å, C-C 1.360(20)-1.380(20) Å.

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Conference "New methods of synthesis, structure and application of organoelemental compounds"
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# Tetraphenylantimony and tetra-*p*-tolylantimony carbonates

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***Keywords:*** tetraphenylantimony carbonate, crystalline modification, tetra-*p*-tolylantimony carbonate, structure.

**Abstract**

The features of the crystal structure of orthorhombic modification carbonate bis(tetraphenylantimony) (**I**) and monoclinic carbonate tetra-*para*-tolylfntimony (**II**). According to X-ray data molecules **I** and **II** present antimony atoms having trigonal-bipyramidal $Sb_{(5)}$, and octahedral coordination $Sb_{(6)}$. For atoms of $Sb_{(5)}$ axial angles CSb(1)O constitute 179.0(2)° and 175.2(1)°, equatorial CSb(1)C angles vary in the intervals 113.6(3) -124.9(3)° and 115.9(1)-124.1(1)° in **I** and **II**, respectively. Bond lengths Sb(1)–O and Sb(1)–C are 2.247(5) and 2.107(8), 2.118(8), 2.124(7), 2.174(8) Å (**I**), 2.264(2) and 2.117(4), 2.120(3), 2.126(3), 2.171(3) Å (**II**). Bond angles at atoms $Sb_{(6)}$ CSb(2)O, CSb(2)C are 163.3(2)°, 152.8(2)°, 161.6(3)° (**I**) и 151.8(1)°, 162.9(1)°, 165.6(1)° (**II**); Sb(2)–O and Sb(2)–C distance equal 2.273(5), 2.246(5) и 2.158(8)-2.179(8) Å (I), 2.217(2), 2.251(2) и 2.159(3)-2.177(3) Å (**II**).

**Short Communication** _____ *Thematic Section:* Preparative Research.
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Conference "New methods of synthesis, structure and application of organoelemental compounds"
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# Reaction of octantetraone-2,4,5,7 with triphenylantimony in the presence of hydrogen peroxide

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***Keywords:*** reaction, octantetraone-2,4,5,7, triphenylantimony, hydrogen peroxide, diacetate triphenylantimony.

**Abstract**

Interaction of octantetraone-2,4,5,7 with triphenylantimony in the presence of hydrogen peroxide in ether triphenylantimony diacetate resulted in 12% yield. Formation of acetic acid in the reaction mixture is explained by oxidative cleavage of the starting tetraketone.

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# Crystal and molecular structure tetra-*p*-tolylantimony dibenzoylmethanate

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*Supervising author; [+]Corresponding author
***Keywords:*** *tetra-p-tolylantimony dibenzoylmethanate, structure.*

**Abstract**

We carried out X-ray analysis of the crystal benzene solvate dibenzoylmethanate tetra-*para*-tolylantimony *p*-$Tol_4SbacacPh_2 \cdot PhH$, in two crystallographically independent molecules which antimony atoms have distorted octahedral coordination (axial angles CSbC and CSbO are 159.9(2)° and 165.24(14)-169.51(15)°). Bond lengths Sb–C vary in the range 2.148(6)-2.165(5) Å, in the heterocycles ($SbO_2C_3$) Sb-O and O-C distance are 2.240(6)-2.313(6) and 1.267(6)-1.281(6) Å, respectively.

**Full Paper** _____ *Thematic Section:* Preparative Research.
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# Reaction of octantetraone-2,4,5,7 with penta-*p*-tolylantimony

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***Keywords:*** reaction, penta-*p*-tolylantimony, octantetraone-2,4,5,7.

**Abstract**

Reaction of *p*-penta-tolylantimony with octantetraone-2,4,5,7 (2:1 mol.) in toluene resulted in the synthesis of binuclear chelate complex $Tol_4Sb[OC(Me)CHC(O)(O)CCH(Me)CO]SbTol_4$. Coordination of atoms Sb(1,2) is distorted octahedral, CSbC and CSbO *trans*-angles vary in the range 158.8(3)-173.2(4)°, bond lengths Sb-C 2.097(10)-2.198(10) Å. In two six-membered metallacycle $[SbO_2C_3]$ Sb-O distances are 2.262(7)-2.290(7) Å, O-C 1.255(12)-1.327(11) Å, C-C 1.318(14)-1.529 (4) Å.

**Full Paper** _____ *Thematic Section:* Preparative Research.
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# Reaction of penta-*p*-tolylantimony with 2,6-di-*tert*-butylphenol. Oxide tri-*p*-tolylantimony structure.

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***Keywords:*** penta-*p*-tolylantimony, 2,6-di-tert-butylphenol, tri-*p*-tolylantimony oxide, molecular structure.

**Abstract**

Reaction of *p*-pentatolylantimony with 2,6-di-*tert*-butylphenol in toluene leads to the formation of tri-*p*-tolylantimony and oxidation product of starting phenol – 2,6,2',6'-tetra-*tert*-butyldiphenoquinone. Minor product of the reaction is tri-*p*-tolyantimony oxide the structure of which was proved by X-ray analysis.

**Short Communication** _____ *Thematic Section:* Preparative Research.
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# Synthesis and structure of tetra-*m*-tolylantimony bromide

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***Keywords:*** tetra-*m*-tolylantimony bromide, synthesis, structure.

**Abstract**

Interaction of the tri-*m*-tolylantimony dibromide with *m*-tolylmagnesiumbromide resulted in obtaining tetra-*m*-tolylantimony bromide (**I**). According to X-ray data, the crystal **I** posess two types of independent trigonal-bipyramidal molecules with a bromine atom in the axial position. Bond lengths Sb-C, Sb-Br, CSbC, equatorial angles and BrSbC axial angles are equal to 2.117(5)-2.165(5); 2.8803(8), 2.9390(8) Å; 118.3(2)-119.6(2)° and 174.9(1)°, 171.9(2)°.

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# The synthesis and structure of *bis*(4-nitrophenoxo)tri-*p*-tolylantimony

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***Keywords:*** tri-*p*-tolylantimony, 4-nitrophenol, *tert*-butylhydroperoxide, oxidative addition, *bis*(4-nitrophenoxo)tri-*p*-tolylantimony, structure.

**Abstract**

Interaction of 4-nitrophenol with tri-*p*-tolylantimony in the presence of *tert*-butyl hydroperoxide resulted in the synthesis of *bis*(4-nitrophenoxo)tri-*p*-tolylantimony (86%) per molecule wherein the antimony atom has a distorted trigonal-bipyramidal coordination. OSbO axial angle and the sum of angles CSbC equatorial plane are equal to 177.8 (1)° and 360°. Bond lengths Sb-O and Sb-C constitute 2.091(3) and 2.091(7), 2.111(4), 2.115(5) Å.

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# Synthesis and crystal structure of acetonyltriphenylphosphonium tetrachloroaurate $[Ph_3PCH_2C(O)CH_3]^+[AuCl_4]^-$

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***Keywords:*** acetonyltriphenylphosphonium tetrachloroaurate, synthesis, structure.

**Abstract**

Reaction of hexahydrate tetrachloroauratehydrogen acid with acetonylphenylphosphonium chloride in acetone resulted in obtaining a complex $[Ph_3PCH_2C(O)CH_3]^+[AuCl_4]^-$ (**I**). According to X-ray data, the crystal of complex **I** consists of four crystallographically independent tetrahedral cations $[Ph_3PCH_2C(O)CH_3]^+$ (bond lengths P-$C_{Ph}$ and P-$C_{Alk}$ are 1.787(6)-1.801(5) and 1.793(6)-1.803(6) Å respectively, angles CPC 106.9(4)°-112.7(3)° and four crystallographically independent planar anions $[AuCl_4]^-$ (angles ClAuCl 88.24(10)°-91.66(9)° and 177.97(9)-179.56(8)°, Au-Cl bond lengths are 2.252(2)-2.281(2) Å).

*Thematic Section:* Preparative Research. **Short Communication**
*Subsection:* Organoelemental Chemistry. *Registration Code of Publication:* 14-38-5-155
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# Synthesis and crystal structure of tetrabutylphosphonium tetrabromoaurate $[Bu_4P]^+[AuBr_4]^-$

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***Keywords:*** tetrabutylphosphonium tetrabromoaurate, synthesis, structure.

**Abstract**

Reaction of hydrate tetrabromoauratehydrogen acid with tetrabutylphosphonium bromide resulted in obtaining the complex $[Bu_4P]^+[AuBr_4]^-$ (**I**). According to X-ray data, the crystal of complex **I** represented tetrahedral cations $[Bu_4P]^+$ (bond lengths P-C 1.75(3)-1.83(3) Å, angles CPC 108.7(16)°-114.8(14)°) and somewhat distorted square planar anions $[AuBr_4]^-$ (*cis*-angles BrAuBr 89.52(7)°-90.40(6)°, *trans*-angles BrAuBr 179.60(7), 179.84(10)°), bond lengths Au-Br 2.3909(18)-2.4126(15) Å ).

**Short Communication** _____ *Thematic Section:* Preparative Research.
*Registration Code of Publication:* 14-38-5-158 *Subsection:* Organoelemental Chemistry.
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# Synthesis and structure of dodecatungstenphosphate tetraphenylphosphonium $[(C_6H_5)_4P]_3[PW_{12}O_{40}]$

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*Supervising author; +Corresponding author
***Keywords:*** dodecatungstenphosphoric acid, tetraphenylphosphonium salt, synthesis, structure.

**Abstract**

Interaction of tetraphenylphosphonium bromide with dodecatungstenphosphoric acid in water was synthesized and structurally characterized salt $[(C_6H_5)_4P]_3[PW_{12}O_{40}]$. Phosphorus atoms in the two types of crystallographically independent cations $[(C_6H_5)_4P]^+$ have a distorted tetragonal coordination (distances P-C 1.74(4)-1.83(3) Å; angles CPC 107.2(15)-110.9(15)°). In centrosymmetric anions $[PW_{12}O_{40}]^{3-}$ (inversion center – phosphorus atom) W-O, W-O($\mu_2$) and W-O($\mu_4$) equal to 1.63(4)-1.71(4), 1.87(4)-1.98(4) and 2.48(3)-2.50 (3) Å.

*Thematic Section:* Preparative Research. **Full Paper**
*Subsection:* Organoelemental Chemistry. *Registration Code of Publication:* 14-38-5-161
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# Synthesis and structure of *bis*(4-nitrophenylacetate) tri-*m*-tolylbismuth

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***Keywords:*** tri-*m*-tolylbismuth, 4-nitrophenylacetic acid, *tert*-butylhydroperoxide, oxidative addition, *bis*(4-nitrophenylacetate) tri-*m*-tolylbismuth, structure.

**Abstract**

Reaction of tri-*m*-tolylbismuth with 4-nitrophenylacetic acid in the presence of *tert*-butylhydroperoxide in ether gives *bis*(4-nitrophenylacetate) tri-*m*-tolylbismuth (**I**). According to the X-ray data, bismuth atom in the molecule **I** has a distorted trigonal-bipyramidal coordination (OBiO axial angle and CBiC equatorial angles are 169.53(18)° and 109.3(6), 110.3(6), 140.3(2)°). The Bi–O and Bi–C bond lengths are 2.228(12), 2.256(13) Å and 2.199(12), 2.223(12), 2.279 (8) Å, respectively. In molecule **I** present close intramolecular contacts Bi···O = C (2.908(8), 2.947(9) Å) on part of the largest equatorial angle CBiC.

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# Tetraorganylphosphonium triiodide $[Ph_3RP]^+[I_3]^-$ ($R = CH_2CHMe_2$, $CH_2Ph$). Synthesis and Structure.

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***Keywords:*** tetraorganylphosphonium triiodide, synthesis, structure.

**Abstract**

Reaction of tetraorganylphosphonium iodides $Ph_3RPI$ ($R = CH_2CHMe_2$, $CH_2Ph$) with antimony triiodide in dimethylsulfoxide resulted in synthesizing complexes $[Ph_3PCH_2CHMe_2]^+[I_3]^-$ (**I**), $[Ph_3PCH_2Ph]^+[I_3]^-$ (**II**). According to the X-ray data, the phosphorus atoms in the cation complex **I-II** have a tetrahedral coordination (CPC 107.2(3)-111.1(2)°), bond lengths P-C are 1.788(5)-1.815(5) Å, respectively. In linear anions $[I_3]^-$ I-I-I angles and I-I bond lengths are equal to 178.31(2)°, 179.15(2)°) and 2.8882(6)-2.9298(8) Å, respectively. Cations and anions in the crystals **I** and **II** are connected with each other through weak hydrogen bonds H···I 3.57 Å (**I**), 3.06 (**II**) Å.

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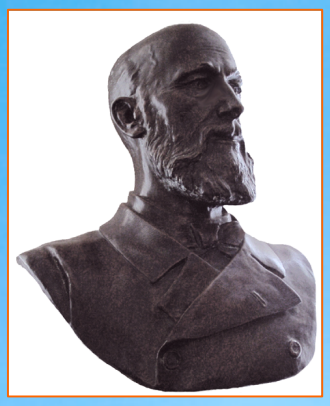

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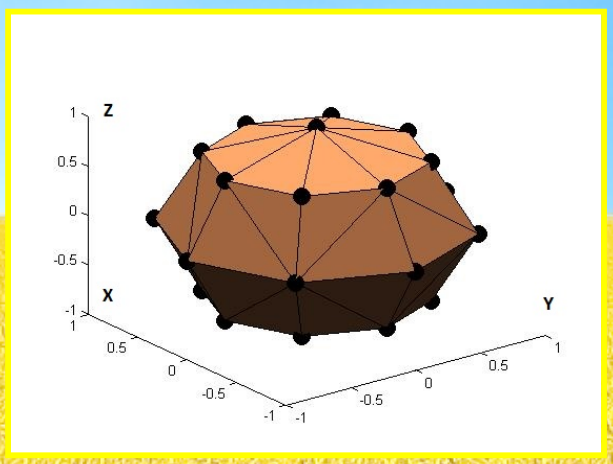


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# Structures of magic clusters of oxyhydrate gels obtained by means of colloidal chemical spectroscopy

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***Keywords:*** Lagrangian maps, electroglobules, fulleroids, multipoles, oxyhydrate gel systems, colloid clusters, spontaneous pulsation flow, diffuse double electric layer, topological continuum, dissociation-disproportion mechanism, Whitney theory, geometry of caustics.

**Abstract**

We have found octahedral formations in the lacework portions of the cluster architecture of oxyhydrate systems; they also contain tetrahedral fragments, complex tetrahedral (and even hexahedral) pyramids, as well as fulleroid-like structures arranged on a Coxeter platform of dispersion colloid medium.

**Full Paper** _____ *Thematic Section:* Theoretical Research.
*Registration Code of Publication:* 14-38-6-8 *Subsection:* Physical Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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# Topology of benzotriazole derivatives

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***Keywords:*** benzotriazole derivatives, topological indices, connectivity, high performance liquid chromatography, sorption-structural correlations.

**Abstract**

Physicochemical and topological characteristics of benzotriazole derivatives were calculated. Results of investigations of the relationship between topological and physicochemical characteristics of these compounds were shown. The influence of the topology of molecules on their chromatographic retention in the conditions of high performance liquid chromatography was analyzed.

*Thematic Section:* Theoretical Research. **Full Paper**
*Subsection:* Organic Chemistry. *Registration Code of Publication:* 14-38-6-15
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# Problems of classification in the estimation of relationship between structure and odor for some organic substances

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***Keywords:*** problems of classification of organic substances, structure-odor relationship, "DENSON" model, structure sensitive "frequency descriptor" $\nu_{cp}$', geometrical structural descriptor $S_d$, calculated relative density $d_4^{20}$.

**Abstract**

We considered problems of classification of some organic substances based on their odor using methods of pattern recognition. Using simple algorithms of classification in descriptor space $\nu_{cp}$', $d_4^{20}$ and $S_d$, organic substances were divided into two odor classes.

*Thematic Section:* Theoretical Research. **Full Paper**
*Subsection:* Physical Chemistry. *Registration Code of Publication:* 14-38-6-21
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# Accounting the concentration of complexes with hydrogen bonds during the kinetic description of reactions with associated compounds

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***Keywords:*** complexes with hydrogen bonds, reactivity, kinetic equations.

**Abstract**

It is shown that between the computed concentrations of the compounds, calculated under the assumption that all of the compounds are in monomeric form, the concentrations of individual associates (complexes with hydrogen bonds) showed a linear dependence. The fact of the possibility of using the calculated concentrations of substances forming associates in the kinetic equations can be an indication that the transformations involved associates.

**Full Paper** _____ *Thematic Section:* The study of catalysts.
*Registration Code of Publication:* 14-38-6-26 *Subsection:* Organic Chemistry.
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# Formation of an active surface of $MoO_3/\gamma$-$Al_2O_3$ catalyst for the metathesis reaction of ethylene and trans-2-butene in propylene

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***Keywords:*** molybdenum oxide, supported catalysts, acid-base surface properties, temperature-programmed reduction, metathesis, propylene.

**Abstract**

The effect of nitric acid addition in the process in preparing the supported Mo-containing alumina catalyst on the nature and distribution of active structures, acid-base properties and catalytic properties in the metathesis reaction of ethylene and trans-2-butene to propylene was investigated in the present work. The object of investigation is a molybdenum oxide supported on the $\gamma$-$Al_2O_3$ (JSK *«SKTB «Katalizator»*, Novosibirsk). It is shown that the addition of nitric acid in the impregnating solution of ammonium heptamolybdate affects the nature of the interaction of the precursor of the carrier component with support surface, the nature of the active component, acid-base properties, morphology and phase composition of the catalyst, that is the reason of the catalytic properties of synthesized systems in the metathesis reaction of ethylene and *trans*-2-butene into propylene.

**Full Paper** _____ *Thematic Section:* Research of Catalysts.
*Registration Code of Publication:* 14-38-6-36 *Subsection:* Organic Chemistry.
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# Influence of palladium precursor nature on the state of metal particles in selective hydrogenation of acetylene

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***Keywords**:* selective hydrogenation of acetylene, Pd/δ-$Al_2O_3$, palladium acetate, palladium acetylacetonate.

**Abstract**

Influence of palladium precursor nature on geometric and electronic properties of supported Pd particles and their adsorption properties in the selective hydrogenation of acetylene was investigated. It has been established that catalysts synthesized from $Pd(Acac)_2$ precursor dispersion is 1.3 times higher than for samples of *acetate* complex. This determines a high conversion of acetylene, catalysts for the former. It is shown that catalysts of $Pd(Ac)_2$ have high electron density on valence orbitals of metal particles compared to samples based on $Pd(Acac)_2$, and characterized by 1.4 times greater selectivity in conversion of acetylene into ethylene.

*Thematic Section:* Preparative Research. **Full Paper**
*Subsection:* Organic Chemistry. *Registration Code of Publication:* 14-38-6-43
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# New dimeric chlorophyll *a* derivatives with di-, tri-and tetraethylene glycol fragments as a spacers between the macrocycles

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***Keywords:*** methylpheophorbide-*a*, chlorin $e_6$, dimers, chlorophyll-*a*.

**Abstract**

Novel phorbin-phorbin and chlorin-chlorin dimers with oligoethylene glycol spacers was synthesized using methylpheophorbide *a* as start matiarial. *Exo* ring ester group transesterification with 2-chloro-*N*-methylpyridinium iodide activation were used for dimeric molecules formation. Chlorin-chlorin dimers was obtained from corresponding phorbin-phorbin dimers by phorbin fragments *exo* rings recovering with methylamine.

*Thematic Section:* Preparative Research. **Full Paper**
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# Synthesis of novel metal complexes based on *meso*-tetrakis(4-hydroxy-3,5-diisobornyl)porphyrin

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***Keywords***: 2,6-diisobornyl-4-methylphenol, porphyrins, porphyrinates, metall complexes.

**Abstract**

Series of novel transition metal porphyrinates ($Zn^{2+}$, $Cu^{2+}$, $Co^{2+}$, $Fe^{3+}$, $Mn^{3+}$) – metalloporphyrin antioxidants with fragments of 2,6-diisobornylphenol using the *meso*-tetrakis(4-hydroxy-3,5-diisobornyl)-porphyrin as ligand was synthesized. These 2,6-diisobornylphenolic fragments at the periphery of macrocycle can participate as an additional reaction sites for interaction with free radicals.

**Full Paper** _____ *Thematic Section:* Preparative Research.
*Registration Code of Publication:* 14-38-6-54 *Subsection:* Organic Chemistry.
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http://butlerov.com/readings/
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# Synthesis of adamantyl containing urea, thiourea and bisurea – monomers for cyclodextrin supramolecular polymers

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***Keywords:*** isocyanate, urea, thiourea, adamantane, adamantyl.

**Abstract**

Adamantyl containing urea and bisurea which may find application as monomers for supramolecular structures cyclodextrin were synthesized. On the basis of synthesized urea supramolecular inclusion complexes with *β*-cyclodextrin were obtained. The article presents data on the synthesis of new adamantly containing urea and bisurea. Reactions were carried out under mild conditions with high yields.

*Thematic Section:* Preparative Research. **Full Paper**
*Subsection:* Organic Chemistry. *Registration Code of Publication:* 14-38-6-59
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# Synthesis and antibacterial activity of 5-aryl-4-acyl-3-hydroxy-1-(2-ethylhexyl)-3-pyrrolin-2-ones

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*Supervising author; +Corresponding author

***Keyword:*** heterocycles, 1,4,5-trisubstituted tetrahydropyrrole-2,3-diones, three-component reaction, ethylhexylamine, antimicrobial activity.

**Abstract**

By the reaction of 1,4,5-trisubstituted 3-hydroxy-3-pyrroline-2-ones from a mixture of aromatic aldehyde and 2-ethylhexylamine we obtained 5-aryl-4-acetyl-1-(2-ethylhexyl) -3-hydroxy-3-pyrroline-2-ones. The antimicrobial activity of these compounds has been studied. The structures of all synthesized compounds were proved by IR, NMR $^1$H spectroscopy.

**Full Paper** _____ *Thematic Section:* Preparative Research.
*Registration Code of Publication:* 14-38-6-64 *Subsection:* Organic Chemistry.
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# Bicyclic anionic σ-adduct of 2-hydroxy-3,5-dinitropyridine in the synthesis of new derivatives of 2,6-diazatricyclododekanes

© **Evgenia V. Ivanova**,[1+] **Irina I. Surova**,[1] **Nikolay V. Hlytin**,[1] **Igor V. Blokhin**,[1] **Irina V. Shahkeldyan**,[1] **Yuriy M. Atroshchenko**,[1*+] and **Konstantin I. Kobrakov**[2*]
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***Keywords**:* anionic *σ*-adducts, complex Yanovsky, 2,6-diazatricyclododekanes, 2-hydroxy-3,5-dinitropyridine.

**Abstract**

Studied the chemical behavior of the 2-hydroxy-3,5-dinitropyridine in reaction with carbanion of acetone in the Yanovsky reaction conditions, identified structure thus formed bicyclic anionic complex by IR and NMR-spectroscopy has been studied.

*Thematic Section:* Preparative Research. **Full Paper**
*Subsection:* Organic Chemistry. *Registration Code of Publication:* 14-38-6-69
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# Synthesis of novel pyrazine derivatives of *p*-hydroxybenzoic acid

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***Keywords:*** pyrazine derivatives, nucleophilic substitution, *p*-hydroxybenzoic acid.

**Abstract**

Reaction of 2-chloro-3-aryloxypirazines with ethyl ester of *p*-hydroxybenzoic acid gives products of nucleophilic substitution of chlorine atom. On the basis of the pyrazine derivatives containing a carboxyl group we have synthesized corresponding carboxamides.

*Thematic Section:* Preparative Research. **Full Paper**
*Subsection:* Organoelemental Chemistry. *Registration Code of Publication:* 14-38-6-73
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# Comparative analysis of powerintensity of processes of purifying of hydrocarbonic gases from sulfur-containing impurities using solid and liquid sorbents

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***Keywords:*** sorbent, ethanolamines, hydrogen sulfide, gas purifying.

**Abstract**

A comparative analysis of an effectiveness of purifying of hydrocarbonic gas from sulfur-containing compounds using solid and liquid sorbents was made. Calculations and comparison of power consumptions necessary for purifying the gas from sulfur-containing compounds using solid and liquid sorbents were carried out.

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# A method for purifying casing-head gas from hydrogen sulfide

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***Keywords:*** complex compound, sorbent, hydrogen sulfide, gas purifying.

**Abstract**

A catalyst for hydrogen sulfide oxidation has been obtained. This catalyst includes a complex compound with the formula $MgCl_2 \cdot AlCl \cdot 3Et_2O$ (where $Et_2O$ – diethyl ether) based on a solid porous carrier. A series of experiments for studying its catalytic properties was carried out.

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*Thematic course*: Hydrochemical synthesis of metal chalcogenides films. Part 19.

# The films $Cu_{2-x}Se$: thermodynamic analysis of the formation conditions, the synthesis, composition, morphology

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***Keywords:*** ionic equilibrium, the boundary conditions of formation, chemical bath deposition, copper(I) selenide.

**Abstract**

The boundary formation conditions of solid phase of copper(I) selenide and copper(I) hydroxide were defined by means of calculation of ionic equilibrium with using of thermodynamic constants for systems "copper(I) chloride − hydroxylamine hydrochloride – sodium selenosulphate" accounting the formation of crystal nucleus with critical radii. It is experimentally shown that the obtaining of copper(I) selenide films with the thickness of 100 to 400 nm of nonstoichiometric composition $Cu_{2-x}Se$ is possible by hydrochemical deposition. The composition and morphology of the obtained layers were investigated. The research revealed that the as-deposited layers $Cu_{2-x}Se$ consist of crystallites polyhedral shape and have *p*-type conductivity.

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*Thematic course*: Hydrochemical synthesis of metal chalcogenides films. Part 20.

# Ion exchange synthesis at the interface "PbS thin film – aqueous solution of cadmium salt", composition and properties of a new phase

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***Keywords:*** ionic equilibrium, thin films, lead sulfide, cadmium sulfide, ion exchange, photoelectric properties.

**Abstract**

For the first time modified PbS layers with cadmium content up to 5.07 at. % were formed in the contacting process of lead sulfide thin films with an aqueous solution of cadmium salt at 368 K. The composition and morphology of the obtained layers were investigated by the methods of energy-dispersive analysis and scanning electron microscopy according to duration of ion-exchange process. Photosensitivity of modified PbS grows with the content of cadmium in these thin films. There is an assumption about the formation of substitution solid solutions $Cd_xPb_{1-x}S$ at the interface of "PbS thin film – an aqueous solution of cadmium salt".

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*Thematic course*: Hydrochemical synthesis of films of chalcogenide metals. Part 21.

# Obtaining substitutional solid solutions in the lead–tin–sulfur system by means of ion-exchange synthesis

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***Keywords****: thin films, lead sulfide, tin sulfide, chemical bath deposition, ion-exchange synthesis, $Pb_{1-x}Sn_xS$ substitutional solid solutions, solubility product.*

## Abstract

The analysis of effective solubility products of lead and tin(II) sulfides at the «$PbS_{solid}$ film– acetate $SnCl_2$ aqueous solution» interface, along with analysis of a change in the Gibbs free energy of PbS → SnS ion-exchange transformation has been performed and confirmed the possibility of formation of $Pb_{1-x}Sn_xS$ substitutional solid solutions in the considered system. The results of scanning electron microscopy and energy-dispersive analyses have revealed changes in the elemental composition and surface morphology of tin-modified PbS layers in relation to duration of contact between a film and an acetate tin(II) chloride aqueous solution. For the first time, tin-containing films based on lead sulfide with the tin content up to 33.3 at % including a phase of $Pb_{1-x}Sn_xS$ solid solutions have been obtained by ion-exchange substitution via incubation of thin polycrystalline PbS films in tin(II) chloride aqueous solutions at 368 K.

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# Features for producing multilayer energy compositions of spherical granulation

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***Keywords:*** multilayer composition, filler, desensitization, armoring, manometric tests.

**Abstract**

The emergence of composite energetic materials causes the need of considering possible ways to increase the progressivity of their combustion. Features for producing multilayer gradient compositions are related to the degree of filling the compounds. The variants of the surface treatment of the pellets (desensitization and armoring), depending on the filler content have been considered. On the basis of water-dispersion technology we developed two methods for applying armoring coatings for low- and high-melting compounds.

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# ESR monitoring of electron transfer to some nickel complexes with α-diimine ligands

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***Keywords:*** nickel complexes; catalysis; cyclic voltammetry; ESR spectroscopy.

**Abstract**

ESR monitoring of the electrochemical reduction process in some nickel complexes with 'non-innocent' ligands such as α-diimines (bpy = 2,2'-bipyridine, tpy = 2,2':6',2''-terpyridine and pybox = (*S,S*)-2,6-bis(4-phenyl-2-oxazolin-2-yl)-pyridine), including sigma-organic nickel complexes, has shown initial heterogeneous electron transfer (first reduction peak) on nickel atom with Ni(I)L formation and gradual appearance of radical anion complex $NiL^{\bullet}$ in time. The transition from metal-centered to ligand-centered electron transfer is discovered. Previously unknown g-factors were calculated for a number of nickel(I) complexes of selected ligands.

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# Structural features of nickel(II) complexes of *bi*- and *ter*-pyridine according to X-ray analysis

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***Keywords:*** nickel, bipyridine, terpyridine complex, X-ray analysis.

**Abstract**

The structure of four previously undescribed nickel(II) complexes of *bi*- and *ter*-pyridine in crystals is determined by X-ray analysis. The $d^2sp^2$ hybridization of nickel atom with coordination number 5 in crystal of compounds **III** Ni(*t*-bu-tpy)$I_2$ was determined. The regularities in the packing of molecules in crystals were found. In particular, in packing of compounds **I** [Nibpy$_2$($H_2O$)Br]Br, **II** [Nibpy$_2$($H_2O$)$_2$]$Br_2$, **III** Ni(*t*-bu-tpy)$I_2$ and **IV** [Ni(*t*-bu-tpy)$_2$] ($H_2O$)$I_2$ the formation of ion and solvate canals was discovered. The simultaneous existence of different forms of nickel(II) complexes of different structure in the presence of α-diimine ligands in solution was assumed to determine some features of their physico-chemical properties, in particular the reduction potentials.

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# Transformations of peroxide olefin ozonolysis products in the system isopropanol-water

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***Keywords:*** monoterpenes, castor oil, ozonolysis and reduction, hydroxylamine hydrochloride, semicarbazide hydrochloride, isopropyl alcohol, water.

**Abstract**

The paper deals with the investigation results on transformations of peroxide olefin ozonolysis products with different structures and degrees of substitution (trisubstituted monoterpenes, castor oil and 1-nonene) under the action of semi-carbazide and hydroxylamine hydrochlorides in isopropanol using water as a co-solvent.

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# Synthesis and structure of $\mu$-oxobis [(trifluoromethanesulfonate)-(tri-*para*-tolyl) antimony][$(4\text{-}C_6H_4Me)_3SbOSO_2CF_3)]_2O$

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***Keywords:*** tri-*para*-tolyl)antimony, trifluoromethanesulfonic acid, tertiary butyl hydroperoxide, $\mu$-oxo-bis[(trifluoromethanesulfonate)(tri-*para*-tolyl)antimony], molecular structure, X-ray analysis.

**Abstract**

Reaction of tri-*para*-tolyl)antimony with trifluoromethanesulfonic acid in presence of tertiary butyl hydroperoxide in water-ether solution produces with the yield 95% $\mu$-oxo-*bis*[(trifluoromethanesulfonate)(tri-*para*-tolyl)antimony] (**I**). In the two types of crystallographically independent binuclear molecules **I*a*** and **I*b*** angles SbOSb make up 137.4(5)° and 137.5(5)° respectively. Antimony atoms have a distorted trigonal-bipyramidal coordination. Distances Sb-C vary in the range of 2.089(5)-2.121(5) Å. Bonds of antimony atoms with the bridging oxygen atom [1.941(4)-1.957(4) Å] are shorter than with oxygen atoms of trifluoromethanesulfonate group [2.356(4)-2.407(5) Å]. Axial angles $O_{bridge}SbO_{therm}$ make up 175.4(2)-177.0(2)°.

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# Acid hydrolysis of brewer grains

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*Supervising author; +Corresponding author
***Keywords:*** brewer grain, acid hydrolysis, xylose, HPLC, IR spectroscopy.

**Abstract**

Brewer grain is a large-capacity waste of brewing industry. The promising field of the brewer grain processing is its use as new raw source for obtaining xylose and xylite – valuable products that found their application as sweeteners for pancreatic diabetes patients nutrition. This work is devoted to the development of ways for acid hydrolysis of brewer grain aimed at the obtaining of pentose hydrolyzates, enriched with xylose. Optimal technological parameters of acid hydrolysis have been determined: hydrolyzing agent ($H_2SO_4$) concentration is 3.0%, temperature – 100 ºC, treatment duration – 5 hours.

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# Comparison of phytotoxicity indices, fungicidal and bactericidal activity of *Streptomices* from different habitats

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***Keywords:*** streptomyces, antibiotical activity, phytotoxicity.

**Abstract**

Five strains of streptomices were compared concerning their antagonistic suppression of test-organisms from various taxonomic groups – bacteria, phycomycetes (yeast), one-cellular green algae and two weed herbs. *Streptomicetes* were isolated from different habitats (potato tubes, soil samples from various regions of the Earth, as well as the wastewater sludge, spoiled with white phosphorus), what determined the difference in their antibiotic activity. In particular, *Streptomyces* species A8 strain, isolated from the toxic sludge, contrary to the other ones, did not suppress at all the growth of the higher plants.

*Thematic Section:* Research of the Biological Activity. **Full Paper**
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# Synthesis and biological activity of some 3-hydroxy-1,5-diaryl-4-pivaloyl-2,5-dihydro-2-pyrrolones

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***Keywords:*** 1,2,4-tricarbonyl compounds, 3-hydroxy-1,5-diaryl-4-pivaloyl-2,5-dihydro-2-pyrrolones, antioxidant activity, oxidative stress, *Escherichia coli*, anti-inflammatory activity, cytotoxic activity.

## Abstract

On the basis of the reaction of pivaloilpiroparatartaric acid and arylidenearylamines different 3-hydroxy-1,5-diaryl-4-pivaloyl-2,5-dihydro-2-pyrrolones were synthesized. Due to the urgency of finding new biologically active compounds, antioxidant, anti-inflammatory and cytotoxic activity of the obtained 2-pyrrolones were investigated. Antioxidant properties of the obtained compounds were studied on the model of oxidative stress, generated 3mm solution of hydrogen peroxide, using as a test system of bacteria *Escherichia coli* strain BW 25113. As reference standard resveratrol was used. The anti-inflammatory activity has been studied *in vivo* on the model of karraginin inflammation. Two compounds were found with moderate antioxidant activity, and four compounds having anti-inflammatory properties activity, one of which exceeds the comparison drug diclofenac sodium. The synthesized 4-pivaloyl-2-pyrrolones are not cytotoxic.

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# Synthesis and antihypoxic activity of some 3-(2-oxoalkyliden)-3,4- dihydro-2*H*-1,4-benzoxazines

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***Keywords:*** 1,3,4,6-tetracarbonyl compounds, 3-(2-oxoalkyliden)-3,4-dihydro-*2H*-1,4- benzoxazine-2-ones, 2-alkanoylmethyl-2-hydroxy-3-(2-oxoylidene)-2*H*-3,4-dihydro-1,4-benzoxazines, antihypoxic activity, normobaric hypoxia, hemic hypoxia, mexidole.

**Аннотация**

On the basis of the reaction of 1,6-dialkyl-3,4-dihydroxy-2,4-hexadiene-1,6-diones with 2-aminophenol there were isolated either (3*Z*)-3-(2-oxoalkiliden)-3,4-dihydro-*2H*-1,4-benzoxazine-2-ones, or 2-alkanoyl methyl-2-hydroxy-3-(2-oxoylidene)-2*H*-3,4-dihydro-1,4-benzoxazines depending on the conditions of synthesis. Due to the urgency of finding new biologically active compounds investigated the acute toxicity and antihypoxic activity of the obtained 1,4-benzoxazines were studied. Antihypoxic properties of the obtained compounds were studied on the model of exogenous normobaric hypoxia with hypercapnia. As a comparator product we used 2-ethyl-6-methyl-3- hydroxypyridine succinate (mexidole). It has been found that the synthesized 1,4-benzoxazines possess high antihypoxic activity significantly higher than the comparison drug. The synthesized compounds are practically non-toxic.

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# Changing the pH of the solution in the system Pb(II)–$H_2O$–$OH^-$ by hydrolysis of precipitation $Pb_5(OH)_xH_2O_y(An)_z$

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***Keywords:*** lead, precipitation, hydrolysis, aqueous solution, equilibrium modeling.

**Abstract**

We studied the kinetics of acidification of the solution in the titration of Pb(II) by the solution NaOH and in the absence of titration. On the basis of experimental data and the provisions on the formation of supersaturated solutions and hydrolysis precipitation of $Pb_5(OH)_xH_2O_y(An)_z$ a mathematical model of pH changes in the solution during the titration of Pb(II) by NaOH solution has been created. An equation of the amplitude of the shift of pH from an acidic solution hold time between additions of titrant portions.

**Short Communication** _____ *Thematic Section:* Chemical and Technological Research.
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# Formation of the acrylonitrile self-associates

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***Keywords:*** acrylonitrile, vinyl monomers, self-associates, AM1, NMR spectroscopy ($^{1}$H, $^{13}$C).

**Abstract**

The structures of the acrylonitrile self-associates (the dimer A3 structure is optimal) were calculated by quantum-chemical methods and proved by NMR $^{1}$H and $^{13}$C spectroscopy. The self-association constants from ~0.070 till 0.103 l/mol were determined by chemical shifts of the *trans*- and *cis*-hydrogen in the $=CH_2$ and carbon in the =CH of the acrylonitrile isomers. It is recommended to use the chemical shift of the carbon in the =CH for the self-association constants calculations. The obtained data are important not only for the further acrylonitrile polymerization, but also for its copolymerization with other vinyl monomers.

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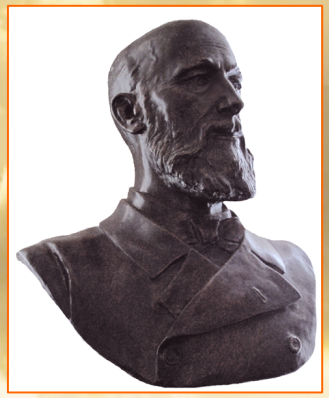

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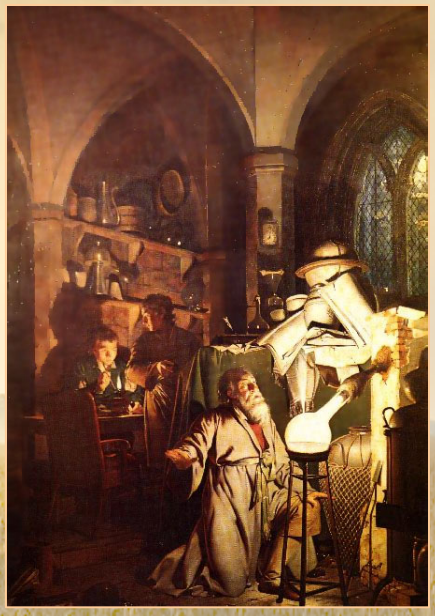

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*Subsection:* Inorganic Chemistry. *Registration Code of Publication:* 14-39-7-1
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# Phosphorus: properties and application

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***Keywords:*** phosphorus, white phosphorus, production, properties, use, chemical industry, raw materials, products, perspectives.

**Abstract**

In the presented review the history of white phosphorus study, as well as extensive field of its application is presented. White phosphorus, being allotropic modification of phosphorus element, can't be considered separately from it, hence significant attention is also paid to the element. The highest risk of white phosphorus in handling causes quite reasonable and well-grounded doubts concerning the necessity of its industrial production and usage. Analyzing the development of scientific interest and practical demand for white phosphorus since the moment of its discovery in the VXII century till the present time, the authors have come to the conclusion that phosphorus production will not be terminated in the nearest future, and, most likely, even never. Thus the study of chemistry, toxicology and methods of neutralization of this substance is still urgent.

*Thematic Section:* Theoretical Research. **Full Paper**
*Subsection:* Thermodynamics. *Registration Code of Publication:* 14-39-7-25
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# Thermodynamic calculation of equilibrium compositions of phases at the hydrochemical production of high-purity thallium halides for IR-ray fiber optics

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***Keywords:*** thallium halides, hydrochemical method, equilibrium compositions of phases, equilibrium constants, activity coefficients, basic reactions, solubility of thallium halides.

## Abstract

The investigated objects represent as heterogeneous systems solid – liquid with brutto-component composition $H_2O$-HX-TlX (X – or Cl, or Br), using in the hydrochemical synthesis of the highpure solid TlX for IR optics. The methodology for the thermodynamic analysis of the equilibrium component compositions of the liquid phases in these systems was developed and realized. It is based on the laws of the phase and chemical equilibriums and requires the using of the handbook data, concerned the equilibrium characteristics of mass-transfer processes between solid and liquid phases and chemical reactions in the liquid phase, as well as the activity coefficients of the liquid-phase components. The reliability of the thermodynamic calculations was confirmed by the experimental data on the solubility of the solid TlX in liquid media.

*Thematic Section:* Theoretical Research. **Full Paper**
*Subsection:* Organic Chemistry. *Registration Code of Publication:* 14-39-7-39
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/ *(English Preprint)*
Contributed: October 6, 2014.

# Presentation of chemical reactions, reagents and their thermo-chemical properties in the intelligence system on physical chemistry of liquid phase radical reactions with the use of the ontological model of the domain

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***Keywords:*** radical reactions, kinetic constant, activation energy, organic molecules, bond dissociation energy, intelligent systems, domain ontology.

**Abstract**

In this paper a fragment of the domain ontology on physical chemistry of liquid phase radical reactions is presented. The presented ontological model of the domain includes about 100 subclasses of radical reactions, more than 50 classes of organic compounds and about 45000 object properties (physical and chemical properties of molecules, radicals and radical reactions). The ontology is developed with the use of ontology editing tool Protégé. The ontology will be used in the scientific intelligence system on physical chemistry of radical reactions.

*Thematic Section:* Chemical and Technological Research. **Full Paper**
*Subsection:* Organic Chemistry. *Registration Code of Publication:* 14-39-7-47
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/ *(English Preprint)*
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# Reactivity indices of alkenes in amino-methylation reactions

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***Keywords:*** amino-methylation of alkenes, aminomethyl carbocation, Mannich reaction, DFT (Density Functional Theory), NBO-analysis, reactivity indices.

**Abstract**

The peculiarities of alkenes interaction with aminomethyl carbocations by quantum and chemical methods were considered. The calculations in the approximation B3LYP/6-31G(d,p) and further NBO analysis demonstrate that the correct reactivity index can be obtained on the basis of atomic orbitals contribution values $Csp^2$ to the multiple bond formation. It accords with the literature data on the alkenes reactivity in the reaction of electrophylic addition of aminomethyl carbocations on multiple bonding.

*Thematic Section:* Theoretical Research. **Full Paper**
*Subsection:* Inorganic Chemistry. *Registration Code of Publication:* 14-39-7-53
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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# Physico-chemical properties of water and its hexameric cluster

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***Keywords:*** water, hexameric cluster, decameric cluster, structure, topological index, physical and chemical properties.

**Abstract**

The value of the product of the molar mass to the value of Wiener topological index to the power 2/3, designated as $J_W$, is used to describe the physical and chemical properties of water and a number of proton donor organic liquids. The structure of water is considered in the form hexameric and decameric cluster. Organic liquids are considered in the form of dimeric and trimeric associates. For the values of $J_W$, corresponding to specified supramolecular structures, correlations are built with saturated steam at a pressure 432.2 K, boiling point, density, surface tension, viscosity, molar heat capacity and enthalpy of melting. In all cases, the values corresponding to water clusters formed a single array with similar values for the associates of organic liquids, which is seen as a natural phenomenon. Aqueous stability of hexameric cluster has been marked. The assumptions are made about the reasons for its stability.

*Thematic Section:* Preparative Research. **Full Paper**
*Subsection:* Organic Chemistry. *Registration Code of Publication:* 14-39-7-61
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/ *(English Preprint)*
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# Novel *N*-hydroxybenzamide derivatives of taurine

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***Keywords:*** hydroxybenzamides, taurine (2-aminoethanesulfonic acid), biological activity, acute toxicity.

**Abstract**

Hydroxybenzamides were obtained by *N*-acylation of 2-aminoethanesulfonic acid (taurine). The structure of the obtained compounds was confirmed by 1H NMR-spectroscopy. The biological activity and acute toxicity of the synthesized compounds were predicted with PASS (Predictor of Activity Spectra for Substance).

**Full Paper** _____ *Thematic Section:* Preparative Research.
*Registration Code of Publication:* 14-39-7-66 *Subsection:* Organic Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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# Synthesis of 1,5-diarylpyrrolidine-2,3-diones and their 3-arylaminoderivatives

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***Keywords:*** threecomponent reaction, 1,5-disubstituted pyrrolidine-2,3-diones, ethyl pyruvate, aromatic aldehydes, arylamines.

**Abstract**

Intereaction of the ethyl pyruvate with a mixture of aromatic aldehyde and arylamine obtained 3-arylamino-1,5-diarylpyrrolin-2-ones, hydrolysis of latters leads to 1,5-diarylpyrrolidin-2,3-diones. Intereaction 1,5-diarylpyrrolidin-2,3-diones with arylamines has been studed. The structures of all synthesized compounds was proved by IR, NMR $^1$H spectroscopy.

*Thematic Section:* Preparative Research. **Full Paper**
*Subsection:* Organic Chemistry. *Registration Code of Publication:* 14-39-7-71
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# Synthesis and antibacterial activity of 5-aryl-4-aroyl-3-hydroxy-1-(4-ethoxycarbonylphenyl)-3-pyrroline-2-ones

© **Vladimir L. Gein**,[1]*+ **Anastasia V. Shmakova**,[1] **Olga V. Bobrovskaya**,[1] **Lyudmila F. Gein**,[2] and **Tatiana F. Odegova**[1]

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***Keywords:*** 3-hydroxy-3-pyrroline-2-ones, synthesis, ethyl 4-aminobenzoate, three-component reaction, antibacterial activity.

## Abstract

A series of 5-aryl-4-aroyl-3-hydroxy-1-(4-ethoxycarbonylphenyl)-3-pyrroline-2-ones were synthesized by the reaction of methyl esters of aroylpyruvic acids with a mixture of ethyl 4-aminobenzoate and aromatic aldehyde. The proposed structures are confirmed by IR, $^1$H NMR spectroscopy. The antibacterial activity of the synthesized compounds was studied.

*Thematic Section:* Preparative Research. _____ **Short Communication**
*Subsection:* Organic Chemistry. *Registration Code of Publication:* 14-39-7-75
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# Synthesis of 5-aryl-4-acyl-1-(3-hydroxypropyl)-3-hydroxy-3-pyrroline-2-ones

© **Vladimir L. Gein**,[1]*+ **Lyudmila F. Gein**,[2] **Andrey N. Korol**,[1] **Irina V. Krylova**,[2] and **Lyudmila I. Varkentin**[1]

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***Keywords:*** heterocycles, 1,4,5-trisubstituted 3-hydroxy-3-pyrroline-2-ones, tricomponent reaction, 3-aminopropanol.

**Abstract**

By intereaction of the methyl esteres of acyl- and aroulpyruvic acids from a mixture of aromatic aldehyde and 3-aminopropanol we obtained 5-aryl-4-acyl-1-(3-hydroxypropyl)-3-hydroxy-3-pyrroline-2-ones. The structures of all synthesized compounds was proved by IR, NMR $^1$H spectroscopy.

**Full Paper** _____ *Thematic Section:* Preparative Research.
*Registration Code of Publication:* 14-39-7-78 *Subsection:* Organic Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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# Hydration of the phtalimide moiety containing allenoates under reflux and ultrasonic irradiation

© **Aynur M. Gumerov**,[+] **Lilia M. Gainetdinova**, **Aisylu F. Muhametyanova**, **Ilshat M. Sakhautdinov**,* **Akhnaf A. Fatykhov**, and **Marat S. Yunusov**
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*Supervising author; [+]Corresponding author
***Keywords:*** allenes, hydration, ultrasound, water.

**Abstract**

Catalyst-free hydration of the phthalimide moiety containing allenoates in neutral media under reflux is demonstrated. Using ultrasonic irradiation in aqueous DMF allowed not only to increase the yield, but also to reduce significantly the reaction time.

**Full Paper** _____ *Thematic Section:* The Study of Catalysts.
*Registration Code of Publication:* 14-39-7-82 *Subsection:* Petrochemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/ *(English Preprint)*
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# The study of the properties of Al-Mo-W-catalysts in hydrotreating of petroleum distillates

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***Keywords:*** hydrodesulfurization activity, Al-Mo-W-catalysts, petroleum fractions, sulfirisation.

**Abstract**

The purpose of this work is to investigate the hydrodesulfurization activity of Al-Mo-W-catalysts, to compare their activity with industrial catalysts and to estimate possibilities of their use for oil fractions deep hydrotreating in petroleum refining.

**Full Paper** _____ *Thematic Section:* Study of Catalysts.
*Registration Code of Publication:* 14-39-7-88 *Subsection:* Organic Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/ *(English Preprint)*
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# Study of physic-chemical properties and catalytic activity of natural iron oxohydroxide

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*Supervising author; [+]Corresponding author
***Keywords:*** nanoscale oxohydroxide iron, catalysis, cumene, the cumene hydroperoxide.

**Abstract**

The paper discusses the iron oxohydroxides, forming the basis of sludge waste water treatment plants with clean water from the iron as a catalyst for the oxidation of cumene with molecular oxygen. It was established by XFA and HRTEM that the main phase in samples annealed up to 300 °C is an amorphous phase with a small amount of crystal structures and just such a pattern is the catalyst of the oxidation process. It is shown that heating of the iron oxohydroxide above 300 °C promotes the formation of crystalline structures, are not active in the oxidation reaction.

*Thematic Section:* Technological Research. **Full Paper**
*Subsection:* Modeling of Chemical Reactors. *Registration Code of Publication:* 14-39-7-93
lication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/ *(English Preprint)*
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# Simulation of the process of makrohydrodynamics of three-component two-phase dispersion-fiber suspension

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***Keywords:*** slurry, mixer, hydrodynamics, modeling.

**Abstract**

Using the ANSYS CFX predicts stirring suspension modes and implement selection of different types of mixing devices, and combinations thereof, to ensure distribution of the components over the volume of the dispersion medium in accordance with their predetermined ratio.

*Thematic Section:* Physicochemical Research. **Full Paper**
*Subsection:* Inorganic Chemistry. *Registration Code of Publication:* 14-39-7-99
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# Features of structural changes in mechanically activated powders of $Nd_{1-x}Ca_xMnO_{3+\delta}$ solid solutions

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***Keywords:*** rare-earth manganites, mechanical activation, polymorphic transitions, cooperative Jahn-Teller effect.

**Abstract**

The influence of mechanical activation on the crystal structure, oxidation properties, the chemical activity of $Nd_{1-x}Ca_xMnO_{3+\delta}$ (x = 0.0; 0.1) solid solutions in the temperature range T = 20-1180 °C was studied. The orbital order–disorder transition (peculiar to rare earth manganites) was found to shift along the temperature axis with increasing grinding duration. The shift of the transition temperature was caused by change in the chemical composition of mechanically activated samples due to either oxidation of the material or change in the cation ratio of the main phase. Change in the chemical composition of the samples was resulted from intensification (under mechanical activation) of chemical reactions between the ions constituting the manganite ($Ca^{2+}$, $Nd^{3+}$, $O^{2-}$) and the air components (water, carbon oxides, oxygen) on the surface of particles. Mechanical activation had a different effect on the sinterability of the samples $NdMnO_{3+\delta}$ and $Nd_{0.9}Ca_{0.1}MnO_{3+\delta}$. Upon heating mechanically activated $NdMnO_{3+\delta}$, the drowth of the coherent scattering regions (CSR) did not occur in the range 20<T<700 °C but it proceeded rapidly when the temperature was increased above 700 °C regardless of the grinding size. As for the sample $Nd_{0.9}Ca_{0.1}MnO_{3+\delta}$, the intensity of CSR growth decreased with increasing duration of grinding. The formation of calcium-containing metastable phases in the surface layer of grains was the factor that retarded the growth of CSR. With the increase in the layer thickness the temperature region of existence of nanostructured state expands.

**Full Paper** _____ *Thematic Section:* Biochemical Research.
*Registration Code of Publication:* 14-39-7-108 *Subsection:* Toxicological Chemistry.
lication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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# Chemical-toxicological research of certain non-steroidal antiinflammatory agents

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***Keywords:*** non-steroidal anti-inflammatory agents, isolation, identification, quantification.

## Abstract

Optimal conditions were defined for isolating nimisulid, meloxicam, ibuprofen and codeine (preparation of Nurofen Plus), Propyphenazone, codeine, and caffeine paratsitamol (kaffetin preparation) from biological fluids and medicines. Test substances were identified using color and sediment reaction by IR, UV spectroscopy, thin-layer and gas chromatography with mass selective detector and high performance liquid chromatography. Quantitative determination in extracts from biological fluids was performed by HPLC chromatography-densitometry and UV spectroscopy. The results of the three methods are similar and reproducible.

*Thematic Section:* Biochemical Research. **Full Paper**
*Subsection:* Bioorganic Composition of Algae. *Registration Code of Publication:* 14-39-7-117
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*Thematic direction:* Bioglycans and lipids of microseaweed. Part I.

# Extracellular bioglycans and intracellular lipids of green microalgae *Scotiellopsis terrestris* (Reisigl) Punč. et Kalina

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***Keywords*:** *bioglycans, total lipids, fatty acids, green microalgae Scotiellopsis terrestris.*

**Abstract**

For green microalgae *Scotiellopsis terrestris* given general chemical characteristics of bioglycans isolated from the culture liquid, as well as total lipids and fatty acids extracted from biomass.

**Full Paper** _____ *Thematic Section:* Biochemical Research.
*Registration Code of Publication:* 14-39-7-122 *Subsection:* Physiological Processes.
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# Age and gender characteristics of biochemical composition of human saliva

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***Keywords:*** saliva, biochemical composition, age and gender characteristics, clinical laboratory diagnostics.

## Abstract

Biochemical composition of human saliva in the norm for the purpose of its use as biosubstrate in clinical laboratory diagnostics has been studied. There were shown correlation interactions of saliva depending on gender, and differences in the composition of saliva in the "norm" for each age group were revealed. We experimentally confirmed the stability of the values of biochemical parameters of saliva in the study with a time interval of 24 hours.

*Thematic Section:* Preparative Research. **Full Paper**
*Subsection:* Organoelemental Chemistry. *Registration Code of Publication:* 14-39-7-127
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# *Tris*(4-fluorophenyl)antimony *bis*(trichloroacetate) And *tris*(4-fluorophenyl)antimony *bis*(bromoacetate): synthesis and crystal structures

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***Keywords:*** *bis*(trichloroacetate), *bis*(bromoacetate), *tris*(4-fluorophenyl)antimony, synthesis, crystal structure.

**Abstract**

*Tris*(4-fluorophenyl)antimony *bis*(trichloroacetate) (**I**) and *tris*(4-fluorophenyl)antimony *bis*(bromoacetate) (**II**) were synthesized by the reaction of *tris*(4-fluorophenyl)antimony with trichloroacetic and bromoacetic acids in the presence of *tert*-butylhydroperoxide. According to the X-ray diffraction data, the antimony atoms in two crystallographically independent molecules **I** have a distorted trigonal bipyramidal geometry with carboxylate ligands in axial positions. The OSbO and CSbC angles are 171.62(17)° (A), 177.97(16)° (B) и 113.8(2)°-127.4(2)° (A), 118.1(2)-123.0(2)° (B). The Sb–O and Sb–C bond lengths are 2.117(4), 2.123(4) и 2.100(6)-2.105(5) Å (A); 2.107(4), 2.115(4) и 2.098(6)-2.106(6) Å (B). In the trigonal bipyramidal molecules **II**, the OSbO and CSbC angles are 176.2(3)° and 107.1(4)°, 110.9(3)°, 142.0(4)°. The Sb–O and Sb–C bond lengths are 2.130(7), 2.130(7) and 2.101(9), 2.102(9), 2.121(9) Å, respectively. The intramolecular $Sb\cdots O_{=C}$ distances in **I** (2.879(6), 2.946(6) Å) are shorter than the analogous distances in **II** (3.197(6), 3.337(6) Å (A), 3.176(6), 3.196(6) Å (B)).

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# Synthesis and structure of μ-oxo-*bis*[(*tert*-butylperoxy) triphenylantimony] and μ-oxo-*bis*[(4-nitrophenoxy) triphenylantimony]

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***Keywords:*** μ-oxo-*bis*[(*tert*-butylperoxy)triphenylantimony], μ-oxo-*bis*[(4-nitrophenoxy) triphenylantimony], synthesis, structure.

## Abstract

Reacting triphenylantimony with *tert*-butyl hydroperoxide and of 4-nitrophenol in the presence of *tert*-butyl hydroperoxide we synthesized μ-oxo-*bis*[(*tert*-butylperoxy)triphenylantimony] (**I**) and μ-oxo-*bis*[(4-nitrophenoxy)triphenylantimony] (**II**), the structure of which was established by X-ray diffraction. Antimony atoms in the binuclear molecules have a distorted trigonal-bipyramidal coordination with oxygen atoms in axial positions. Bond lengths Sb-C are 2.111(3)-2.119(3) Å, Sb-$O_{bridge}$1.9698(2) Å, Sb-$O_{terminal}$ 2.078(2) Å, angles $O_{bridge}SbO_{terminal}$ 170.17(6)°, SbOSb 180° for **I** and Sb-C 2.085(6)-2.108(5) Å, Sb-$O_{bridge}$ 1.979(3), 1.982(3) Å, Sb-$O_{terminal}$ 2.143(3), 2.141(3) Å, $O_{bridge}SbO_{terminal}$ 177.12(16)°, 177.70(14)°, SbOSb 138.0(2)° for **II**.

**Short Communication** _____ *Thematic Section:* X-ray Diffraction Research.
*Registration Code of Publication:* 14-39-7-136 *Subsection:* Organoelemental Chemistry.
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# Structural features of the triaryl antimony compounds

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***Keywords:*** triaryl antimony compound, structure.

**Abstract**

According to X-ray analysis the antimony atoms in the two types of triphenylantimony crystallographically independent molecules (**1*a,b***) have a distorted tetragonal coordination with the carbon atoms of the phenyl substituent and the unshared electron pair of the vertices of the tetrahedron. Sb–C bond lengths and CSbC angles are equal to 2.151(3), 2.156(3), 2.161(4) Å (***a***); 2.150(3), 2.154(3), 2.158(3) Å (***b***) and 97.60(12)°, 94.87(13)°, 95.82(12)° (***a***); 95.58(12)°, 96.24(12)°, 97.81(12)° (***b***) respectively. We analyzed the geometric characteristics of molecules of triaryl antimony compounds, and identified factors affecting the value of the Sb–C bond lengths and CSbC bond angles.

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*Subsection:* Organoelemental Chemistry. *Registration Code of Publication:* 14-39-7-139
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# Synthesis and structure of tetraphenylantimony hydrogen succinate

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***Keywords****:* tetraphenylantimony hydrogen succinate, synthesis, structure.

**Abstract**

Interaction of equimolar amount of pentaphenylantimony with succinic acid in benzene resulted in obtaining tetraphenylantimony hydrogen succinate (**I**) with the yield of 97%, According to the data of X-ray, the atom of antimony in molecule **I** has a deformed trigonal-bipyramidal coordination, the atoms of oxygen and carbon being located in the axial positions. The distances $Sb–C_{ekv}$, $Sb–C_{ax}$, Sb–O and angle $C_{ax}SbO_{ax}$ are equal to 2.111(2), 2.111(2), 2.121(2); 2.169(2), 2.302(1) Å and 175.78(7)° respectively.

**Short Communication** _____ *Thematic Section:* Preparative Research.
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Conference "New methods of synthesis, structure and application of organoelemental compounds"
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# Crystal and molecular structure of *bis*(2-furancarboxylate) tri-*o*-tolylantimony

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***Keywords****: bis*(2-furancarboxylate) tri-*o*-tolylantimony, structure.

**Abstract**

Crystal and molecular structure of *bis*(2-furancarboxylate) tri-*o*-tolylantimony (**I**) was defined by X-ray. In the molecule, the antimony atom has a distorted trigonal-bipyramidal coordination with axially spaced carboxylate ligands and equatorial phenyl groups, OSbO and CSbS angles are 174.2(1)° and 116.3(4)°, 117.9(4)°, 125.8(1)° respectively. The Sb–O and Sb–C bond lengths are equal to 2.055(8), 2.191(8) and 2.110(7), 2.118(3), 2.124(7) Å. Intramolecular distances Sb···$O_{(=C)}$ make up 3.274(12) and 3.319(13) Å.

*Thematic Section:* Preparative Research. **Short Communication**
*Subsection:* Organoelemental Chemistry. *Registration Code of Publication:* 14-39-7-145
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Contributed: September 24, 2014.

# Synthesis and structure of $\mu_2$-oxo-*bis*[(*tert*-butylperoxy)tri(*m*-tolyl) antimony] (*m*-$Tol_3SbOOBu$-*t*)$_2$O

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***Keywords***: $\mu_2$-oxo-*bis*[(*tert*-butylperoxy)tri(*m*-tolyl) antimony](*m*-$Tol_3SbOOBu$-*t*)$_2$O, synthesis, structure.

**Abstract**

By the interaction of three-meta-tolylantimony with *tert*-butylhydroperoxide in ether there has been synthesized $\mu_2$-*oxo-bis*[(*tert*-butylperoxy)tri(*m*-tolyl) antimony], in centrosymmetric dinuclear molecule of which (the inversion center – bridging oxygen atom), the antimony atoms have trigonal-bipyramidal environment with oxygen atoms in axial positions (CSbC 115.95(17)°, 118.11(16)°, 125.41(17)°; SbOSb 180°, OSbO 175.63(13)º, Sb–C 2.109(4), 2.115(4), 2.121(4) Å, Sb-$O_{bridge}$ 1.9904(12) Å, Sb–$O_{term}$ 2.089(3) Å, O–O 1.462(5) Å).

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Contributed: October 2, 2014.

# Synthesis and structure of solvate *μ*-oxo-*bis*[(nitrato)triphenylantimony] with benzene

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***Keywords:*** *μ*-oxo-*bis*[(nitrato)triphenylantimony], solvate, benzene, synthesis.

**Abstract**

Interaction of *μ-oxo-bis*[(chloro)triphenylantimony] with silver nitrate produced the solvate of *μ-oxo-bis*[(nitrato)triphenylantimony] with benzene, the structure of which was established by X-ray diffraction. Antimony atoms in binuclear molecule have a distorted trigonal-bipyramidal coordination with bridging oxygen atom and a nitro group in the axial positions. Bond lengths of Sb-C are 2.105(2)-2.113(2) Å, Sb-$O_{bridg}$ 1.968(2), 1.962(2) Å, Sb-O($NO_2$) 2.241(2), 2.301(2) Å, OSbO 174.37(6)°, 177.59(7)°, SbOSb 142.22(6)°.

*Thematic Section:* Preparative Research. **Short Communication**
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# Interaction phenylanthranilic acid with antimony tri(4-fluorophenyl) in presence of *tert*-butylhydroperoxide

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***Keywords**:* reaction, *tris*(4-fluorophenyl)antimony, phenylanthranilic acid, *tert*-butylhydroperoxide, structure.

**Abstract**

Interaction of *tris*(4-fluorinephenyl)antimony with phenylanthranilic acid in presence of *tret*-butylhydroperoxide in tetrahydrofuran obtained solvate of triphenylantimony *bis*(phenylanthranilate) with tetrahydrofuran, the structure of which was proved by X-ray structure analysis. The atoms of antimony are in a trigonal-bipyramidal coordination with the oxygen atoms in axial positions (Sb–C 2.110(2), 2.111(2), 2.116(2) Å; Sb–O 2.127(2), 2.127(2) Å; Sb···O=C 2.752(4), 2.842(5) Å; OSbO 174.99(5)º, CSbC 104.19(8)º, 109.11(8)º, 146.69(7)º).

**Short Communication** _____ _____ *Thematic Section:* Preparative Research.
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# Synthesis and structure of 2,4-dimetylbenzolsulfonate tetraphenylbismuth

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***Keywords:*** *2,4-dimetylbenzolsulfonate tetraphenylbismuth, synthesis, structure.*

**Abstract**

Interaction of pentaphenylbismuth with 2,4-dimetylbenzolsulfonate diphenylantimony received 2,4-dimetylbenzolsulfonate tetraphenylbismuth, whose structure was established by X-ray diffraction. Bi atoms in the compound has a distorted trigonal-bipyramidal coordination c arensulfonate ligand in the axial position. Bi-C bond lengths are equal to 2.198 (3)-2.208(3) Å, Bi-O distance and magnitude of the axial angle CBiO up 2.658(3) Å и 174.24(12)° respectively.

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# Synthesis and structure of *bis*(bromoacetate) *tris*-(*meta*-tolyl)bismuth

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***Keywords****: tris*-(*meta*-tolylbismuth, bromoacetic acid, *tert*-butyl hydroperoxide, oxidative addition, *bis*(bromoacetate) *tris*-(*meta*-tolyl)bismuth, structure.

**Abstract**

Reaction of *tris*-(*meta*-tolyl)bismuth with bromoacetic acid in the presence of a tertiary butyl hydroperoxide in ether resulted in obtaining bis(bromoacetate) *tris*-(*meta*-tolyl)bismuth (**I**). According to the X-ray data, bismuth atoms in the two crystallographically independent molecules **Ia** and **Ib** have a distorted trigonal-bipyramidal coordination (angles OBiO and CBiC are 173.4(4)° and 109.4(5)-139.1(4)° (***a***), 172.7(3)° and 109.2(5)-140.1(5)° (***b***). The bond lengths Bi–C and Bi–O are equal to 2.174(12)-2.222(12) Å and 2.266(9)-2.307(9) Å. Carbonyl oxygen atoms are located opposite the largest angle of the equatorial CbiC (109.4(5), 111.3(4), 139.1(4)° (***a***) and 109.2(5), 110.7(5), 140.1(5)° (***b***).

**Short Communication** _____ _____ *Thematic Section:* Preparative Research.
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# Crystal and molecular structure of iodide triphenylbutylphosphonium

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***Keywords**:* iodide triphenylbutylphosphonium, structure.

**Abstract**

With X-ray spectral analysis method we determined the crystal structure of triphenylbutylphosphonium iodide, which consists of a crystal of tetrahedral cations $[Ph_3BuP]^+$ and anions $[I]^-$. P atoms in the cation $[Ph_3BuP]^+$ have the usual tetrahedral coordination (CPC 106.32(12)–111.09(12) Å, P-$C_{Ph}$ 1.796(3)-1.797(3) Å, P-$C_{Bu}$ 1.798(2) Å).

*Thematic Section:* X-ray Diffraction Research. **Letter to the Editor**
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# Crystal and molecular structure of 4-dimetylaminobenzaldoxime

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***Keywords:*** 4-dimetylaminobenzaldoxime, structure.

**Abstract**

Crystal structure of 4-dimetylaminobenzaldoxime has been determined by X-ray spectral analysis method. C=N distances are 1.265(2) Å, O-N 1.407(2) Å, $C_{Ar}$-N 1.376(2) Å, $C_{Me}$-N 1.426(2), 1.433(3) Å.

# Butlerov Communications

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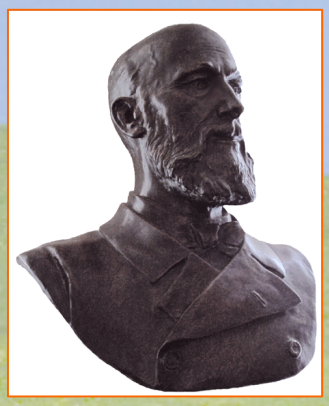

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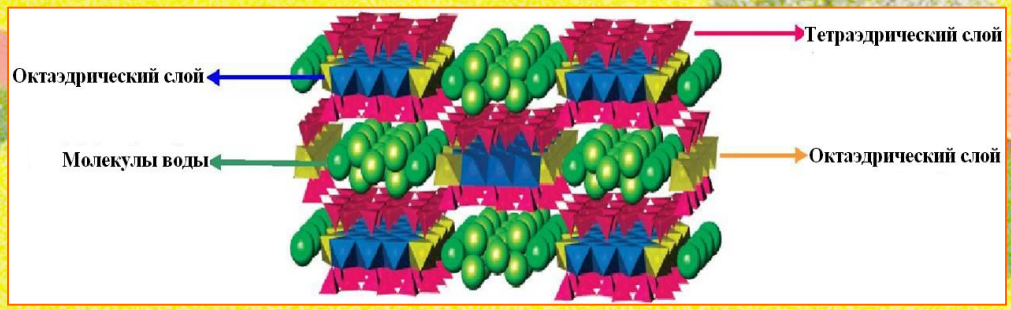


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# Percolation in mixed energy materials. Characteristics of burning, ignition and sensitivity of mixtures to mechanical stress.

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***Keywords:*** mixed energy materials, particulate filler, degree of filling, percolation cluster, burning rate, ignition, sensitivity to mechanical stress.

**Abstract**

The paper presents the research results of the content of powdered fillers (oxidants, energy supplements, metal fuel) on the ignition, burning rate and sensitivity to mechanical stress of composite energetic materials. The concentrations of powder components, corresponding to the critical content which yields a percolation cluster and the observed changes in functional dependencies properties of materials. Comparison of the experimental data with the theoretical results has been carried out.

*Thematic Section:* Physicochemical Research. **Full Paper**
*Subsection:* Inorganic Chemistry. *Registration Code of Publication:* 14-39-8-17
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# Glauconite of Saratov region, properties, composites based on it, the application

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***Keywords****:* inorganic sorbents, glauconite, sorption, composites.

**Abstract**

Elemental, granulometric, morphological composition of natural mineral glauconite (Belozersky field of Saratov region) have been studied. Finely dispersed (60 and 5 μm) and granulated fractions of enriched glauconite and nanocomposites based on them were obtained. Sorption, physico-chemical properties and environmental safety of them were studied. The expediency of using of glauconite and composites based on it for water purification, soil remediation and components of premixes for animals was considered.

*Thematic Section:* Physicochemical Research. **Full Paper**
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# Thermal decomposition of tetraaminecuprosulfate monohydrate

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***Keywords:*** copper, complex, thermal decomposition, degradation kinetics, TGA, IR spectra, topochemical models.

**Abstract**

By thermogravimetric analysis (TGA) we studied the thermal decomposition of tetraaminecuprosulfate monohydrate in linear rise in temperature and isothermal conditions in the atmosphere of the stationary atmosphere of the own vapor and in the stream of dry air. It has been established that degradation proceeds under isothermal conditions within 4 successive temperature stages.The effective kinetic parameters of the process in each stage have been defined. By IR spectroscopy solids were studied at each of the complex decomposition temperature stages.It was shown that the surface of these products has an increased adsorption capacity for water vapor in air.It has been established that for the kinetic description of the results of thermogravimetric analysis of the complex $[Cu(NH_3)_4]SO_4 \cdot H_2O$ in isothermal conditions topochemical models Kolmogorov-Erofeev, Garner-Prout-Tompkins, Roginskii-Schultz are applicable.

**Full Paper** _____ *Thematic Section:* Technological Research.
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*Thematic course:* Disposal of chromium waste. Part 2.

# Conditions of deposition of chromium(VI) with metal shavings from sulfuric acid solutions of chromium within hydronium jarosite production

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***Keywords:*** hexavalentchromium, wastewatersutilization, galvanic shops wastes, kinetic of hydroniumjarosite synthesis reaction.

**Abstract**

The innovation way to solve of galvanic shops chromium waste waters neutralization problem, in base of one lies hexavalent chromium reaction with steel shavings in acid, is considered in this paper. In the result of kinetic studies of hydroniumjarosite production from model solution optimal process conditions were obtained with achieving the minimal residual chromium concentration in aqueous solutions.

**Full Paper** _____ *Thematic Section:* Thermodynamic Research.
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# Phase complex of stable tetrahedron LiF–RbI–$Rb_2CrO_4$–$Li_2CrO_4$ of quaternary reciprocal system Li,Rb||F,I,$CrO_4$

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***Keywords**:* phase equilibria, differential thermal analysis, united stable tetrahedron, quasi-quaternary system, congruently melting compound, liquid compound stratification, concentrated model of phase complex.

**Abstract**

Experimentally researched quasi-quaternary system LiF–RbI–$Rb_2CrO_4$–$Li_2CrO_4$ is a united stable tetrahedron of quaternary reciprocal system Li,Rb||F,I,$CrO_4$. Two quaternary eutectics are formed in the system, compound $LiRbCrO_4$ (D 604) doesn't change the congruent type of melting. Liquid compound stratification is realized in two concentrated fields of limited solubility of liquid phases abutting to the sides $Li_2CrO_4$–RbI and LiF–RbI of tetrahedron in the system. On the basis of experimental data, 3D computer model of phase complex has been constructed in the form of concentrated tetrahedron.

**Full Paper** _____ *Thematic Section:* Physicochemical Research.
*Registration Code of Publication:* 14-39-8-50 *Subsection:* Petrochemistry.
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http://butlerov.com/readings/ *(English Preprint)*
Contributed: November 14, 2014.

# Integrated approach of the structural-group composition and oil type analysis study at the Udmurtia fields

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***Keywords:*** IR-spectrometry, spectral coefficients, study of oil, the molecular weight distribution of n-alkanes.

**Abstract**

A detailed analysis of crude oils from different deposits of the Udmurtia using complex of physico-chemical and instrumental methods is carried out. Basic properties and structural composition are determined by means of HPLC, GC and IR-spectroscopy the distribution of structural groups contamination and spectral coefficients are identified for crude oils and different fractions, which allowed us to describe the composition of cruds and identify the most important relations between pour point, tendency to the formation of deposits and the hydrocarbon composition.

*Thematic Section:* Preparative Research. **Full Paper**
*Subsection:* Supramolecular Chemistry. *Registration Code of Publication:* 14-39-8-57
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http://butlerov.com/readings/ *(English Preprint)*
Contributed: November 19, 2014.

# Synthesis of new types of PAMAM-dendrimers based on *p-tert*-butylthiacalix[4]arene

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***Keywords:*** thiacalixarenes, oligoamines, PAMAM, synthesis.

## Abstract

For the first time *p-tert*-butylthiacalix[4]arene functionalized at the lower rim with *N*-(2-aminoethyl)propanamide and *N*-(3-(3-aminopropylamino)propyl)propanamide fragments in *cone* and *1,3-alternate* conformations have been synthesized. The structure and composition of the new derivatives were characterized by a set of physical and chemical methods. It has been shown that the high reaction rates and quantitative product yields of aminolysis makes the initial esters good building blocks for introducing shorter chain oligoamino groups into the thiacalix[4]arene platform.

*Thematic Section:* Preparative Research. **Full Paper**
*Subsection:* Supramolecular Chemistry. *Registration Code of Publication:* 14-39-8-65
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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Contributed: December 06, 2014.

# Synthesis of *p-tert*-butylthiacalix[4]arene derivatives functionalized in the lower rim with *N*-(2-hydroxyethyl)ethylenediamine fragments in the *cone* and *1,3-alternate* conformation, and their interaction with DNA

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***Keywords:*** thiacalixarenes, oligoamines, synthesis, DNA.

## Abstract

For the first time *p-tert*-Butylthiacalix[4]arene derivatives functionalized in the lower rim with *N*-(2-hydroxyethyl)ethylenediamine fragments in the *cone* and *1,3-alternate* conformations have been synthesized. The structure and composition of the new derivatives have been characterized by physico-chemical methods. The ability of the synthesized macrocycles to interact with calf thymus DNA, and the formation of "macrocycle/DNA" aggregates have been demonstrated. It has been shown that the formation of monodisperse systems occurs only at specific stoichiometric ratios of "macrocycle / DNA".

**Full Paper** _____ *Thematic Section:* Physicochemical Research.
*Registration Code of Publication:* 14-39-8-72 *Subsection:* Petrochemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/ *(English Preprint)*
Contributed: November 14, 2014.

# Immobilization of hemoprotein in multilayer matrix of thiacalix [4] arene

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***Keywords:*** substituted thiacalix[4] arenes, monolayers on the substrate ITO, cytochrome *c*, Biomimetics.

**Abstract**

Research has been conducted on the formation of films *tetrakis*-(3-cyanopropoxy)-*n-tret*-butyl-thiacalix[4]arene in the conformation *1,3-alternate* on the surface of solid support of indium tin oxide (ITO) by atomic force microscopy (AFM). Calixarene films were obtained by Langmuir-Schaefer method through horizontal transfer of the layer formed at the phase interface water-air with the surface pressure $\pi$ = 30 $mN \cdot m^{-1}$, on the surface of the solid substrate. By AFM and nanolithography methods we established the capacity of Langmuir-Blodgett films of Calix [4] arene to immobilize the cytochrome enzyme *c* (*cyt c*) on the surface of the indium tin oxide.

**Full Paper** _____ *Thematic Section:* Preparative Research.
*Registration Code of Publication:* 14-39-8-76 *Subsection:* Organic Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/ *(English Preprint)*
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# Synthesis and biological activity of *N*-arylbenzamidines

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***Keywords:*** benzonitrile, arylamines, *N*-arylbenzamidines, acute toxicity, antimicrobial activity, anti-inflammatory activity, analgesic activity.

**Abstract**

A new technological method of *N*-arylbenzamidines synthesis has been worked out. Electronic nature of the substitute within arylamine molecules determines the probability and direction of a chemical reaction of benzonitrile with arylamines. This reaction being thermodynamically controlled allows to get *N*-arylbenzamidines with maximal yield at t = 180 °C. The derived amidines show signified antimicrobial, anti-inflammatory and analgesic activity.

**Full Paper** _____ *Thematic Section:* Preparative Research.
*Registration Code of Publication:* 14-39-8-82 *Subsection:* Organic Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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# Three-component synthesis of 9-(1-alkylhydroquinolin-6-yl)acridine-1,8(2H,5H)-diones

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*Supervising author; [+]Corresponding author
***Keywords:*** Three-component reaction, hydroquinoline, Acridinediones.

**Abstract**

Synthesis of new acridine-1,8(2*H*,5*H*)-dione derivatives containing hydroquinoline group via a three-component cyclocondensation reaction of 1-alkylhydroquinoline-6-carbaldehyde, ammonium acetate, and cyclohexane- 1,3-dione compound is described. The products were obtained in high yields in refluxing ethanol. The newly synthesized compounds were characterized by $^{1}$H NMR, and elemental analysis techniques.

*Thematic Section:* Preparative Research. **Full Paper**
*Subsection:* Biochemistry. *Registration Code of Publication:* 14-39-8-87
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: December 08, 2014.

# Synthesis, structure and biological activity of some amidrazones

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***Keywords:*** amidrazones, hydrazonoylchlorides, biological activity.

## Abstract

Some amidrazone derivatives were synthesized and their structure was established with the help of modern physico-chemical methods of analysis (TLC, mass spectrometry, elemental analysis, $^{1}$H NMR spectrometry and infrared spectroscopy). As starting compounds for the preparation of substituted amidrazones, hydrazonoylchlorides were used as the most available compounds. Antimicrobial activity was studied by the method of two-fold serial dilutions of the sample in the meat-broth and Sabouraud medium. As test cultures, microorganisms were used recommended by the State Pharmacopoeia of the Russian Federation XII. The resulting compounds had a pronounced antimicrobial activity.

*Thematic Section:* Preparative Research. **Short Communication**
*Subsection:* Organic Chemistry. *Registration Code of Publication:* 14-39-8-91
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http://butlerov.com/readings/ *(English Preprint)*
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# Imines with fragments of (aza,tio)xanthenes

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***Keywords:*** imines, 5*H*-benzopyrano[2,3-b]pyridine-5-ol, 9*H*-xanthene-9-ol, 9*H*-thioxanthene-9-ol, *N*-arylmethylene-4-(5*H*-chromeno[2,3-b]pyridine-5-yl)aniline, *N*-arylmethylene-4-(9*H*-xanthene-9-yl)aniline, *N*-arylmethylene-4-(9*H*-thioxantene-9-yl)aniline.

**Abstract**

Ternary synthesis of imines – *N*-arylmethylene-4-(5*H*-chromeno[2,3-*b*]pyridin-5-yl)anilines, *N*-arylmethylene-4-(9*H*-xanthene-9-yl)aniline, *N*-arylmethylene-4-(9*H*-thioxanthene-9-yl)anilines, comprising reacting aniline, aromatic aldehyde, 5*H*-benzopyrano[2,3-*b*]pyridin-5-ol, (9*H*-xanthene-9-ol, 9*H*-thioxanthen-9-ol) has been developed with the advantages of reducing the number of steps and having high purity of the resulting imines.

**Short Communication** _____ *Thematic Section:* Preparative Research.
*Registration Code of Publication:* 14-39-8-94 *Subsection:* Organoelemental Chemistry.
Publication is available for discussion within the functioning of the permanent internet-
Conference "New methods of synthesis, structure and application of organoelemental compounds"
http://butlerov.com/synthesys/ *(English Preprint)*
Contributed: November 17, 2014.

# Synthesis and structure of solvate *bis*(2,6-dichlorophenoxy) triphenylantimony with hexane

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***Keywords****:* triphenylantimony, 2,6-dichlorophenol, *tert*-butyl-hydroperoxide, oxidative addition, solvate, hexane, *bis*(2,6-dichlorophenoxy) triphenylantimony, structure.

**Abstract**

With the reaction of 2,6-dichlorophenol with triphenylantimony in the presence of tertiary butyl hydroperoxide in hexane in 95% yield solvate with hexane we synthesized *bis*(2,6-dichlorophenoxy) triphenylantimony (**I**), in which the molecules are antimony atoms distorted trigonal-bipyramidal coordination. OSbO axial angles and the sum of the angles CSbC in the equatorial plane are 178.4(6)° and 360°. The bond lengths Sb-O and Sb-C constitute 2.079(3), 2.084(2) Å and 2.095(4), 2.102(5), 2.111(5) Å. Distances C–O are 1.324(5), 1.338(5) Å; angles CSbC (114.5(6)°, 122.2(6)°, 123.6(6)°) are close to the ideal value (120°).

*Thematic Section:* Preparative Research. _____ **Short Communication**
*Subsection:* Organoelemental Chemistry. *Registration Code of Publication:* 14-39-8-97
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http://butlerov.com/synthesys/ *(English Preprint)*
Contributed: November 25, 2014.

# Synthesis and structure of a silver complex $[p\text{-Tol}_4P]^+_3[Ag_3I_6]^{3-}$

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***Keywords:*** reaction, tetra-*para*-tolylphosphonium iodide, silver iodide, dimethylsulfoxide, complex, $[p\text{-Tol}_4P]^+_3[Ag_3I_6]^{3-}$, structure.

**Abstract**

By the reaction of tetra-para-tolylphosphonium iodide with silver iodide in dimethylsulfoxide we synthesized silver ionic complex $[p\text{-Tol}_4P]^+_3[Ag_3I_6]^{3-}$. According to X-ray analysis, this complex is composed of tetra-para-tolylphosphonium cations and trinuclear silver anions. Phosphorus atoms have a tetragonal coordination (CPC 106.6(4)°-110.3(2)°, C–P 1.782(5)-1.802(5) Å), terminal silver atoms in the anion $[Ag_3I_6]^{3-}$ are three-coordinated (Ag-I 2.653 (2)-2.8032(12) Å), central silver atom is bound with the terminal atoms of silver through four atom bridge **I** and has a coordination number 4 (Ag-I 2.9014(14)-2.9049(15) Å). The angle between the planes of two rhombic fragments $Ag_2I_2$ [AgIAg 77.60(4)°], connected in whole through the central silver atom in anions makes up 59.53°.

**Letter to the Editor** _____ *Thematic Section:* Preparative Research.
*Registration Code of Publication:* 14-39-8-100 *Subsection:* Organometallic Chemistry.
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Conference "New methods of synthesis, structure and application of organoelemental compounds"
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Contributed: November 28, 2014.

# Synthesis and structure of solvate hexabromoosmate sodium with dimethyl sulfoxide $[Na_2(DMSO)_8][OsBr_6]$

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***Keywords:*** hexabromoosmate sodium, dimethyl sulfoxide, solvate, structure.

**Abstract**

Interaction of hexabromoosmate sodium with dimethyl sulfoxide produced solvate hexabromoosmate sodium with dimethyl sulfoxide $[Na_2(DMSO)_8][OsBr_6]$ (**I**), which structure was established by X-ray analysis. Crystal **I** consists of centrosymmetric octahedral anions $[OsBr_6]^{2-}$ (Os-Br 2.4796(9), 2.4799(9), 2.4885(11) Å; BrOsBr 180°, 89.72(4)-90.26(4)°) and centrosymmetric binuclear cations $[Na_2(DMSO)_8]^{2+}$, where sodium atoms are linked by bridging oxygen molecules of dimethylsulfoxide (Na···DMSO···Na 2.353(7), 2.381(7) Å). Each sodium atom is coordinated by three oxygen atoms of terminal molecules of dimethyl sulfoxide (Na···$OSMe_2$ 2.176(9), 2.341(8), 2.380(8) Å). Cycles $Na_2O_2$ flat, angle NaONa is 97.9(2)°.

**Short Communication** _____ *Thematic Section:* Biochemical Research.
*Registration Code of Publication:* 14-39-8-102 *Subsection:* The Composition of Vegetable Raw Materials.
Publication is available for discussion in the framework of the on-line Internet conference "*Chemical basis for the rational use of renewable natural resources*". http://butlerov.com/natural_resources/ *(English Preprint)*
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# Method for quantitation of phenolic glycosides (eleuterosides B and E) in dry extract of Eleuterococcus

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***Keywords:*** eleutherosides, chromatography, quantitation, validation method.

## Abstract

The article presents a modified method for the quantitation of eleutherosides B and E in the dry extract of Eleutherococcus senticosus (Rupr. Et Maxim.) Maxim, in that the dry extract of Eleutherococcus contains the greatest number of these phenolic glycosides. Pharmacological effect is also associated with the action of these eleutherosides. In connection with the above, it is important to develop and validate a method for determining eleutherosides B and E. Quantification of eleutherosides B and E was performed by HPLC. Chromatography was conducted in parallel with the standard sampling of eleutherosides B and E as described below. Validation method is presented by the following characteristics: specificity, linearity and limit of quantification.

*Thematic Section:* Biochemical Research. **Full Paper**
*Subsection:* Human Biochemistry. *Registration Code of Publication:* 14-39-8-105
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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Contributed: December 04, 2014.

# Homocysteine – a probable substrate for glutathione peroxidase of human serum

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***Keywords**:* homocysteine, homocystine, glutathione, hydrogen peroxide, thiol peroxidase, Ellman reagent.

**Abstract**

Using hydrogen peroxide as a reduction substrate**,** the distribution of two thiol peroxidase activities (with reduced homocysteine and glutathione as thiol substrates) within the human serum protein fractions was studied. Both activities were identified for fractions precipitated by low ammonium sulfate saturation (0-35%) that corresponds to literature data on the human extracellular glutathione peroxidase (Gpx3). When the concentration of reduced homocysteine is increased, the $K_{M\ app}$ for $H_2O_2$ and $V_{max\ app}$ increase proportionally to each other (retaining the ratio $V_{max\ app} / K_{M\ app}$) that is indicative of the ping-pong mechanism. Sigmoid dependence of the enzymatic reaction rate upon thiol concentration was revealed in cases of homocysteine and glutathione, confirming cooperative binding of thiol, that is a predictable property of homotetrameric enzyme. The data obtained indirectly support the hypothesis that the homocysteine peroxidase activity, found earlier in human serum, belongs to Gpx3.

*Thematic Section:* Chemical and Technological Research. **Full Paper**
*Subsection:* Organic Chemistry. *Registration Code of Publication:* 14-39-8-109
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# Theoretical study of 3-(4-chlorophenyl)-2,1-benzisoxazole-5-carbonyl chloride structure

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***Keywords:*** 3-(4-chlorophenyl)-2,1-benzisoxazole-5-carbonyl chloride, quantum chemical modeling, ab initio and semi-empirical quantum chemistry methods.

**Abstract**

Optimized molecular geometry, bond order, charges on each atom of 3-(4-chlorophenyl)-2,1-benzisoxazole-5-carbonyl chloride were modeled by different quantum chemistry methods. Results of modeling by semi-empirical quantum chemistry methods PM3 and PM6, *ab initio* HF and MP2 methods were compared with X-Ray Structural Analysis data. Mulliken atom charge analysis was done. Intermolecular interactions were detected.

*Thematic Section:* Chemical-Technological Research. **Full Paper**
*Subsection:* Supercritical Technologies. *Registration Code of Publication:* 14-39-8-113
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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# Energy analysis of prospects for the use of supercritical technologies in the ethylene oxide production

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***Keywords:*** supercritical extraction, ethylene oxide, supercritical carbon dioxide, distillation column, separation technology.

**Abstract**

The paper presents an analysis of the prospects for the use of supercritical technologies in the purification of ethylene oxide after preparation thereof in a reactor and single water absorption. Comparison of the proposed technology with the technology developed by the firm *Scientific Design* has been considered. It is shown that the use of the new technology can reduce both energy and capital costs for the implementation of the process.

*Thematic Section:* Physicochemical Research. **Full Paper**
*Subsection:* Kinetics of Interfacial Interactions. *Registration Code of Publication:* 14-39-8-119
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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# Adsorption kinetics of sulfide ions on the carbon surface

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***Keywords**:* carbon adsorbent, carbon surface, sulfide ions, adsorption, adsorption kinetics, functional groups.

**Abstract**

In the work, the chemical structure of the surface of carbon materials was investigated. Kinetic curves of sulfide ions adsorption for all studied materials were obtained. Time of adsorption equilibrium onset was determined. The dependence of sulfide ions equilibrium adsorption from the amount of alkaline groups on the surface of the carbon material was detected. The sulfide ions rate of adsorption in all taken materials was calculated.

**Full Paper** _____ *Thematic Section:* Research into New Materials.
*Registration Code of Publication:* 14-39-8-124 *Subsection:* Radio Reflective Materials.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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# Obtaining textile materials with bismuth nanoparticles for protection against microwave radiation influence

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***Keywords:*** nanoparticles, bismuth, materials, fabric, radiation, radio protective clothes.

**Abstract**

Synthesis of metal nanoparticles which consisted in chemical restoration of bismuth nitrate solution is carried out. Optimum parameters of bismuth restoration to zero-valent metal state and its drawing on fabric are developed. The modified fabric subjected to radiation allows to lower the radiation dose. The material can be used in radio protective clothes with the strengthened partial protection which includes overalls, helmets, gloves, boot covers made of radio reflecting materials.

*Thematic Section:* Biochemical Research. **Full Paper**
*Subsection:* Composition of Plant Raw Materials. *Registration Code of Publication:* 14-39-8-127
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Contributed: December 11, 2014.

# Ellagitannins in Rosaceous plants from the flora of Sakha (Yakutia) Republic

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***Keywords:*** ellagitannins, chemo-diversity, Sakha (Yakutia), HPLC.

## Abstract

A study of ellagitannins chemo-diversity in the aerial part of members of Rosaceae family from the Republic of Sakha (Yakutia) was carried out. Among 29 investigated species the presence of ellagitannins was detected only in 18 species belonging to subfamily Rosoideae. Some compounds were discovered in species at the first time, including agrimoniin in *Fragaria orientalis* and *Comarum palustre*, gemin A in leaves of *Geum urbanum*; pedunculagin in *Rubus idaeus*, sanguiin H-6, lambertianins C, D and pedunculagin in *Rubus arcticus*, *R. matsumuranus* and *R. saxatilis*, rugosins A, $B_1$, $B_2$, D, $E_1$, $E_2$, tellimagrandins $I_1$, $I_2$ and II in *Rosa acicularis*, *R. majalis* and leaves of *R. rugosa*, rugosins A, D, $E_1$ and $E_2$ in leaves of *Rosa canina*.

*Thematic Section:* Technological Research. **Full Paper**
*Subsection:* Membrane gas separation *Registration Code of Publication:* 14-39-8-139
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# Experimental installation for studying nonstationary hydrogen permeation through the membranes of metals and alloys

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***Keywords:*** *alloy, hydrogen, hydrogen permeability, pressure, diffusion, boundary conditions.*

## Abstract

The economic production of high-purity hydrogen is required to make possible the transition to environment oriented power systems. In the coming years, rapid increase in the proportion of membrane gas separation is expected. Interest in the processes of hydrogen transfer through metals and alloys has quickened in the past few decades. That is why reliable data concerning hydrogen permeability in materials are required and they allow to approximate the processes of hydrogen transfer by adequate models. The apparatus for studying non-stationary hydrogen permeation through structural and functional material was constructed. Vacuum scheme, principle of operation, key characteristics of the apparatus are presented, and some tentative research results of hydrogen permeability through the $Ta_{77}Nb_{23}$ (wt.%) alloy are submitted.

*Thematic Section:* Preparative Research. **Full Paper**
*Subsection:* Supramolecular Chemistry. *Registration Code of Publication:* 14-39-8-143
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# Interaction of Pillar[5] – and Pillar[6]arenes with $NO_2/N_2O_4$ and $NO^+$ donors

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***Kewwords:*** *pillar[n]arenes, $NO_x$, incapsulation, nitration.*

**Abstract**

The interaction of pillar[5]- and pillar[6]arenes with gaseous $NO_2/N_2O_4$, and with alkyl nitrites in the presence of a Lewis acids in organic solvents has been studied. Experimental data support the reversible formation of inclusion complexes between pillararenes and nitrosonium cations. Upon the prolonged standing on the reaction mixture the degradation of pillararene macrocycles has occurred as a result of nitration/ pillararene macrocycle degradation products.

**Full Paper** _____ *Thematic Section:* Biochemical Research.
*Registration Code of Publication:* 14-39-8-150 *Subsection:* Chemical-toxicological analysis.
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# Identification of 5F-AB-PINACA cannabimimetic metabolites in urine by GC-MC

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***Keywords:*** *5F-AB-PINACA, cannabimimetics, metabolism, enzymic hydrolysis, solid-phase extraction, gas chromatography – mass spectrometry.*

**Abstract**

The metabolites, allowing to establish the fact of using cannabimimetic of *N*-[1-carbamoyl-2-methylpropyl]-1-(5-fluoropentyl)-1*H*-indazole-3-carboxamide (5F-AB-PINACA) in the procedure of screening the urine on drugs and medicinal substances with the application of methods of solid-phase extraction and gas chromatography with mass spectrometry are described. Identification of the main metabolites of 5F-AB-PINACA in urine of consumers of smoking mixes was performed. It is established that the metabolism of 5F-AB-PINACA passes, generally through hydrolysis of amide bonds, the main metabolites are removed with urine in the conjugated form. Gas chromatographic and mass-spectrometric characteristics of derivative main metabolites which can be useful in practice of the forensic-chemical and chemical-toxicological analysis are received.

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*Subsection:* Physiological processes. *Registration Code of Publication:* 14-39-8-161
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# Determination of copper and ceruloplasmin in saliva

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***Keywords:*** *saliva, copper, ceruloplasmin, clinical laboratory diagnostics.*

**Abstract**

Experimental methods are developed to determine the concentration of copper and ceruloplasmin in saliva, the applicability of the calculation method is shown for determining the activity of ceruloplasmin. Increasing concentrations of copper and ceruloplasmin in the saliva of patients with cancer has been confirmed experimentally.

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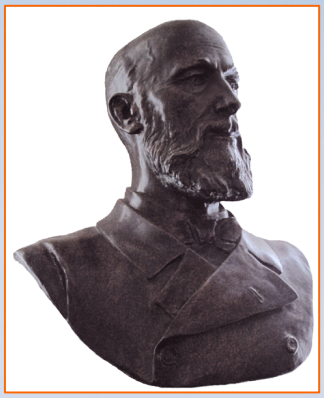

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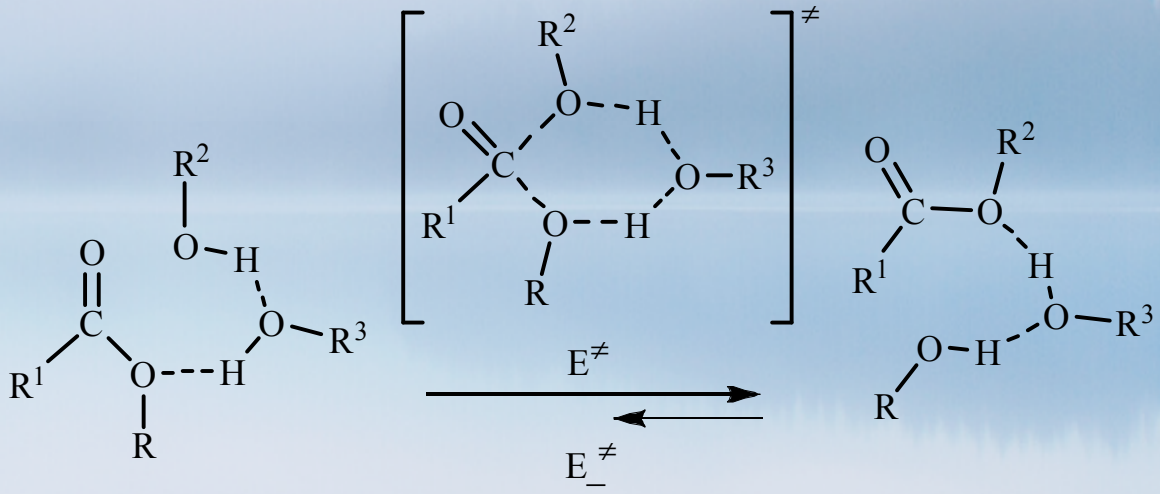


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*Thematic course:* Quantum-chemical study of the transformations of triglycerides. Part 1.

# Elementary acts of noncatalytic transesterification reaction of triglycerides and their analogs under the conditions of supercritical fluids

© **Alexandre I. Kourdioukov**,[1]*+ **Asiya R. Gabitova**,[2]*+ **Farid M. Gumerov**,[2]* **Evgeny N. Ofitserov**,[3] and **Ainur F. Mingaliev**[1]

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***Keywords:*** triglycerides of fatty acids, ethanol, methanol, methyl acetate, triacetin, associates, transesterification, reaction mechanism, elementary acts, quantum-chemical modeling, supercritical fluids, the method of DFT.

**Abstract**

Using quantum-chemical DFT method with density functional PBE in the basis 3z (comparable basis set cc-pVTZ) realizing the programs *Priroda 4.11* and B3LYP/6-311++g(df,p) applying the program *Gaussian09* we have studied the reactions of transesterification of triglycerides in methanol in the physical conditions of supercritical fluids, that is at T = 623 K and P = 30 MPa. Detailed consideration of the energy specificity of the following reaction systems was carried out: 1) The simplified gas phase reaction systems with triglyceride (or its analogues) and monomeric form of methanol in which the reaction proceeds by a one-step reaction mechanism involving alkoxycarbonyl bonds or two-step mechanism involving a carbonyl group in a first step of the alkoxy quaternary intermediate in the second step; 2) The reaction systems in which the elementary event involve carbonyl or alkoxy carbonyl group of triglyceride and dimer or trimer form of methanol and its substitution analogs.

It is shown that the simplified gas phase reaction systems involving methanol monomeric form are hypothetical and those with dimeric and trimeric forms of methanol are actually proceeding reaction directions, still not having a pronounced potential trap for target products – methyl esters of fatty acids and their substitution analogs that means equiprobable flow direction of most of the competitive transesterification of triglycerides, i.e., reaction systems described are in equilibrium with each other.

However, the presence of a few percent of water in in dry alcohol leads to the fact that for the associate pair glycerol-water at the interaction with alkoxy carbonyl bond of triglyceride there is observed a rather big potential trap (10.33 kkal/mol) for the forward direction reaction products, namely the hydrolysis products – aliphatic monocarboxylic acids with open chain that transfer the given transformation from a model category to the category of the real direction of the reaction.

It is concluded that in order to explain the experimental fact of the formation of the desired product - methyl ester of fatty acids in the transesterification reaction of triglycerides in the physical conditions of supercritical fluids it is required to conduct a detailed exploration of the potential promoter effect of fatty acids, which are the equilibrium products of a competitive hydrolysis reaction of triglycerides.

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*Thematic course:* Quantum-chemical study of the transformation of triglycerides. Part 2.

# Elementary acts of the hydrolysis reaction of triglycerides and catalytic role of intermediately authentic aliphatic carboxylic acids in the formation of their methyl esters in the physical conditions of supercritical fluids

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***Keywords:*** triglycerides of fatty acids, methanol, methyl acetate, triacetin, hydrolysis, aliphatic carboxylic acids, transesterification, methyl esters of fatty acid, acid catalysis, reaction mechanism, elementary acts, quantum chemical simulation, supercritical fluids, DFT method.

**Abstract**

By the quantum-chemical method DFT with the functional density PBE in the basis 3z (comparable basis set cc-pVTZ) using the program *Priroda 4.11* we studied the reactions of transesterification and hydrolyses of triglycerides in methanol at a promoter the assistance of the fatty acid analogues in the physical conditions of supercritical fluids, that is, when T = 623 K and P = 300 atm.

It is shown that in the conditions of a supercritical fluids the thermodynamic equilibrium of various reaction systems takes place that implements elementary acts of methanolysis and the hydrolysis of triglycerides to the side of accumulation of catalytically significant amounts of fatty acids. Thus associates of carboxylic acid – ethanol (or water) in a single reaction step of methanolysis (or hydrolysis) on the alkoxycarbonyl group of triglyceride analogues in supercritical fluids provide a promoter effect, which in combination with the presence of potential pitfalls, makes the directions of the reactions with their participation the main channel for accumulation of target products of the process of methanolysis of triglycerides, i.e. methyl esters of fatty acids..

It is noted that at high temperatures and pressures there is an unusual type of catalysis, due to a variety of thermodynamic equilibrium shift reaction systems realizing elementary acts of methanolysis and hydrolysis of triglycerides in the direction of the accumulation of catalytically significant amounts of fatty acids. In the transition to normal conditions the same thermodynamic equilibrium transfers fatty acids into their methyl esters.

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# Singlet and triplet transitions in the optical UV absorption spectrum of perylene

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***Keywords****:* condensed aromatic compounds, perylene, electronic structure, electron-excited singlet state, triplet states, UV optical absorption spectroscopy, photoelectron spectroscopy.

**Abstract**

UV–Vis optical absorption spectra were obtained for perylene in different solvents. The survey UV-spectrum of singlet transitions in cyclohexane and UV-spectrum of triplet transitions in bromopropane were recorded. The method of registration of triplet transitions was employed, based on the use of a cell with a large optical path length and bromo-substituted solvent. The presence of a heavy Br atom increases the spin-orbit interaction in the investigated molecule and thus the probability of excitation to triplet states. Assignment of the singlet and triplet electronic excited states and their attribution to the specific dominating electronic configurations were carried out using TD DFT B3LYP/6-31G quantum chemical calculations. The specific features of the occupied and vacant molecular orbitals involved into electron transitions were characterized via consideration of the photoelectronic spectra of perylene, found in the literature, and assigning the observed photoionization bands to the calculated B3LYP/6-31G orbitals. The energy of the first (lowest) vertical triplet transition was shown to be 1.92 eV, lying by ca. 0.4 eV higher than corresponding adiabatic transition known from the luminescence measurements made by other authors.

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# The generalized force constants of $NF_3$ and $ONF_3$ molecules in $X_\delta^0$ coordinates

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***Keywords:*** $NF_3$, $ONF_3$, generalized force constants, coordinates $X_\delta^0$, calculations DFT, vibration frequencies.

**Abstract**

Within the framework of the approach B3LYP6-311++G(3df,3pd) the force field of $NF_3$ and $ONF_3$ molecules in coordinates $X_\delta^0$ for the first time is obtained. Frequencies of normal vibrations were calculated. Comparison of the obtained generalized force constants with those of molecules was carried out.

*Thematic Section:* Physicochemical Research. **Full Paper**
*Subsection:* Physical Chemistry. *Registration Code of Publication:* 14-39-9-39
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# The possibility of proton magnetic relaxation in the analysis of the Gibbs adsorption of water on plant polymers

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***Keywords****:* surface phenomena, Gibbs adsorption, NMR relaxation, cellulose.

**Abstract**

Possibility of a nuclear magnetic resonance relaxation in studying of the interphase superficial phenomena in biopolymer-water system in the framework of Gibbs thermodynamics is established. Link of times of a nuclear magnetic relaxation is established with the chemical potential and coefficient of a superficial tension on limit of the section of phases in the adsorptive system. Nature of change of thermodynamic and relaxation parameters in the course of formation of the adsorptive layer of Gibbs in various samples of cellulose at their moistening is shown. The analysis of a condition of water in the adsorptive layer is given and its average width is determined.

**Full Paper** _____ *Thematic Section:* Physicochemical Research.
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# Study of influence of biological effects on the nature of structural changes of cellulose by $^1$H NMR relaxation

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***Keywords:*** cellulose, NMR relaxation, enzymatic hydrolysis, supramolecular structure.

**Abstract**

The possibility of using the pulsed NMR method for the analysis of the enzymatic hydrolysis of cellulose has been established. It has been shown that when processing pulp alcohol, ether and urea, the surface becomes more capable of enzymatic hydrolysis. The effect of such components of cellulose complex as *endo*-1,4-*β*-glucanase, pulp causes an abrupt change in its supramolecular structure, resulting in the reduction of translational molecular mobility of water.

**Full Paper** _____ *Thematic Section:* Physicochemical Research.
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# Effect of ultrasonic cavitation on reactivity of lignocellulosic substrates during the bioconversion of plant biomass

© **Andrey G. Dontsov**,[1]*+ **Anatoliy P. Karmanov**,[1] **Lyudmila S. Kocheva**,[2] **Alexey V. Rudkovskiy**,[3] **Svetlana A. Kuznetsova**,[3,4] and **Vladimir V. Volodin**[1]

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***Keywords:*** bioconversion, lignocellulosic substrates, enzymatic hydrolysis, ultrasonic cavitation.

**Abstract**

The use of ultrasound for the pretreatment of lignocellulose substrates in a heterogeneous medium leads to an increase their reactivity during the bioconversion in the sugars using cellulolytic enzymes. Under the influence of ultrasonic cavitation the process proceeds of lignin depolymerization, which facilitates its dissolution at the alkaline extraction stage. Lignin exhibits a protective effect with respect to the amorphous phase of cellulose, that allows to carry out the activation of substrates due to their delignification.

**Full Paper** _____ *Thematic Section:* Physicochemical Research.
*Registration Code of Publication:* 14-39-9-58 *Subsection:* Physical Chemistry.
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# Exploring the optical and mechanical properties of $AgCl_xBr_{1-x}$, $Ag_{1-x}Tl_xBr_{1-x}I_x$, $Ag_{1-x}Tl_xCl_yI_zBr_{1-y-z}$ crystals and IR fibers based on them

© **Liya V. Zhukova**,*+ **Akexandr S. Korsakov**, **Alexandr E. Lvov**,
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***Keywords:*** crystals of silver and monadic thallium halides, refractive index, spectral transmission, optical losses, light stability, Young's modulus, Poisson's ratio, rigidity modulus, rapture strength of IR fibers.

**Abstract**

We investigated the physical and chemical properties of new crystals and IR fibers on their basis: chemical composition, impurities content, refractive index, spectral transmission and optical losses, light stability, far-field distribution of the modes effluent from the fiber's end, Poisson's ratio, Young's modulus and rigidity one, as well as rapture strength of the IR fibers. In order to explore the characteristics above, we designed the corresponding setups.

*Thematic Section:* Physicochemical Research. **Full Paper**
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# Formal kinetics of high-temperature thermal decomposition of polyurethanes and their mixtures with flame retardants

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***Keywords:*** Polyurethanes, the kinetics of the thermal decomposition, flame retardants, decomposition products, toxicity.

**Abstract**

The thermal destruction of different purposes polyurethanes and rigid polyurethane foam are considered, formal kinetic equation of thermal decomposition is obtained. The dependence of the thermal properties of molded polyurethane on the structure of polyester and diisocyanate component is found. It is shown that the use of the principle of trimerization of isocyanates for polyurethanes allows to increase the resistance of the polymer to elevated temperatures. The efficiency of applying a number of fire retardant additives is analyzed. The mechanism of preparing hydrocyanic acid in the pyrolysis products is shown.

**Full Paper** _____ *Thematic Section:* Physicochemical Research.
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# Gibbs energy dependence on temperature and concentration during the crystallization of binary crystal hydrate solutions

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***Keywords:*** Gibbs energy, crystal hydrates, sodium acetate trihydrate, sodium carbonate decahydrate, geometrical thermodynamics, equilibrium and non-equilibrium crystallization.

**Abstract**

On the example of equilibrium and non-equilibrium phase diagrams of $Na_2CO_3 \cdot 10H_2O$ – $NaCH_3COO \cdot 3H_2O$ system, ways of Gibbs energy changes are shown for liquid and liquid – solid phases when cooling pure components and alloys in binary system.

**Full Paper** _____ *Thematic Section:* Physicochemical Research.
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*Thematic course:* Hydrochemical synthesis of metal chalcogenide films. Part 22.

# Thermal stability of hydrochemically deposited $Cd_xPb_{1-x}S$ supersaturated solid solutions

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*Supervising author; +Corresponding author

***Keywords:*** hydrochemical deposition, thin films, supersaturated solid solution, lead sulfide, cadmium sulfide, thermal stability.

**Abstract**

It was found that the upper temperature limit of stability of hydrochemical deposited supersaturated solid solutions $Cd_xPb_{1-x}S$ ($0 < x \leq 0.18$) is 405-410 K. At higher temperatures, heating decomposes these compounds in two phases: a solid solution with the equilibrium at a given temperature sulfide content cadmium and X-ray amorphous CdS. The greatest changes in the photovoltaic properties of the films of supersaturated solid solutions $Cd_xPb_{1-x}S$ during the first two years of storage at room conditions were observed in the first 2-3 months. Dark resistance varied by 20-40% during this period, the maximum change in voltage sensitivity was 20-25% of the original value.

**Full Paper** _____ *Thematic Section:* Physicochemical Research.
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# Investigation of surface electrical properties and agregate stability of monodisperse polystyrene latexe particles with aminated surface

© **Irina Yu. Shirokova**,[1+] **Marima S. Tereshchenko**,[1] **Irina D. Shpilina**,[1]
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***Keywords:*** *collidal stability, sols coagulation, electrokinetic potential,electrophoretic mobility, polystyrene latex.*

## Abstract

The dependences of the electrokinetic potential of monodisperse polystyrene latex with particle size of 0.19 microns and 0.42 microns were obtained at variation pH (3.0-9.0) and electrolyte concentration ($C_{NaCl}$ $=10^{-2}$-$10^{-3}$mol/l and 0.15 mol/l). Coagulation kinetics of latex was investigated in these conditions by direct ultramicroscopy method and the spectroturbidimetry method. It wass shown that the aggregate stability depended on the dispersion medium composition (pH and NaCl) and the polystyrene particles size.

*Thematic Section:* Physicochemical Research. **Full Paper**
*Subsection:* Inorganic Chemistry. *Registration Code of Publication:* 14-39-9-107
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# Metastable defects concentrated near growth dislocations in cadmium sulfide

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***Keywords:*** the metastable defects, dislocations in cadmium sulfide, capacitive spectroscopy of deep levels, compressive stress.

**Abstract**

The article examines the metastable defects concentrated near the growth dislocations in cadmium sulfide. Using the methods of transient capacitive spectroscopy of deep levels it has been revealed that the concentration of these defects depends on the shape of etch pits of dislocations, i.e. on the ratio between the depth and width of holes. In the work, with the help of different models, we calculated the stress state of the surface region. We came to the conclusion that the appearance of deep levels in the spectra is due to the onset of compressive stress at a certain profile of etch pit.

*Thematic Section:* Physicochemical Research. **Full Paper**
*Subsection:* Analytical Chemistry. *Registration Code of Publication:* 14-39-9-113
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# New methodical approach to the potentiometric analysis of natural water

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***Keywords:*** potentiometry, ion-selective electrodes, addition method, dilution method.

**Abstract**

We propose a potentiometric analysis method of the ion concentration in aqueous solutions, based on measurement of the electrode potential change rate after a controlled change in the concentration, as well as design of semi-automatic device that implements this method. The described approach significantly reduces the time of potentiometric measurements and allows to reduce the systematic error of the method due to considering the sample matrix. Created semi-automatic device allows to measure the ions concentration in such a methodical approach.

*Thematic Section:* Physicochemical Research. **Full Paper**
*Subsection:* Phase Equilibria. *Registration Code of Publication:* 14-39-9-117
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# Phase equilibria and heat storage materials in the system Li,Ca//F,$SO_4$,$MoO_4$

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***Keywords:*** physical and chemical analysis, phase equilibria, eutectic, peritectic, heat of fusion, the entropy of fusion.

**Abstract**

Differential thermal, visual-polythermal and X-ray phase methods of physical and chemical analysis were used to study the system Li,Ca//F,$SO_4$,$MoO_4$. It has been found that stable secant triangle LiF-$Li_2SO_4$-$CaMoO_4$ prism splits compositions of the system on a tetrahedron LiF-$Li_2SO_4$-$Li_2MoO_4$-$CaMoO_4$ and pentahedron LiF-$Li_2SO_4$-$CaF_2$-$CaSO_4$-$CaMoO_4$. We identified the compounds and the melting temperature of four invariant points, defined heat and entropy of melting alloys of invariant twenty four-reciprocal system.

*Thematic Section:* Thermodynamic Research. **Full Paper**
*Subsection:* Phase Equilibria. *Registration Code of Publication:* 14-39-9-125
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# About some features of description and determination of thermodynamic properties of substances near critical point

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***Keywords:*** Equation of state, compressibility factor, critical point, isochoric specific heat capacity, one-parameter law of corresponding states, normal un-dissociated substances.

**Abstract**

It is shown that the difficulties of determining the critical parameters from the lines of phase equilibrium – specific volume dependences of pressure and temperature – can be easily overcome by examining the specific volume dependencies of some complexes consisting of the dependencies and the specific volume, and having no broad maximum near the critical point. In particular, such complexes can be compressibility factor, the products of pressure and temperature on the specific volume, ratios of specific volume to pressure and temperature, which can determine the critical volume, pressure and temperature.

The relationship between the conditions imposed on thermal equation of state at the critical point and parameters of the equation of state is discussed.

Three new equations of state were proposed satisfying the conditions of stability at the critical point and describing the critical point.

It is shown that most widely used equations of state equal to the sum of products of functions of temperature on the functions of the volume, in principle, can not describe the singularity of the isochoric heat capacity at the critical point.

It is proved that all critical amplitudes and exponents depend only on one parameter for normal un-dissociated substances, that is, there must be relations between all the critical amplitudes and exponents, and they must depend on only one of them.

The classification of substances according to the value of the critical exponent $\beta$ is suggested.

The uniqueness of this classification for normal un-dissociated substances is proved.

Relation is found between the critical exponent $\beta$ and the critical amplitude $B$.

*Thematic Section:* Thermodynamic Research. **Full Paper**
*Subsection:* Phase Equilibria. *Registration Code of Publication:* 14-39-9-135
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# Phase equilibrium of Van der Waals gas

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***Keywords:*** phase transition, phase equilibrium line, Van der Waals equation of state.

**Abstract**

Critical analysis of the literature data on phase equilibrium of Van der Waals gas is carried out. The necessity of obtaining reliable and more accurate data is substantiated. The data on the densities of the liquid and the gas, the saturation pressure was obtained for temperature interval from the absolute zero to the critical temperature. It is shown that: 1) the absolute zero temperature of this gas is an analogue of the triple point temperature of real systems; 2) the volume of fluid per particle at the triple point is equal to the parameter $b$ of the Van der Waals equation of state; 3) the unit compressibility line is tangential to the liquid branch of phase equilibrium line at the triple point on the temperature-density plane; 4) the liquid branch of phase equilibrium line has tangent line with zero slope angle at the triple point on the density-pressure plane.

**Full Paper** _____ *Thematic Section:* Thermodynamic Research.
*Registration Code of Publication:* 14-39-9-144 *Subsection:* Phase Equilibria.
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# Positivity of pressure in the canonical Gibbs ensemble

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***Keywords***: *Negative pressure, interaction potential, triple point, equation of state of hard spheres, Van der Waals equation of state, equilibrium, interaction with the wall, density dependence of potential.*

**Abstract**

It is proved within the framework of the classical canonical Gibbs ensemble *(N,V,T) = const* that the equilibrium pressure is non-negative for any potential independent of density. It is shown that: 1) the pressure can be negative in a macroscopic system if the interaction potential depends on the density; 2) the pressure is non-negative if the density-dependent interaction potential does not include attraction; 3) the pressure can be negative only if the potential depends on the density and it is not fully repulsive.

Physical consistency criterion (inequality) obtained for exact and approximate solutions of the equations for the pair correlation function.

It is shown that if we assume that Van der Waals equation of state obtained for a system of particles interacting via the potential energy independent of density, than there is a triple point in this system at which the temperature and pressure are not equal to zero. Formula was obtained for estimating the temperature and density of the liquid at the triple point.

It is shown that the equation of state of hard spheres with interaction energy described by Katz potential is not exact, its theoretical derivation contains a hidden error, and this equation must be supplemented by condition of positivity of the pressure at finite temperature and density.

*Thematic Section:* Thermodynamic Research. **Letter to the Editor**
*Subsection:* Phase Equilibria. *Registration Code of Publication:* 14-39-9-149
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# On the significance of the second partial derivatives of thermodynamic quantities at the critical point

© **Ikhtiyor H. Umirzakov**
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***Keywords:*** phase transition, the equation of state, critical point.

**Abstract**

The second partial derivative of specific volume on pressure have been analytically studied with the help of the Van der Waals equation of state. It has been shown that this derivative at the critical point of the liquid-gas phase transition does not have a definite value. It has also been shown that the second partial derivative of the specific volume on pressure is not a continuous function and therefore it is not a function of the state.

*Thematic Section:* Thermodynamic Research. **Letter to the Editor**
*Subsection:* Phase Equilibria. *Registration Code of Publication:* 14-39-9-151
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# A method to determine the virial coefficients from the height dependence of the pressure of gas in the gravitational field

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***Keywords:*** virial coefficient, gravitational field.

**Abstract**

A method for determining the virial coefficients from the data on the height dependence of the pressure of gas in the gravitational field at the constant temperature is suggested. The method allows to determine the virial coefficients from the experimental data for a single density value for a given temperature, unlike conventional methods requiring the experiment for each value of pressure or density for a given temperature.

*Thematic Section:* Technological Research. _____ **Letter to the Editor**
*Subsection:* Constructions of Chemical Apparatus. *Registration Code of Publication:* 14-39-9-153
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# Resistive furnace for single crystals growth

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***Keywords:*** crystal growth equipment, crystallization, crystal growth.

**Abstract**

The description of the experimental furnace for bulk single crystals growth of oxide materials in air at temperatures up to 1300 °C is presented. In the paper, there is also given the scheme of thermal units that allow to control the crystallization conditions with changing the axial temperature gradient in both cases of spontaneous crystallization, as well as grown on a seed.

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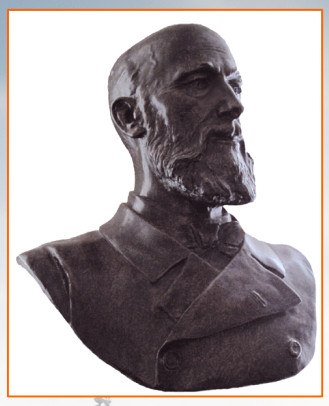

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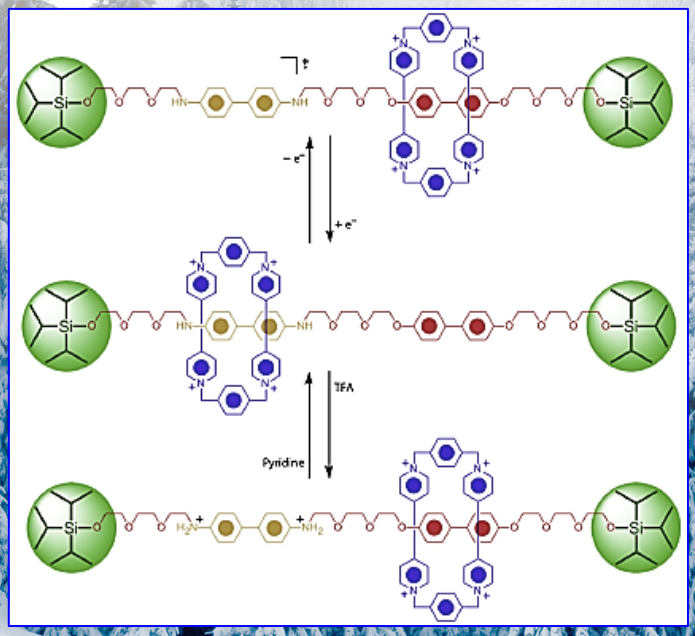


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# Molecular machines based on supramolecular systems

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***Keywords:*** supramolecular chemistry, molecular machines, nanotechnology, photochemistry, catenanes, rotaxanes.

**Abstract**

The paper describes the design and construction of multicomponent nanoscale systems that can perform certain functions or to perform any kind of work like macroscopic devices under the influence of an external pulse. There are discussed the basic principles of molecular machines based on supramolecular systems, and also shown the classification methods of controlling the state of the system.

*Thematic Section:* Preparative Research. **Full Paper**
*Subsection:* Supramolecular Chemistry. *Registration Code of Publication:* 14-39-10-23
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# Sorption of bovine serum albumin with hybrid organo-inorganic material based on silicon dioxide nanoparticles, functionalized with organosilicon derivative of thiacalix[4]arene

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***Keywords:*** thiacalixarenes, nanoparticles, proteins, sorption.

**Abstract**

New sorbent, combining high specific surface area, formed by silicon dioxide nanoparticles and high effectivity of biopolymer binding, which is specific for derivatives of thiacalix[4]arene was proposed. Modification of silicon dioxide nanoparticles with organosilicon derivatives of thiacalixarene was carried out. Removal of water from colloidal suspension of superficially functionalized nanoparticles of silicon dioxide has allowed to obtain water-insoluble sorbent, for which high effectivity of bovine serum albumin was shown. Study of sorption kinetics and capacity of bovine serum albumin shows, that high sorption capacity is attained – up to 160 mg of protein per 1 g of sorbent, in correspondence with experiments on sorption kinetics – saturation of sorbent with protein is attained in the course of 60 minutes.

*Thematic Section:* Preparative Research. **Full Paper**
*Subsection:* Supramolecular Chemistry. *Registration Code of Publication:* 14-39-10-29
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# Synthesis of *p-tert*-butylthiacalix[4]arene modified with glucosamine fragments at the lower rim

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***Keywords:*** thiacalixarene, polyhydroxy-derivatives, synthesis, glucosamine.

**Abstract**

Synthesis methods are developed of stereoisomers of *p-tert*-butylthiacalix[4]arenes (*cone* and *1,3-alternate*), containing residues of *D*-glucosamine as sensory and structure-forming groups. Three derivatives of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis-[(*β-D*-glucopyranosylamidocarbonyl)-metoxy]-2,8,14,20-tetrathiacalix[4]arene were synthesized. The synthesized compounds were characterized by a complex of physical methods: $^{1}$H and $^{13}$C NMR and IR spectroscopy, mass spectrometry, and elemental analysis.

*Thematic Section:* Preparative Research. **Full Paper**
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# Interaction of methylpheophorbide (a) with ethylenediamine

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***Keywords:*** Methylpheophorbide-a, chlorin $e_6$, ethylenediamine, aminochlorins.

**Abstract**

Chlorin $e_6$ amide derivatives with one, two and three amino groups were synthesized by the action of ehtylenediamine on methylpheophorbide (a). Ester group in position 17 has being shown to react first in the amidation with ehtylenediamine and then in position 15. Amidation of the ester group in position 15 without the reaction in position 17 does not occur. The higher reaction ability of the ester group in position 17 can be explained with the lower steric hindrance.

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# Nucleophylic substitution of the allilic amino group in double aminomethylated chlorophyl *a* derivates

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***Keywords:*** Methylpheophorbide-a, chlorin $e_6$, nucleophylic substitution, aminomethylated chlorophyll *a* derivatives, 3(1),3(2)-*bis*-(*N,N*-dimethylaminomethyl)-chlorin $e_6$ 13(1)-*N*-methyl amide-15(2),17(3)-dimethyl ester.

## Abstract

Nucleophylic substitution reaction of 3(1),3(2)-*bis*-(*N,N*-dimethylaminomethyl)-chlorin $e_6$ 13(1)-*N*-methyl amide-15(2),17(3)-dimethyl ester as a substrate with a series of alcohols, phenol and some amines as a nucleophiles using different ways of carbcatione from allilic dimethylamino groups formation were studied. Nucleophylic substitution was realized in case of $Zn(OAc)_2$ and some *O*-nucleophyles.

**Short Communication** _____ *Thematic Section:* Preparative Research.
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# Levoglucosenone in the synthesis of chiral benzodecanolide

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***Keywords:*** levoglucosenone, 1,6-anhydro sugar, tetralone, the Michael reaction, lactone, salicyligalomides.

**Abstract**

The reaction of levoglucosenone with tetralone gave Michael adducts, the treatment of which with HCl-MeOH gave the corresponding ketals. Oxidation of pyridinium by chloro-chromate of the mixture of ketals completed the synthesis of the target decanolide annulated by benzene ring.

*Thematic Section:* Preparative Research. **Short Communication**
*Subsection:* Organic Chemistry. *Registration Code of Publication:* 14-39-10-43
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# The structure of 4-(7-cyclohepta-1,3,5-trienyl)aniline and synthesis of 4-(7-cyclohepta-1,3,5-trienyl)-*N*-(1-cyclohepta-2,4,6-trienyl) aniline

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***Keywords:*** X-ray analysis, 4-(7-cyclohepta-1,3,5-trienyl)aniline, 4-(7-cyclohepta-1,3,5-trienyl)-*N*-(1-cyclohepta-2,4,6-trienyl)aniline.

**Abstract**

The method of X-ray analysis was used to investigate the molecular and crystal structure of 4-(7-cyclohepta-1,3,5-trienyl)aniline. The method of synthesis of 4-(7-cyclopepta-1,3,5-trienyl)-*N*-(1-cyclohepta-2,4,6-trienyl)aniline by the interaction of 4-(7-cyclohepta-1,3,5-trienyl)aniline with tetra-fluoroborate of tropylium has been worked out.

**Full Paper** _____ *Thematic Section:* Preparative Research.
*Registration Code of Publication:* 14-39-10-54 *Subsection:* Structural Chemistry.
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# Synthesis and structure of silver complexes $[Ph_3PCH=CHPPh_3]^{2+}[Ag_2Br_4]^{2-}$ and $[Ph_3P(CH_2)_3PPh_3]^{2+}{}_2[Ag_5Br_9]^{4-}\cdot DMSO$

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***Keywords:*** complex, silver, tetraorganylphosphonium, synthesis, structure.

**Abstract**

By reacting 1,2-dibromide vinylenbis(triphenylphosphonium) dibromide and trimethylenbis (triphenylphosphonium) with silver bromide we synthesized silver complexes $[Ph_3PCH=CHPPh_3]^{2+}[Ag_2Br_4]^{2-}$ (**I**), $[Ph_3PCH_2CH_2CH_2PPh_3]_2^{2+}[Ag_5Br_9]^{4-}\cdot DMSO$ (**II**), whose structure was established by X-ray analysis. Crystals I and **II** consists of binuclear cations of tetraorganilphosphoniumin in which phosphorus atoms are tetrahedrally coordinated (P-C 1.787(3)-1.907(12) Å; CPC 104.1(6)-112.1(9)° (**I**), P-C 1.758(8)-1.815(8) Å; CPC 107.1(4)-112.1(4)° (**II**)). In crystals of the complexes, there are present centrosymmetric anions $[Ag_2Br_4]^{2-}$ (**I**) (Ag-Br 2.4855(5)–2.6633(6) Å, BrAgBr 79.30(2)-132.76(2)°) and $[Ag_5Br_9]^{4-}$ (II) (Ag-Br 2.6603(13)-2.9355(12) Å, BrAgBr 71.63(3)-126.79(5)°).

**Full Paper** _____ *Thematic Section:* Preparative Research.
*Registration Code of Publication:* 14-39-10-58 *Subsection:* Structural Chemistry.
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# Quantum-chemical study of ozone protonation

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***Keywords:*** ozone, quantum chemistry, B3LYP, protonation, DFT.

**Abstract**

The process of protonation of ozone in the singlet and triplet states was studied using B3LYP/6-311++G(df,p) quantum-chemical method. The geometric structure of the products of protonation were studied. The thermodynamic parameters of the reaction of protonation of ozone in the singlet and triplet electronic configurations were described. It was shown that the process of protonation of ozone in all cases is exothermic and proceeds with free energy and entropy decrease.

**Full Paper** _____ *Thematic Section:* Studies of Catalytic Processes.
*Registration Code of Publication:* 14-39-10-62 *Subsection:* New Technologies.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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# Features of dry methane reforming on $MoO_3$, $MoO_x$-C and β-$Mo_2C$

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***Keywords:*** carbon dioxide reforming of methane, carbon dioxide, catalytic systems, carbides, molybdenum.

**Abstract**

The catalytic activity of systems based on molybdenum oxides and carbides in carbon dioxide reforming of methane were investigated, the research showing the prospects of this direction. It was found that the differences in the catalytic activity with the nature and structure of the particles, the maximum conversion of methane and carbon dioxide are observed when multi-faced β-$Mo_2C$-particles (with a hexagonal close-packed lattice) are used as a catalyst. The authors suggest that carbon dioxide conversion of methane on oxide and reduced catalysts take place by different routes: either through the formation of carbonate complexes or through the formation of particles $CH_X$ and C.

**Full Paper** _____ *Thematic Section:* Biochemical Research.
*Registration Code of Publication:* 14-39-10-68 *Subsection:* Physical Chemistry.
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# Influence of salts of single and double charged metal cations on the sorption of $H^+$ and $OH^-$ ions on the mycelium of basidiomycetes

© **Aleksander S. Chukhno**,* **Elena P. Ananeva**, **Svetlana V. Gurina**, **Anastasia N. Bankina**,+ **Elizaveta Yu. Brilliantova**, and **Irina B. Dmitrieva**
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***Keywords:*** Basidiomycetes, potentiometric titration, point of zero charge.

**Abstract**

The paper presents the study of colloidal properties of mycelium of basidiomycetes.

The aim is to study the adsorption on the mycelia of basidiomycetes *Abortiporus biennis* and *Poliporus ciliatus*, as well as determining the point of zero charge of the mycelium, and studying the effect of electrolytes on its value. The studies were conducted by potentiometric titration. Point of zero charge mycelium *Polyporus ciliatus* is 5.0, and the point of zero charge of mycelium *Abortiporus biennis* is 6.5. It was established that specifically adsorbed on the mycelium cations of simple electrolytes evidenced shift point of zero charge in an acidic electrolyte solution in the region. With increasing either concentration or a cationic charge the effect on the point of zero charge increases. This shows the selective sorption on the surface of the mycelium. Mycelium and basidiomycetes *Abortiporus biennis* and *Poliporus ciliatus* can be used both as a carrier, and as a sorbent of metal cations.

**Full Paper** _____ *Thematic Section:* Biochemical Research.
*Registration Code of Publication:* 14-39-10-76 *Subsection:* Physical Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/ *(English Preprint)*
Contributed: December 23, 2014.

# Investigation of the properties of colloidal mycelium of basidiomycetes with the aim of using it as a carrier of BAS

© **Aleksander S. Chukhno**,* **Svetlana V. Gurina**, **Elena P. Ananeva**, **Anastasia N. Bankina**,+ **Elizaveta Yu. Brilliantova**, and **Irina B. Dmitrieva**
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*Supervising author; +Corresponding author
***Keywords:*** Basidiomycetes, isoelectric point, amino acids, azoles.

**Abstract**

The paper presents the study of colloidal properties of mycelium of basidiomycetes. The aim is to study the adsorption on the mycelia of basidiomycetes Abortiporusbiennis and Poliporusciliatus, as well as the possibility of using mycelium as a carrier for drugs. The effect of glycine, aspartic acid, imidazole and tetrazole on the surface properties of mycelium were studied. pHiep value in the presence of an amino acid or an azole shifted to the acidic region, indicating a predominance of anionic amino acids of specific adsorption or azole. It has been shown that at pH greater than 3.0 the mycelium surface both in amino acid solutions and in the solution of azoles is negatively charged due to the dominance of the adsorption of the anionic form. It is known that amino acids and the azoles are present in the solution as both cations and anions. The predominance of the sorption of the anionic form speaks of selective sorption on the surface of the mycelium. Therefore, as the transported drug substance it is better to use a drug substance in the solution of which anionic form prevails.

*Thematic Section:* Physicochemical Research. **Full Paper**
*Subsection:* Biochemistry. *Registration Code of Publication:* 14-39-10-83
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# Application of the method of thermal analysis for the study of eggs

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***Keywords:*** thermal analysis, egg, chemical composition, protein yolk.

**Abstract**

The chemical composition of proteins and yolk of eggs from 10 regions of Russia was studied by thermal analysis. According to the experiments for three years studies have shown that using the developed techniques in protein and egg yolks can determine the content of water, ash and up to 4 organic macro-components in 1 hour, with the account of time for sample preparation. Macro components can be characterized by the temperature of exothermic or endothermic effect, it is recommended to use this indicator in the identification of eggs to their areas of origin, as well as the quality of feeding chickens. Calculated according to the thermal analysis of the activation energy for each of the components in the composition of albumen and yolk, and this figure can also be used to characterize the individual components of eggs from different manufacturers from different regions and assessing their energy and nutritional value.

*Thematic Section:* Biochemical Research. **Full Paper**
*Subsection:* The Elemental Composition of Plants. *Registration Code of Publication:* 14-39-10-89
Publication is available for discussion in the framework of the on-line Internet conference "*Chemical basis for the rational use of renewable natural resources*". http://butlerov.com/natural_resources/ *(English Preprint)*
Contributed: December 14, 2014.

# Elemental composition of the aerial part of *Pteridium pinetorum*

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***Keywords****:* elemental composition, *Pteridium pinetorum, Hypolepidaceae.*

**Abstract**

In this paper, the elemental composition of the aerial part of *Pteridium pinetorum* (*Hypolepidaceae*), assembled in the territory of South-Eastern Pribaikalye in different plant communities is considered. A content of 9 of trace elements, including toxic metals – lead and cadmium is determined by atomic absorption method. Elemental composition of the aerial part of *Pteridium pinetorum* is studied for the first time.

**Review** _____ *Thematic Section:* Biochemical Research.
*Registration Code of Publication:* 14-39-10-94 *Subsection:* Chemistry of Plant Raw Materials.
Publication is available for discussion in the framework of the on-line Internet conference "*Chemical basis for the rational use of renewable natural resources*". http://butlerov.com/natural_resources/ *(English Preprint)*
Contributed: December 22, 2014.

# Chemical modification of dihydroquercetin (taxifolin) and biological activity of its derivatives

© **Mikhail P. Koroteev**,[1]*+ **Anton O. Pozdeev**,[1] **Alexander M. Koroteev**,[1] **Harry Z. Kaziev**,[1] **Andrey T. Teleshev**,[1] and **Evgeny N. Ofitserov**[2]*+

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***Keywords*:** flavonoids, link structure – biological activity, 2,3-dihydro-3,5,7-trihydroxy-2-[3',4-dihydroxyphenyl]-4*H*-1-benzopyran-4-on or taxifolin or dihydroquercetin, UV-spectra, NaOH, $H_2O_2$, acylation, phosphorylation, oximation, benzoylation, inclusion compounds, aminomethylation, mixed esters of Taxifolin, cytotoxicity, antioxidant, antiproliferative activity, actoprotective action.

## Abstract

This review covers the latest data, mainly of the authors, on the structure and chemical properties of dihydroquercetin (taxifolin) as one of the representatives of the plant flavonoids (FL). The latter are the excellent means for not only the prevention and health care activities, but also for the treatment of many diseases caused by imbalance in the enzymes. In addition, FL have antibacterial, antioxidant, membran-and-immuno-stabilizing, anti-inflammatory, decongestant, anti-cancer and other properties which turn them into quite valuable synthons for chemical modification, research of biological activity and development of new preparations. Based on the structural features and biological activity, the class of plant flavonoids in their reactivity, especially in relation to oxygen, dissociates into two groups: having the three conjugated rings and the group with the absence of conjugation between cycles A and B. These differences are manifested in the UV-spectra with respect to oxygen, complexation with metals in the biological activity - inhibitory concentrations may differ by two to three orders of magnitude. Literature data shows that in contrast to the previously described processes of complexation, dihydroquercetin (DHQ) forms complexes with oxygen, which once were taken as complexes with metals. In those cases where the DHQ concentration used were less than 0.01%, the authors had artifacts – DHQ complexes of reversible interaction with oxygen, which determined the properties studied. It is suggested that these complexes change the conductivity of the capillaries under the action of DHQ.

*Thematic Section:* Study of Reactivity. **Full Paper**
*Subsection:* Colloidal Chemistry. *Registration Code of Publication:* 14-39-10-121
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# Supramolecular complexes of squalene in electrophilic addition

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*Supervising author; [+]Corresponding author

***Keywords:*** squalene, electrophilic addition, supramolecular structures, vesicles, mechanism of electrophilic addition.

**Abstract**

There were obtained supramolecular formations of squalene, tetrahydrofuran in the presence of hydrogen halides, which as well as natural vesicles have a membrane that protects the contents from the external environment. On this basis, we can assume that many of the details of natural behavior of vesicles can be modeled using supramolecular complexes obtained by us on the basis of a new type of squalene and polar solvent molecules On the other hand, the scheduled path finding new supramolecular structures based on squalene and polar molecules of low molecular weight for use in the manufacture of a new generation medicinal products lacking drawbacks phosphatidylcholine based vesicles.

*Thematic Section:* The Study of Biological Activity. **Full Paper**
*Subsection:* Organic Chemistry. *Registration Code of Publication:* 14-39-10-127
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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# Comparative evaluation of tests for determining antioxidant activity on the examples of biologically active 3-substituted-3-hydroxy-6-phenyl-3,4-dihydro-2*H*-1,3-oxazines

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***Keywords:*** 1,3,4,6-tetracarbonyl compounds substituted oxazines, oxidative stress, antiradical activity, diphenyl, antioxidant activity.

**Abstract**

Based on the reaction of 1,6-diaryl-3,4-dihydroxy-2,4-hexadiene-1,6-dione and arilidenarilmines we have synthesized various 3-substituted-3-hydroxy-6-phenyl-3,4-dihydro-2*H*-1,3-oxazines. Due to the urgency of finding new biologically active compounds, there were studied the antioxidant activity of oxidative stress on the model of the culture of bacteria *Escherichia coli* M17 by the coulometric method, as well as the antiradical activity of the obtained oxazines. Antiradical properties of the compounds were studied in the coupling reaction of stable free radical 2,2-diphenyl-1-picrylhydrazyl. As a comparison standard Trolox was used. Four compounds with moderate anti-radical activity were found. Among most of the samples investigated antioxidant activity was demonstrated by (2Z)-3-hydroxy-3-[4-hydroxy-2-(4-methylphenyl)-2-(4-methylphenyl-3,6-diphenyl-3,4-dihydro-2*H*-1,3-oxazin-4-yl]-1-phenylprop-2-en-1-one.

*Thematic Section:* Physicochemical Research. **Full Paper**
*Subsection:* Physical Chemistry of Explosives. *Registration Code of Publication:* 14-39-10-135
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# Properties and stability of furazan-1,2,3,4-tetrazin-1,3-dioxide and co-crystals on its basis

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***Keywords:*** furazan-1,2,3,4-tetrazin-1,3-dioxide, co-crystals, thermal decomposition, sensitivity to mechanical influences, thermal explosion, stability of burning.

**Abstract**

In the work, thermal decomposition, sensitivity parameters to mechanical influences, characteristics of thermal explosion and burning of furazan-1,2,3,4-tetrazin-1,3-dioxide and two co-crystals on its basis is considered. The first (known) co-crystal consists of furazan-1,2,3,4-tetrazin-1,3-dioxide and a dinitrazapentan with equimolar ratio of components, the second (new) co-crystal includes furazan-1,2,3,4-tetrazin-1,3-dioxide and benzotrifurocsan with the ratio of components 2/1 in moles. Possibilities for regulating the complex of characteristics of furazan-1,2,3,4-tetrazin-1,3-dioxide are shown at co-crystallization with the specified substances.

**Full Paper** _____ *Thematic Section:* Physicochemical Research.
*Registration Code of Publication:* 14-39-10-148 *Subsection:* Physical Organic Chemistry.
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# Research of the associated stable tetrahedral $LiF-Li_2CrO_4-KBr-K_2CrO_4$ of quaternary reciprocal system $Li,K||F,Br,CrO_4$

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***Keywords:*** differential thermal analysis, T-x diagram, eutectic, phase equilibria.

**Abstract**

Phase equilibria in the associated tetrahedral $LiF-Li_2CrO_4-KBr-K_2CrO_4$ of quaternary reciprocal system $Li,K||F,Br,CrO_4$ have been studied by the differential thermal analysis. The compositions of two quaternary eutectic (equiv. %) have been determined: 3% LiF, 42.7% $Li_2CrO_4$, 9.7% KBr, 44.6% $K_2CrO_4$ with melting point 455 °C and 1% LiF, 77.1% $Li_2CrO_4$, 7% KBr, 14.9% $K_2CrO_4$ with melting point 350 °C.

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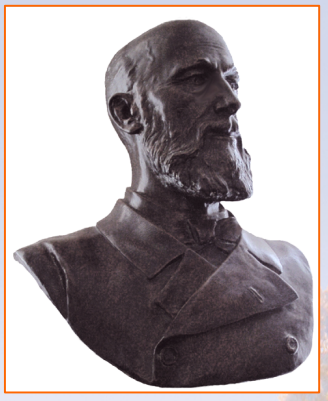

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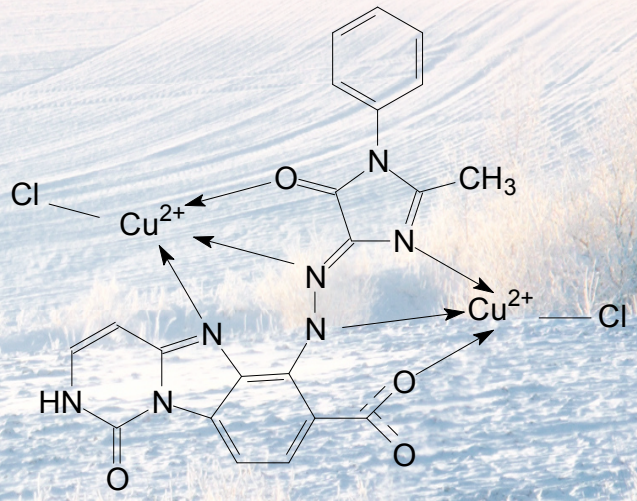


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# Thermodynamic investigation of relations between equilibrium compositions of phases at hydrochemical synthesis of solid solutions {AgCl, AgBr}(s)

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***Keywords****:* silver halide solid solutions, hydrochemical synthesis, equilibrium compositions of phases, thermodynamic equilibrium laws of basic in phase and interfacial reactions, equilibrium constants, activity coefficients of components.

**Abstract**

The object of investigation is new, more advanced in handling, method of hydrochemical synthesis of solid solutions {AgCl, AgBr}(s), which are used as a demanded raw material at growth of monocrystals for the IR-fiber optics. It is based on the phenomenon of solid solution formation under isothermal interaction of individual AgCl($s^o$) and/or AgBr($s^o$) with the liquid mixture of hydrochloric and hydrobromic acids {$H_2O$, HCl, HBr}(l), and we named it the method of acid influence on individual halides (AIIH).

For the creation of method AIIH scientific foundation, which provides theoretical account and strict implementation of formation conditions of solid solutions {AgCl, AgBr}(s) with required relative contents of components, it is necessary to determine the relations between equilibrium component compositions of solid solution and liquid phase in analytical form.

Thermodynamic investigation of the mentioned relations has a complex nature and includes the following main stages: the introduction of the concept of hydrochemical system (HCS) and consideration of it's composite parts; the construction of stoichiometric models of inphase chemical transformations and interphase mass-exchange processes in HCS in terms of basic reactions; the consideration of thermodynamic laws of equilibrium of such reactions; the determination of activity coefficients in analytical form and determining the temperature dependences of equilibrium constants.

*Thematic Section:* Theoretical Research. **Full Paper**
*Subsection:* Thermodynamics. *Registration Code of Publication:* 14-40-11-15
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# Exact solutions of Gibbs-Tolman-Koenig-Buff equation for spherical dividing surface and exactly solvable models of interfacial layer

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***Keywords:*** surface tension, curvature radius, liquid drop, bubble, tension surface, break surface, Gibbs surface, dividing surface, equimolar surface, Tolman's length, Tolman's parameter, Tolman's formula, boundary of interface, coexisting phases, ideal thermodynamic system of comparison.

**Abstract**

Exact solutions of the Gibbs-Tolman-Koenig-Buff equation for the dependence of the surface tension on the radius of the spherical liquid droplet in the vapor and spherical vapor bubble in a liquid are found. Five well-known formulae for this dependence are theoretically justified. New approximate formulae for this dependence are obtained using method of sequential approximations. The approximate formulae are compared with the exact formula. A simple approximated theoretically based formula for the dependence of the surface tension on the radius is suggested. The method to restore the radius and temperature dependences of the Tolman's length using the radius and temperature dependences of the surface tension is suggested. The radius dependence of the Tolman's length, when Tolman's formula and this simple formula become accurate, and the asymptotic behavior of this dependence in the limits of small and large radii of curvature are obtained.

**Full Paper** _____ *Thematic Section:* Theoretical Research.
*Registration Code of Publication:* 14-40-11-36 *Subsection:* Thermodynamics.
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# Connection of the critical parameters of phase transition liquid-vapor with low-temperature elastic properties of solid body

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***Keywords****:* equation of state, the critical point, the bulk modulus, liquid, gas, solid, crystal, tensile strength, fluctuation theory, scaling, scale invariance, critical exponent, critical amplitude, critical parameter, isotropic body.

**Abstract**

Wehavefound relations between critical parameters, critical exponents and critical amplitude characteristics of the substance, readily identifiable at low temperatures and pressures on the basis of the fundamental equation of state of the fluctuation theory of phase transitions of liquid-gas.

*Thematic Section:* Theoretical Research. **Short Communication**
*Subsection:* Thermodynamics. *Registration Code of Publication:* 14-40-11-47
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# Determination of gas pressure using Rayleigh scattering of light on clusters

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***Keywords:*** Rayleigh scattering, nanoparticle, size distribution function of clusters, liquid drop model of cluster, fraction of condensate.

**Abstract**

It is shown that the gas pressure and the fraction of condensate (clusters) in gas can be determined using Rayleigh scattering of light on clusters. Formula relating gas pressure with the mean value of sixth degree of the radius of the cluster (determined using size distribution function of clusters) which is proportional to the intense of Rayleigh scattering of the light by clusters in gas is obtained. Formulae are obtained to determine fraction of condensate using data on Rayleigh scattering of the light on clusters in gas.

**Full Paper** _____ *Thematic Section:* Theoretical Research.
*Registration Code of Publication:* 14-40-11-50 *Subsection:* Physical Chemistry.
The article is published on the materials of report presented at the "International Scientific Forum Butlerov Heritage – 2015". http://foundation.butlerov.com/bh-2015/ *(English Preprint)*
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# Observation of fractional charges in the mass spectroscopic experiments

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***Key words:*** chemical bond energy, dissociative electron attachment, dissociative photoionization, Yukawa potential, fractional charges.

**Abstract**

In previous publications dealing with experimental mass spectrometry of tungsten hexacarbonyl, hexafluoroacetylacetone and its bidentate metal complexes $M(hfac)_2$; M = Cu, Pd the obtained data have not been adequately systematized. In this paper, we analyse the previously published experimental data of the various bond dissociation energy. A modified Yukawa potential is used to analyse the experimental data. Experimental results of the formation of ions can be interpreted only in terms of the formation of fractionally charged quasi-particles. As an experimental technique, mass spectrometry of negative ions in electron resonance capture mode ranks next to the fractional quantum Hall effect in which fractional values of the charge quantization are observed.

*Thematic Section:* Theoretical Research. **Full Paper**
*Subsection:* Physical Chemistry. *Registration Code of Publication:* 14-40-11-59
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*Thematic course:* Kinetics and mechanism of acyl transfer reactions. Part 9.

# Influence of ester structures on kinetics of piperidine and morfoline *N*-acylation in aqueous-organic solvents

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***Keywords:*** acylation, piperidine, morfoline, phenyl benzoates, water–1,4-dioxane, water–2-propanol, quantum chemical descriptors.

**Abstract**

The kinetics of piperidine and morfoline reactions with mono- and dinitrosubstituted phenyl benzoates in phenoxide ring is investigated in binary solvents water–2-propanol and water–1,4-dioxane. It is shown that Hammet's equation is true for the compounds of this class. Linearity is established between logarithms of the reactions rate constants and $pK_a$ values of the ester leaving groups. Linearity is established between logarithms of rate constants of the amines reactions with 4-nitrophenyl benzoate and phenyl salicilate. Values of activation parameters of piperidine reactions with esters agree with results of investigations of temperature dependence of dibutyl amine and diethyl amine reactions with 4-NPhB in the same conditions. It is shown that $E_{LUMO}$ values of the substituted phenyl benzoates can be descriptors of their reactivity in reaction with piperidine.

*Thematic Section:* Theoretical Studies. **Full Paper**
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# Application of three rules of solubility and selection rule of sediment priority to calculate areas of solid phase in aqueous solutions of metal salts

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***Keywords:*** heterogeneous equilibrium, aqueous solutions, saturation condition, simulation of equilibrium.

**Abstract**

For calculating the formation areas of a large amount of solid phases in the same system with overlapping areas, the mathematical model of equilibrium in aqueous solutions of metal salts has been created. The model is used as a classical condition of saturation in the solution on the basis of the product solubility rules and rule of molecular solubility as well as the rule of solubility for intermediates. Selection rule of priority sediment is used to calculate the transition point from one sediment to the another in supersaturated solution with several precipitations. The model is used for planning the experiment, calculating the constants of homogeneous and heterogeneous equilibrium, planning conditions of synthesis of target compounds in the precipitations form or thin films.

**Full Paper** _____ *Thematic Section:* Theoretical Research.
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# Kinetic modeling of hydrocarbons conversion on the high-silica zeolite system Ga-ZSM-5

© **Raisa I. Kuzmina**,*+ **Sergey V. Ignatyev**, **Anton Yu. Pilipenko**, and **Yaroslav A. Rybkin**
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*Supervising author; +Corresponding author
***Keywords****:* n-hexane, ZSM-5, kinetics, model, rate equation.

**Abstract**

The kinetic scheme of hydrocarbons conversion on the high-silica zeolite system Ga-ZSM-5 were proposed. A system of differential rate equations for each of the reaction components were compiled. Methods for solving direct and inverse kinetic problem with the use of parallel computing systems and technologies to speed up calculations are developed.

**Full Paper** _____ *Thematic Section:* Quantum-Chemical Research.
*Registration Code of Publication:* 14-40-11-84 *Subsection:* Physical Chemistry.
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# Solution of a spectral problem for molecules $NH_2NO_2$, $CH_3NO_2$ and $N_2O_4$ in coordinates $X_\delta^0$

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***Keywords:*** molecules $NH_2NO_2$, $CH_3NO_2$, $N_2O_4$, the generalized force constants, coordinates $X_\delta^0$, calculations DFT, vibration frequencies.

**Abstract**

Within the framework of approach B3LYP 6-311 ++ G (3df, 3pd) the force field of $NH_2NO_2$, $CH_3NO_2$ and $N_2O_4$ molecules in coordinates $X_\delta^0$ for the first time is obtained. Frequencies of normal vibrations were calculated. Comparison of the obtained generalized force constants with those of molecule was carried out.

*Thematic Section:* Quantum-Chemical Research. **Full Paper**
*Subsection:* Physical Chemistry. *Registration Code of Publication:* 14-40-11-91
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# Generalized force constants of hydrazine molecule

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***Keywords:*** hydrazine, generalized force constants, coordinates $X_\delta^0$, DFT calculations, vibration frequencies.

**Abstract**

Within the framework of the approach B3LYP6-311++G(3df,3pd) the force field of hydrazine molecule in coordinates $X_\delta^0$ for the first time is received. Frequencies of normal vibrations were calculated. Comparison of the received generalized force constants with those of tetrafluorohydrazine molecule was carried out.

*Thematic Section:* Quantum-Chemical Research. **Full Paper**
*Subsection:* Organic Chemistry. *Registration Code of Publication:* 14-40-11-95
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# Tautomeric composition as one of the most important characteristics of a substance

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***Keywords:*** tautomerism, rotating isomerism, absorption electronic spectra, quantum-chemical calculations, σ-constants of the substituents, correlation analysis, intramolecular hydrogen bond, anthraquinones, p-acenquinones.

**Abstract**

The properties of substances possessing the ability to tautomeric transformations strongly depend on their tautomeric composition. A method for determination of tautomeric composition based upon correlation analysis of the position of $\pi_l,\pi^*$ absorption bands in the electronic absorption spectra is proposed.

*Thematic Section:* Kinetic Research. **Full Paper**
*Subsection:* Organic Chemistry. *Registration Code of Publication:* 14-40-11-101
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# Chain reaction of *N,N'*- diphenyl -1,4- benzoquinonediimine with 2-mercaptobenzothiazole

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***Keywords:*** 2-mercaptobenzothiazole, *N,N'*-diphenyl-1,4-benzoquinonediimine, chain reaction, kinetics, the effect of the initiator.

**Abstract**

The kinetics of the reaction N, N'-diphenyl-1,4-benzoquinonediimine with 2-mercaptobenzoxazole in chlorobenzene at 343 K was studied. The reaction orders were defined on the components by the way of by introducing the initiator (tetraphenylhydrazine) found that the reaction is characterized by a chain mechanism of quadratic chain termination. There was defined the value of the parameter $k_{pr}/(2k_t)^{1/2} = 12.4 \pm 1.1$ (l mol $^{-1}$c$^{-1}$)$^{1/2}$, where $k_{pr}$ – the rate constant for the rate-limiting step of continuing, and $2k_t$ – speed constant of chain termination step. It is shown that both specified steps proceed with 2-mercapto benzoxazolyl thiyl radicals.

*Thematic Section:* Preparative Research. **Analytical Review**
*Subsection:* Organic Chemistry. *Registration Code of Publication:* 14-40-11-107
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# From insect pheromone synthesis to preparations

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***Keywords:*** Pest insect and honey bee pheromones, synthesis, pheromone preparations.

**Abstract**

The paper summarizes the results obtained by the Laboratory of Insects' Bioregulators (Ufa Institute of Chemistry of the Russian Academy of Sciences) in the streamlined synthesis of honey bee and pest insect pheromones and development of preparations on their basis for beekeeping and pest population control.

Progress has been achieved in a promising research area, namely, a streamlined synthesis of low-molecular-weight insect bioregulators, including the development of high-tech procedures for obtaining a large group of universal acyclic-type block-syntones and designing original and efficient schemes on their basis to synthesize acetogenin, isoprenoid and macrolide pheromones of more than 60 species of agricultural and forest insect pests.

Using the theory of insect communication by pheromones, a promising research area has been formed and developed to create beekeeping medications on the basis of synthesized honey bee metabolites [multifunctional pheromone of the honey bee – 9-oxo-2*E*-decenoic acid (9-ODA) – and the active component of royal jelly – 10-hydroxi-2*E*-decenoic acid (10-HDA)], including the development of efficient methods for their synthesis and investigations into pharmacological activity and application techniques.

*Thematic Section:* Preparative Research. **Full Paper**
*Subsection:* Organic Chemistry. *Registration Code of Publication:* 14-40-11-117
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# Radical binding activity product of interaction of methyl ester of 3,4-dihydroxy-6-oxo-2,4-hexadiene acid with 1,2-diaminobenzene

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***Keywords:*** 1,3,4,6-tetracarbonyl compounds, methyl 3,4-dihydroxy-6-oxo-2,4-hexadiene acid, methyl (2*Z*)-[3-(2-oxopentyl)quinoxalin-2-(1*H*)-ylidene] etanoat radical binding activity.

**Abstract**

Reaction of methyl 3,4-dihydroxy-6-oxo-2,4-hexadiene and 1,2-acid diaminobenzene was performed to obtain methyl (2Z)-[3-(2-oxopentyl) quinoxalin-2(1*H*)-ylidene] etanoat. On the basis of IR and $^1$H NMR spectroscopy and mass spectroscopy the structure of the synthesized compounds was found out. Its radical binding activity in the reaction with DPPH (DPPH) was studied, which was at the level of the standard anti-radical activity - water-soluble form of vitamin E (Trolox).

**Full Paper** _____ *Thematic Section:* Preparative Research.
*Registration Code of Publication:* 14-40-11-122 *Subsection:* Coordination Chemistry.
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# Complex compounds of metals with some azo-derivatives of benzo[4,5]imidazo[1,2-c]quinazoline carboxylic acids

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***Keywords****:* benzo[4,5]imidazo[1,2-c]quinazoline carboxylic acids, azo-derivatives, metal complexes, synthesis, electron absorption spectra, IR absorption spectra, structure, formation constants.

**Abstract**

Complex compounds of metals with some azo derivatives of benzo[4,5]imidazo[1,2-c]quinazoline carboxylic acids are isolated in the crystalline state and studied by a set of analytical methods. The processes of complex formation in solutions are studied, the ionization constants of the ligands and the formation constants of the complexes are determined. The efficiency of the organic molecules and their metal complexes as dyes for polyamide fibers is shown.

**Full Paper** _____ *Thematic Section:* Preparative Research.
*Registration Code of Publication:* 14-40-11-128 *Subsection:* Coordination Chemistry.
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# Spectrophotometric study of the complexing of pyrazolelyazopyrazolone derivatives

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***Keywords:*** pyrazolelyazopyrazolone, metal complexes, electronic absorption spectra, equilibrium in solutions, formation constants.

**Abstract**

The processes of complex formation of some derivatives of pyrazolylazopyrazolones in ethanol aqueous solutions were studied by the method of spectrophotometric titration. As it was shown, the processes of complexing are accompanied by a batochrome shift of long wave absorption bands in the electronic absorption spectra of the organic molecules. The metal-to-ligand ratios are determined, and the ionization constants of the ligands and formation constants of the complexes are calculated. The correlation curves of the formation constants of the metallic complexes vs the physical characteristics of the complexing ions are obtained.

**Full Paper** _____ *Thematic Section:* Preparative Research.
*Registration Code of Publication:* 14-40-11-132 *Subsection:* Electrochemistry.
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# Electric properties of $Li_{2-2x}Sr_xZrO_3$ solid solutions

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***Keywords:*** Lithium-ion conductors, solid electrolytes, conductivity, resistance to molten lithium.

**Abstract**

The novel lithium-conductive solid electrolytes based on the $Li_{2-2x}Sr_xZrO_3$ lithium metazirconate have been synthesized as a result of carried out experiments. The transport properties of the $Li_{2-2x}Sr_xZrO_3$ solid solutions have been studied. The strontium implementation into the lithium sublattice, unlike $Li_{8-2x}Sr_xZrO_6$ solid solution, was found to decrease the $Li_{2-2x}Sr_xZrO_3$ conductivity. Possibly, it occurs due to disorder of the lithium cations migration ways. Practical resistance of the $Li_{2-2x}Sr_xZrO_3$ ceramics to molten lithium has been investigated.

*Thematic Section:* Research into New Technologies. **Full Paper**
*Subsection:* Inorganic Chemistry. *Registration Code of Publication:* 14-40-11-137
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# Removal of copper by organo-mineral composite sorbents infused with hydroxide or sulfide based active phase

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***Keywords:*** composite sorbent, cation exchanger KU-2×8, iron(III) hydroxide, tin(II) hydroxide, tin(IV) hydroxide, titan(II) hydroxide, zinc sulfide, copper sulfide(II), lead sulfide, sorption of heavy non-ferrous metals.

## Abstract

Research has been carried out on copper(II) sorption by composite organo-mineral sorbents based on cation resin KU-2×8 with hydroxide and sulfide based active phase with structures as follows: KU-2×8-$Fe(OH)_3$, KU-2×8-$Sn(OH)_2$, KU-2×8-$Sn(OH)_4$, KU-2×8-$Ti(OH)_3$, KU-2×8-CuS, KU-2×8-ZnS, KU-2×8-PbS. There have been identified the number and strength of ionic groups within composite sorbents, and determined the nature of active phase distribution, the size of its particles, the composite sorbents elemental composition. It is shown that the full dynamic adsorption capacity of composite sorbents for copper(II) exceeds the capacity of cation resin KU-2×8, reaching 10.9 mEq/g while maintaining high kinetics of the sorption process. Experiments were conducted on copper removal from ammonia etching process in the manufacture of printed circuit boards.

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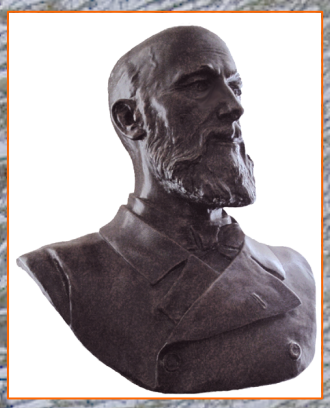

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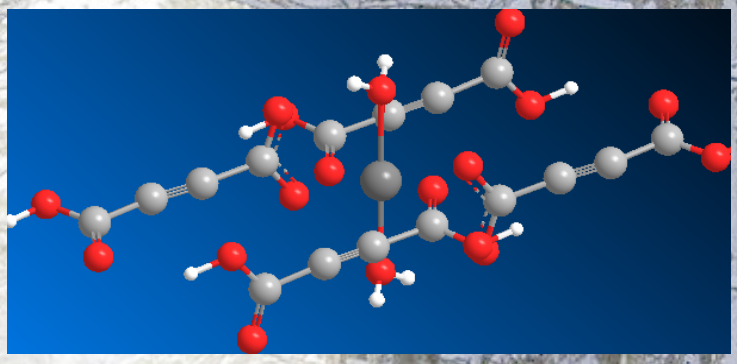

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# White phosphorus as a new object of biological destruction

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***Keywords:*** detoxication, white phosphorus, sewage sludge, anaerobic conditions, gas secretion kinetics, gas chromatography–mass spectrometry, metabolic pathway, metabolites, nuclear magnetic resonance, sulfate reducers, Bacillus, Streptomyces, phytotoxicity, culture medium, chemical equilibrium.

## Abstract

Possibility of white phosphorus degradation under the effect of waste water sludge (WWS) of waste-water treatment facilities is shown for the first time. White phosphorus suppresses the micro-organisms growth not immediately after application, but in several days or even weeks. It means that toxic effect is caused by the presence of intermediate products of degradation, which are accumulated in substrates. Considering the change in evolved gaseous products composition one can make a conclusion about greater stability of eubacteria to white phosphorus compared to that of methanogens. Micro-organism cultures are obtained, growing on substrate with white phosphorus content of 0.01 and even 0.1%. The $P_4$ concentration decrease in media is in inverse proportion to the duration of microflora growth lag-phase, as it was demonstrated by GCMS method. This fact indicates the white phosphorus biodegradation process. Besides, in the present work the research work is presented, devoted to the search for the white phosphorus metabolites, and the probable way of the phosphorus metabolism is proposed for the first time. Inoculation of stable bacteria on synthetic medium, containing white phosphorus as a unique source of phosphorus, has demonstrated the possibility of their growth in such conditions. *Streptomyces* species A8 strain, isolated from the white phosphorus containing sludge, contrary to the other ones, did not suppress at all the growth of the higher plants, i.e. habitat affected this antibiotic activity.

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# Transdermal procaine delivery in the presence of dimethylsulfoxide

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***Keywords:*** transdermal drug delivery, procaine, dimethylsulfoxide.

**Abstract**

The article considers transdermal drug delivery of procaine and its mixtures with dimethylsulfoxide (DMSO). The parameters of drug transport via the human skin, such as J (μg·cm$^{-2}$·h$^{-1}$), D (cm$^{-2}$·h), P (cm/h). have been calculated. It is shown that DMSO increases the activity of penetration – enhancement ratio (ER) 15 times.

**Full Paper** _____ *Thematic Section:* Biochemical Research.
*Registration Code of Publication:* 14-40-12-32 *Subsection:* Chemistry of Plant Raw Materials.
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# Flavonoids in the grass Tribulus Terrestris

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***Keywords:*** acetonitrile, Tribulus Terrestris – *TribulusterrestrisL*, MC-detector TQD (Waters), analysis of the test sample materials, chromatograms and spectra.

**Abstract**

In this article, you can appreciate raw Tribulus terrestris as a promising model for the study. An example is presented of the detection method of flavonoids by ultra performance liquid chromatography /MC on a chromatograph *WatersAcquility* with tandem quadrupole MC-detector *TQD* (*Waters*).

*Thematic Section:* Biochemical Research. **Full Paper**
*Subsection:* Analytical Chemistry. *Registration Code of Publication:* 14-40-12-37
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# Peculiarities of chemical composition of juvenile perch in the Volga reach of the Kuibyshev reservoir

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***Keywords****:* aquatic ecosystem, Kuibyshev reservoir, environmental pollution, heavy metals, perch underyearlings, X-ray fluorescence analysis, concentration of pollutants.

**Abstract**

The features of the chemical composition of perch underyearlings caught in the Volga reach of the Kuibyshev reservoir were investigated. The accumulation of heavy metals in muscle tissue was shown. Excess of permissible levels of copper and zinc has been noted.

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*Registration Code of Publication:* 14-40-12-42 *Subsection:* Analytical Chemistry.
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# Features of the mineral composition of worms *Eisenia foetida* as soil-forming organisms

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***Keywords:*** soil, humus, environmental pollution, heavy metals, vermiculture, earthworms, Eisenia foetida, X-ray fluorescence analysis, concentration of the chemical elements.

**Abstract**

The features of the mineral composition of earthworms as organisms that form the humus layer of the soil were investigated. The features of the chemical composition of *Eisenia foetida* were shown as a basis for vermiculture in comparison with species. The characteristic of the chemical composition of coprolites and vermiculture contribution in removing heavy metals during the formation of humus was shown.

**Full Paper** _____ *Thematic Section:* Physicochemical Research.
*Registration Code of Publication:* 14-40-12-50 *Subsection:* Analytical Chemistry.
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# Chemical characteristics of flue gases when disposing of liquid and gaseous wastes of chemical industry

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***Keywords:*** flue gases, chemical composition, atmospheric air, photocolorimetric and chromatographic methods of analysis, concentration of pollutants.

**Abstract**

Results of a study conducted to reveal the chemical characteristics of flue gas processing and disposal of liquid and gaseous wastes are presented in the paper. It is shown that the chemical composition of the flue gas is determined by the environmental conditions of their formation and man-made features.

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*Subsection:* Hydrochemistry. *Registration Code of Publication:* 14-40-12-55
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# Investigation of the features of chemical composition of different types of soil in the Kazan lakes of Middle and Upper Kaban

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***Keywords:*** bottom sediments, heavy metals, water ecosystem, coarse silts, fine silts, sand.

**Abstract**

In the article, there is given the analysis of bottom sediments in the Kazan lakes of Middle and Upper Kaban. These lakes are tested for different degree of anthropogenic stress. Three types of soil were allocated in these lakes which characterized by certain features and properties. The research of chemical composition of allocated types of soil and the analysis of heavy metals in them were carried out. Determination the quantity of loss on ignition allowed to identify the amount of organic composition in samples analyzed.

**Full Paper** _____ *Thematic Section:* Physicochemical Research.
*Registration Code of Publication:* 14-40-12-62 *Subsection:* Physical Chemistry.
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# Effect of temperature on ethanol conversion over surface of Zr-modified zeolite system of ZSM-5 type

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***Keywords****:* ethanol, zeolite, ZSM-5, alcohol, ethylene, alkylation, isomerization, aromatization.

**Abstract**

A modification of high-silicon zeolite ZSM-5 by zirconium is carried out and a direction defined for chemical conversion of ethanol on the surface of this system. The paper shows the influence of the process parameters on the direction of the transformation of the products of ethanol dehydration. It discusses the surface state of the catalyst and the mechanism of the formation of aromatic hydrocarbons comprising dehydrogenation, dehydrocyclization and alkylation of intermediates on the surface of the system.

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*Subsection:* Physical Chemistry. *Registration Code of Publication:* 14-40-12-69
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# Adsorption features of hydrocarbon vapors on the surface of the carbon adsorbent modified by polyvinylpyrrolidone monolayer

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***Keywords:*** gas-adsorption chromatography, carbon adsorbents, modified adsorbents, polymer modifiers, polyvinylpyrrolidone.

**Abstract**

In this paper by the reverse gas-adsorption chromatography method, there were defined thermodynamic characteristics of adsorption (TCA) of a number of hydrocarbons on the carbon graphite-solid support Carbopack Y (CpY) modified by polar polymer polyvinylpyrrolidone (PVP). Analysis of the TCA showed that PVP is adsorbed in the form of globules on the surface of the carbon adsorbent CpY. The intervals between these may be the centers of localization for the appropriate size of the adsorbed molecules.

**Full Paper** _____ *Thematic Section:* Physicochemical Research.
*Registration Code of Publication:* 14-40-12-74 *Subsection:* Chemical Technologies.
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# Investigation of the effect of the ratio of technical carbon and silica in the tread of the automobile tires on its technological, vulcanization and performance properties

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***Keywords:*** tread, carbon black, silica, processing and performance properties.

## Abstract

In the work, it is shown that partial substitution of carbon black with silica has a positive effect on most of the technological and vulcanization properties of the tread rubber mixture. Furthermore it is established that the introduction of silica in the tread together with carbon black increases the tire resistance, dynamic endurance, grip with dry road at medium and high speeds. It is found that the wear is a complicated function of the tire. In severe conditions, wear increases with the content of silica dioxide and in mild conditions, on the contrary, decreases. In the case of traction on the ice, the introduction of silicon dioxide has a positive effect in the range of temperatures -5° ÷ -25 °C.

**Full Paper** _____ *Thematic Section:* Physicochemical Research.
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# The influence of the ratio of carbon black: silicon dioxide on the structure of the tread rubber

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***Keywords:*** structure of the tread rubber compound and vulcanizate, transmission electron microscopy, dynamic mechanical analysis, stress relaxation.

**Abstract**

Using a penetrating electron microscope we discovered a three-tier structure of silica in the tread rubber composition. It is established that in case of joint use of silicon and carbon black, the surface of carbon black particles is covered with a layer of particles of silicon dioxide of primary structure. There was estimated the effective activation energy of structural processes occurring in the tread rubber with different ratio of carbon: silica at different amplitudes of shear deformation. Using the method of tension relaxation there were revealed the structural features of the tread rubber containing only carbon black or only silica dioxide.

**Analytical Review** _____ *Thematic Section:* Physicochemical Research.
*Registration Code of Publication:* 14-40-12-94 *Subsection:* Colloidal Chemistry.
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# Micellar extraction by surfactants as a way for concentrating organic compounds

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***Keywords:*** surfactants, micellar extraction, organic analytes, concentrating.

**Abstract**

The methodology of extraction in "cloud point" on the basis of surfactant solutions of different types for concentrating organic analytes in environmental, biological liquids, food etc. was considered. Influence of different factors (concentration, temperature, pH, electrolytes, organic additives) on phase separation of surfactant aqueous solutions was discussed.

*Thematic Section:* Physicochemical Research. **Full Paper**
*Subsection:* Analytical Chemistry. *Registration Code of Publication:* 14-40-12-103
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# Test method for the determination of Fe(III) ions and their metrological characteristics

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***Keywords:*** test-method, Fe(III), surfactants, technique of binary respond.

**Abstract**

The test-method for determination of Fe(III), based on the use of immobilized indicator paper potassium thiocyanate and cetylpyridinium chloride, has been proposed. The metrological characteristics of the test-method using detection techniques with a binary respond: lower determined limit of Fe(III)content – $1 \cdot 10^{-4}$ mol/l, interval unreliability reaction $1 \cdot 10^{-4} – 1 \cdot 10^{-5}$ mol/l and $c_{min}(Fe^{3+}) = (3.5 \pm 0.2) \cdot 10^{-5}$ mol/l were determined.

**Full Paper** _____ *Thematic Section:* Physicochemical Research.
*Registration Code of Publication:* 14-40-12-110 *Subsection:* Electrochemistry.
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# Studies of reasons for the effective use of lignosulfonates in the electrolysis of zinc

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***Keywords:*** zinc, electrochemical studies, lignosulfonate, sulfates, electrolysis, polarization, the exchange current, the discharge rate, anionic surfactants , the anodic and cathode current, potential, current efficiency.

**Abstract**

Curves of potentiostatic and polarization for solutions of zinc sulfate (0.25 mol/l) and 0.025 mol/l with the background electrolyte of $Na_2SO_4$ (0.5 mol/l) in the potential range from -400 to -1400 mV (for Ag/AgCl) are obtained. The calculation of the current exchange on the results of cathode polarization upon receipt of chronopotentialmetric curves was performed. The effect of additives on electrochemical processes of anionic surfactants of lignosulfonate was studied. The possibility of efficient use of lignosulfonate in admixture with the bone glue into the zinc electrolysis process was shown.

*Thematic Section:* Physicochemical Research. **Short Communication**
*Subsection:* Petrochemistry. *Registration Code of Publication:* 14-40-12-117
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# Methods of extracting thermal bitumen from oil shale deposit Kotsebinsk

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***Keywords:*** oil shale, asphalt concrete, thermal bitumen, methods of extraction.

**Abstract**

Two methods of extracting liquid thermobitumen from oil shale deposits Kotsebinsk were developed. Resulting liquid thermobitumen can be used in road construction as an astringent element in asphalt concrete with the purpose of improving the adhesive properties of the substrate.

**Full Paper** _____ *Thematic Section:* Geochemical Research.
*Registration Code of Publication:* 14-40-12-120 *Subsection:* Catalytic Processes.
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# Gas fluids of low permeable rocks as a potential source of hydrocarbons

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***Keywords:*** gas fluids, low-permeable rock, Ashalchinskoye area, South-Tatar arch, clay minerals, activation, intercalation, the catalytic transformation, low molecular weight hydrocarbons.

**Abstract**

The possibility of the catalytic transformation of gaseous fluids of low permeable cap rocks oil fields in the low molecular weight hydrocarbons with the yield to 5% at the temperature 250 °C and a pressure of 12 atm in the presence of natural clays, activated by thermal or chemical action, as well as intercalation hydroxo aluminum salts as Keggin structures, while the highest activity is reached in the latter case.

**Full Paper** _____ *Thematic Section:* Technological Research.
*Registration Code of Publication:* 14-40-12-126 *Subsection:* Chemical Technology.
The article is published on the materials of report presented at the "International Scientific Forum Butlerov Heritage – 2015". http://foundation.butlerov.com/bh-2015/ *(English Preprint)*
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# Simulation and modeling complex for vinyl chloride polymerization by suspension method

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***Keywords:*** polymer, vinyl chloride, polymerization, initiator, medium molecular weight.

## Abstract

This article describes the results of investigations of the physico-chemical properties of polyvinyl chloride using a simulation-modeling complex of polymerization process by vinyl chloride suspension method. Simulation and modeling system allows you to define the technological parameters of the process, not amenable to direct measurement (amount of polymer-monomer particles, the temperature distribution inside the particles, the distribution of molecular mass of the polymer); provides automatic control and maintenance of optimal modes of carrying out chemical transformations. Simulation and modeling software operating in the training mode allows to acquire the skills of process control and in supervisory mode to evaluate the level of training of operating personnel.

*Thematic Section:* Kinetics Research. **Full Paper**
*Subsection:* Physical Chemistry. *Registration Code of Publication:* 14-40-12-133
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# Mechanically stressed structures and thermal degradation kinetics of zinc and cobalt acetylenedicarboxylates dehydrates

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***Keywords:*** crystalline hydrates of acetylenedicarboxylate zinc and cobalt, the kinetics of mass loss, a critical value of the mass loss, mechanochemical destruction of crystals and initiation reactions, quantum chemical calculation of strain energy.

**Abstract**

The mass loss kinetics of Zn and Co acetylenedicarboxylates was investigated in the temperature range of 263-313 K and at residual pressure of 1.3 Pa. It was shown that mass loss observed was due to dehydration that had only lasted until special critical value of residual water was reached. With a small change in that value during further dehydration the rapid collapse of ZnAC and CoAC took place involving chemical bonds destruction and formation of active particles that initiated solid state polymerization. Dehydration enthalpy was calculated using DFT methods. Model clusters of different size were considered and in every case substantial enthalpy values of 70-100 kJ/mole for each molecule of water removed were obtained. Such considerable values indicate mechanochemical activation for observed collapse of ZnAC and CoAC structures.

*Thematic Section:* Preparative Research. **Full Paper**
*Subsection:* Organic Chemistry. *Registration Code of Publication:* 14-40-12-141
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# Peculiarities of the reaction of sterically hindered nitrones with Grignard reagents

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***Keywords:*** nitroxide radicals, fluorescence, nitrones, pyrroline N-oxide, Grignard reagents.

**Abstract**

New routes of the interaction of Grignard reagents with sterically hindered nitrones pyrroline *N*-oxide series have been founded. The addition of organometallic compound was shown to proceed to formally non-activated double carbon-carbon bond with preservation of C=N at the same molecule. Hypothetical mechanism of this reaction was proposed.