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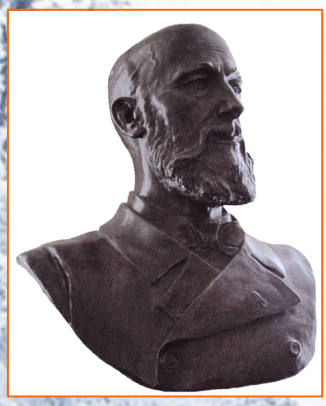

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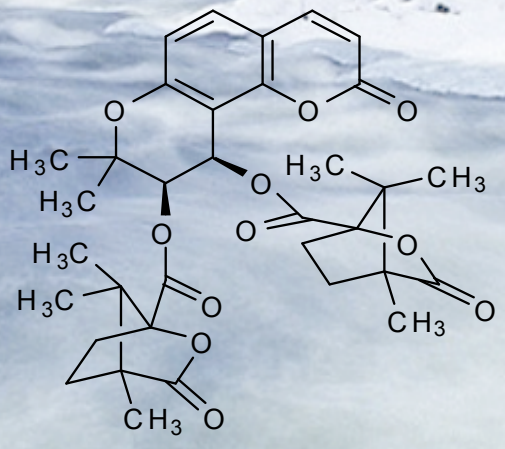

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Contributed: December 24, 2012.

Current state of synthesis and research into anti-HIV activity of the series of 2*H*-1-benzopyran-2-one compounds

© Azad Z. Abyshev,[1]*+ **Rashid A. Abyshev**,[2] **Stanislav V. Gadzikovsky**,[1] **V.H. Nguen**,[1] and **Victoria A. Morozova**[1]

[1] *Department of Pharmaceutical Chemistry. Saint-Petersburg Chemical-Pharmaceutical Academy of the Ministry of Health. Prof. Popov St., 14. Saint-Petersburg, 197376. Russia. Phone: +7 (812) 234-13-59. E-mail: azabyshev@mail.ru*

[2] *St. Petersburg Centre for the Prevention and Control of AIDS and Infectious Diseases. Emb. Obvodnoy Kanal St., 179. Saint-Petersburg, 198103. Russia. Phone: +7 (812) 251-08-53.*

*Supervising author; +Corresponding author

Keywords: *anti-HIV coumarins, kalanolid.*

Abstract

Pandemia of Human Immunodeficiency Virus (HIV) / Acquired Immune Deficiency Syndrome (AIDS) is a serious threat to the health and human development, and the search for effective compounds with anti-HIV activity was, is and will be a serious problem. In recent years there has been considerable progress in the development of drugs against HIV. A great number of heterocyclic organic compounds of different classes of natural and synthetic origin were produced, including derivatives of 2*H*-1-benzopyran (coumarin) with different structures, which showed anti-HIV activity. This survey demonstrates the diversity of structures and activity, namely, coumarin synthetic and natural origin with unique mechanisms of action, referring to the various stages of HIV replication. Recent studies using a variety of coumarins have shown that some of them are strong non-nucleoside reverse transcriptase inhibitors, and others – inhibitors of HIV-integrase or HIV-protease. Therefore, in a number of research centers abroad actively conducting research on the development of new drugs and their combined forms for the treatment of HIV-infection that would be useful for first-line therapy, and in relation to resistant mutants. Research conducted on compounds possessing anti-HIV activity give hope and optimism in this regard. This review, we describe recent advances in the discovery, study and structural modifications of the dependence structure-activity in relation to some of coumarin derivatives, showing pronounced anti-HIV activity.

Full Paper _____ *Thematic Section:* Biochemical Research.
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Conference "New methods of synthesis, structure and application of organoelemental compounds"
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Possibility of anaerobic detoxication of white phosphorus

© **Anton Z. Mindubaev**,[1]*+ **Farida K. Alimova**,[2] **Serge C. Ahossiyenagbe**,[2]
Chuluun Bolormaa,[2] **Alexandra D. Voloshina**,[1] **Natalia V. Kulik**,[1]
Salima T. Minzanova,[1] **Lubov G. Mironova**,[1] and **Dmitry G. Yahvarov**[1]*
[1] *Institution of RAS. A.E. Arbusov Institute of Organic and Physical Chemistry KazSC RAS. Arbuzov St., 8. Kazan, 420088. Republic of Tatarstan. Russia. E-mail: mindubaev@iopc.ru*
[2] *Department of Biochemistry. Kazan (Volga Region) Federal University. Universitetskaya St., 18. Kazan, 420008, Republic of Tatarstan. Russia.*

*Supervising author; +Corresponding author

Keywords: *detoxication, white phosphorus, waste water slurges, anaerobic conditions, kinetics of gas evolution.*

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. It has been established that as a result of the toxic effects of white phosphorus decomposition products the process of inhibition of methanogenic activity of microorganisms takes place, with the subsequent adaptation of microorganisms to the action of fluorine which leads to the complete biodegradation and recycling of white phosphorus into non-toxic products. White phosphorus is clearly established to suppress the microorganisms growth not immediately after application, but in the course of several days or even weeks. This means that the degradation intermediates that accumulate in the substrates possess the toxic action. Considering the change in evolved gaseous products composition one can make a conclusion about greater stability of eubacteria to white phosphorus as compared to that of methanogens. White phosphorus aggregative state and thermostating mode (mesophilic or thermophilic) do not significantly effect the vital activity of anaerobic microorganisms in the presence of white phosphorus. NMR method allowed us to establish that white phosphorus oxidizes to water-soluble compounds as a result of interaction with active sludge. White phosphorus degradation rate is demonstrated to be inversely proportional to the activity of metabolic processes in microflora that gives the evidence of biological destruction. The effect of white phosphorus on the microbe metabolites is manifested in abrupt increase of skatole and *n*-cresol content as compared to the control data, detected by GCMS method. Microorganism cultures are obtained, growing on substrate with white phosphorus content of 0.01 and even 0.1%.

Thematic Section: Biochemical Research. **Full Paper**
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Isolation of plasma blood drugs using solid phase extraction

© **Natalia A. Chuvina**, **Olga Yu. Strelova**,[+] and **Vladimir N. Kuklin***
Department of Pharmaceutical Chemistry. St. Petersburg Chemical-Pharmaceutical Academy of the Ministry of Health. Prof. Popov St., 14, Lit. A. St. Petersburg. 197376. Russia.
Phone: +7 (812) 234-13-59, 8-921-912-7257. E-mail: ous.chim-tox@yandex

*Supervising author; [+]Corresponding author

Keywords: *blood plasma, drugs, solid-phase extraction cartridges of Waters Oasis, high performance liquid chromatography.*

Abstract

The paper is devoted to studying the possibility of using the method of solid phase extraction on the basis of Oasis cartridges to isolate certain medicinal substances of different chemical structures to carry out the chemical and toxicological analysis. The cartridge Oasis HLB can be recommended for non-purposeful research on toxic substances from the group of drugs. For targeted research on the biological fluid for derivatives of barbituric acid, you should not use cartridges of the brand Oasis MAX, cartridges Oasis WAX and WCX should not be used for isolation of the studied medicinal substances from blood plasma, since they do not stay on the sorbent of the cartridge.

Thematic Section: Biochemical Research. **Full Paper**
Subsection: Cellular Metabolism. *Registration Code of Publication:* 13-33-1-43
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: December 12, 2012.

Study of oxidative stress manifestations in vetch seedlings in the presence of nickel chloride

© **Elvira A. Abramova**,[+] and **Victor V. Ivanishchev***
Department of Botany and Agricultural Technology. L.N. Tolstoy Tula State Pedagogical University. Lenin pr. St., 125. Tula, 300026. Russia. E-mail: abramea@mail.ru

*Supervising author; [+]Corresponding author

Keywords: *nickel, oxidative stress, hydrogen peroxide, lipid peroxidation, catalase, peroxidase.*

Abstract

Indicators of stress impact of nickel ions on the vetch seedlings have been defined. It has been studied Features of functioning the components of antioxidant protection in the emerging seedlings during early ontogeny have been studied.

Thematic Section: Biochemical Research. **Full Paper**
Subsection: Spectroscopy. *Registration Code of Publication:* 13-33-1-47
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: January 28, 2013.

Sample tabletting influence on the metrological parameters in the NIR-analysis of mixed fodders

© **Alexander P. Bayunov**,* and **Sergey N. Smaryguin**[+]
Department of Inorganic and Analytical Chemistry. Russian State Agrarian University - MTAA K.A. Timiryazev. Timiryazevskaya St., 49. Moscow, 127550. Russia.
Phone: +7 (499) 976-03-81. E-mail: ssmarygin@timacad.ru

*Supervising author; [+]Corresponding author

Keywords: *near infrared, reproducibility, mixed fodders, tabletting.*

Abstract

This article deals with sample tabletting as a method of sample preparation and its influence on mixed fodder NIR-analysis. Sample tabletting allows to reduce the factors that influence the reproducibility of spectra in the nearest infrared spectra and to improve sample quality. A method based on the correlation of standard deviation with spectral intensity analysis has been developed to control the sample quality.

Thematic Section: Preparative Chemistry. **Full Paper**
Subsection: Organic Chemistry. *Registration Code of Publication:* 13-33-1-55
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: January 28, 2013.

Functionalization of the pyrrol ring in naphtho[1,2,3-*cd*]indol-6(2*H*)-ones

© **Olga I. Kargina**, **Anna V. Bindareva**, and **Leonid M. Gornostaev***[+]
Department of Chemistry. Astaf'ev Krasnoyarsk State Pedagogical University. A. Lebedevoy St., 89. Krasnoyarsk, 660049. Russia. Phone: +7 (391) 217-17-29. E-mail: gornostaev@kspu.ru

*Supervising author; [+]Corresponding author

Keywords: *aminomethylation, 1-amino-2-methylnaphtho[1,2,3-cd]indol-6(2H)-one, 1-nitro-2-methylnaphtho[1,2,3-cd]indol-6(2H)-one, 1-chloroacetylamino-2-methylnaphtho[1,2,3-cd]indol-6(2H)-one, nucleophilic substitution, functionalization of naphtho[1,2,3-cd]indol-6(2H)-one.*

Abstract

The functionalization of the pyrrol ring in naphtho[1,2,3-*cd*]indol-6(2*H*)-ones was studied. The reaction of nucleophilic substitution of nitro group in 1-nitro-2-methylnaphtho[1,2,3-*cd*]indol-6(2*H*)-one under the influence of arenols, arentiols and mercaptoacetic acid was examined. The aminometylation of naphtho[1,2,3-*cd*]indol-6(2*H*)-one to give *N*-substituents of naphtho[1,2,3-*cd*]indol-6(2*H*)-one proceeds by the atom of nitrogen. Based on 1-amino-2-methylnaphtho[1,2,3-*cd*]indol-6(2*H*)-one and cloroacetyl chloride we obtained 1-chloroacetylamino-2-methylnaphtho[1,2,3-*cd*]indol-6(2*H*)-one. The chlorine atom in 1-chloroacetylamino-2-methylnaphtho[1,2,3-*cd*]indol-6(2*H*)-one was substituted by secondary amines.

Thematic Section: Preparative Chemistry. **Full Paper**
Subsection: Organic Chemistry. *Registration Code of Publication:* 13-33-1-61
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http://butlerov.com/readings/
Contributed: December 19, 2012.

trans-2-[2-(1-Naphtyl)vinyl]- and *trans*-2-[2-(2-fluorenyl)vinyl]-3-phenyl-*3H*-quinazolin-4-ones: synthesis and photo-physical properties

© **Emilia V. Nosova**,[1+] **Tatiana V. Stupina**,[1] **Galina N. Lipunova**,[2]
and **Valery N. Charushin**[1,2]*
[1] *Department of Organic Chemistry. Chemical Technology Institute. Urals Federal University Named After the First President of Russia Boris N. Yestsin. Mira St., 19. Ekaterinburg, 620002. Russia. Phone: +7 (343) 375-45-01. E-mail: emily74@rambler.ru*
[2] *I. Ya. Postovsky Institute of Organic Synthesis. Ural Division of the Russian Academy of Sciences. S. Kovalevskoy St., 22. Ekaterinburg, 620219. Russia. Phone: +7 (343) 362-30-65. E-mail: lipunova@ios.uran.ru*

*Supervising author; +Corresponding author

Keywords: *styryl dyes, photoluminescence, styrylbenzazines, quinazolin-4-ones, 2-methyl-3,1-benzoxazin-4-one, (aryl) methylenephenylamines.*

Abstract

Synthesis of novel styrylquinazolinones has been performed by means of transformation of hetero-ring of 2-methyl-3,1-benzoxazin-4-ones under the action of (naphtalin-1-yl)- and (9*H*-fluoren-2-yl)-methylenephenylamines upon heating under reflux in glacial acetic acid in the presence of sodium acetate. Adsorption and fluorescence spectra of compounds obtained have been studied.

Thematic Section: Preparative Chemistry. **Full Paper**
Subsection: Organic Chemistry. *Registration Code of Publication:* 13-33-1-65
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: January 31, 2013.

Synthesis of 1,3-disubstituted ureas and bisureas – structural elements for supramolecular compounds

© **Ekaterina A. Zubovich**,[1+] **Vladimir V. Burmistrov**,[1]* **Boris A. Lysich**,[1]
Sergey V. Dyakonov,[1] **Dmitry V. Danilov**,[1] and **Gennady M. Butov**[2]*
[1] *Volgograd State Technical University. VSTU. Pr. Lenin St., 28. Volgograd, 400005. Russia. Phone: +7 (917) 848-49-18. E-mail: ekamneva@rambler.ru*
[2] *Volzhsky Polytechnic Institute (branch) Volgograd State Technical University. Engels St., 42a. Volzhsky, 404121. Volgograd region. Russia. Phone: +7 (8443) 22-19-59 E-mail: butov@volpi.ru*

*Supervising author; +Corresponding author

Keywords: *isocyanate, adamantane, adamantyl, urea, 1,3-dimethyladamantane.*

Abstract

We synthesized 1,3-disubstituted ureas and bisureas of adamantane series that can be used as molecular components for the synthesis of supramolecular complexes, in particular, rotaxanes or as monomers for supramolecular cyclodextrine polymers. The reactions were carried out under mild conditions with high yields. The article presents data on the synthesis of new 1,3-adamantyldisubstituted ureas and bisureas.

Thematic Section: Preparative Chemistry. **Full Paper**
Subsection: Coordination Chemistry. *Registration Code of Publication:* 13-33-1-69
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: January 28, 2013.

Synthesis and composition of complexes of transitive metals with some α-carbonyl-containing arylhydrazones

© **Olga V. Kovalchukova**,[1]*+ **All TahanRana Abdulila Abbas**,[1,2] **Boris E. Zaitsev**,[1]* **Svetlana B. Strashinova**,[1] **Oleg V. Volyansky**,[3] and **Dmitry N. Kuznetsov**[3]
[1] *Department of General Chemistry. Peoples' Friendship University of Russia. Miklukho-Maklay St., 6. Moscow, 117198. Phone: +7 (495) 955-08-60.*
[2] *Chemistry Department. Technological Institute. Baghdad. Iraq.*
[3] *Department of Organic Chemistry. Moscow State University of Design and Technology. Sadovnicheskaya St., 33. Moscow, 117997. Russia. E-mail okovalchukova@mail.ru*

*Supervising author; +Corresponding author

Keywords: *complexes, arylhydrazones, synthesis, spectral characteristics, formation constants, correlation.*

Abstract

We have isolated in crystalline state and studied with a set of spectral methods of investigation 8 complexes of manganese(II), nickel(II), copper(II) and cadmium(II) with some α-carbonyl-containing arylhydrazones. On the basis of spectral characteristics (IR, electron spectroscopy) we defined the character of coordination and suggested the schemes of composition of coordination compounds.

Full Paper _____ *Thematic Section:* Quantum-Chemical Research.
Registration Code of Publication: 13-33-1-74 *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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The electronic absorption spectra and the structure of 6-(2-methyl-5-oxo-1-phenyl-4,5-dihydro-1*H*-imidazole-4-ilazo)-1-oxo-2,5-dihydro-1*H*-benzo[4,5]imidazo[1,2-c] pyrimidine -7- carboxylic acid

© **Olga V. Kovalchukova**,[1]*+ **Mikhail A. Ryabov**,[1] **All TahanRana Abdulila Abbas**,[1,2]
Boris E. Zaitsev,[1]* **Svetlana B. Strashinova**,[1] and **Oleg V. Volyansky**[1]
[1] *Department of General Chemistry. Peoples' Friendship University of Russia. Miklukho-Maklay St., 6. Moscow, 117198. Phone: +7 (495) 955-08-60. E-mail okovalchukova@mail.ru*
[2] *Chemistry Department. Technological Institute. Baghdad. Iraq.*

*Supervising author; +Corresponding author

Keywords: *electron spectroscopy, quantum-chemical calculations, PPP, PM3, benzo[4,5]imidazo[1,2-c] quinazoline, derivatives.*

Abstract

Using spectral (electron spectroscopy) and quantum-chemical (PPP, PM3) methods we studied tautomeric and ionic forms 6-(2-methyl-5-oxo-1-phenyl-4,5-dihidro-1*H*-imidazole-4-ilazo)-1-oxo-2,5-dihidro-1*H*-benzo[4,5]imidazo[1,2-c]pyrimidine-7-carboxxylic acid. Its primary existence as non-flat CH-azo tautomer has been shown.

Full Paper _____ *Thematic Section:* Quantum-Chemical Research.
Registration Code of Publication: 13-33-1-78 *Subsection:* Organic Chemistry.
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Quantum-chemical modeling of the metal chelate cycles of methylphloroglucine phenylazo derivatives

© **Svetlana B. Strashinova**,*+ **Olga V. Kovalchukova**,* **Ekaterina P. Romashkina**, **Oksana V. Avramenko**, and **Oleg V. Volyansky**
Department of General Chemistry. Peoples' Friendship University of Russia. Miklukho-Maklay St., 6. Moscow, 117198. Phone: +7 (495) 955-08-60. E-mail sstrashnova@mail.ru

*Supervising author; +Corresponding author

Keywords: *metalchelate cycle, methylphloroglucine, quantum-chemical modeling, density functional theory.*

Abstract

We performed quantum-chemical modeling of five- and sixmembered metalchelate cycles of the complex Ni^{2+} with 2-phenyl-4-nitro-2,4,6-trihydroxytoluene H_4L.

Based on the relevant changes of the experimental and calculated electronic absorption spectra upon complexation we determine the most preferable type of coordination.

Thematic Section: Thermodynamic Research. **Full Paper**
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http://butlerov.com/readings/
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Thermodynamic properties of lead-scandium alloys enriched by fusible component

© **Alexey B. Shubin**,[1+] **Konstantin Yu. Shunyaev**,[1]* and **Leonid F. Yamshchikov**[2]
[1] *Institute of Metallurgy, Urals Branch of RAS. Amundsen St., 101. Ekaterinburg, 620016. Russia.*
Phone: +7 (343) 232-91-38. E-mail: abshubin@gmail.com
[2] *Urals Federal University. Mira St., 19. Ekaterinburg, 620002. Russia.*

*Supervising author; +Corresponding author

Keywords: *scandium, lead, alloy, thermodynamic properties, structure.*

Abstract

In this paper, we studied thermodynamic properties of scandium in its liquid alloys with lead in the temperature range of 650-1040 K. Two modifications of the electromotive forces (EMF) method were used for measurements. The first (classical EMF method) included the potential determination during long time interval (about 1-2 h) for each temperature point. The second (chronopotentiometric method) allowed us to investigate the potential of galvanic elements within comparatively short time interval and, further, to carry out large number of measurements at different temperatures. The results of both methods are in good agreement. This fact allows us to merge EMF data to one linear dependence. Partial Gibbs energy of scandium in liquid two-phase alloy of the composition (L + Pb_6Sc_5) (where L is liquid solution of Sc in Pb) can be determined by the equation: $\Delta G_{Sc} = - (90.93 \pm 2.1) + (6.7 \pm 2.3) \cdot 10^{-3}$ T, kJ/mol Sc.

Thematic Section: Chemical and Technological Research. **Full Paper**
Subsection: Organic Chemistry. *Registration Code of Publication:* 13-33-1-87
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http://butlerov.com/readings/
Contributed: January 17, 2013.

Purification of octene-1 from vinylidene compounds by oligomerization reaction

© **Mikhail S. Ahmedyanov**,[1+] **Raisa A. Ahmedyanova**,[1] **Alexander G. Liakumovich**,[1]*
Oleg I. Gnezdilov,[1] and **Vladimir G. Uryadov**[2]

[1] *Department of Synthetic Rubber. Kazan National Research Technological University.*
K. Marx St., 68. Kazan, 420015. Republic of Tatarstan. Russia.
Phone: +7 (843) 231-43-91. E-mail: limarsel@mail.ru

[2] *Department of Organic Chemistry. Kazan National Research Technological University.*
K. Marx St., 68. Kazan, 420015. Republic of Tatarstan. Russia.
Phone: +7 (843) 231-43-81. E-mail: vguryadov@mail.ru; uryadov@kstu.ru

*Supervising author; +Corresponding author

Keywords: *polyethylene, α-olefins, vinylidene compounds.*

Abstract

The process of purification of alpha-olefins C_8 fractions from vinylidene compounds based on separation of α-olefin from vinylidene compounds oligomerized under mild conditions. The efficiency of the proposed technology is shown.

Thematic Section: Chemical Technology. **Full Paper**
Subsection: Polymer Chemistry. *Registration Code of Publication:* 13-33-1-93
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 aromatic oligoesterdiols and thermally stable polyurethane coatings on their basis

© **Maria A. Paserb**,[+] **Indira N. Bakirova**,* and **Alexander Ya. Samuilov**
Department of Technology of Synthetic Rubber. Kazan National Research Technological University.
K. Marx St., 68. Kazan, 420015. Republic of Tatarstan. Russia.
Phone: +7 (843) 231-95-89. E-mail: paserbm@mail.ru

*Supervising author; [+]Corresponding author

Keywords: *diphenylolpropane oxyethylated; aromatic oligoesterdiols; heat-resistant polyurethane coatings.*

Abstract

Aromatic oligoesterdiols were synthesized from bis-2-hydroxyethyl ether of 4,4′-dioxydiphenyl-2,2-propane and then used to obtain polyurethane coatings. It was established that these coatings are characterized by high thermal stability, hardness, durability and adhesion. It was shown that the hardness of coatings increase naturally with the increase in concentration of a polyisocyanate and reduction of molecular weight of oligoesterdiol.

Thematic Section: Physicochemical Research. **Full Paper**
Subsection: Inorganic Chemistry. *Registration Code of Publication:* 13-33-1-97
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
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Thematic course: Hydrochemical synthesis of metal chalcogenide films. Part 16.

The chemical bath deposition and study of thin films in the system $Cu_2S–In_2S_3$

© **Stanislav S. Tulenin**,[1] **Vyacheslav F. Markov**,[1]*
Larisa N. Maskaeva,[2+] and **Mikhail V. Kuznetsov**[3]
[1] *Department of Physical and Colloidal Chemistry. Ural Federal University Named After the First President of Russia B.N. Yeltsin. Mira St., 19. Ekaterinburg, 620002. Sverdlovsk area. Russia. Phone: +7 (343) 375-93-18. E-mail: mln@e-sky.ru*
[2] *Department of Chemistry and Burning Processes. UISFS of EMERCOM of Russia. Mira St., 22. Ekaterinburg, 620022. Russia. Phone: +7 (343) 360-81-68. E-mail: mln@e-sky.ru*
[3] *Institute of Chemistry of Solid State. Ural Branch of the Russian Academy of Sciences. Pervomaiskaya St., 91. Ekaterinburg, 620990. Russia. Phone: +7 (343) 362-33-56. E-mail: kuznetsov@ihim.uran.ru*

*Supervising author; +Corresponding author

Keywords: *chemical bath deposition, copper sulfide(I), indium sulfide(III), thin films, type of conductivity, x-ray photoelectron spectroscopy.*

Abstract

For the first time the thin films of $In_xCu_{1-x}S_yO_{1-y}$ composition with the content of indium up to 9.63 at% were obtained by means of a chemical bath deposition from the system "indium chloride − copper chloride − sodium hydroxide − tiourea" and "indium chloride − copper chloride − sodium hydroxide – trilon B − tiourea". The experimental data on the distribution and the atomic ration of elements in synthesized patterns obtained by the x-ray photoelectron spectroscopy were discussed. The change in the surface microstructure of thin films depending on the temperature and the composition of reaction bath were determined by means of scanning electron microscopy. The structure of the obtained thin films has *n*-type of conductivity.

Full Paper _____ *Thematic Section:* Physicochemical Research.
Registration Code of Publication: 13-33-1-104 *Subsection:* Inorganic 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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Platinum(IV) sorption by the modified carbon-mineral sorbent

© **Tatiana A. Kovalenko**,[+] and **Ludmila N. Adeeva***
Department of Inorganic Chemistry. Omsk State University. Mira St., 55A.
Omsk, 644077. Russia. Phone: +7 (3812) 26-81-99. E-mail: kovalenko_85@list.ru

*Supervising author; [+]Corresponding author

Keywords: *sorption, platinum, modified sorbent, polyaniline, carbon-mineral sorbent, desorption.*

Abstract

Results of research of selective extraction of platinum(IV) with the use of the synthesized modified carbon-mineral sorbent are given. The sorbent is modified by polyaniline in the form of the emeraldin-basis. Capacity of the obtained sorbent on platinum(IV) makes 62 mg/g, and is not lowered in the presence of the ions of copper(II), nickel(II), iron(III), being in concentrations of the order greater than the concentration of platinum. By IR-spectroscopy it is shown that platinum sorption on the modified sorbent proceeds by amino groups. As the eluent we can use the hydrochloric acid solution of thiourea.

Thematic Section: Thermodynamic Research. **Full Paper**
Subsection: Physical Chemistry. *Registration Code of Publication:* 13-33-1-109
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Equilibrium distribution of clusters in the size of the finite system

© Ihtiyor H. Umirzakov
Simulation laboratory. Institute of Thermal Physics at SB RAS. Pr. Lavrent'eva St., 1. Novosibirsk, 630090. Russia. Phone: +7 (383) 354-20-17. E-mail: tepliza@academ.org

Keywords: *isolated and isothermal systems, microcanonical and canonical ensembles, cluster, nanoparticle, size distribution function, thermodynamic equilibrium.*

Abstract

Methods of statistical thermodynamics were used to find the equilibrium distribution of clusters (nanoparticle) by sizes in the system formed of finite numbers of molecules (atoms), being in the long confinement at constant total energy (isolated system). On the basis of the kinetic nucleation equation using single droplet approximation the distribution function was found both for isolated and for the isothermal systems. The results are compared with the data of computer simulation of finite two-dimensional systems.

Full Paper _____ *Thematic Section:* Thermodynamic Research.
Registration Code of Publication: 13-33-1-122 *Subsection:* Phase Equilibria.
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The significance of the isochoric heat capacity at the critical point of phase equilibrium gas-liquid

© Ihtiyor H. Umirzakov
Simulation laboratory. Institute of Thermal Physics SB RAS. Pr. Lavrent'eva St., 1. Novosibirsk, 630090. Russia. Phone: +7 (383) 354-20-17. E-mail: tepliza@academ.org

Keywords: *heat capacity, speed of sound, one-component material, phase equilibrium gas-liquid critical point*

Abstract

The popular viewpoint is that the speed of sound at the critical point of phase equilibrium gas-liquid of one-component material is zero, which is a consequence of the treatment in the infinity of isochoric heat capacity on the critical isochore at the critical temperature. Still there is no experimental proof of the latter, since nobody managed to obtain experimentally the infinite value of the specific heat at the critical point. We have shown that the behavior of isochoric heat capacity at the critical point can be described by nonanalytic function критической точки может быть описано неаналитической функцией, having a finite value at the critical point, so that the sound speed at the critical point is not zero. This function gives a finite value for the jump of isochoric heat capacity at the critical density of the transition through the critical point.

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Characteristic features of task statement at the numerical research of metallized condensed substance ignition by a local power source

© **Dmitry O. Glushkov**,[+] and **Pavel A. Strizhak***
National Research Tomsk Polytechnic University. Lenin St., 30. Tomsk, 634050. Russia.
Phone: +7 (3822) 70-17-77 (1910). E-mail: dmitriyog@tpu.ru

*Supervising author; [+]Corresponding author

Keywords*: ignition, metallized condensed substance, heat transfer, particle, plate, mathematical modeling.*

Abstract

Comparison of ignition results of the heterogeneous condensed substance of the small single particle heated to high temperatures and a "hot" massive plate within models of two-dimensional and one-dimensional heat transfer was carried out. Ignition time delays of the metallized condensed substance were defined. Scales of local power source heat content influence on process characteristics are established. It has been shown that the use of heat transfer model with first boundary condition leads to greater deviations of local ignition time delay than with the two-dimensional model.

Thematic Section: Physicochemical Research. **Full Paper**
Subsection: Chemistry of Complex Compounds. *Registration Code of Publication:* 13-33-1-133
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Contributed: December 20, 2012.

The study of the solubility of complexes with general formula $aM^nCl_n \cdot mZnCl_2 \cdot pEt_2O$ in the media of diethyl ether (where M = Li, Mg, Ca, Sr, Ba; a = 1-2; n = l-2; m = l.2; p = 2-6; Et_2O – diethyl ether)

© **Yury M. Mikhailov**,[1]* **Roza F. Gatina**,[1]* **Zalimkhan K. Omarov**,[2+] and **Oksana N. Shakurskaya**[1]
Federal State Enterprise "State Scientific-Research Institute of Chemical Products". Svetlaya St., 1. Kazan, 420033. Russia. Phone: Phone: +7 (843) 544-07-21. E-mail: gniihp@bancorp.ru;
[2)] *Phone: +7 (843) 541-76-02. E-mail: omarov@mail.ru*

*Supervising author; [+]Corresponding author

Keywords: *complex compounds, diethyl ether, solvent.*

Abstract

For isothermal solubility studies in systems M^nCl_n-$ZnCl_2$-Et_2O, 298K we have established the regions of equilibrium crystallization of complexes: $aM^nCl_n \cdot mZnCl_2 \cdot pEt_2O$ (where M = Li, Mg, Ca, Sr, Ba; n = 1-2; m = l.2; p = 2-6; Et_2O – diethyl ether) and the formation of chloride complexes: $LiCl \cdot ZnCl_2 \cdot 4Et_2O$, $LiCl \cdot ZnCl_2 \cdot 4Et_2O$, $MgCl_2 \cdot ZnCl_2 \cdot 2Et_2O$, $CaCl_2 \cdot ZnCl_2 \cdot 4Et_2O$, $SrCl_2 \cdot ZnCl_2 \cdot 4Et_2O$, $2BaCl_2 \cdot ZnCl_2 \cdot 6Et_2O$.

Discovered complexes were isolated. By elemental analysis we established the composition of phases formed in the system $aM^nCl_n \cdot mZnCl_2 \cdot pEt_2O$.

Thematic Section: Research into New Materials. **Full Paper**
Subsection: Coordination Chemistry. *Registration Code of Publication:* 13-33-1-139
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Sorbent of hydrogen sulfide on the basis of complex compound with the formula $MgCl_2 \cdot ZnCl_2 \cdot 2Et_2O$ (where Et_2O – diethyl ether)

© **Yury M. Mikhailov**,[1]* **Roza F. Gatina**,[1]* and **Zalimkhan K. Omarov**[2+]
Federal State Enterprise "State Scientific-Research Institute of Chemical Products".
Svetlaya St., 1. Kazan, 420033. Russia. Phone: [1)] *+7 (843) 544-07-21,* [2)] *+7 (843) 541-76-02.*
E-mail: [1)] *gniihp@bancorp.ru,* [2)] *omarov@mail.ru*

*Supervising author; [+]Corresponding author

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

Abstract

Sorbent of hydrogen sulfide, composed of the complex compound with the formula $MgCl_2 \cdot ZnCl_2 \cdot 2Et_2O$ (where Et_2O – diethyl ether) on the solid porous substrate has been obtained.

A number of experiments have been conducted to study the sorption properties of the obtained sorbent of hydrogen sulfide.

Thematic Section: Research into New Materials. _____ **Short Communication**
Subsection: Kinetics and Catalysis. *Registration Code of Publication:* 13-33-1-143
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Oxidation catalyst of hydrogen sulfide, composed of a complex compound with the formula $LiCl \cdot ZnCl_2 \cdot 4(C_2H_5)_2O$ on the substrate

© **Yury M. Mikhailov**,[1]* **Roza F. Gatina**,[1]* and **Zalimkhan K. Omarov**[2+]
Federal State Enterprise "State Scientific-Research Institute of Chemical Products".
Svetlaya St., 1. Kazan, 420033. Russia. Phone: [1)] *+7 (843) 544-07-21,* [2)] *+7 (843) 541-76-02.*
E-mail: [1)] *gniihp@bancorp.ru ,* [2)] *omarov@mail.ru*

*Supervising author; [+]Corresponding author

Keywords: *complex compounds, diethyl ether, catalyst, hydrogen sulfide.*

Abstract

Oxidation catalyst of hydrogen sulfide, composed of a complex compound with the formula $LiCl \cdot ZnCl_2 \cdot 4(C_2H_5)_2O$ on the solid porous substrate have been obtained.

A number of experiments have been conducted to study the catalytic properties of a new catalyst under various conditions.

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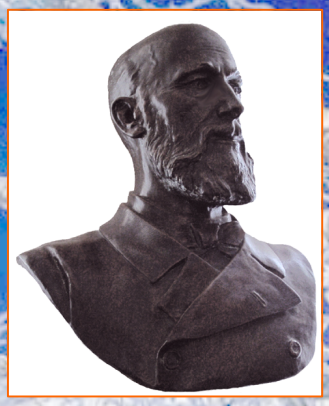

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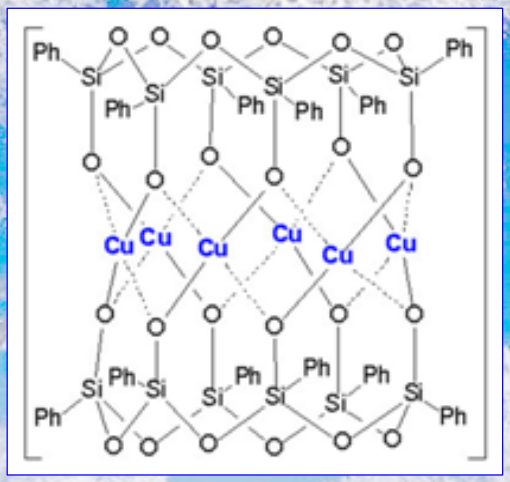

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Fundamental bases of the structure of substance

© Alexey A. Potapov
Irkutsk. Russia. Phone: +7 (395) 246-30-09. E-mail: aleksey.potapov.icc@gmail.com

***Keywords**:* substance, atom, molecule, model, covalent bond, intermolecular structure, crystals, intermolecular interactions.

Abstract

New approach to creation of the predictive theory of substance in a logic-genetic linkage of hierarchical levels in a chain is offered: atom – a molecule – substance. Fundamental difference of the offered approach is the theory of an electronic structure of atom which cornerstone the dipole- shell model of multielectronic atoms within which the nature and the mechanism of formation of electronic structure of atoms is established is so-called. The understanding of an electronic structure of atoms predetermined understanding of the nature and the mechanism of formation of molecules as structural elements of substance. A basis of formation of molecules is covalent bond which quantitative description found in universal model of a ring on a molecule axis.

Full Paper _____ *Thematic Section:* Technological Research.
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Molecular brownian motors or stochastic transport in ratchet-potential, forming structural features oxyhydrated clusters

© **Yuriy I. Sukharev**, and **Inna Yu. Apalikova**

Department of Chemistry of Solids and Some Processing Stages. Chelyabinsk State University. Br. Kashirinyh St., 129. Chelyabinsk, 454000. Russia. Tel.: (351) 799-70-63. E-mail: Yuri_Sucharev@mail.ru

*Supervising author; +Corresponding author

Keywords: Lagrangian mapping oxyhydrate gel systems, colloidal clusters, spontaneous pulsating flow, diffuse electric double layer topological continuum-dissociative disproportionate mechanism Whitney theory, geometry caustics.

Abstract

Understanding of the formation of the structuring element oxihydrate heavy metals in non-equilibrium conditions allows us to hope for a sorbents based on oxihydrate with specified sorption characteristics. Study of nonlinear properties of gel oxyhydrate systems found the following features: dilatant oscillating, oscillating (pulsation) electrical conductivity, electric current spontaneous self-organization on the background of the gel polarization phenomena stained gel systems, vibrational, optical and sorption properties and much more.

In our data the behavior of charged fragments around some center. According to our previous papers, the part oxyhydrated fragments have the property itself centers around a gel clusters having a specific electric moment. This raises the important question of the interaction of colloidal clusters in the dispersion medium. Suppose that in a certain spatial region oxyhydrate clusters do not interact with the gel microheterogeneous environment, as large macromolecular education hardly move in volume. Diffusion of them very delayed, the centers of mass are inactive. In the limited space of the same area of the colloidal clusters intensively interact with the environment and with each other. This interaction occurs through conformational motion gel cluster-cluster formations or close to processes (polymerization-peptization), due to the dynamic phenomena "chlopyvaniya" or "break" DES macromolecules with emission in the dispersion medium-flowing nanoclusters and the creation of quasi-stable intermediate DES different capacity. These processes can be called dissociative-disproportionate effects.

Thematic Section: Theoretical Research. **Full Paper**
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Giant clusters of distilled water in ratchet forming coxeter space

© **Yury I. Sukharev**, **Inna Yu. Apalikova**, and **Oksana M. Shamina**
Department of Chemistry of Solids and Some Processing Stages. Chelyabinsk State University.
Br. Kashirinyh St., 129. Chelyabinsk, 454000. Russia.
Tel: +7 (351) 799-70-63. E-mail: Yuri Sucharev@mail.ru

*Leader of the thematic course; +Corresponding author

Keywords: Lagrangian mapping, electroglow, fulleroid, multipoles, oxyhydrates system, colloidal clusters, spontaneous pulsation flow, the diffuse electric double layer, topological continuum, dissociation disproportionate mechanism, theory of Whitney, the geometry of caustics.

Abstract

Whenever a moving cluster is in a cell containing an obstacle or obstacles, a reaction occurs, which needs those obstacles. That is, point reflex maps of those interacting fragments form. Those maps are Coxeter polygons, including individual megaclusters, as with water clusters. The following giant formations can be discerned on calculated giant clusters: fulleroid polytopes of giant clusters of, e.g., water or oxyhydrates (with 17 or more vertexes) can be clearly observed; and pyramidal polygons with 10 vertexes and octahedral with six vertexes are also observable.

Full Paper _____ *Thematic Section:* Technological Research.
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Thematic course: Numerical characteristic of the organic molecule structure. Part 18.

On the issue of the motion of nonelectrolyte molecules

© Vladimir G. Uryadov
Department of Organic Chemistry. Kazan National Research Technological University.
K. Marx St., 68. Kazan, 420015. Russia. Phone: +7 (8432) 63-87-95. E-mail: uryadov@kstu.ru

Keywords: topological index, rotational movement, force of gravity, heat capacity, viscosity.

Abstract

Certain forms of molecular motion of non-electrolytes, as well as the role of the Earth's gravity forces in the nature of intermolecular interactions have been studied. On the basis of the ideal gas equation and the expression of universal gravitation law, a formula have been obtained for the relationship of linear temperature of the molecular ensemble and the weight of the constituting molecules. The actual dependence of the experimental values of the boiling point of a series of alkanes of normal structure on the molecular weight is given by a smooth convex curve. Based on the analysis of the boiling point of alcohols, cycloalkanes, poly halogen alkanes, including hydrogen atoms in the molecule, and per-halogen alkanes, it has been suggested that the basis of the interaction of molecules in the liquid phase, perceived as the dispersion, is the balance between the force of attraction to the Earth and repulsion of electronic shells of molecules. Based on the above ideas about the manifestation of intermolecular interactions we derived regression equations defining the boiling point of alkanes of normal structure as a function of molar mass and previously introduced by us energy and structural parameter and as a function of molar mass, energy and structural attributes and values J_W, – a parameter entered by us with the rotational positions of molecular motion in order to describe the physical and chemical properties of fluids. In addition to the rotational motion we considered the motion of the molecules in the liquid along closed trajectories, the limiting case of it being the circle. For a number of normal structure alkanes we defined the values of the circle radius basing on the density data at various temperatures. The presence of the relationship of square radius with the heat capacity of alkanes has been established. The plotted dependence curves include two distinct sections. One is practically parallel to the axis of abscissas indicating the absence of the specific heat dependence on the radius. The other section represents a linear dependence of the specific heat on the square of the radius. The first portion of plots is related to the quasi fluid. The second section is regarded as a gas-like liquid. We have also obtained the dependences of the reverse viscosity of alkanes on the cube of the radius. These dependences are regarded as an indication of the intensification of heat transfer in a liquid with the temperature rise. On the basis of the obtained dependences a supposition has been suggested on the features of the nature of the liquid phase.

Full Paper _____ *Thematic Section:* Technological Research.
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Simulation of a scrubbing process in a passing filter with a random packing

© **Andrew A. Permyakov**,[+]* **Tatiana A. Eneykina**,[+]* **Zalimhan K. Omarov**, and **Rose F. Gatina**
State Research Institute of Chemical Products. Federal State Enterprise.
Svetlaya St., 1. Kazan, 420033. Russia. Phone: +7 (843) 544-07-21. E-mail: gniihp@bancorp.ru

*Supervising author; [+]Corresponding author
Keywords: sorbent, hydrogen sulphide, scrubbing, simulation.

Abstract

A computer simulation of the process of gas distribution to a filter volume during its clearing off hydrogen sulphide was carried out using an Ansys code. An analysis of a distribution of gas streams depending on a diameter of an inlet nozzle was carried out for estimating of a sorbent consumption during scrubbing.

Full Paper _____ *Thematic Section:* Quantum-Chemical Research.
Registration Code of Publication: 15-41-2-82 *Subsection:* Organic Chemistry.
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Study of chemical bonding in the complexes of interhalogen based on density functional theory

© **Oleg Kh. Poleshchuk**,[1]*+ **Anna G. Yarkova**,[2] **Alexander V. Fateev**,[2] **Myrzabek N. Ermakhanov**,[3] and **Pulat A. Seidakhmetov**[3]
[1] *National Research Tomsk Polytechnic University. Lenin Ave., 30. Tomsk, 634050. Russia.*
[2] *Tomsk State Pedagogical University. Kievskaya St., 60. Tomsk, 634061. Russia.*
[3] *South Kazakhstan State University Named after M. Auezov. Tauke Khan Ave., 5. Shymkent. Republic of Kazakhstan. E-mail: poleshch@tspu.edu.ru*

*Supervising author; +Corresponding author
Keywords: microwave spectroscopy, density functional theory, chemical bonding, quadrupole interaction, molecular orbitals.

Abstract

The density functional theory analysis was used for a number XYL complexes, formed between molecules I_2, ICl, IBr and pyridine. The calculated geometrical parameters, IR spectra and nuclear quadrupole interaction constants of iodine are consistent with the data of microwave spectroscopy and nuclear quadrupole resonance. The good correlation between the experimental and calculated binding energies of the inner electrons of iodine, chlorine and nitrogen atoms were found with the calculation of Gaussian and Slater functions. The comparison of experimental and calculated changes in the electron density on the atoms upon complex formation allowed choosing the scheme of calculating the effective charge on the atoms, which allow us to interpret the experimental spectra. It is shown that the use of both calculated schemes allows calculating the enthalpy of complex formation, close to the experimental values. The energy analysis shows that in the complexes the electrostatic binding is of dominates to that of covalent binding.

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New approach to Boulton-Katritzky rearrangement

© **Timofey V. Rybin**,[+] and **Aleksandr V. Belik***[+]
Chelyabinsk State University. Department of Chemistry. Chair of Chemical Engineering and Computational Chemistry. Kashyrinikh Bros. St., bld.129. Chelyabinsk, 454001. Russia.
Phone: +7 (351) 799-70-66. E-mail: rybintv@csu.ru

*Supervising author; [+]Corresponding author
***Keywords**:* heterocycles, furoxan, Boulton-Katritzky rearrangement, DFT calculations.

Abstract

The charge-changing analysis of atoms during molecular vibrations in compounds, participating in Boulton-Katritzky rearrangement, was conducted. The correlation between reaction pathways and charge's behavior of certain atoms during molecular vibrations was found for initial compounds and products of reaction. A novel approach was proposed for analysis of reaction direction.

Thematic Section: Quantum-Chemical Research. **Full Paper**
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Computation of vibration spectra of 4-nitro-benzofuroxan in coordinates X_{δ}^{0}

© **Alexander V. Belik**
Faculty of Chemical Technology and Computing Chemistry. Chelyabinsk State University.
Kashyrinykh Brothers St., 129. Chelyabinsk, 454001. Russia.
Phone: +7 (351) 799-70-66. E-mail: belik@csu.ru

Keywords: 4-nitro-benzofuroxan, the generalized force constants, coordinates X_{δ}^{0}, calculations DFT, vibration frequencies.

Abstract

Within the framework of approach B3LYP 6-311++G(3df,3pd) the force field of 4-nitro-benzofuroxan molecule in coordinates X_{δ}^{0} for the first time is received. Frequencies of normal vibrations were calculated. Generalized force constants of molecule was carried out.

Thematic Section: Quantum-Chemical Research. **Full Paper**
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Kinetics and mechanisms of the ozonolysis of 1,3-butadiene according to quantum chemical calculations

© **Anastasia A. Vyazovaya**,[1]*+ **Boris E. Krisyuk**,[2,3]*+
Alexey V. Mayorov,[1,4]* and **Anatoly A. Popov**[1,3]

[1] *Laboratiry of Physics and Chemistry of Synthetic and Nature Polymer Blends. N.M.Emanuel Institute of Biochemical Physics of the Russian Academy of Sciences. Kosygina St., 4. Moscow, 119334. Russia.*
[2] *Laboratory of Kinetic of Thermal Transformations. The Institute of Problems of Chemical Physics of the Russian Academy of Sciences. Academician Semenov pr., 1. Chernogolovk ,142432. Russia.*
Phone: +7 (905) 503-69-33. E-mail: bkris@mail.ru
[3] *Department of Chemistry and Physics. Plekhanov Russian University of Economics. Stremyanny per., 36. Moscow, 117997. Russia.*
[4] *Biomolecular Measurement Division. National Institute of Standards and Technology. Gaithersburg, USA. Phone: +7 (301) 975-40-12. E-mail: hruk78@gmail.com, alexey.mayorov@nist.gov*

*Supervising author; +Corresponding author

Keywords: quantum-chemical calculations, ozone, butadiene, activation energy, rate constant.

Abstract

The mechanisms of the initial step of the ozonolysis of 1,3-butadiene in the *trans*-configuration were studied by density functional theory methods (DFT) B3LYP, double hybrid B2PLYP method based on both DFT and MP2 approaches and couple-cluster CCSD method. Two possible reaction channels were considered: concerted 1,3-cycloaddition of ozone to the double bond of 1,3-butadiene leading to the primary ozonide (Criegee mechanism) and stepwise addition by the biradical mechanism (DeMore mechanism). Predicted structures of intermediate and transition states, the energies of elementary steps, and activation barriers were reported. For the rate-determining steps of both mechanisms, the full geometry optimization of stationary points was performed at the b3lyp/aug-cc-pVDZ and b2plyp/aug-cc-pVDZ theory level. The rate constants and their ratio for reaction channels calculated for both mechanisms demonstrate that Criegee mechanism competes with DeMore one. The proportion of the competition is approximately 1:6 with the prevalence of Criegee mechanism. According to B2PLYP/aug-cc-pvdz, a total reaction rate constant is equal to 3664 L/mol·sec for both channels of the Ozone binding, whereas a total reaction rate constant calculated with CCSD/aug-cc-pvdz is equal to 2848 L/mol·sec.These results are in agreement with the experimental data ($3 \cdot 10^3$) and previous computational results.

Thematic Section: Quantum-Chemical Research. **Full Paper**
Subsection: Organic Chemistry. *Registration Code of Publication:* 15-41-2-109
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Mechanism of isomerization radical adducts of addition of thiophenol radical to quinone imine

© **Boris E. Krisyuk**,[1,3+] and **Vladimir T. Varlamov**[2*+]
[1] *Laboratory of Kinetics of Heterophase Processes;* [2] *Laboratory of Radical Liquid-Phase Reactions. Institute of Problems of Chemical Physics RAS. Akademika Semenova Ave., 1. Chernogolovka, 142432. Russia. E-mail: bkris@mail.ru, varlamov@icp.ac.ru*
[3] *Department of Chemistry and Physics. Russian Economic University Named after. G.V. Plekhanov. Stremyannoy per., 36. 117997, Moscow. Russia.*

*Supervising author; +Corresponding author

Keywords*:* quinone imines, thiyl radicals, radical adducts, isomerization, thiophenol participation, transition state, quantum-chemical calculations.

Abstract

On the example of adducts appearing at thiophenol radical addition to the cyclohexadiene moiety of the quinone imine, the methods of quantum chemistry are consider the possible mechanisms of isomerization of mentoned intermediates to corresponding phenoxyl and aromatic aminyl radicals. It is shown that the value of activation energy of intramolecular transfer of atom H of C-H bond from the point of connection of radical $PhS^{\cdot}$ so large, that can equal or even exceed C-H bond dissociation energy. Thus the intramolecular rearrangement of radical adducts appears to be improbable. The alternative bimolecular mechanism of atoms H transfer is considered with participation the additional molecule of thiol, that executes the role of reaction catalyst because of formation of the six-member transition state and the high exothermicity of reaction. The obtained data show that such mechanism can provide the rapid transfer of atom H.

Thematic Section: Quantum-Chemical Research. **Full Paper**
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Reaction of aromatic hydrodechlorination: quantum-chemical diagnostics of the mechanism

© **Matvei S. Gruzdev**,[1] **Lyudmila V. Virzum**,[2+] and **Evgeny N. Krylov**[3]*
[1] *G.A. Krestov Institute of Solution Chemistry. Russian Academy of Sciences. Akademicheskaya St., 1. Ivanovo, 153045. Russia. Phone: +7 (4932) 33-62-59.*
[2] *Ivanovo State Agricultural Academy Named after Academician D.K. Belyaev. Sovetskaya St., 45. Ivanovo, 153012. Russia. Phone: +7 (4932) 32-81-44. E-mail:virzum@list.ru*
[3] *Chemistry Department. Ivanovo State University. Ermak St., 39. Ivanovo, 153025. Russia. Phone: +7 (4932) 37-37-03. E-mail: enk2000S @yandex.ru*

*Supervising author; +Corresponding author

Keywords*:* hydrodehalogenation, aryl halogenides, electrophilicity, Fukui function, Pearson`s hard and soft acids and bases.

Abstract

The dehydrohalogenation process of aryl- and heteroaryl haligenides is described on base of the Pearson`s hard and soft acids and bases theory. It Is discovered electrophilic nature of limiting velosity stage. The correlation between logarithm of the catalytic hydrodehalogenation velocities constants and local electrophilicity of the reactions centre are exists. Function Fukui and local electrophilicity as a factor of electron-donating abilities of the reactionary centre introduces reliable descriptor to reactionary ability of aryl halogenides in process of dehidrogalogenation.

Thematic Section: Quantum-Chemical Research. **Short Communication**
Subsection: Organic Chemistry. *Registration Code of Publication:* 15-41-2-121
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Quantum-chemical modeling of the interaction of 1,2-di-phenylcyclopropyl with *N*-benzylideneaniline

© **Victoria V. Esenbaeva**,[1] **Alexander N. Vasyanin**,[2]
Sergey N. Shurov,[2+] and **Lidia P. Yunnikova**[1*+]
[1] *Perm State Agricultural Academy n.a. Academician D.N. Pryanishnikov. Petropavlovskaya St., 23. Perm, 614000. Perm Region. Russia. Phone: +7 (342) 212-95-68. E-mail: yunnikova@yahoo.com.*
[2] *Perm State National Research University. Bukerev St., 15. Perm, 614990. Perm Region. Russia. Phone: +7 (342) 239-64-35. E-mail: seshurov@yandex.ru*

*Supervising author; +Corresponding author

Keywords: *N*-benzylideneaniline, 1,2-diphenylcyclopropyl, 1*a*,2,7*b*-triphenyl-1*a*,2,3,7*b*-tetrahydro-1*H*-cyclopropa[c] quinoline, quantum-chemical calculations.

Abstract

Mechanism has been suggested for the formation of 1*a*,2,7*b*-triphenyl-1*a*,2,3,7*b*-tetrahydro-1*H*-cyclopropa[*c*]quinoline in the reaction of 1,2-diphenylcyclopropyl with *N*-benzylideneaniline in the presence of zinc chloride.

Full Paper _____ *Thematic Section:* Quantum-Chemical Research.
Registration Code of Publication: 15-41-2-124 *Subsection:* Spectroscopy.
The article is published on materials of the report on "International Scientific Forum Butlerov Heritage – 2015". http://foundation.butlerov.com/bh-2015/ *(English Preprint)*
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Singlet and triplet transitions in UV optical absorption spectra of pyrene

© **Laysan Z. Khatymova**,[+] **Olga G. Khvostenko**,* and **Rustem V. Khatymov**
Laboratory of Negative Ion Mass Spectrometry and Molecular Spectroscopy.
Institute of Molecule and Crystal Physics. Ufa Research Center of Russian Academy of Sciences.
Prospekt Oktyabrya, 151. Ufa, 450075. Bashkortostan Republic. Russia.
Phone: +7 (347) 231-91-68. E-mail: lesya0706@ya.ru

*Supervising author; [+]Corresponding author
Keywords*:* condensed aromatic compounds, pyrene, electronic structure, electron-excited singlet state, triplet states, UV optical absorption spectroscopy, photoelectron spectroscopy.

Abstract

Optical absorption UV–Vis spectra were obtained for pyrene. The survey UV-spectrum depicting the transitions into singlet electron-excited states in the range 1-6 eV was recorded using cyclohexane as solvent. With the aid of a cuvette with a large optical path length and by dissolving the pyrene sample in bromopropane, the spectrum was registered from which the direct vertical transitions into triplet states were distinguished. The experimental value 2.75 eV was determined for the energy of lowest vertical triplet transition, by ca. 0.6 eV lying higher than corresponding adiabatic transition energy measured by the other groups using phosphorescence technique. Assignment of the bands observed in UV spectra was accomplished using TD DFT B3LYP/6-31G level quantum chemical calculations. The pyrene molecular ground state electronic structure, namely the configuration of occupied and virtual molecular orbitals involved in electron excitation processes of interest, was considered on the basis of photoelectron spectrum taken from literature. The photoionization bands observed in this spectrum were attributed to the specific occupied molecular orbitals obtained from B3LYP/6-311G level calculations. The symmetries and electronic configurations of the studied singlet and triplet electron-excited states of pyrene were specified as well.

Full Paper _____ *Thematic Section:* Quantum-Chemical Research.
Registration Code of Publication: 15-41-2-130 *Subsection:* Physics Chemistry of Fullerenes.
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Structure and IR spectra of Me@C_{60} (Me = Cu, Ag, Au, Sc, Y, La) endofullerenes according to quantum-chemical calculation data

© **Dmitry A. Machnev**, **Igor V. Nechaev**,[+] and **Aleksander V. Vvedensky***
Department of Physical chemistry. Voronezh State University. Universitetskaya sq., 1. Voronezh, 394006. Russia. E-mail: nechaev_iv@chem.vsu.ru

*Supervising author; [+]Corresponding author

Keywords: endohedral fullerenes, IR spectra, quantum-chemical modeling.

Abstract

The results Ib- and IIIb-groups metal endofullerenes Me@C_{60} DFT-simulation are presented. It has been found that the copper subgroup metals are positioned in the center of the carbon cage without forming chemical bonds to carbon atoms, while the scandium subgroup metals are linked to six-membered ring forming a structure with C_s symmetry. With the encapsulation of Cu, Ag and Au atoms in C_{60}, IR spectrum endofullerene consists of four lines, as well as pure C_{60}. The spectra of scandium subgroup metal endofullerenes includes lines forbidden by symmetry for pure fullerene, which makes their experimental determination by IR spectroscopy in mixture with C_{60} possible.

Thematic Section: Quantum-Chemical Research. **Full Paper**
Subsection: Inorganic Chemistry. *Registration Code of Publication:* 15-41-2-135
The article is published on materials of the report on "International Scientific Forum Butlerov Heritage – 2015". http://foundation.butlerov.com/bh-2015/ *(English Preprint)*
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Quantum-chemical modeling of the hydroxide ion gas-phase adsorption on IB metal clusters Me_n (n = 2-8)

© **Alexander A. Doroshenko**,[+] **Igor V. Nechaev**, and **Alexander V. Vvedensky***
Department of Physical Chemistry. Voronezh State University. Universitetskaya sq., 1. Voronezh, 394006. Russia. Phone: +7 (473) 220-85-46. E-mail: doroshenko@chem.vsu.ru

*Supervising author; [+]Corresponding author

Keywords: quantum-chemical modeling, IB-metals clusters, hydroxide ion, chemisorption, IR spectra.

Abstract

The gas-phase adsorption of hydroxide ion on small IB-metals clusters simulation has been carried out within the framework of the density functional theory. The enthalpies and Gibbs energy of metal-cluster interaction was calculated. Similarities in geometry and charge states of he adsorbed OH-radical and OH-anion were revealed. The analysis of the vibrational spectra of adsorption complexes was carried out. It was established that the hydroxide ion is chemisorbed on small IB-metals clusters on top or in bridge position. It was shown that the OH bond frequency of adsorbed OH-ion is increased relative to the corresponding values in the isolated state, while the intensity of the oscillations is considerably reduced.

Thematic Section: Quantum-Chemical Research. **Full Paper**
Subsection: Inorganic Chemistry. *Registration Code of Publication:* 15-41-2-141
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Submitted on March 31, 2015.

Quantum-chemical modeling of process iron and zinc sulfides synthesis from their chlorides

© **Linara R. Baraeva**,[1+] **Guzelya I. Sabahova**,[2] and **Rezida T. Akhmetova**[1,3]*
[1] *Technology of Inorganic Substances and Materials Division. Institute of Petroleum, Chemistry and Nanotechnologies. Kazan National Research Technological University. Karl Marx St., 68. Kazan, 420015. Republic of Tatarstan. Russian Federation. Phone: +7 (843) 238-56-94. E-mail: office@kstu.ru, baraeva.linara@yandex.ru*
[2] *Enhanced Oil Recovery Department. Tatar Oil Research and Design Institute of Tatneft Company (TatNIPIneft). M. Jalil St., 32. Bugulma, 423230. Republic of Tatarstan. Russia. Phone: +7 (855) 947-85-55. E-mail: sabahova.guzel@yandex.ru*
[3] *Chemistry and Engineering Ecology in Engineering Division. Institute of Engineering Technologies and Engineering-Ecological Systems. Kazan State University of Architecture and Engineering. Zelenaya St., 1. Kazan, 420043. Republic of Tatarstan. Russian Federation. Phone: +7 (843) 510-47-42. E-mail: info@ksaba.ru*

*Supervising author; +Corresponding author

***Keywords**:* iron sulfide, zinc sulfide, Lewis acid, quantum-chemical program *Priroda 6*.

Abstract

Quantum-chemical calculations are executed with use of the Priroda 6 program by means of a hybrid method of functionality of density of DFT functional = PBE, basis of basis 4.in. High temperature of sulfides synthesis is a condition of chemical interactions between components as steady cyclic sulfuric molecules pass into radicals. However also other way of radical transformations of sulfur is known and it is connected with activation of sulfur under elektrophilic components. Calculations proved formation of difficult sulfides, the containing S_n (n = 1, 2, 4, 6, 8) in process iron and zinc sulfides synthesis from their chlorides. The activating effect of chlorides on sulfur consisting in destabilization and disclosure of cyclic molecules is established.

Thematic Section: Study the Specifics of the Processes._____ **Full Paper**
Subsection: Physical Chemistry. *Registration Code of Publication:* 15-41-2-147
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The role of non-ionogenic surfactants in formation of porous structure of active aluminium oxide

© **Irina I. Lebedeva**,[+] **Dmitriy M. Kiselkov**, and **Viktor A. Valtsifer***
Institute of Technical Chemistry. Ural Branch of the RAS.
Academician Korolev St., 3. Perm, 614013. Russia.
Phone: +7 (342) 237-82-81. E-mail: irene.i.lebedeva@gmail.com

*Supervising author; [+]Corresponding author

Keywords*:* aluminium oxide, porous structure, non-ionogenic surfactants, bi-modal pore size distribution.

Abstract

In this work, regularities in formation of porous structure of active aluminium oxide under conditions of hydrothermal synthesis (HTS) in the presence of non-ionogenic surfactants (NIS), namely of poly(ethylene oxide)-poly(propylene oxide)-poly(ethylene oxide) (Pluronic) have been ascertained. Formation of a NIS-based organo-inorganic gel-precursor and of hydroxonic forms of aluminium oxide (precursor forms of aluminium oxide) formed either during precipitation from soluted aluminium salts or as hydrolyzed aluminium alkoxides has been evinced to be the key moment in HTS of active aluminium oxide with bi-modal porous structure. Spatial organization of the organo-inorganic gel-precursor has been ascertained to be determined by interaction between particles of precursor forms of aluminium oxide and NIS which, in turn, is determined by their phase composition. A mechanism to form the NIS-based organo-inorganic gel-precursor and hydroxonic forms of aluminium oxide has been proposed. The influence of type and quantity of NIS on parameters of porous structure of aluminium oxide was ascertained. The structure of aluminium oxide, as hydrophilic-lipophilic balance of NIS increases, was shown to change from the homogeneously porous structure characterized by cone-shaped pores to the structure with bi-modal pore size distribution.

Thematic Section: Research Ultralow Temperatures._____ **Full Paper**
Subsection: Physical Chemistry of Semiconductors. *Registration Code of Publication:* 15-41-2-155
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Crystallization of cadmium telluride on single crystal substrates cooled with liquid nitrogen

© **Alexey P. Belyaev**,[1+]* **Vladimir P. Rubets**,[2] and **Svetlana A. Belyaeva**[2]
[1] *Department of Phisical and Colloidal Chemistry. St. Petersburg State Chemical-Pharmaceutical Academy. Professor Popov St., 14. St. Petersburg, 197376. Russia. Phone: +7 (820) 234-11-28. E-mail: Alexei.Belyaev@pharminnotech.com.*
[2] *Department of Analitical Chemistry. Saint Petersburg State Institute of Technology (Technical University). Moscovskiy pr. 26. Saint-Petersburg, 190013. Russia. Phone: +7 (812) 494-93-71. E-mail: vladimir@mail.ru*

*Supervising author; +Corresponding author

Keywords*:* heteroepitaxy, ultralow temperatures, thin films, synthesis from vapor phase, structural studies, II-VI compounds.

Abstract

Heteroepitaxy at ultralow temperatures is reported. Formation of an ordered monocrystalline state was for the first time observed in condensation of semiconductor films from vapor phase on crystalline substrates cooled with liquid nitrogen. Feasibility of targeted impact on structural type and crystalline perfection of the synthesized materials has been demonstrated

Results are presented of technological experiments and structural studies of II-VI compounds formed on mica and silicon substrates.

Condensation diagrams, micrographs, electron diffraction patterns and X-ray diffraction spectra are presented.

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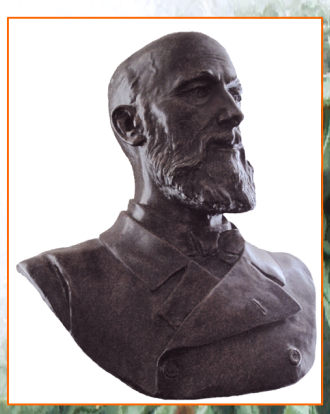

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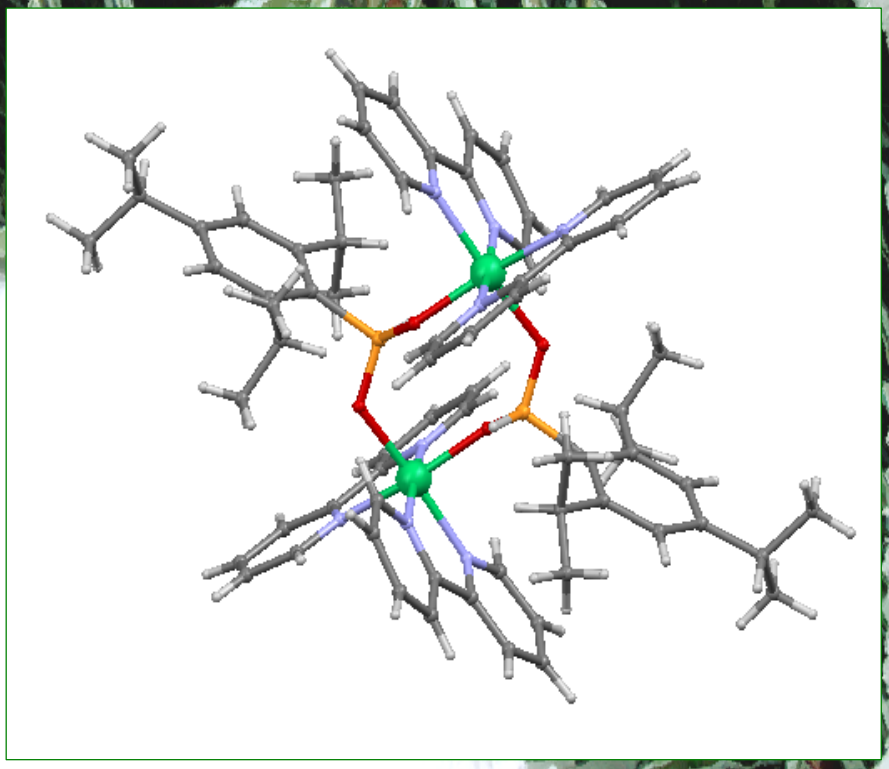

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Subsection: Chemistry of Xenobiotics. *Registration Code of Publication:* 13-33-3-1
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http://butlerov.com/readings/
Contributed: March 1, 2013.

Thematic course: Biodegradation as a method for waste processing. Part 1.

Biodegradation of xenobiotics

© **Anton Z. Mindubayev** and **Dmitry G. Yakhvarov**
Institution of RAS, A.E. Arbuzov Institute of Organic and Physical Chemistry.
Arbuzov St., 8. Kazan, 420088.Tatarstan Republic. Russia. E-mail: mindubaev@iopc.ru
State Budgetary-Funded Institution of Science A.E. Arbuzov Institute of Organic and Physical Chemistry of Kazan Scientific Center of Russian Academy of Sciences

*Supervising author; +Corresponding author

Keywords: *biodegradation, detoxication, industrial toxic waste.*

Abstract

One of the most significant probems of modern civilization is waste processing. Among the ways of its solving is biodegradation method, which is the most natural and environmentally friendly way for the destruction of waste of the cities, industry and agriculture. This review is aimed at the elucidation of biodegradation possibilities, its strength and weakness and the reasons of biodegradation insufficient application at present. The review contains the describtion of a number of specific examples of biodegradation of various classes of substances, many of biodegradation methods have already become customary.

Full Paper _____ *Thematic Section:* Physicochemical Research.
Registration Code of Publication: 13-33-3-42 *Subsection:* Thermal Physics of Energetic Materials.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: February 26, 2013.

Thermal explosion of mixed energy materials on the basis of various combustible binders and oxidizers

© **Vladimir N. Popok**,*+ and **Konstantin F. Il'inykh**
Open Joint Stock Company «Federal Research and Production Center "ALTAI". Sotsialisticheskaya St., 1. Biysk, 659322. Altai region. Russia. Phone: +7 (3854) 30-19-37. E-mail: vnpopok@mail.ru

*Supervising author; +Corresponding author

Keywords: *thermal explosion, composition energy materials, bindings, oxidizers.*

Abstract

Results of defining the parameters of thermal explosion of mixed energy materials are presented in the article on the basis of inert binder and two types of the active binders: on the basis of triazoles and mixed nitroester plasticizers. Perchlorate and ammonium nitrate were considered as oxidizers. It is shown that the most perspective fuel binder in respect to thermal stability and parameters of thermal explosion is the binder with triazole plasticizer.

Thematic Section: Study of Reactivity. **Full Paper**
Subsection: Supramolecular Chemistry. *Registration Code of Publication:* 13-33-3-49
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Investigation of the influence of reaction conditions on the process of dinuclear nickel(II) complexing

© **Ekaterina A. Trofimova**,[1] **Alexey B. Dobrynin**,[1] **Oleg G. Sinyashin**,[1] and **Dmitry G. Yakhvarov**[1,2]

[1] *Department of Coordination Chemistry and Nanomaterials. A.E.Arbuzov Institute of Organic and Physical Chemistry of the Russian Academy of Sciences. Arbuzov St., 8. Kazan, 420088. Tatarstan Republic. Russia. Phone: +7 (843) 273-48-93. E-mail: fomina@iopc.ru*

[2] *Physical Chemistry Division. A.M. Butlerov Institute of Chemistry. KFU. Kremlevskaya St., 18. Kazan, 420008. Tatarstan Republic. Russia. Phone: +7 (843) 233-73-46. E-mail: yakhvar@iopc.ru*

*Supervising author; +Corresponding author

Keywords*: arylphosphonic acids, bridging ligands, 2,2'-bipyridine, crystallisation, dinuclear nickel(II) complexes, solvothermal synthesis.*

Abstract

The influence of the reaction conditions on the formation of binuclear nickel complexes of the type $[Ni_2(\mu\text{-}O_2P(H)Ar)_2(bpy)_4]Br_2$, where Ar = Ph (**1**), 2,4,6-trimethylphenyl (Mes, **2**), 2,4,6-triisopropylphenyl (Tipp, **3**), 9-antryl (Ant, **4**), bpy = 2,2'-bipyridine, by interaction of $[NiBr_2(bpy)_2]$ with arylphosphinic acids ArP(O)(OH)H, where Ar = Ph (**1a**), Mes (**2a**), Tipp (**3a**), Ant (**4a**), was investigated. It was established that crystallization of complexes **2** and **4** proceeds at room temperature in solution, while the formation of the crystal samples of complexes **1** and **3** requires the conditions of solvothermal synthesis at high temperature.

Thematic Section: Preparative Chemistry. **Full Paper**
Subsection: Nanochemistry. *Registration Code of Publication:* 13-33-3-55
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: February 22, 2013.

Synthesis of nanoscale aluminum and zirconium oxides from aqueous and aqueous-alcoholic solutions with polyethylene glycol

© **Galina V. Lyamina**,[1]*+ **Ilela Alfa Edison**,[1] **Edgar S. Dvilis**,[1]
Irina A. Bozhko,[1] and **Antonina P. Gerdt**[2]
[1] *Department of Nanomaterials and Technology. Institute of Physics of High Technologies. Tomsk Polytechnic University. Pr. Lenina St., 30. Tomsk, 634050. Russia. Phone: +7 (3822) 41-91-47. E-mail: lyamina@tpu.ru*
[2] *Department of Organic Chemistry. Chemistry Faculty. Altai State University. Pr. Lenina St., 61. Barnaul, 656049. Russia. Phone: +7 (3852) 66-66-82. E-mail: csycdtnf@mail.ru*

*Supervising author; +Corresponding author

Keywords: *aluminum oxide, zirconium oxide, nano-powders, nano spray drying.*

Abstract

In this paper, the feasibility of the use of nano of spray drying (*Nano Spray Dryer B-90*) for obtaining the powders of Al_2O_3 and ZrO_2 has been shown. It was found that the use of alcoholic solutions and stabilizer (polyethylene glycol) for the synthesis of zirconium oxide can increase the content of the tetragonal phase. The use of water-alcohol solutions can increase the amount of granular product.

Thematic Section: Technological Research. **Full Paper**
Subsection: Regeneration of Water in Industrial Processes. *Registration Code of Publication:* 13-33-3-63
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: March 13, 2013.

Some aspects of the process water regeneration in the conversion of acidic tars

© **Elena N. Fedoseeva**,[1]*+ **Arkady D. Zorin**,[1]* **Valentina F. Zanozina**,[1]
Evgeny V. Zhebryakov,[1] **Vasily N. Batsinin**,[1] **Tatiana V. Kuznetsova**,[1]
Elena A. Gushchina,[2] **Marina L. Markova**,[1] and **Natalia M. Goryacheva**[1]
[1] *Laboratory of Applied Chemistry and Ecology. Research Institute of Chemistry. N.I. Lobachevsky Nizhni Novgorod State University. Gagarin St., 23, b.5. Nizhni Novgorod, 603950. Russia.*
Phone: +7 (831) 465-81-66. E-mail: enfedoseeva@front.ru
[2] *Department of Chemistry at NNSAA. Nizhni Novgorod State Agricultural Academy (NNSAA).*
Gagarin St., 97. Nizhni Novgorod, 603107. Russia. Phone: +7 (831) 462-65-08, (831) 462-78-17.
E-mail: adzorin@mail.ru

*Supervising author; +Corresponding author

Keywords*: acidic tar, sulphonic acids, renewable water, colloidal solution, colloidal particle, coagulation, flocculation, stability of dispersion, surface-active properties.*

Abstract

Treatment of acidic tars with water is one of the stages of the method developed by the authors to obtain bituminous materials out of the waste of oil refining industry. We have studied the causes for the stability of colloidal solution formed during the phase separation of the mixture of the acidic tar and water, the composition and surface-active properties of this dispersion. The process selection for regenerating the dispersion medium, water, in order to return the latter to the cycle of the acidic tar treatment has been reported.

Thematic Section: Preparative Chemistry. **Full Paper**
Subsection: Organic Chemistry. *Registration Code of Publication:* 13-33-3-81
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
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Coordination compounds of sodium and potassium 4,6-dinitro-5,7- diamino benzofuroxan

© **Luiza M. Yusupova**,*+[1] **Tatiana A. Eneykina**,*[2] **Ekaterina A. Vasyutina**,[1] **Roza F. Gatina**,[2] and **Nikolay A. Pokalyukhin**

[1] *Kazan National Research Technological University. K. Marx St., 68. Kazan, 420015. Tatarstan Republic. Russia. Phone: +7 (343) 231-40-88.*
[2] *State Scientific-Research Institute of Chemical Products. Svetlaya St., 1. Kazan, 420033. Tatarstan Republic. Russia. Phone: +7 (843) 541-76-02. E-mail: hgm1961@ rambler.ru*

*Supervising author; +Corresponding author

Keywords: *coordination compounds, synthesis, derivatives of dinitrobenzofuroxans, infrared spectroscopy.*

Abstract

For the first time the coordinating compounds of sodium and potassium of 4,6-dinitro-5,7-diaminobenzofuroxan were synthesized by the «assembly» method from 4,6-dinitro-5,7-dichlorobenzofuroxan, sodium bicarbonate (potassium) and ammonium chloride in aqueous medium. By elemental, X-ray diffraction, IR spectroscopy and differential scanning calorimetry we found out. The structure complexes of chelate type and their sensitivity to mechanical and thermal stress were studied.

Full Paper _____ *Thematic Section:* Preparative Chemistry.
Registration Code of Publication: 13-33-3-88 *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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Reactions of 4-*R*-amino-7-nitro-2,1,3- benzoxadiazoles with nitrifying and nitrosating reagents

© **Anastasia S. Kuznetsova**, and **Leonid M. Gornostaev***[+]
Department of Chemistry. Astaf'ev Krasnoyarsk State Pedagogical University.
A. Lebedeva St., 89. Krasnoyarsk, 660049. Russia.
Phone: +7 (391) 217-17-29. E-mail: gornostaev@kspu.ru

*Supervising author; [+]Corresponding author

Keywords: *2,1,3-benzoxadiazoles, nitration, nitrosation, heterocyclization, regrouping.*

Abstract

4-Aryl- and benzylamino-7-nitro-2,1,3-benzoxadiazoles interact with nitriting and nitrosating reagents with participation of aryl and benzofurazans carbocycles or secondary amino groups depending on the type of reagent.

Thematic Section: Preparative Chemistry. **Full Paper**
Subsection: Chemistry of Dyes. *Registration Code of Publication:* 13-33-3-93
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http://butlerov.com/readings/
Contributed: March 4, 2013.

Synthesis of new nitrogen of methyl phluoroglucinol – potential dyes and pigments for textiles

© **Andrey I. Alafinov**,[1] **Konstantin I. Kobrakov**,[1]*[+]
Dmitry N. Kuznetsov,[1] and **Maria B. Dmitrieva**[2]
[1] *Department of Organic Chemistry. Moscow State University of Design and Technology. Malaya Kaluzhskaya St., 1.Moskow, SSE-1, 119991. Russia. Phone: +7 (495) 955-35-58. E-mail: occd@mail.ru*
[2] *Center for Biological Control Laboratory Microfilming and Document Restoration. Russian State Archive of Scientific and Technical Documentation. Profsoyuznaya St., 82. Moscow, 117393. Russia. Russia: +7 (495) 335-00-95. E-mail: biorest.maria@gmail.com*

*Supervising author; [+]Corresponding author

Keywords: *2,4,6-tri-hydroxytoluene, methyl phloroglucinol, azo combination, dyeing, fungicidal activity.*

Abstract

The article presents data on the synthesis and properties of previously undescribed azo-derivatives 2,4,6-tri-hydroxytoluene, which are of interest as potential azodyes for textile materials of different composition.

Full Paper _____ *Thematic Section:* Biochemical Research.
Registration Code of Publication: 13-33-3-98 *Subsection:* Additives to Fish Fodder.
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: March 10, 2013.

Thematic direction: Feed additives of amaranth for fish. Part 2.

Features of the mineral composition of amaranth leaves

© **Anatoly A. Lapin**,[1]*+ **Valery N. Zelenkov**,[2] and **Lilia G. Grechuhina**[1]
[1] *Department of Water Bioresources and Aquaculture. Kazan State Power Engineering University. Krasnoselskaya St., 51. Kazan, 420066. The Republic of Tatarstan. Russia.*
Phone: +7 (843) 519-43-53. E-mail: lapinanatol@mail.ru
[2] *Department of Physico-chemical Biology and Innovations. Russian Academy of Natural Sciences, All-Russian Research Institute of Vegetable Crops Russian Academy of Agricultural Sciences, Moscow. Russia.*

*Supervising author; +Corresponding author

Keywords: *amaranth, amaranth stalks and leaves, amaranth seeds, biologically active supplements, macro - and microelements, a forage production, animal husbandry, pisciculture.*

Abstract

The review shows promising use of feed additives from amaranth for growing fish. The high concentration of macro-elements, such as calcium, magnesium, phosphorus, and microelements, as manganese, silicon, iron, zinc and copper are typical for plants from amaranth. There are prospects of application of amaranth as feed additive in forages for fishes as a source of biogene mineral elements in order to prevent the diseases connected with their deficit.

Full Paper _____ *Thematic Section:* Biochemical Research.
Registration Code of Publication: 13-33-3-108 *Subsection:* Chemistry of Dyes.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
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Effective express method for testing preparations to protect textiles from biological damage

© **Maria B. Dmitrieva**, **Dmitry N. Kuznetsov**,[2]*[+]
Konstantin I. Kobrakov,[2] and **Valentin V. Safonov**[3]
[1] *Center for Biological Control Laboratory Microfilming and Document Restoration. Russian State Archive of Scientific and Technical Documentation. Profsoyuznaya St., 82. Moscow, 117393. Russia. Phone: +7 (495) 335-00-95. E-mail: biorest.maria@gmail.com*
[2] *Department of Organic Chemistry. Moscow State University of Design and Technology. Malaya Kaluzhskaya St., 1. Moscow, GSP-1, 119991. Russia. Phone: +7 (495) 955-35-58. E-mail: occd@mail.ru*
[3] *Department of Chemical Technology of Fibrous Materials. Moscow State University of Design and Technology. Malaya Kaluzhskaya St., 1. Moscow, GSP-1, 119991. Russia. Phone: +7 (495) 955-35-58.*

*Supervising author; [+]Corresponding author

Keywords*: biological stability of tissues, biocide, fungicide protection, fungicide dyes, nanoparticles of silver and copper.*

Abstract

In this article we are proposing modified version of the disco-diffusion method for testing biocidal activity. This method, widely used in antibiotics, was adapted for assessing the fungicidal stability in textiles. It allows us to obtain information from many samples within a short time (3-7 days) and to use certain species of fungi for certain aims. In our case we tested samples of fabrics stained and treated with synthesized chemical substances, particularly pyrazole contained azodyes and colloidal silver nano particles. Test cultures for artificial infestation were chosen from a list of ones frequently found on damaged textiles. Two examples of the application of this express method are provided, and advantages and disadvantages are discussed.

Full Paper _____ *Thematic Section:* Biochemical Research.
Registration Code of Publication: 13-33-3-116 *Subsection:* Chemistry of Polysaccharides.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: February 21, 2013.

Thematic course: Fruit polysaccharides. Part I.

General chemical characteristics of polysaccharides of pomegranate fruits (*Punica granatum* L.)

© **Evgeny G. Shakhmatov**,[1]* **Elena N. Makarova**,[1]* **Elena A. Mikhailova**,[2]*
Anatoly A. Shubakov,[2+] and **Yury S. Ovodov**

[1] *Laboratory of Chemistry of Phytopolymers. Institute of Chemistry. Komi Science Centre. Urals Branch of the Russian Academy of Sciences. Pervomaiskaya St., 48. Syktyvkar, 167982. Komi Republic. Russia. Phone: +7 (8212) 21-99-16. E-mail: shachmatow-eg@ya.ru*

[2] *Department of Molecular Immunology and Biotechnology. Institute of Physiology. Komi Science Centre. Urals Branch of the Russian Academy of Sciences. Pervomaiskaya St., 50. Syktyvkar, 167982. Komi Republic. Russia. Phone: +7 (8212) 24-10-01. E-mail: shubakov@physiol.komisc.ru*

*Supervising author; +Corresponding author

Keywords: *polysaccharides, pectins, hemicelluloses, sugar composition, protein content, Punica granatum, biological activity of polysaccharides.*

Abstract

A number of polysaccharide fractions were isolated from peels and partitions of the pomegranate fruit with the aid of the previously developed method of isolation of polysaccharides from plant raw materials by means of successive extraction with water, with ammonium oxalate and with alkali solutions. The general chemical characteristics of isolated polysaccharides is given and their biological activity is determined. The fractions extracted with water and with ammonium oxalate belong to the class of pectic polysaccharides. The fractions extracted with alkali solutions belong to the hemicelluloses. The highest biological activity in regard to the effect on the germination and energy of germination and the rate of growth of seedlings and roots of the cereal crops (wheat, rye, oats) has fraction of pectins, isolated from the pomegranate fruit by extraction with ammonium oxalate.

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http://butlerov.com/readings/
Contributed: March 14, 2013.

Comparative assessment of indicators of blood and the mixed saliva of patients against acute parenchymatous parotitis

© **Lyudmila V. Belskaya**,[1]*+ **Andrey S. Korshunov**,[2]* and **Peter I. Ivasenko**[2]
[1] *Department of Chemical Technology. Omsk State University. Pr. Mira St., 55-a. Omsk, 644077, Russia.*
Phone: +7 (3812) 64-24-10. Fax: +7 (3812) 64-24-10. E-mail: LudaB2005@mail.ru
[2] *Department of Maxillofacial Surgery. Omsk State Medical Academy. Lenin St., 12. Omsk, 644043. Russia.*

*Supervising author; +Corresponding author

Keywords: *parenchymatous parotitis, abscess formation, saliva, chemical composition.*

Abstract

A comparative evaluation of serum biochemical parameters in patients with primary parenchymatous parotitis aggravation with those of mixed saliva of the patients was carried out. We found high correlations in biological fluids in terms of total protein, chloride, ALT, AST, phosphatase, amylase and creatinine. The obtained informative parameters of the saliva can be used when inspecting the patients with primary exacerbation of parenchymatous parotitis on the pre-hospital stage for establishing severity, forecasting and for efficiency of therapeutic measures of high-precision, noninvasive pathognomonic tests.

Full Paper _____ *Thematic Section:* Physico-Chemical Reserch.
Registration Code of Publication: 13-33-3-126 *Subsection:* Toxicological Chemistry.
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Synthetic cannabinoid A-836, 339 – methods of identification

© Peter S. Mashchenko
Department of Toxicological Chemistry. Perm State Pharmaceutical Academy.
Polevaja St., 2. Perm, 614990. Russia. Phone: +7 (342) 282-58-65. E-mail: kaftox@mail.ru.

Keywords*: synthetic cannabinoid; A-836, 339; drugs.*

Abstract

Synthetic cannabinoids are a relatively large group of organic compounds of great interest to science. Relatively recently, A-836, 339, another representative of the group of synthetic cannabinoids, having psychoactive properties, appeared on the Russian illegal market. As part of the study of new psychoactive substances we obtained main qualitative characteristics of the matter (mass spectrum, IR spectrum, UV spectrum).

Full Paper _____ *Thematic Section:* Physoco-Chemical Research.
Registration Code of Publication: 13-33-3-130 *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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Features of molecular interactions in the binary system of cellulose nitrate-filler

© **Rinat O. Almashev**,* **Tatiana A. Eneykina**, **Lilia Selivanov**, **Nadezhda A. Romanko**, **Anna V. Kiprova**,+ **Elvira N. Tarazova**, **Roza F. Gatina**, and **Yury M. Mikhailov**
State Scientific-Research Institute of Chemical Products. Svetlaya St., 1. Kazan, 420033. Tatarstan Republic. Russia. E-mail: anekolab@mail.ru

*Supervising author; +Corresponding author

Keywords: *IR spectroscopy, filler, cellulose nitrate, molecular interactions, octogen, hexogen.*

Abstract

Using IR-spectrometry we studied intermolecular interaction in systems cellulose nitrate (CN) – octogen (hexogen). It has been established that the stability of the molecular complexes CN-octogen (hexogen) depends on the properties of CN, the type and the content of the filler and the characteristics of hydrogen bonds (E) in the interval 12.1-33.2 kJ/mol. The strongest intermolecular interactions in the considered range of the input of fillers (0-80 % weight.) is observed in the compositions hexogen- colloxylin, starting with the component ratio 60:40 due to the great number of the molecular complexes being formed (E = 33.2 kJ/mol). For compositions octogen – colloxylin the similar dependence is preserved, but at the lower energies of hydrogen bonds (E = 16.1-25.1 kJ/mol). In the compositions of hexogen (octogen) – pyroxylin the optimal compositions, from the point of view of steady molecular complexes, are those with the filler content ~60 % weight (E = 27.1 and 25.1 kJ/mol, accordingly).

Full Paper _____ *Thematic Section:* Physico-Chemical Research.
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Molecular mobility of chitosan-based hydrogel components

© Tatiana V. Smotrina,[1]*+ and **Natalia R. Kildeeva**[2]*
[1] *Department of Physics. Volga State Technological University. Lenin Sq., 3. Yoshkar-Ola, 424000. Mari El Republic. Russia. Phone: +7 (8362) 68-68-04. E-mail: tatyana-smotrina@yandex.ru*
[2] *Department of Analytical, Physical and Colloidal Chemistry. A.N. Kosygin Moscow State Textile University M. Kaluzhskaya St., 1. Moscow, 119071, Russia. Phone: +7 (495) 955-33-77. E-mail: kildeeva@mail.ru*

*Supervising author; +Corresponding author

Keywords: *chitosan, hydrogels, nuclear magnetic relaxation, molecular mobility.*

Abstract

The processes of spin-lattice and spin-spin relaxation of the proton magnetized water in chitosan-based hydrogels synthesized on varying pH-factor and concentration of crosslinking agent were investigated by the method of nuclear magnetic relaxation. The correlation between hydrogel structure and mobility of the retained water was shown. The character of structure changes of dried hydrogels during their reswelling in water steam was analyzed. The correlation between sorption data and NMR data was shown.

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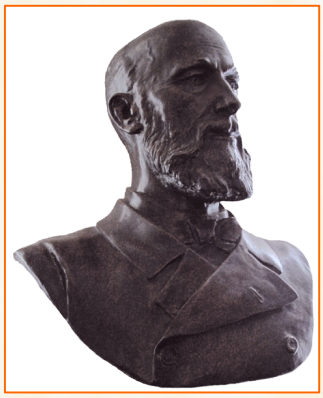

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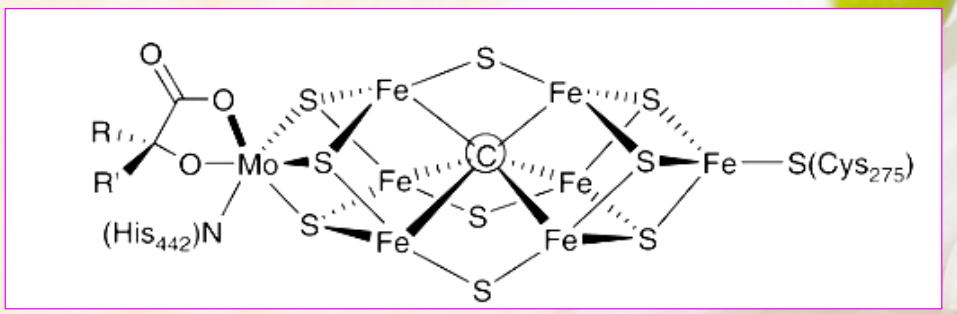

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Synthesis of partially hydrogenated nitrogen heterocycles. How does the heterocyclization on Ritter proceed?

© **Yury V. Shklyaev**,*+ **Tatiana S. Vshivkova**, **Yulia S. Rozhkova**, **Olga G. Stryapunina** and **Andrew A. Smolyak**

Institute of Technical Chemistry, Ural Branch of the Russian Academy of Sciences. St. Academician KorolevSt., 3. Perm, 614013. Russia. Phone: (342) 237-82-89. E-mail: yushka@newmail.ru

*Supervising author; +Corresponding author

Keywords: Ritter reaction, nitrogen-containing heterocycles, spiro-σ-complex stabilization, 3,4-dihydroisoquinoline, spirain, neospiran.

Abstract

On the vast experimental material the authors propose the concept on of heterocyclization proceeding by Ritter reaction through the formation of spiro-σ-complex, the different ways of stabilization of which produce 3,4-dihydroisoquinolines,spirains, neospirains and other heterocyclic systems.

Full Paper _____ *Thematic Section:* Preparative Research.
Registration Code of Publication: 15-42-4-16 *Subsection:* Organic Chemistry.
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Natural pectins: oxidative destruction and interaction with uracils

© **Yury S. Zimin**,[1]* **Natalia S. Borisova**,[1+] **Guzel R. Timerbaeva**,[2]
Alfia R. Gimadieva,[3] and **Akhat G. Mustafin**[1]
[1] *Department of Physicla Chemistry and Chemical Ecology. Bashkir State University.*
Zaki Validi St.,32. Ufa, 450074. Republic of Bashkortostan. Russia.
Phone: +7 (347) 229-96-94. E-mail: ZiminYuS@mail.ru
[2] *Department of General Subjects. Branch of Ufa State Aviation Technical University.*
Molodeznhyj micro-district, 5. Tujmazy, 452750. Republic of Bashkortostan. Russia.
[3]*Laboratory of Pharmacophore Cyclic Systems. Ufa Institute of Chemistry RAS.*
Oktyabrya St., 71. Ufa, 450054. Republic of Bashkortostan. Russia.

*Supervising author; +Corresponding author
Keywords: cytrous pectin, apple pectin, oxydative desctruction, ozon-oxygen mixture, complexes formation, uracil and its derivatives.

Abstract

On the basis of studying the kinetics of oxydative desctruction of cytrous and apple pectins we find the conditions for obtaining oxidative fractions of polysaccharides with prescribed molecular masses. By means of spectral methods, we study the interactions of pectins and its oxidative fractions ($M_{aver.}$ ~ 20-25 kDa) with uracil and its derivatives (UD). We define the composition and stability constants of creating complex compounds. It is found that the compounds' composition is equal to 1 : 1, i.e., one carboxyl group of pectin (or of its oxidized fraction) interacts with one molecula of UD. It is shown that electricdonor substitutents located at the fifth position of 6-methyluracil increase the stability of its complexes with apple pectins and its oxydative fraction.

Thematic Section: Preparative Research. **Full Paper**
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Development of a synthesis method of arylaliphatic diamino alcohols. The influence of the solvent on the process regioselectivity.

© **Alexander V. Krylov**,[1]*+ **Elena Ya. Borisova**,[2]* **Alexandra I. Ivanova**,[2]
Dyk Quang Hoang,[2] and **Nadejda Y. Borisova**[2]
[1] *Y.K. Sirkin Department of Physical Chemistry. Lomonosov Moscow University of Fine Chemical Technology. Vernadskogo pr., 86. Moscow, 119571. Russia.*
Phone: +7 (495) 246-05-55 (916). E-mail: allylnmr@yandex.ru
[2] *I.N. Nazarov Department of Organic Chemistry.*
Phone: +7 (495) 246-05-55 (908). E-mail: seacastle@mail.ru

*Supervising author; +Corresponding author

Keywords*:* epoxide, ring opening, *N*-nucleophiles, regioselectivity.

Abstract

The synthesis method of arylaliphatic amino alcohols based on reaction of styrene oxide ring opening by diamines was developed. It is shown that in conditions of low polarizing ability of the solvent the formation of α-substituted products of normal structure is the main process direction. For *N,N*-diethylethylenediamine the solvent influence on the reaction regioselectivity was investigated. It has been established that the ratio of the products is good correlated with the value of the dielectric constant for the mixed aqueous-organic solvents and with the polarity parameters E_T and AN for the pure solvents.

Thematic Section: Preparative Research. **Full Paper**
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The bis-thioethers based on 3,4-dichloro-2(5*H*)-furanone and propane-1,3-dithiol

© **Hoang Thi Lien**, **Almira R. Kurbangalieva**,*+ **Anna S. Yezhova**, **Evgeny A. Berdnikov**, and **Galina A. Chmutova***
Department of Organic Chemistry. A.M. Butlerov Institute of Chemistry. Kazan (Volga) Federal University. Kremlevskaya St., Kazan 18, 420008. Republic of Tatarstan. Russia.
Phone: +7 (843) 233-74-62. E-mail: Almira.Kurbangalieva@ksu.ru

*Supervising author; +Corresponding author
***Keywords*:** heterocycles, 2(5*H*)-furanone, mucochloric acid, propane-1,3-dithiol, bis-thioethers, diastereomers, NMR spectroscopy.

Abstract

We studied the reactivity of 3,4-dichloro-2(5*H*)-furanone in relation to propane-1,3-dithiol in the conditions of the basic or acid catalysis. При взаимодействии mucochloric acid and its 5-alkoxy derivatives with propane-1,3-dithiol in the presence of triethylamine there were obtained new bis-thioethers, in which two molecules of the fragment 2(5*H*)-furanone are bound on its carbon atoms C^4 through $-S(CH_2)_3S-$ chains. Under acid catalysis the reaction of mucochloric acid with propane-1,3-dithiol proceeds with substitution of the hydroxyl group and the formation of the bis-thioether bound with carbon atoms by C^5 γ-lactone cycles. There have been revealed similarities and differences in the reactions of 3,4-dichloro-2(5*H*)-furanone with propane-1,3-dithiol and 1,2-ethane-dithiol in the conditions of basic and acidic catalysis. The structures of all newly synthesized bis-thioethers 2(5*H*)-furanone were proved by IR spectroscopy, ^{1}H NMR and ^{13}C {^{1}H}.

Thematic Section: Preparative Research. **Full Paper**
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Some transformation of adducts of levoglucosenone and 1,3-diens in approaches to iridoides

© **Ilgiz M. Biktagirov**, **Liliya Kh. Faizullina**,[+]
Shamil M. Salihov, and **Farid Abdullovich Valeev***
Ufa Institute of Chemistry of the Russian Academy of Sciences.
Oktyabrya pr., 71. Ufa, 450054. Fax: +7 (3472) 35-60-66. E-mail: sinvmet@anrb.ru

*Supervising author; [+]Corresponding author

Keywords*:* levoglucosenone, 1.6-anhydro sugar, iridoides, the Diels-Alder adducts, cyclopentanoides.

Abstract

On the base of the Diels-Alder adduct of levoglucosenone and piperylene studied the possibility of modification of cyclohexane ring to cyclopentane by ozonolysis cleavage and intermolecular aldol cyclization.

It was carried out reaction of allyl oxidation of the Diels-Alder adducts of levoglucosenone and 1,3-dienes by action $CrO_3 \cdot 2Py$ in CH_2Cl_2. It was found that this transformation occurs upon prolonged storage on atmospheric oxygen and to light.

Full Paper _____ *Thematic Section:* Preparative Research.
Registration Code of Publication: 15-42-4-48 *Subsection:* Organic Chemistry.
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Receiving derivative fulvic acids and research of their complex formation with copper ions

© **Ekaterina V. Burova**,* **Irina A. Potapova**,*+
Petrovich P. Pyotr, and **Vasily V. Vishnyakov**
Chair of Organic, Bioorganic and Medicinal Chemistry. Samara State University.
Akad. Pavlova, 1. Samara, 443011. Samara region. Russia.
Phone: +7 (846) 334-54-59. E-mail: potap59.59@mail.ru

*Supervising author; +Corresponding author

***Keywords**:* fulvic acids, humic substances, brown coal, oxime of fulvic acids, hydroxymethyl derivative of fulvic acids, complex formation, copper ions.

Abstract

The new method of allocation of fulvic acids from brown coal is developed. Methods of synthesis of derivative fulvic acids are described and developed: oxime and hydroxymethyl derivatives of fulvic acids are synthesized. Reactions of a complex formation of fulvic acids and their derivatives with copper ions are for the first time studied and is shown that balance of sorption is established in 110 minutes, and the greatest absorbability in relation to copper ions possesses oxime of fulvic acids.

Thematic Section: Preparative Research. **Full Paper**
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Synthesis of 2-alkoxy-4,6-(2-phenylvinyl)pyrimidines incorporating terminal TTF-fragments

© **Ekaterina A. Komissarova**,[1+] **Igor V. Lunegov**,[1] **Olga A. Mayorova**,[4] **Elena V. Shklyaeva**,[1,3] and **George G. Abashev**[1,4*+]

[1] *Department of Organic Chemistry. Perm State University. Bukireva St., 15. Perm, 614990. Russia. Phone: +7 (342) 239-66-12. Email: seshurov@yandex.ru*

[2] *Department of Radio Electronics and Information Security. Perm State University. Bukireva St., 15. Perm, 614990. Russia. Phone: +7 (342) 239-62-31. Email: lunegov@psu.ru*

[3] *Laboratory of Organic Semiconductors. Natural Scientist Institute. Perm State University. Genkel St., 4. Perm, 614990. Russia. Email: gabashev@psu.ru*

[4] *Laboratory of Active Reagents' Synthesis. Institute of Technical Chemistry. Russian Academy of Sciences, Ural Division. Academician Korolev St., 3. Perm, 614990. Russia. Phone: +7 (342) 237-82-89. Email: gabashev@psu.ru*

*Supervising author; +Corresponding author

Keywords: tetrathiafulvalene, Y-shaped pyrimidine, electrochemical oxidation, bridging structure.

Abstract

There were synthesized novel 4,6-disubstituted 2-alkoxypyrimidines including two tetrathiafulvalenes fragments which are connected with pyrimidine core via S-CH_2-C_6H_4-CH=CH-bridges. Their photovoltaic properties have been studied.

Thematic Section: Preparative Research. **Full Paper**
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Synthesis of ferrocene-containing 4,6-disubstituted 2-(1*H*-Pyrrole-1-yl)pyrimidines

© **Alexandra D. Antuvjeva**,[1+] **Tatiana V. Shavrina**,[2] **Elena V. Shklyaeva**,[2,3] and **Georgy G. Abashev**[1,2]*[+]

[1] *Laboratory of Active Reagents' Synthesis. Institute of Technical Chemistry, Russian Academy of Sciences, Ural Division. Academician Korolev St., 3. Perm, 614990. Russia. Phone: +7 (342) 237-82-89. Email: gabashev@psu.ru 2*

[2] *Department of Organic Chemistry. Perm State University. Bukireva St., 15. Perm, 614990. Russia. Phone: +7 (342) 239-66-12. Email: seshurov@yandex.ru*

[3] *Laboratory of Organic Semiconductors. Natural Scientist Institute. Perm State University. Genkel St., 4. Perm, 614990. Russia. Email: gabashev@psu.ru*

*Supervising author; [+]Corresponding author

Keywords: ferrocene, 2-aminopyrimidine, 2-(2-pyrrole-1-yl)pyrimidine, electrochemical oxidation, bridge structures.

Abstract

There are several key areas of ferrocene-containing compounds application in the chemistry of materials: ferrocene-containing chemosensors; electroconducting compounds, electro- and photochromic compounds; ferrocene-containing metal complexes; ferrocene-containing liquid crystal compounds; polymers with ferrocene moieties; the surfaces chemically modified with compounds including ferrocene fragments. The structure of these compounds often contains heterocycles, in particular azines, such as pyridines, pyrimidines, quinolines, triazines. The paper submitted here includes the material concerning synthesis and electrochemical properties of newly substituted pyrimidines, which central pyrimidine core is surrounded with several electron donating cyclic moieties, one of which is ferrocene.

Full Paper _____ *Thematic Section:* Preparative Research.
Registration Code of Publication: 15-42-4-66 *Subsection:* Organic Chemistry.
The article is published on materials of the report on "International Scientific Forum Butlerov Heritage – 2015". http://foundation.butlerov.com/bh-2015/ *(English Preprint)*
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Preparation of 5-[4-(carbazol-9yl)phenyl]thiophene-2-carbaldehyde and its condensation with malonic acid derivatives. Optical properties and electrochemical polymerization.

© **Artur N. Bakiev**,[4+] **Alexey A. Gorbuov**,[4] **Igor V. Lunegov**,[2]
Elena V. Shklyaeva,[1,3] and **Georgy G. Abashev**[1,4]*[+]

[1] *Department of Organic Chemistry. Perm State University. Bukireva St., 15. Perm, 614990. Russia. Phone: +7 (342) 239-66-12. E-mail: seshurov@yandex.ru*

[2] *Department of Radio Electronics and Information Security. Perm State University. Bukireva St., 15. Perm, 614990. Russia. Phone: +7 (342) 239-62-31. E-mail: lunegov@psu.ru*

[3] *Laboratory of Organic Semiconductors. Natural Scientist Institute. Perm State University. Genkel St., 4. Perm, 614990. Russia. Email: gabashev@psu.ru*

[4] *Laboratory of Active Reagents Synthesis. Institute of Technical Chemistry, Russian Academy of Sciences, Ural Division. Academician Korolev St., 3. Perm, 614990. Russia. Phone: +7 (342) 237-82-89. E-mail: gabashev@psu.ru*

*Supervising author; [+]Corresponding author

Keywords: carbazole, chromophores, optical properties, electrochemical oxidation.

Abstract

There have been synthesized a new series of carbazole-containing chromophores with the structure D-π-A, as electron-acceptor moieties we used fragments of aldehyde and ethyl ether of 2-cyanoacrylic acid. 5-[4-(Carbazole-9-yl)phenyl] thiophene-2-carbaldehyde (**1**) was obtained with the help of с помощью cross-coupling reaction of Suzuki, further modification was carried out by the reaction of Knoevenagel. For the compounds produced we obtained absorption and fluorescence spectra, based on the values of the red boundary of the calculated value of the optical width of the prohibited zone, and the electrochemical behavior was investigated. We have shown that the aldehyde **1** and ethyl-3-{5-[4(9*H*-carbazole-9-yl)phenyl]thiophene-2-yl}-2- cyanoprop-2-enoate capable of electrochemical polymerization.

Thematic Section: Preparative Research. **Full Paper**
Subsection: Organic Chemistry. *Registration Code of Publication:* 15-42-4-71
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Synthesis of the novel chalcones containing the ethylenedioxythiophene moiety

© **Anna N. Ignaishevich**,[1] **Daria G. Selivanova**,[3+] **Alexey A. Gorbunov**,[3] **Elena V. Shklyaeva**,[1,2] and **George G. Abashev**[1,3]*
[1] *Department of Organic Chemistry. Perm State University. Bukireva St., 15. Perm, 614990. Russia. Phone: +7 (342) 239-66-12. Email: seshurov@yandex.ru*
[2] *Department of Radio Electronics and Information Security. Perm State University. Bukireva St., 15. Perm, 614990. Russia. Phone: +7 (342) 239-62-31. Email: lunegov@psu.ru*
[3] *Laboratory of Organic Semiconductors. Natural Scientist Institute. Perm State University. Genkel St., 4. Perm, 614990. Russia. Email: gabashev@psu.ru*
[4] *Laboratory of Active Reagents' Synthesis. Institute of Technical Chemistry, Russian Academy of Sciences, Ural Division, Academician Korolev St., 3. Perm, 614990. Russia. Phone: +7 (342) 237-82-89. Email: gabashev@psu.ru*

*Supervising author; +Corresponding author

Keywords: 3,4-ethylenedioxythiophene, chalcone, π-conjugated systems, cross-coupling.

Abstract

With an aim to prepare electroconducting polymer films there was prepared a series of chalcones including 3,4-ethylenedioxythiophene and thiophene moieties. Optical properties of all the synthesized compounds were investigated. It has been shown that the lengthening of the conjugation chain results in the bathochromic shift of absorption maxima if compared with those of the parent compounds. The band gaps (E_g^{opt}) have been calculated using the values of the longest absorption wavelengths (λ_{onset}); they comprises 2.58 eV for 2,5-di{4-[1-oxo-3-(thiophen-2-yl)-prop-2-enyl]phenyl}-3,4-ethylenedioxythiophene and 1.93 eV - for 5,5′′-di[3-oxo-3-(thiohen-2-yl)-prop-1-enyl]-$(EDOT)_3$.

Thematic Section: Preparative Research. **Full Paper**
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Synthetic possibilities sulfenyl chlorides group in β-diketonate chelates

© **Irina V. Svistunova**,[+] and **Nikolay P. Shapkin***
Department of General, Inorganic and Organometallic Chemistry. School of Natural Sciences. Far Eastern Federal University. October St., 27. Vladivostok, 69000. Russia.
Phone: +7 (8423) 245-76-69. E-mail: svistunova.iv@dvfu.ru; irasvist@gmail.com

*Supervising author; [+]Corresponding author

***Keywords**:* sulfenyl chlorides, β-diketonates, unsaturated compounds, organosilicon compounds, CH-acid pyrazoles polynuclear dendrimers.

Abstract

Sulfenilhlorid's derivatives of β-diketonate complexes were obtained and the reactions of sulfenilhlorid's group were studied. The reactions of addition and substitution of β-diketonates sulphenylchlorides showed that similar interactions as for SCl-groups in organic compounds are occurring. That enables the synthesis of a wide range of γ-thiosubstituted diketonates. Chromium(III) acetylacetonate sulphenylchlorides were used for dendrimers obtaining. With using of boron difluoride sulfenilhlorid complex new pyrazoles and diketones were synthesized.

Thematic Section: Preparative Research. **Full Paper**
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Thematic course: Alkylation of phenols by β-pinene using phenolate and aluminum isopropylate. Part 4.

Alkylation of resorcinol by β-pinene at the presence of aluminum-containing catalysts

© **Olga A. Shumova**, **Irina Yu. Chukicheva**,[+]
Tatiana A. Kolegova, and **Alexandr V. Kutchin**
Institute of Chemistry, Komi Science Center. Ural Branch of the Russian Academy of Sciences. Pervomaiskaya, St., 48. Syktyvkar, 167982. Russia. E-mail: chukicheva-iy@chemi.komisc.ru

*Supervising author; [+]Corresponding author

Keywords: phenol, resorcinol, β-pinene, aluminum phenoxide, aluminum isopropoxide, terpenphenols.

Abstract

Studied alkylation of resorcinol by β-pinene in the presence of $(PhO)_3Al$ and $(i\text{-}PrO)_3Al$ at 120 and 160 °C. It was found that on the alkylation resorcinol of β-pinene affect the structure carbocation formed from β-pinene. The use of equimolar amounts of the starting components (or excess resorcinol) contribute to the formation of esters of the chroman type. Use of excess β-pinene leads to the formation of product *O*- and *C*-alkylation with bornyl structure of substituent.

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Effective ways the synthesis of pyrrolo[3,2,1-*ij*]quinoline-1,2-dione and the products of its oxidative transformations

© **Svetlana M. Medvedeva**,*+ and **Khidmet S. Shikhaliev**
Chair of Organic Chemistry. Chemical department. Voronezh State University.
Universitetskaja pl., 1. Voronezh, 394006. Russia.
Phone: +7 (473) 220-84-33. E-mail: SMMedvedeva@rambler.ru

*Supervising author; +Corresponding author

Keywords: 1,2,3,4-tetrahydroquinoline, oxalylchloride, reaction Stolle, pyrrolo[3,2,1-ij]quinoline-1,2-dione, oxidation, [1,3]oxazino[5,4,3-ij]quinolin-1,3-dione, [1,4]oxazino[2,3,4-ij]quinoline-2,3-dione.

Abstract

Developed an effective way to obtain 5,6-dihydro-4*H*-pyrrolo[3,2,1-*ij*]quinoline-1,2-dione. With gradual addition of a solution of 1,2,3,4-tetrahydroquinoline to a solution of oxalyl chloride in toluene, followed by reflux for 1-1.5 h., Along with a simple acylation, cyclization proceeds at Stolle type of reaction, resulting in a mixture of 5.6-dihydro-4*H*-pyrrolo[3,2,1-*ij*]quinoline-1,2-dione and 1,1'-(1,2-dioxoethane-1,2-diyl)bis-1,2,3,4-tetrahydroquinoline in the ratio 3: 1. The resulting mixture was treated with an excess of 20% solution of NaOH, the insoluble by-product was separated, by acidification of the solution obtained by major product. The optimum conditions for the selective oxidation of the resulting pyrrolo[3,2,1-*ij*]quinoline-1,2-dione: at the last action of *meta*-chloroperbenzoic acid, a 6,7-dihydro-1*H*,5*H*-[1,3]oxazino[5,4,3-*ij*]quinoline-1,3-dione, and the action of sodium peroxodisulfate in sulfuric acid produced its isomer – 6,7-dihydro-1*H*,5*H*-[1,4]oxazino[2,3,4-*ij*] quinoline-2,3-dione.

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Synthesis 6-thiosubstituted 3,5-dinitro-1,2,3,4-tetrahydropyridines

© **Irina I. Surova**,[1] **Evgenia V. Ivanova**,[1] **Igor V. Blokhin**,[1]
Iryna V. Shahkeldyan,[1] **Yury M. Atroshchenko**,[1]* **Konstantin I. Kobrakov**,[2]
Dmitry Nikolaevich Kuznetsov,[2]*[+] and **Ivan V. Fedyanin**[3]
[1] *Department of Chemistry. Tula State Lev Tolstoy Pedagogical University. Lenin pr., 125. Tula, 300026. Russia. Phone: +7 (4872) 35-78-08. E-mail: reaktiv@tspu.tula.ru*
[2] *Department of Organic Chemistry. Moscow State University of Design and Technology. Sadovnicheskaya St., 33. Moscow, 115035. Russia. Phone: +7 (495) 955-35-58. E-mail: occd@mail.ru*
[3] *A.N. Nesmeyanov Institute of Organoelement Compounds of Russian Academy of Sciences. Vavilova St., 28, V-334. Moscow, 119991. Russia. Phone: +7 (499) 135-92-14. E-mail: octy@xrlab.ineos.ac.ru*

*Supervising author; [+]Corresponding author

Key words: 3,5-dinitro-1,2,3,4-tetrahydropyridine, 2-chloro-3,5-dinitropyridine, nucleophilic substitution, selective hydrogenation, *o*-thiocresol, 1*H*-benzimidazol-2-thiol.

Abstract

Reaction of 2-thiosubstituted 3,5-dinitropyridine with $NaBN_4$ and orthophosphoric acid to synthesize the corresponding 3,5-dinitro-1,2,3,4-tetrahydropyridine. By IR and NMR spectroscopy and X-ray diffraction data proved the structure of the compounds obtained.

Full Paper _____ *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 15-42-6-96 *Subsection:* Phase Equilibrium.
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Phase equilibria in condensed systems with cyclododecane and *n*-alkanes

© **Ivan K. Garkushin**,[1]* **Alexander V. Kolyado**,[2+] **Evgeny P. Petrov**,[3+] and **Alexander A. Shamitov**[4+]
Department of General and Inorganic Chemistry. Samara State Technical University. Molodogvardeiskaya St., 244, Samara, 443100. Samara Region. Samara. [1)] *Phone: +7 (846) 278-44-77.*
E-mail: [1)] *baschem@samgtu.ru;* [2)] *kolyado@rambler.ru;* [3)] *e.p.petrov@yandex.ru;* [4)] *sansher@mail.ru;*

*Supervising author; [+]Corresponding author

Keywords: *n*-decane, *n*-octadecane, cyclododecane, phase equilibria, liquidus, eutectics.

Abstract

By low-temperature differential thermal analysis using a differential scanning calorimeter of heat flow the systems of *n*-decane–*n*-octadecane–cyclododecane, *n*-decane–cyclododecane, *n*-octadecane–cyclododecane have been investigated. All of the studied systems belong to the eutectic type. The eutectic composition alloys contain 10.0 % wt in the system *n*-decane–*n*-octadecane–cyclododecane; eutectic composition alloy contains 84.5 % wt. *n*-$C_{10}H_{22}$; 5.5 % wt. *n*-$C_{18}H_{38}$; 10 % wt. $C_{12}H_{24}$ and has the melting point of 34.9 °C.

Full Paper _____ *Thematic Section:* Preparative Research.
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Interaction of 1-germatranol hydrate with *D*-tartaric acid in water medium

© **Victor Petrovich Baryshok**,[1+]* and **Nhat Thuy Giang Le**[2]
[1] *Cathedra of Chemical Technology. Irkutsk State Technical University. Lermontova St., 83. Irkutsk, 664074. Russia. Phone: +7 (3952) 40-55-13. E-mail: baryvik@yandex.ru*
[2] *Baria-Vung Tau University, Vung-Tau, Vietnam. 80 Trương Công Đinh, Phường 3, TP. Vũng Tàu*

*Supervising author; [+]Corresponding author

Keywords*:* 1-Germatranol hydrate, *D*-tartaric acid, triethanolamine, bis(μ-tartrato)di-(hydroxo)germanate(IV) triethanolammonium, bis(μ-tartrato)di(hydroxo)germanate(IV) pyridinium.

Abstract

When interacting hydrate 1-germatranol, $N(CH_2CH_2O)_3GeOH \cdot H_2O$, with D-tartaric acid in an aqueous medium germatrane cycle collapses and forms a bis(μ-tartrato)di(hydroxo)germanate(IV) triethanolammonium. The reaction of bis(μ-tartrato)di(hydroxo)digermanium acid with triethanolamine leads to the same binuclear complex of pentacoordinated Ge atom. Pyridine ligands in bis(μ-tartrato)di(hydroxo)germanate(IV) can be easily substituted triethanolamine, also forming bis(μ-tartrato)di(hydroxo)germanate(IV) triethanolammonium.

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Synthesis of diadamantyl diureas – new class of target-oriented soluble epoxide hydrolase inhibitors

© **Vladimir V. Burmistrov**,[+] and **Gennady M. Butov***
Volzhsky Polytechnic Institute (branch) Volgograd State Technical University. Engels St., 42a. Volzhsky, 404121. Volgograd region. Russia.
Phone: +7 (8443) 22-19-59. E-mail: butov@volpi.ru

*Supervising author; [+]Corresponding author
Keywords: *isocyanate*, urea, adamantane, adamantyl, soluble epoxide hydrolase.

Abstract

Series of adamantylcontaining 1,3-disubstituted diureas containing various spacers between urea group and adamantane part were synthesized. Compounds obtained show high inhibitory activity against human soluble epoxide hydrolase. Reactions were carried out in mild conditions with high yield.

Full Paper _____ *Thematic Section:* Preparative Research.
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Ethoxycarbonyl(acetyl)cyclohexanones in reactions with *C*- and *N*-aminotriazole

© **Natalia O. Vasilkova**,[+] **Nadezhda V. Zaraeva**,[1] **Vitaly Viktorovich Sorokin**,* and **Adele P. Krivenko**

Department of Organic and Bioorganic Chemistry. Saratov State University them N.G. Chernyshevsky. Astrakhanskay St., 83. Saratov, 410012. Russia. Phone: +7 (8452) 27-14-91.
[1] Saratov State Medical University. VI Razumovsky. E-mail: vasilkovano@mail.ru

*Supervising author; [+]Corresponding author

***Keywords**: C*-amino-1,2,4-triazole, *N*-amino-1,2,4-triazole, cyclocondensation, oksocyclohexandikarboksilate, diatsetilcyclohexanone, triazoloquinazoline, *N*-triazoliliminocyclohexane, spectre.

Abstract

By reaction polycarbonyl compounds – oksocyclologeksandikarboksilate, diatsetiltsiklogeksanonov *C*- and *N*-amino-1,2,4-triazoles. At the same time, depending on the structure of reagents obtained Functionally triazoloquinazoliny or *N*-triazoliliminotsiklohexanes, the structure of which is set by spectral methods.

Full Paper _____ *Thematic Section:* Preparative Research.
Registration Code of Publication: 15-42-4-112 *Subsection:* Organic Chemistry.
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Arylamines with a moiety of 1-azaxanthene

© Valery Yu. Gorokhov
Department of General Chemistry. FSBEI HPE «Perm State Agricultural Academy" n.a. Academician D.N. Pryanishnikov. Petropavlovskaya St., 23, Perm, 614000. Perm region. Russia.
Phone: (3422) 12-95-68. E-mail: gorokhov_v.yu@mail.ru

Keywords: arylamines, *N*-benzylidene-4-methoxyaniline, 5*H*-chromeno[2,3-*b*]pyridin-5-ol-(1-azaksantgidrol), 4-substituted-*N*-(5*H*-chromeno[2,3-b]pyridine-5-yl)anilines *N*-benzylidene-2-(5*H*-chromeno[2,3-*b*]pyridin-5-yl)-4-methoxy aniline.

Abstract

For the first time we synthesized new 4-substituted-*N*-(5*H*-chromeno[2,3-*b*]pyridin-5-yl)anilines by the interaction of 5*H*-chromeno[2,3*b*]pyridin-5-ol with arylamines. A new *ortho*-product *N*-benzylidene-2-(5*H*-chromeno[2,3-*b*]pyridin-5-yl)-4-methoxyaniline has been produced by the interaction of 5*H*-chromeno[2,3*b*]-pyridin-5-ol with *N*-benzylidene-4-methoxyaniline.

Short Communication _____ *Thematic Section:* Preparative Research.
Registration Code of Publication: 15-42-4-116 *Subsection:* Organic Chemistry.
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Selectivity of the reaction of chalcones with aniline derivatives

© **Yaroslav V. Bykov**, **Vikentiy D. Pak**, and **Nadezhda N. Yaganova**
Department of General Chemistry. Perm State Agricultural Academy n.a. Academician D.N. Pryanishnikov. Petropavlovskaya St., 23, Perm, 614000. Perm region. Russia.
Phone: +7 (3422) 12-95-68. E-mail: BykovJaV@mail.ru

*Supervising author; +Corresponding author

Keywords: chalcones, benzylideneacetophenone, Schiff bases, chalcone anils, *N*-(1,3-difenilalliliden) anilines β-arylamino ketones, 1,3-diphenyl-3-(phenylamino) propane-1-ones.

Abstract

Interaction of chalcones with 4-substituted anilines in anhydrous ethanol in the presence of the appropriate amine hydrochloride results in the formation of the products of coordination at the ethylene bond or carbonyl group. The formation of synthetically inaccessible *N*-(1,3-diphenylallylidene) anilines depends on the nature of the substituents in chalcone and arylamine.

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Synthesis of complex oxides transitive metal powders in aqueous media

© **Vladimir I. Ivanenko**,*+ **Svetlana V. Vladimirova**, **Svetlana V. Aksenova**, **Ekaterina N. Yakubovich**, and **Efroim P. Lokshin**
A Federal State Budgetary Institution of Science, I.V. Tananaev Institute of Chemistry and Technology of Rare Elements and Mineral Raw Materials. Kola Science Centre, RAS (ICTREMRM KSC RAS). Akademgorodok St., 26a. Apatity, Murmaks region, 184209. Russia.
Phone: +7 (8155) 57-92-40. E-mail: ivanenko@chemy.kolasc.net.ru

*Supervising author; +Corresponding author

***Keywords**:* complex transitive metal oxides, titanium(IV), niobium(V), tantalum(V), complexformation, ion exchange, synthesis.

Abstract

On the basis of regularities of complexation and ion exchange in aqueous media, there have been developed a strategy and principles of directed synthesis of materials as monophase nano-size powders of alkali metal metaniobates (metatantalates), as well as metatitanates of di-valent metals (strontium, barium and lead). We have found ways for obtaining precursors that preclude the development of olation-oxolation processes and studied the effect of reagent concentration and temperature on the composition of solid phases formed. The basis for the approaches to the formation of solid phases of desired composition became a study into the processes of cation displacement using inorganic precursors. The values of constants of the process of the alkali metal cation displacement by hydrogen ions in hydrated niobates(tantalates) and titanates have been determined. The affinity of the alkali metal cation to the hydrated matrix of titanium(IV), niobium(V) and tantalum(V) depends on the degree of alkali metal cation hydration. We determined the conditions for the existence in aqueous media of solid phases with the ratios M:Nb(Ta) = 1 and M:Ti = 2 (M - Li^+, Na^+, K^+), corresponding to the composition of hydrated alkali metal metaniobates, metatantalates and metatitanates. Thermal treatment of these precursors results in monophase crystalline nano-size or superdispersed powders of alkali metal metaniobates, metatantalates and metatitanates of stoichiometric composition. By using hydrated titanates of singly charged cations with M:Ti = 2 (M - NH_4^+, Li^+, Na^+, K^+) as precursors in aqueous media was studied the process of the formation of monophase crystalline nano-size powders and superdispersed powders of stoichiometric barium, strontium and lead metatitanates. The effective way of synthesis providing obtaining of monophase nanosized powders of complex oxides of transitive metals of the stoichiometric composition and solid solutions on their basis is developed.

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Registration Code of Publication: 15-42-4-130 *Subsection:* Supramolecular Chemistry.
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Amphiphilic thiacalixarenes in supramolecular systems

© **Ivan I. Stoikov**,*+ **Elena A. Andreyko**, and **Pavel L. Padnya**
A.M. Butlerov Chemical Institute. Kazan Federal University. Kremlevskaya St., 18. Kazan, 420008. Russia. Phone: +7 (843) 233-74-62. E-mail: ivan.stoikov@mail.ru

*Supervising author; +Corresponding author
Keywords: thiacalixarenes, supramolecular chemistry, amphiphilic compounds, self-assembly.

Abstract

The formation of supramolecular associates based on water-soluble *p-tert*-butylthiacalix[4]arenes with organic acids has been studied. Two approaches have been used to create supramolecular structures due to the formation of hydrogen bonds: self-association of amphiphilic p-*tert*-butylthiacalix[4]arenes and aggregation of macrocycles with organic acids. It was found that the increasing size of the substituents at the ammonium nitrogen atom of *p-tert*-butylthiacalix[4]arenes led to decrease the concentration at which self-associates can be formed. It has been shown by DLS that in most cases self-associates represent the oblate spheroid. It has been shown by UV-spectroscopy that hydroxy acids are able to interact with *p-tert*-butylthiacalix[4]arenes containing small methyl and ethyl substituents at the ammonium nitrogen atom or macrocycles containing phthalimide and ester substrates with additional coordination centers.

Full Paper _____ *Thematic Section:* Preparative Research.
Registration Code of Publication: 15-42-4-138 *Subsection:* Supramolecular Chemistry.
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A pulsed field gradient NMR diffusion investigation of water-soluble *p-tert*-butyl-thiacalix[4]arene derivatives

© **Elizaveta A. Arkhipova**,[1,2] **Lilia B. Magomedova**,[1,2] **Andrey B. Konov**,[3]
Pavel Leonidovich Padnya,[2] **Ivan Ivanovich Stoikov**,[2]
Bulat I. Khairutdinov,[1,2,*+] and **Yury F. Zuev**[1*]
[1] *Kazan Institute of Biochemistry and Biophysics. Lobachevsky St., 2/31. Kazan, 420111. Republic of Tatarstan. Russia.*
[2] *Kazan Federal University. Ul. Kremlevskaya, 18. Kazan, 420008. Republic of Tatarstan. Russia.*
[3] *Kazan Physical-Technical Institute. Siberian trakt, 10/7. Kazan, 420029. Republic of Tatarstan. Russia.*
Phone.: +7 (843) 231-90-30. E-mail: khayrutdinov@yahoo.com

*Supervising author; +Corresponding author
Keywords: calixarenes, conformation, NMR, self-diffusion, micelle formation.

Abstract

Micellization process of 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis[(*N*-(3',3'-dimethyl-3'-{(ethoxy-carbonylmethyl)amidocarbonylmethyl}ammoniumpropyl)carbamoylmethoxy]-2,8,14,20-tetrathiacalix[4]arene tetrabromide in *cone* and *1,3-alternate* conformations by pulsed field gradient NMR diffusion was investigated. Self diffusion coefficient dependency from concentration was explained by phenomenological approach. Thiacalix[4]arene in *cone* conformation have shown canonical micelle formation with clear monomer-micelle transition. Critical micellization concentration of micelle formation for this compound has been calculated. Micelle transition was absent for thiacalix[4]arene in *1,3-alternat* conformation when concentration was increased. Only slow increasing of aggregation degree was observed.

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Subsection: Electrochemistry. *Registration Code of Publication:* 15-42-4-143
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The electrochemical oxidation of organometallic diphosphonate-bridged palladacycles

Tatiana V. Gryaznova, and **Yulia H. Budnikova***[+]
A.E. Arbuzov Institute of Organic and Physical Chemistry. Kazan Scientific Center of Russian Academy of Sciences. Arbuzov St., 8. Kazan, 420088. Russia. Fax: +7 (8432) 75-22-53. E-mail yulia@iopc.ru

*Supervising author; [+]Corresponding author

***Keywords**:* palladium complex, oxidation, electrolysis.

Abstract

The redox properties of new diphosphonate-bridged dipalladacycles $[(phpy)Pd(EtO)_2P(O)]_2$, $[(phpy)Pd(EtO)_2P(O)]_2$, $[(phpy)Pd(EtO)_2P(O)]_2$ (phpy = 2-phenylpyridine, bhq = benzo[h]quinoline, phpz = 1-phenylpyrazole) derived from acetate analogues were studied. It is found that the electrochemical oxidation of a number of dipalladacycles $[PdL(EtO)_2P(O)]_2$, in acetonitrile afforded corresponding arylphosphonates at a potential -1.1–1.4 V ref.Fc/Fc^+. For complete convertion of dipalladacycles into arylphosphonates 8*F* electricity per each palladium atom is required This oxidation process can be used in the synthesis of new arylphosphonate from different arenas in the ligand-directed reaction of aromatic CH phosphonation.

Full Paper _____ *Thematic Section:* Preparative Research.
Registration Code of Publication: 15-42-4-148 *Subsection:* Physical Chemistry of Explosives.
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Synthesis and properties of CL-20crystals with inclusions of dispersed aluminum

© **Georgy V. Teplov**,*+ **Vladimir N. Popok**, **Alena V. Kireeva** and **Nikolay V. Bychin**
Joint Stock Company "Federal Research and Production Center" Altai ". Sotsyalisticheskaya St., 1. Biysk, 659322. Altay region. Russia.Phone: +7 (3854) 30-19-37. E-mail: teplov_georgii@mail.ru

*Supervising author; +Corresponding author

Keywords: cyclic nitramine, CL-20, the dispersed aluminum complex with inclusions.

Abstract

As a result of the work there have been obtained the crystals of hexanitrohexaazaisowurtzitane with inclusions of dispersed aluminum.Their surface and microstructure were studied by optical and electron microscopy, thermoanalytical parameters were identified. The sensitivity of the samples to mechanical stress, as well as specific electrical resistance and the minimum ignition energy of crystals have been studied.

Full Paper _____ *Thematic Section:* Preparative Research.
Registration Code of Publication: 15-42-4-152 *Subsection:* Organic Chemistry.
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Convenient synthesis of aryl-substituted 3-(pyrazin-2-yl)- and 3-(pyrimidine -2-yl)-1,2,4- triazines

© **Dmitry S. Kopchuk**[1,2]*+, **Albert F. Khasanov**[2], **Igor L. Nikonov**[2], **Alexey P. Krinochkin**[2], **Sogata Santra**[2], **Igor S. Kovalev**[2], **Gregory V. Zyryanov**[1,2], **Olga S. Tania**[2], **Dmitriy E. Pavlyuk**[2], **Vladimir L. Rusinov**[1,2] and **Oleg N. Chupahin**[1,2]
[1] *I.Ya. Postovsky Institute of Organic Synthesis. UB RAS.*
Kowalewskiy St., 22 / Academicheskaya St., 20. Ekaterinburg, 620990. Russia.
Phone/Fax: +7 (343) 369-30-58. E-mail: dkopchuk@mail.ru
[2] *Ural Federal University. St. Mira, 19, Ekaterinburg, Russia 620002. Phone/fax: (343) 375-45-01.*

*Supervising author; +Corresponding author

Keywords: heterocyclization, 1,2,4-triazine, cyanodiazines, iminoethers, amidrazones.

Abstract

There were developed two effective method for obtaining arylsubstituted 3-(pyrazin-2-yl)- and 3-(pyrimidine-2-yl)-1,2,4-triazines as a result of heterocyclization of the appropriate amidrazones and 1,2-diones (we proposed an optimized method in comparison with earlier published versions through easier procedures for obtaining amidrazones based on the corresponding nitrites due to the lack of the need for additional purification), as well as through condensation of the obtained *in situ* iminoethers of diazines with hydrazones of izonitrozoacetophenones.

Full Paper _____ *Thematic Section:* Physicochemical Research.
Registration Code of Publication: 15-42-4-158 *Subsection:* Physical Chemistry of Cellulose.
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The influence of amphiphilic substances and enzymes on resin components of wood pulp

© **Regina A. Kopnina**,[+] **Elena Yu. Demyantseva**,* **Il'ya A. Karpov**, and **Ol'ga S. Andranovicha**

Physical and Colloid Chemistry Department. Institute of technology. Saint Petersburg State Technological University of Plant Polymers. Ivana Chernykh St., 4. Saint-Petersburg, 198095. Russia.
Phone: +7 (904) 638-37-57. E-mail: zz1234567@yandex.ru

*Supervising author; [+]Corresponding author

***Keywords**:* nonionic surfactants, lipase enzymes, pulp wood, deresination, cellulose.

Abstract

This study demonstrates the influence of nonionic surfactants, commercial lipase enzyme and their mixtures on the content of resin components in various wood pulps. Optimal deresination compositions were selected then examined their colloid-chemical characteristics and estimated extent of pitch removal. Among individual surfactants, the most surface active is sintanol DS-10. The most synergetic mixtures were recommended for pulp deresination. Influence of ones on pulp residual pitch content was determined.

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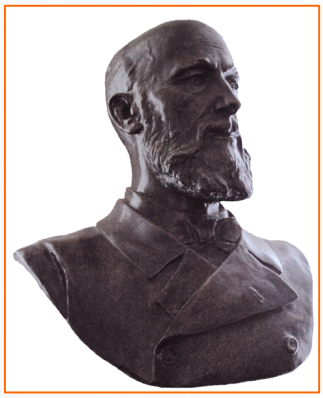

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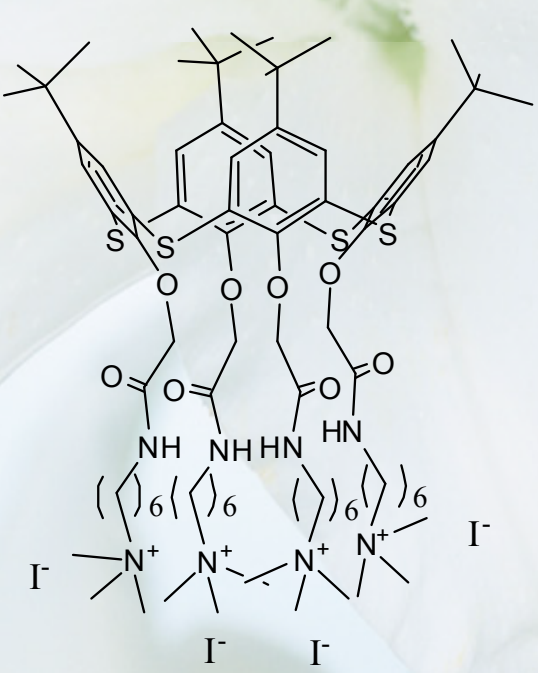

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Synthesis of new water soluble *p-tert*-butylthiacalix[4]arene derivatives containing quaternary ammonium fragments

© **Pavel L. Padnya**,[1] **Elena A. Andreyko**,[1] **Alisa Z. Harisova**,[1]
Yury F. Zuev,[2] and **Ivan I. Stoikov**[1,2]*[+]

[1] *Organic Chemistry Department. A.M. Butlerov Chemical Institute. Kazan (Volga Region) Federal University. Kremlevskaya St., 18. Kazan, 420008. Tatarstan Republic. Russia. Phone: +7 (843) 233-74-62. E-mail: ivan.stoikov@mail.ru*

[2] *Kazan Institute of Biochemistry and Biophysics, Russian Academy of Science. Lobachevskogo St., 2/31. Kazan, 420111. Tatarstan Republic. Russia.*

*Supervising author; [+]Corresponding author

Keywords: *dynamic light scattering, thiacalix[4]arenes, synthesis, synthetic receptors, molecular recognition, supramolecular chemistry.*

Abstract

p-tert-Butylthiacalix[4]arenes tetrasubstituted at the lower rim containing primary amino groups, quaternary ammonium and cyclic amide fragments have been synthesized. It has been shown that the formation of cyclic amide fragments in thiacalix[4]arenes occurs in the case of aliphatic diamines with ethylene bridge fragments.

Thematic Section: Preparative Chemistry. **Full Paper**
Subsection: Organic Chemistry. *Registration Code of Publication:* 13-34-5-11
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Synthesis of dibazole derivatives

© **Natalia V. Meshcheryakova**, **Sergey I. Bobrovsky**,
Zoya P. Belousova,*+ **Yury P. Zarubin**, and **Pyotr P. Purygin**
Department of Organic, Bioorganic and Medicinal Chemistry. Samara State University. Akad. Pavlov St., 1. Samara, 443011. Samara region. Russia. Phone: +7 (846) 334-54-59. E-mail: zbelousova@mail.ru

*Supervising author; +Corresponding author

Keywords*: dibazole, 4-(2-benzyl-1H-benzimidazole-1-ylmetyl)phenol, 2-(2-benzyl-1H-benzimidazole-1-ylmethyl)phenol, 4-(2-benzyl-1-benzimidazole-1-ylmethyl)phenyl-2,3,4,6-tetra-O-acetyl-β-D-glucopyranoside.*

Abstract

The synthesis of dibazole derivatives: 2-(2-benzyl-1*H*-benzimidazole-1-ylmethyl)phenol, 4-(2-benzyl-1*H*-benzimidazole-1-ylmethyl)phenol, 4-(2-benzyl-1*H*-benzimidazole-1-ylmethyl)phenyl-2,3,4,6-tetra-*O*-acetyl-β-*D*-glucopyranoside was implemented. The structure of the compounds was confirmed by IR and ^{1}H NMR spectroscopy. Using the program *HyperChem 7.52* we built the models of molecules of synthesized derivatives of benzimidazole and calculated their physicochemical properties. According to the estimation of the alleged biological activity by the program *PASS Professional 2007* the synthesized compounds may possess some types of biological action useful in pharmacology.

Full Paper _____ *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 13-34-5-16 *Subsection:* Colloidal Chemistry.
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http://butlerov.com/readings/
Contributed: April 24, 2013.

The problem of stochastic flow cluster caustics in oxyhydrate systems

© **Boris A. Markov**, **Yury I. Sukharev**,*+ and **Inna Yu. Apalikova**
Department of Solids and Nanoprocesses. Chelyabinsk State University.
Bratiev Kashirinykh St., 129. Chelyabinsk, 454000. Russia.
Phone: +7 (963) 460-27-75. E-mail: Yuri_Sucharev@mail.ru.

*Supervising author; +Corresponding author

Keywords: *Lagrangian maps, caustics, oxyhydrate gel systems, oxyhydrate noise, colloid clusters, spontaneous pulsation current, spike surge, diffuse double electrical layer.*

Abstract

It is common knowledge that the equation for the motion of particles in a gel is subject to viscous equations of hydrodynamics. This means that a system of equations that describes motions of particles in a gel can be put down in a form that is similar to that of the equations for plasma dynamics. A caustic is a set of degenerated critical points of the function that describes the phenomenon. Therefore, one can find those points by formulating a solution to the equation that is a simple linear equation.

Full Paper _____ *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 13-34-5-22 *Subsection:* Physical Chemistry of High Temperatures.
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Mathematic simulation of ignition process for gelled condensed substance by single heated metallic and non-metallic particles

© **Dmitry O. Glushkov**,[+] **Alena O. Zhdanova**, and **Pavel A. Strizhak***
National Research Tomsk Polytechnic University. Lenin St., 30. Tomsk, 634050. Russia.
Phone: +7 (3822) 70-17-77, 1910. E-mail: dmitriyog@tpu.ru

*Supervising author; [+]Corresponding author

Keywords*: ignition, melting, evaporation, crystallization, oxidation, gelled condensed substance, heated particle, simulation.*

Abstract

Mathematic simulation of main physical and chemical processes and phase exchanges at the ignition of gelled condensed substance (fuel) by local heating is performed. Conditions of interaction between near-surface layer of fuel and heated till high temperature metallic (steel, aluminum) and non-metallic (ceramic, carbon) particles from various origin are investigated. Values of main integral characteristic process – ignition time delay are determined. Dependences of ignition time delay from energy source temperature are established. Comparison of ignition conditions for gelled, liquid and solid condensed substances at local heating is performed.

Full Paper _____ *Thematic Section:* Physoco-Chemical Research.
Registration Code of Publication: 13-34-5-34 *Subsection:* Physical Chemistry of Explosives.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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Analysis of the predictive capability of rheological characteristics of filled lacquer compositions based on cellulose nitrate

© **Lilia I. Selivanova**, **Tatiana A. Eneykina**,* **Natalia S. Gainutdinova**,+ **Anatoly P. Pavlov**, **Dilara R. Ibneeva**, **Alexey I. Hatsrinov**, **Roza F. Gatina**, and **Yury M. Mikhailov**
Federal State Enterprise "State Research Institute of Chemical Products". Svetlaya St., 1. Kazan, 420033. Tatarstan Republic. Russia. Phone: +7 (843) 544-07-21, 544-09-82. E-mail: 173gniihp@gmail.com

*Supervising author; +Corresponding author

Keywords: *cellulose nitrate lacquer, filler, volume fraction, effective viscosity, relative viscosity.*

Abstract

The dependence of the effective viscosity of filled 2% solutions of cellulose nitrates the concentration of HMX, which has an extreme character with pronounced minima at the filler concentration ~15 and ~50 wt.% has been presented. It is established that due to the multifactorial nature of the rheological properties of heterogeneous nitrate cellulose lacquer compositions, none of the known mathematical functions can be used to predict the rheological behavior of systems in the formation of the spherical powder.

Thematic Section: Physico-Chemical Research. **Full Paper**
Subsection: Physical Chemistry. *Registration Code of Publication:* 13-34-5-41
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http://butlerov.com/readings/
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Study of physico-chemical properties of the azido-containing oligomers and polyurethanes based on them

© **Rinat O. Almashev**,* **Anastasia A. Orekhova**, **Nadezhda Roman'ko**, **Anna V. Kiprova**,+ **Elena V. Nurullina**, **Elvira N. Tarazova**, **Roza F. Gatina**, and **Yury Mikhailov**
Federal State Enterprise "State Research Institute of Chemical Products". Svetlaya St., 1. Kazan, 420033. Tatarstan Republic. Russia. E-mail: anekolab@mail.ru

*Supervising author; +Corresponding author

Keywords: *IR-spectroscopy, azido-containing oligomers.*

Abstract

It has been shown that with the help of IR-spectroscopy you can expressways and with high confidence establish if the synthesis proceeds according to the theoretical assumptions, and if as a result azido-containing oligomers are formed with high content of N_3 groups. It has been shown that azido-containing oligomers are easily identified by the absorption band of the azide group which has the frequency 2100±20 cm^{-1}, chlorine-containing oligomers, the absence of the IR spectra of absorption bands characteristic of the azide groups and the presence of intense absorption bands in the region of 710-730 cm^{-1} (υ_{C-Cl}) and υ = 1240 cm^{-1} (ω_{CH2Cl}).

Thematic Section: Physico-Chemical Research. **Full Paper**
Subsection: Physical Chemistry. *Registration Code of Publication:* 13-34-5-49
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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Contributed: April 10, 2013.

Hydrochemical deposition of polyvinyl acetate from aqueous dispersion

© **Rinat O. Almashev**,* **Nadezhda Roman'ko**, **Anna V. Kiprova**,+
Elena V. Nurullina, **Tatiana A. Eneykina**, **Sergey V. Soldatov**,
Anna V. Kiprova,+ **Elvira N. Tarazova**, **Roza F. Gatina**, and **Yury M. Mikhailov**
Federal State Enterprise "State Research Institute of Chemical Products". Svetlaya St., 1. Kazan, 420033. Tatarstan Republic. Russia. E-mail: anekolab@mail.ru

*Supervising author; +Corresponding author

Keywords: *polyvinyl acetate, aluminum sulfate, intermolecular interaction, IR spectroscopy, UV spectroscopy.*

Abstract

The interaction of aqueous dispersions of polyvinyl acetate with aluminum sulfate at different ratios of reactants has been studied. The optimum concentration of aluminum sulfate, which provides a complete replanting of the aqueous dispersion of polyvinyl acetate. There was discussed the associates formation mechanism of the type $Al^{3+}\ldots{}^{-}O=C<$, which quantitatively fall out of dispersion as a precipitate. The course of complexing is confirmed by IR and UV spectra of aqueous solutions and precipitates.

Thematic Section: Chemical and Technological Research. **Full Paper**
Subsection: Kinetics and Catalysis. *Registration Code of Publication:* 13-34-5-55
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
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Studies of kinetic parameters of the process of solution purification from impurities of cobalt and nickel by metallic zinc

© **Alexander V. Kolesnikov**,*+ and **Vladimir A. Burmistov**
Department of Analytical and Physical Chemistry. Chelyabinsk State University.
Brothers Kashirinykh St., 129. Chelyabinsk, 454001. Russia. E-mail: avkzinc-gu@yandex.ru

*Supervising author; +Corresponding author

Keywords: *purification, restoration, cobalt, nickel, hydrogen, activating additives, copper, antimony, kinetics, speed, energy of activation, category of cations.*

Abstract

The values of kinetic solutions purification parameters from impurities of cobalt, nickel and hydrogen restoration by the metallic zinc have been obtained. The process of purification took place in water solutions without zinc sulfate and in its presence. The activating additives of copper and antimony were added into the solutions. It is shown that the obtained kinetic curves of the category of hydrogen cations are characteristic for topochemical reactions, and processes proceed on the interface of a solid and liquid phase. The experimental data allows to explain the reason for accelerated discharge of hydrogen cations in solutions containing zinc sulphate and increased consumption, while zinc metal (zinc dust) in industrial purification of zinc sulfate solutions from impurities.

Full Paper _____ *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 13-34-5-60 *Subsection:* Nanochemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: April 23, 2013.

Particular properties of micron size powder particles

© **Igor E. Ignat'ev**,* and **Ivan S. Sipatov**[+]
Institute of Metallurgy. Ural branch of Russian Academy of Science. Amundsen St., 101. Ekaterinburg. Russia. Phone: +7 (343) 232-90-42. E-mail: ivan.sipatov@gmail.com

*Supervising author; [+]Corresponding author

Keywords: *powder agglomeration, powder conglomeration, mathematical simulation, vibro-treatment.*

Abstract

The relations of the deformation resistance of powder particle, the powder pressing density, the particle conglomeration of dry powder, the agglomeration of powder particles and their ability for breakage due to vibration in melt environment on the particle diameter are presented. Based on the obtained relations, it is shown that the boundary between the properties passes within the narrow range of 1-15 microns. In further fragmentation of the object its size in mathematical models should be taken into account starting exactly from this range.

Thematic Section: Chemical Cybernetics. **Full Paper**
Subsection: Physical Chemistry. *Registration Code of Publication:* 13-34-5-67
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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Program with elements of artificial intelligence to evaluate the enthalpy of formation of radicals on the kinetic data

© **Vladimir E. Tumanov**,* **Andrey I. Prokhorov**,+ and **Maina E. Solov'va**
Institute of Problems of Chemical Physics RAS. Chernogolovka, 142432.
Moscow Region. Russia. Fax: +7 (496) 522-35-07. E-mail: tve@icp.ac.ru

*Supervising author; +Corresponding author

Keywords: *intelligent software agent, enthalpy of formation of free radical, enthalpy of formation of molecule, intersecting parabolas model, bond dissociation energy, radical stabilization energy.*

Abstract

We have developed the intellectual software agent, which implements the evaluation algorithm of the enthalpy of formation of free radical on kinetics data which is based on hybrid knowledge base. Logical structure of knowledge base and the algorithm of intellectual software agent have been described. The results of numerical experiments on predicting the values of enthalpies of the formation of free radicals derived from acetals have been presented. We conducted the comparison of the calculated values of enthalpy of the radicals formation, derivatived from acetals, nitriles and nitro compounds with literary data. The comparison shows good agreement with the published data. Linear correlations have been constructed between the formation enthalpy of free radicals derived from a series of substituted acetals. The radical stabilization energy of substituted phenyl radicals has been calculated. It is shown that the conjugated system of π-electrons near the radical center destabilizes the radical, both for electron-donor substituents, and for electron-acceptor substituents.

Thematic Section: Thermodynamic Research. _____ **Discussion Column**
Subsection: Phase Equilibria. *Registration Code of Publication:* 13-34-5-75
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Relationship of parameters of the critical point of phase gas-liquid transition with boyle temperature

© Ihtiyor H. Umirzakov
Laboratory for Simulation. Institute of Thermal Physics SB RAS. Lavrentyev Pr., 1. Novosibirsk, 630090. Russia. Phone: +7 (383) 354-20-17. E-mail: tepliza@academ.org

Keywords: *critical temperature, critical volume, critical pressure, Boyle temperature, state equation of van der Waals, liquid-gas phase transition.*

Abstract

It is shown that for 21 real substances the relation of Boyle temperature to the product of critical temperature and critical compressibility factor with high precision is equal to number 9, predicted by the state equation of van der Waals. We proposed the ratio for finding the critical volume through the relation of Boyle temperature to critical pressure. We also suggest a formula for determining the critical volume through the critical temperature and parameters of straight line of single compressibility.

Full Paper _____ *Thematic Section:* Methodological Research.
Registration Code of Publication: 13-34-5-80 *Subsection:* Analytical Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: April 15, 2013.

Investigation of the metrological characteristics of quantitative multi-element analysis of inorganic nanomaterials by mass spectrometry with inductively coupled plasma with electrothermal vaporization

© **Albert Kh. Gilmutdinov**,[1] **Alexander V. Voloshin**,[2]* and **Konstantin Yu. Nagulin**[2+]
[1] *Kazan State Technical University Tupolev-KAI. K. Marx St., 10. Kazan, 420111. The Republic of Tatarstan. Russia. Phone: +7 (843) 231-01-06.*
[2] *Department of General Physics. Institute of Physics. Kazan (Volga) Federal University. Kremlin St., 18. Kazan, 420008. The Republic of Tatarstan. Russia. Phone: +7 (843) 233-72-20.*
E-mail: alexandr.voloshin@kpfu.ru,

*Supervising author; +Corresponding author

Keywords: *metrological characteristics, mass spectrometry, electrothermal vaporizer addition method.*

Abstract

Metrological characteristics are investigated by mass spectrometry with inductively coupled plasma entering the analyte by its electro-thermal evaporation. It is shown that the direct sublimation provides better metrological characteristics when compared to the traditional method of sample preparation for the "wet chemistry".

Thematic Section: Research into New Materials. **Full Paper**
Subsection: Chemistry of Polymers. *Registration Code of Publication:* 13-34-5-85
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Study of supramolecular structure of metal coordinated polyurethanes

© **Ilsia M. Davletbaeva**,[1+]* **Ruslan S. Davletbaev**,[2]
Olesya R. Gumerova,[1] **Ilnaz I. Zaripov**,[1] and **Viktor V. Parfenov**[3]
[1] *Department of Synthetic Rubber Technology. Kazan National Research Technological University. K. Marx St., 68. Kazan, 420015. Tatarstan Republic. Russia. Phone: +7 (843) 231-95-88. E-mail: davletbaeva09@mail.ru*
[2] *Department of Materials Science & Technology. Kazan National Research Technical University, K. Marx St., 10. Kazan, 420111. Tatarstan Republic. Russia. Phone: +7 (843) 238-44-10. E-mail: Darus@rambler.ru*
[3] *Department of Solid State Physics. Kazan Federal University. Kremlyovskaya St., 18. Kazan, 420008. Tatarstan Republic. Russia. Phone: +7 (843) 233-71-48. E-mail: Viktor.Parfenov@ksu.ru*

*Supervising author; [+]Corresponding author

Keywords*: metal complex structuring, urethane prepolymer, bulky coordination copper compounds, stuck structures, coordination bound azogroups, thermo mechanical analysis, dielectric losses, rigid block.*

Abstract

Bulky coordination compounds of copper were designed, showing the catalytic activity in the low-temperature dissociation of urethane groups and the ability to interact with the isocyanate groups with the subsequent formation of azoaromatic derivatives. Formation of stack ordered structures due to the formation of the azo groups and their subsequent coordination binding was a condition of charge transport through the stacks, which led to the possibility of an abrupt fall of volume resistivity of polyurethanes (ρ_v) by more than 10,000 times. It was found that the rigid blocks of coordination bound azo groups were formed in the polymer matrix having a significant influence on the supramolecular organization of polyurethanes, and on the complex of their physical and mechanical properties.

Thematic Section: Physico-Chemical Research. **Full Paper**
Subsection: Biochemistry. *Registration Code of Publication:* 13-34-5-91
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Investigation of interaction of proteins with bioactive nitrogenated heterocyclice compounds at various pH

© **Aleksandr S. Chukhno**,[+] **Irina B. Dmitriyeva**,*
Anastasia N. Bankina, and **Elizaveta Yu. Brilliantova**
Department of Physical and Colloid Chemistry. Saint-Petersburg State Chemical-Pharmaceutical Academy. Professor Popov St., 14. Saint-Petersburg, 197376. Russia.
Phone: +7 (812) 234-11-38. E-mail: alex-chuhno@yandex.ru, amylee2208@mail.ru

*Supervising author; [+]Corresponding author

Keywords: *nitrogenated heterocyclice compounds, sorption, isoelectric point.*

Abstract

In this work several nitrogenated heterocyclices were selected for investigation. Proteins were used such as serum albumin, casein, gelatine. Experiments were conducted in aqueous solutions.

Changes in value of isoelectric point were observed in water solutions with nitrogenated heterocyclic compounds, which means that nitrogenated heterocyclic compounds can specifically sorb on the surface of proteins. This is accompanied by the cationic form of nitrogenated heterocyclic compounds moving the isoelectric point into the alkaline area, and the anionic form – doing so into the acidic area. In certain cases, two isoelectric points were detected, one of them in the alkaline area, another in the acidic area. The ability of nitrogenated heterocyclic compounds to react with proteins depends on variation of the isoelectric point. Occurrence of a complex was detected with the help of absorption spectrum.

Full Paper _____ *Thematic Section:* Research into New Materials.
Registration Code of Publication: 13-34-5-100 *Subsection:* Biochemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: April 16, 2013.

The bactericidal action of experimental composite material of protective and decorative purposes

© **Vsevolod N. Bogdanov**, **Vladimir D. Buhanov**,
Alexander I. Vesentsev,* and **Olga A. Vorontsova**[+]
Department of General Chemistry. Belgorod National Research University. Pobeda St., 18. Belgorod, 308015. Russia. Phone: +7 (4722) 30-11-50. E-mail: vorontsova@bsu.edu.ru.

*Supervising author; [+]Corresponding author

Keywords*: bactericidal action, Escherichia coli, Staphylococcus aureus, nanodispersed hydrosilicate potassium, protective-decorative coating.*

Abstract

Bacteriostatic activity increases with increasing mass fraction of nanodispersed hydrosilicate potassium. We have recommended the ratio of film-forming materials for bactericidal coatings: 75-90 wt. % of nanodispersed hydrosilicate potassium, 10-25 wt. % of styrene acrylic dispersion, 0.5-1.0 wt.% of Zinc Pyrithione.

Full Paper _____ *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 13-34-5-106 *Subsection:* Physical Chemistry of Explosives.
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http://butlerov.com/readings/
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Mechanical activation of co-crystallization of some nitro compounds

© **Vladimir N. Popok**,*+ **Nikolay V. Bichyn**, **Nikolay I. Popok**, and **Nikolay V. Shein**
Open Joint Stock Company «Federal Research and Production Center "ALTAI".
Sotsialisticheskaya St., 1. Biysk, 659322. Altai region. Russia.
Phone: +7 (3854) 30-19-37. E-mail: vnpopok@mail.ru

*Supervising author; +Corresponding author

Keywords: *co-crystals, mechanical activation, solution, fusion, thermal methods of analysis, IR-spectroscopy.*

Abstract

Results of researches of physical and chemical properties of co-crystals obtained by mechanical activation, in comparison with the data for co-crystals, obtained from solutions and melts are presented in the article. The wide nomenclature of nitrocompounds – trinitrotoluene, trinitrobenzole, HMX, HNIW, *N,N*-dimethylmethylenedinitramine is considered. High efficiency of mechanical activation, as the method of obtaining co-crystals, in comparison with the production methods from solution and melt is shown.

Full Paper _____ *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 13-34-5-124 *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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Sorption of H + and OH-on chlorophyll, the effect of pH on the stability of aqueous dispersions of chlorophyll

© **Alexander S. Chukhno**, **Irina B. Dmitrieva**,* **Daria S. Silaeva**,+ **Anna S. Senina**, **Anastasia S. Koshevenko**, and **Albina R. Nazipova**
Department of Physical and Colloid Chemistry. St. Petersburg State Chemical-Pharmaceutical Academy. Professor Popov St., 14. St. Petersburg, 197376. Russia.
Phone: +7 (812) 234-11-38. E-mail: dasha.com.92@mail.ru , alex-chuhno@yandex.ru

*Supervising author; +Corresponding author

Keywords: *chlorophyll, the point of zero charge, isoelectric point.*

Abstract

The effect of single-charged electrolytes (KC1, HC1) on the sorption of H+ and OH- ion on chlorophyll, depending on the composition of the aqueous phase (KC1 and pH concentration) have been studied with the method of continuous potentiometric titration. All studies were performed after purifying the solution from carbon dioxide.

It has been found out that the point of zero charge of chlorophyll in the solutions of KC1 changes in the pH range from 4.0 to 3.0. The isoelectric point of chlorophyll was determined by using the viscosimeter and the spectrophotometric method. It was shown that pH isoelectric point and pH point zero charge coincide. It is proved that the change in pH value affects the coagulation threshold.

Thematic Section: Preparative Chemistry. **Full Paper**
Subsection: Supramolecular Chemistry. *Registration Code of Publication:* 13-34-5-131
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Efficient synthesis of pillar[5]arenes and pillar[6]arenes as the new synthetic acetylcholine receptors

© **Gregory V. Zyryanov**,[1,2]* **Alice A. Meyer**,[2] **Oleg S. Eltsov**,[2] **Dmitry S. Kopchuk**,[1,2+] **Igor S. Kovalev**,[2] **Igor L. Nikonov**,[2] **Albert F. Hasanov**,[2] **Dmitry Rudkevich**,[3] **Vladimir L. Rusinov**,[1,2] and **Oleg N. Chupahin**[1,2]

[1] *I.Ya. Postovsky Institute of Organic Synthesis UrB RAS. Kovalevskaya St., 22.Akademicheskaya St., 20. Ekaterinburg, 620990. Russia. Phone/fax: +7 (343) 369-30-58. E-mail: dkopchuk@mail.ru*

[2] *Ural Federal University.Mira St., 19. Ekaterinburg, 620002. Russia. Phone/fax: +7 (343) 375-45-01.*

[3] *University of Texas at Arlington. Nedderman St., 701. Arlington, Texas, 76013. USA. Phone/fax: +7 (817) 272-2011*

*Supervising author; +Corresponding author

Keywords: *synthetic receptors, pillararenes, acetylcholine, encapsulation.*

Abstract

An efficient synthesis of pillar [5] - and pillar [6] arenes with alkyl substituents of various lengths from commercially available reagents (1,4-dialkoxybenzene and paraformaldehyde or 1,3,5-trioxane in the presence of Lewis acids) has been worked out. Cyclooligomerization products were isolated in high yields and with high oligoselectivity. In the presence of acetylcholine 1,4-bis(dodecyloxy)pillar[5]arene forms the inclusion complex in the ratio 1:1, which is observed by ^{1}H NMR method.

Full Paper _____ *Thematic Section:* Theoretical Simulation.
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A simplified mathematical model of the impact assessment of thermal modes of ignition on the layer of soil after the stage of ignition of forest combustible material

© **Nikolay V. Baranovskiy**,[1]*+ and **Rakhmanbek M. Toichuev**[2]
[1] *Department of Theoretical and Industrial Heating Engineers.*
National Research Tomsk Polytechnic University. Lenin St., 30.
Tomsk, 634050. Russia. Phone: +7 (3822) 56-36-13. E-mail: firedanger@narod.ru
[2] *Institute of Medical Problems of Southern Branch of National Academy of Sciences of the Kirghiz Republic.*
Uzgensky St., 130-A. Osh, Kirghiz Republic.

*Supervising author; +Corresponding author

Keywords: *forest fire, thermal mode, soil, forest combustible material, ignition, influence of raised temperatures.*

Abstract

The simplified model of forest combustible material ignition is considered and the base mathematical model of an estimation of influence of thermal modes of forest fire on soils is presented in article. The model is presented by a set of the equations of heat conductivity with corresponding initial and boundary conditions. The numerical analysis of influence of various centres of forest fire on temperature distribution in the top soil layers is carried out. Results can be applied for the analysis of border regimes of vital activity of microorganisms in the soil.

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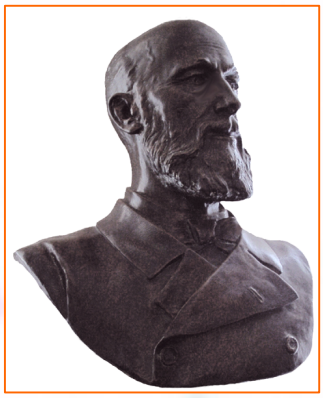

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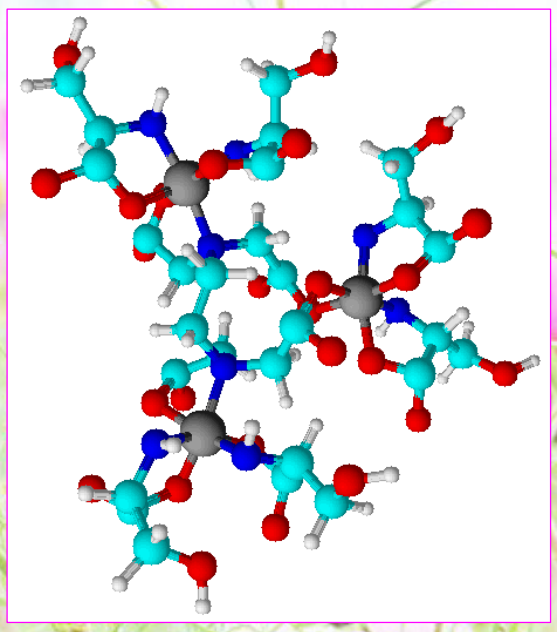

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http://butlerov.com/readings/
Contributed: May 6, 2013.

Biochemical activity of metal nanoparticles of hyperbranched polyester polyol composites

© **Marianna P. Kutyreva**,[1]*+ **Alfiya R. Gataulina**,[1] **Olga I. Medvedeva**,[1]
Ivan I. Stoikov,[2] and **Nikolay A. Ulakhovich**[1]

[1] *Department of Inorganic Chemistry. A.M. Butlerov Chemical Institute. Kazan Federal University. Kremlevskaya St., 18. Kazan, 420008. Tatarstan Republic. Russia. Phone: +7 (843) 233-74-65. E-mail: Marianna.Kutyreva@kpfu.ru*

[2] *Department of Organic Chemistry. A.M. Butlerov Chemical Institute. Kazan Federal University. Kremlevskaya St., 18. Kazan, 420008. Tatarstan Republic. Russia. Phone: +7 (843) 233-74-62. E-mail: ivan.stoikov@kpfu.ru*

*Supervising author; +Corresponding author

Keywords: *antimycotics, proteinase of Candida albicans, metal nanoparticles, hyperbranched polyester polyols.*

Abstract

Copper and cobalt nanoparticles have been synthesised on the platform of hyperbranched third-generation polyesterpolypropionic acid $H30(CH_2CH_2COOH)_{22}$ by the method of chemical reduction in the media of stabilizer. According to results of X-Ray phase analysis and transmission electron microscopy it was established that samples of $Cu/H30(CH_2CH_2COOH)_{22}$ nanoparticles consist of 10±4 nm particles, while $Co/H30(CH_2CH_2COOH)_{22}$ samples consist of 4±1 nm for metallic cobalt and 2-5 nm for its oxide phase. We estimated and compared antiproteinase activity of stabilizers – hyperbranched polyesterpolyol H30, $H30(CH_2CH_2COOH)_{22}$ and composition nanoparticles of copper and cobalt on their basis towards secretory aspartic proteinase *Candida albicans*.

Thematic Section: Physicochemical Research. **Full Paper**
Subsection: Supramolecular Chemistry. *Registration Code of Publication:* 13-34-6-9
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http://butlerov.com/readings/
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Encapsulation of volatile organic substances from their binary mixtures by macrocyclic receptor

© **Marat A. Ziganshin**,[+] **Rada I. Sinichkina**,
and **Valery V. Gorbatchuk***
A.M. Butlerov Institute of Chemistry. KFU. Kremlevskaya St., 18. Kazan, 420008. Tatarstan Republic. Russia. Phone: +7 (843) 233-73-09. E-mail: Marat.Ziganshin@ksu.ru.

*Supervising author; [+]Corresponding author

Keywords*: calixarene, polymorphism, clathrate, molecular recognition. enthalpy, thermogravimetry, differential scanning calorimetry, mass-spectrometry.*

Abstract

In this article, the clathrate formation of *tert*-bytilcalix[6]arene with vapors of binary mixtures of organic compounds was studied using the simultaneous thermogravimetry and differential scanning calorimetry analysis combined with mass spectrometric evolved gas analysis. The temperature ranges of stability and decomposition of the obtained mixed clathrates were determined. The content of each organic component of the binary mixture in inclusion compounds was calculated. The mutual influence of the two 'guests' on the thermal properties of the clathrates was analyzed. The calculated values of the enthalpy of the process of 'guest' removal from the clathrate were compared with the enthalpy of vaporization of these 'guests' at their boiling temperatures.

Thematic Section: Physico-Chemical Research. **Full Paper**
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Primary, secondary, tertiary, and quaternary structural organization of gel oxyhydrates

© Yury I. Sukharev
Department of Solid State Chemistry and Nanoprocesses. Chelyabinsk State University.
Br. Kashirinykh St., 129. Chelyabinsk, 454000. Russia.
Phone: +7 9634602775. E-mail: Yuri_Sucharev@mail.ru.

Keywords: *Lagrangian mappings, oxyhydrate gel systems, colloidal clusters, spontaneous pulsating stream, spike splash, diffuse double electric layer, dissociative-disproportionate destruction of macromolecules, theory of Whitney, geometry of caustics*

Abstract

As we see it now, the structural organization of gel oxy hydrate is very similar to the protein structure. It was K. Lindstrom-Lang who in his time suggested to distinguish 4 levels of structural organization of proteins: primary, secondary, tertiary and quaternary structures. Although this division is somewhat outdated, we still use it. For proteins the primary structure is natural when there is observed the sequence of amino acid residues of polypeptide determined by the structure of the gene and its genetic code. That is, the primary structure is the sequence of amino acid residues in the polypeptide chain. It is quite the other thing with oxyhydrates of *d*- and *f*-elements. The primary structure of oxyhydrate should be regarded as a kind of critical points of some complex smooth functions (by V.I. Arnold). Physically, these features are related to the geometry of destruction and binding of diffuse double electrical layer of macromolecules of gel oxyhydrates and their aging.

Thematic Section: Physico-Chemical Research. **Full Paper**
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PETN crystals decomposition at heat treatment up to melting point

© **Nadezhda L. Aluker**,[1]* **Gennadiy S. Denisov**,[2] **Ekaterina V. Ivanova**,[1+]
Mustafa M. Kidibaev,[2]* and **Alexander S. Pashpekin**[1]
[1] *Department of Physical Chemistry. Kemerovo State University. Krasnaya St., 6. Kemerovo, 650043. Russia. Phone: +7 (384-2) 58-81-17. E-mail: lira@kemsu.ru*
[2] *Crystalophysics Laboratory. Institute of Physical and Technological Problems and Materials Science. Chui St., 265. Bishkek, 720071. Kyrgyz Republic. Phone: +996 (312) 65-76-98. E-mail: kidibaev@mail.ru*

*Supervising author; [+]Corresponding author

Keywords*: pentaerythritol tetranitrate, decomposition, melting, absorption spectra, fluorescence spectra.*

Abstract

The absorption spectra of single crystals of PETN in a wide spectral range from 190 to 3300 nm, and the luminescence spectra before and after annealing of single crystals are measured. We conducted the measurements of absorption spectra in the heating process at certain temperatures up to the melting point. The absorption spectrum of the melt and the luminescence of the melted PETN were measured. This allowed to make a supposition about the mechanism of the slow decomposition of PETN during thermal treatment.

Full Paper _____ *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 13-34-6-38 *Subsection:* Physical Chemistry of Explosives.
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Laser initiation of PETN at low luminosity

© **Edward D. Aluker**,[1+] **Alexander G. Krechetov**,[1]*
Mustafa M. Kidibaev,[2]* and **Tatiana S. Koroleva**[2]*
[1] *Department of Physical Chemistry. Kemerovo State University.*
Krasnaya St., 6. Kemerovo, 650043. Russia. Phone: +7 (384-2) 58-81-17. E-mail: lira@kemsu.ru
[2] *Crystalophysics Laboratory. Institute of Physical and Technological Problems and Materials Science.*
Chui St., 265. Bishkek, 720071. Kyrgyz Republic. Phone: +996 (312) 65-76-98. E-mail: kidibaev@mail.ru

*Supervising author; [+]Corresponding author

Keywords*: pentaerythritol tetranitrate, laser initiation, hot spots.*

Abstract

We propose a method for separate determination of the efficiency of photochemical and thermochemical mechanisms of laser initiation of energetic materials. The method is based on the difference of initiation inertia of actual photo- and thermo-chemical processes leading to the different efficiency dependence of these mechanisms on the duration of the initiating pulse with sharply differing capacities of initiation. The experimental verification of the method was performed for PETN initiating at luminosity of 10^9 W/cm^2 at λ = 1064 nm and 10^4 W/cm^2 at λ = 1070 nm. The results allow us to compare the effectiveness of photo and thermo-chemical mechanisms for the case of pure PETN (photochemical mechanism) and PETN, 0.1% black (thermochemical mechanism), the threshold for initiating the photochemical mechanism being ~ 4 J/cm^2 , for thermochemical ~ 14 J/cm^2.

Thematic Section: Physico-Chemical Research. **Full Paper**
Subsection: Physical Chemistry of Explosives. *Registration Code of Publication:* 13-34-6-43
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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Time optimization of mixing octogene and cellulose nitrate lacquer during the formation of composite materials

© **Natalia S. Gainutdinova**,[+] **Tatiana A. Eneykina**,* **Lilia I. Selivanova**, **Anatoly P. Pavlov**, **Dilara R. Ibneeva**, **Rosa F. Gatina, Alexey I. Hatsrinov**, and **Yury M. Mikhailov**
State Scientific-Research Institute of Chemical Products. Svetlaya St., 1. Kazan, 420033. The Republic of Tatarstan. Russia. Phone: +7 (843) 544-07-21, 544-09-82. E-mail: gniihp@bancorp.ru

*Supervising author; [+]Corresponding author

Keywords: *stirring, octogene, torque.*

Abstract

The results have been presented of the study of the mixing process of octagene with 25% cellulose nitrate lacquer, obtained on the basis of acetate by two technologies: in the twin-rotor mixer and in volume device with mixer. The uniform distribution of the filler (the quality of mixing) was evaluated according to two criteria: on achieving a constant torque and on the minimum value of the arithmetic mean error of filler concentration measurement in the volume of lacquer. By comparing the torque on the example of mixing HMX and carbon we established the influence of the nature of the filler on the nature of mixing. The possible reasons for the fundamental difference between the nature of HMX mixing (extreme dependence) and carbon (symbatic dependence) at a constant concentration of polymer lacquer.

Thematic Section: Physico-Chemical Research. **Full Paper**
Subsection: Physics and Chemistry of liquid Crystals. *Registration Code of Publication:* 13-34-6-51
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http://butlerov.com/readings/
Contributed: June 17, 2013.

Dynamics of phase transitions in lyotropic liquid crystal based on *N*-dodecyl-*N*-(2-hydroxyethyl)-*N*,*N*-dimethylammonium bromide

© **Aydar A. Akhmadiyarov**,[1] **Alexander E. Vandyukov**,[2] **Alina F. Saifina**,[2] **Svetlana S. Lukashenko**,[3] **Lucia Ya. Zakharova**,[3] and **Valeri I. Kovalenko**[1,2]*

[1] *Department of Engineering Ecology. Kazan National Research Technology University. K. Marx St., 68. Kazan, 420015. Tatarstan Republic. Russia. Phone: +7 (843) 238-56-94. E-mail: koval@iopc.ru*

[2] *Physico-Chemical Research Division. A.E. Arbuzov Institute of Organic and Physical Chemistry. Akad. Arbuzov St., 8. Kazan, 420088. Tatarstan Republic. Russia. Phone: +7 (843) 273-93-65. E-mail: koval@iopc.ru*

[3] *Supramolecular Chemistry Division. A.E. Arbuzov Institute of Organic and Physical Chemistry. Akad. Arbuzov St., 8. Kazan, 420088. Tatarstan Republic. Russia. Phone: +7 (843) 273-93-65.*

*Supervising author; +Corresponding author

Keywords: *lyotropic liquid crystal, lamellar phase, FT-Raman spectroscopy, X-ray powder diffraction.*

Abstract

Series of mesomorphic phase transitions (hexagonal → bicontinuous cubic → lamellar) of *N*-dodecyl-*N*-(2-hydroxyethyl)-*N*,*N*-dimethylammonium bromide have been observed by polarizing optical microscopy using spontaneous water evaporation from a droplet of dilute solution of mesogen in water. The same technique of spontaneous water evaporation has been used in X-ray diffractometry and Raman experiments. The conformational changes of the hydrocarbon tail during phase transitions were shown. Structural peculiarities of the lamellar lyotropic liquid crystal phase were defined.

Thematic Section: Physico-Chemical Research. **Full Paper**
Subsection: Physical Chemistry of High Temperatures. *Registration Code of Publication:* 13-34-6-57
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: June 4, 2013.

Influence of inorganic salts on kinetics of catalytic pyrolysis of wood

© **Vladimir A. Beliy**,[+] and **Elena V. Udoratina***
Institute of Chemistry. Komi Scientific Center. Ural Branch of RAS. Pervomayskaya St., 48. Syktyvkar, 167982. Russia. Phone.: +7 (8212) 43-19-77. E-mail: skeyling@yandex.ru

*Supervising author; [+]Corresponding author

Keywords: *pyrolysis, biomass, inorganic salts, kinetics.*

Abstract

The thermogravimetry and differential scanning calorimetry methods were used to study the pyrolysis of coniferous and deciduous species of wood. The effect of catalysts – inorganic salts – on the temperature of thermal degradation beginning and output of coal was reported. Kinetic studies have revealed the order of reaction and the activation energy of the initial stage of pyrolysis of wood.

Thematic Section: Applied Research. **Full Paper**
Subsection: Biochemistry. *Registration Code of Publication:* 13-34-6-65
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: July 2, 2013.

Humic acids from siliceous sapropel: IR spectroscopy and thermal analysis

© **Ludmila N. Adeeva**,* **Daria S. Platonova**, **Mikhail S. Masorov**, and **Tatiana A. Didenko**+
Department of Inorganic Chemistry. Omsk State University. Mir St., 55A. Omsk, 644077. Russia.
Phone: +7 (3812) 26-81-99. E-mail: kovalenko_85@list.ru

*Supervising author; +Corresponding author

Keywords*: humic acid, sapropel, coefficient of share of stable groups, infrared spectroscopy.*

Abstract

It has been shown that humic acids can be isolated by the action of alkali on the sapropel with subsequent precipitation by acid. We used varying experimental conditions for the most complete extraction of humic acid from sapropel. The equations of regression showing the influence of concentration of alkali, temperature and process duration on efficiency of allocation of humic acids and their ash-content are derived. Transformations of the humic acids emitted from sapropel in the range of temperatures 40-1000 ºC on air by means of the thermal analysis are studied. IR spectroscopy confirmed the existence of humic acids of sapropel of various functional groups in the composition. The number of oxygen-containing functional groups is determined by Boem's technique. Large number of groups allows to assume that humic acids can be used as a sorbent of heavy metals.

Full Paper _____ *Thematic Section:* Research into New Materials.
Registration Code of Publication: 13-34-6-70 *Subsection:* Water Treatment Technology.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: June 20, 2013.

Bifunctional sorbent for sewage treatment obtained from sapropel

© **Ludmila N. Adeeva**,[1]* **Darya S. Platonova**,[1] **Alexander V. Puzhel**,[1]
Nikolay A. Belykh,[2] and **Tatiana A. Didenko**[1+]
[1] *Department of Inorganic Chemistry. Omsk State University. Mir St., 55A. Omsk, 644077. Russia.*
Phone: +7 (3812) 26-81-99. E-mail: kovalenko_85@list.ru
[2] *A.S. Popov Omsk Production Association. 10 let Oktyabrya St., 195. Omsk, 644009. Russia.*
Phone: +7 (3812) 66-63-69.

*Supervising author; +Corresponding author

Keywords*: bifunctional sorbent, sapropel, sorption capacity, petroleum products, nickel (II) ions.*

Abstract

It has been shown that by heat treatment of sapropel on air at the temperature of 300-350 °C the bifunctional sorbent can be obtained. The sorbent is capable of extracting organic substances and ions of metals from water solutions. Sorbent capacity on ions of nickel(II) makes up 51.0±2.0 mg g^{-1}, the sorption value of petroleum products is equal to 33.1±1.2 of mg/g^{-1} at their initial concentration of 1.0 mg ml^{-1}. On the example of washing water of nickeling workshop section of radio plant it is established that bifunctional sorbent is capable to extract at the same time ions of metal and petroleum products from water solutions. Comparison is made of characteristics of the sorbent obtained during thermal treatment of sapropel in the air environment at the temperature of 300 °C and the sorbent obtained by carbonization of sapropel in the inert environment at the temperature of 700 °C.

Full Paper _____ *Thematic Section:* Research into New Materials.
Registration Code of Publication: 13-34-6-76 *Subsection:* Building Materials.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
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Influence of retarders on the base of 1-hidroksyethilidene-1,1-diphosphonium acids on gypsum plasters properties

© **Irina V. Berdnik**,[1]*+ **Sergey A. Krasnov**,[2] and **Ildar M. Magdeev**[1]
[1] *Technology Laboratory.* [2] *Laboratory of Coordination Chemistry and Nanomaterials.*
A.E. Arbuzov Institute of Organic and Physical Chemistry. Kazan Scientific Center.
Russian Academy of Sciences. Arbuzov St., 8. Kazan, 420088. The Republic of Tatarstan. Russia.
Phone: +7 (843) 272-73-84. Faxc: +7 (843) 272-73-34. E-mail: berdnik@iopc.ru

*Supervising author; +Corresponding author

Keywords*: gypsum, gypsum-limy mixtures, curing retarder for gypsum, 1-hidroksyethilidene-1,1-diphosphonium acid, three-ethanolamine, microphoto.*

Abstract

Using the method of graphical vizualization in Statistica program the influence of gypsum setting from additives of 1-hydroxyethylidene-1,1-diphosphonic acid salts was investigated. The synergy of salt components, for example of thriethanolamine salt retarding action, on gypsum was examined. Stronger effect was found for gypsum half-hydrated forms, including gypsum-limy mixes. Using electron-radiographic microphoto, the mechanism based on adsorption of 1-hydroxyethylidene-1,1-diphosphonic acid complexes on crystallizing surface was proposed.

Thematic Section: Chemical and Technological Research. **Full Paper**
Subsection: Organoelemental Chemistry. *Registration Code of Publication:* 13-34-6-83
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Optimization of some parameters in syntheses of methyl-*O,O*-di(oxyrantlmethyl)phosphonate

© Irina V. Berdnik
Enterprise of Russian Academy of Sciences. A.E. Arbuzov Institute of Organic and Physical Chemistry. Kazan Scientific Center of Russian Academy of Sciences. Arbuzov St., 8. Kazan, 420088. Tatarstan Republic. Россия. Phone: +7 (843) 273-93-44. Fax: +7 (843) 272-73-34. E-mail: berdnik@iopc.ru

Keywords: *methyl-O,O-di-(oxyranylmethyl)phosphonate, hydroxymethyloxyran, technological experiment, optimization, graphical visualization.*

Abstract

With mathematical processing of technological experiments we studied the dependences of methyl-*O,O*-di(oxyranylmethyl)phosphonate yield on the parameters characterizing the starting material quality and synthesis conditions. The results are used to optimize the process.

Thematic Section: Theoretical Research. **Full Paper**
Subsection: Analytical Chemistry. *Registration Code of Publication:* 13-34-6-91
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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Method for defining the equivalence point from potentiometric mesurements

© **Irina V. Berdnik**,*+ and **Vladimir V. Berdnik**
Technology Laboratory. A.E. Arbuzov Institute of Organic and Physical Chemistry, Kazan Scientific Center, Russian Academy of Sciences. Arbuzov St., 8. Kazan, 420088. Tatarstan Republic. Russia.
Phone: +7 (843) 272-73-84. Faxc: +7 (843) 272-73-34. E-mail: berdnik@iopc.ru

*Supervising author; +Corresponding author

Keywords: *potentiometric titration, approximations of a titration curve, analysis of errors, methyl-O,O-di-(oxyranylmethyl)phosphonate.*

Abstract

Six-parameter function for approximation of potentiometric titration curves is offered. It is shown, that this function describes the real titration curves rather well. The algorithm of equivalence point definition, based on determination of parameters for this function from the results of the potentiometric titration by the method of least squares is developed. Estimates of stability for the offered way of defining the measurement errors have been done. Practical suitability of the method is shown on the example of defining methyl-*O,O*-di-(oxyranylmethyl)phosphonate main substance content.

Full Paper _____ *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 13-34-6-98 *Subsection:* Physical Chemistry of Complex Compounds.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
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Poly-nuclear complexes of nickel(II) with 2-amino-3-hydroxypropanoic acid in water solutions

© **Victor I. Kornev**,* and **Nadezhda S. Buldakova**[+]
Department of Inorganic and Analytic Chemistry. Udmurt State University. Universitetskaya St., 1. Izhevsk, 426034. Udmurt Republic. Russia. Phone: +7 (3412) 91-64-34. E-mail: nah@uni.udm.ru

*Supervising author; [+]Corresponding author

Keywords*: complex compounds, complex, ligand, nickel(II), ethylenedeminetetraacetic acid, serine, stability constant, complex structure.*

Abstract

Formation of complexes containing nickel(II) salts, as well as ethylenedeminetetraacetic acid (EDTA, $Edta^{4-}$) and 2-amino-3-hydroxypropanoic acid (serine, HSer) were studied by absorption spectrophotometry and pH-metry. The mathematical modelling was used to discover the fact that the most expected mathematical models for absorption correlation between pH and reacting components concentration include dissociation constants of ligands(K_i), metal hydrolysis constants(K_{ig}) and stability constants (β) of homoligands, heteroligands and polynuclear complexes of the general composition $[Ni_mSer_nEdta_r]^{2m-n-4r}$ (m = 1-4, n = 0-8, r = 0-1). We calculated the equilibrium constants of reactions and the stability constants of the complexes formed. The limits of pH values of the existence of complexes were found.

Thematic Section: Research into New Materials. **Full Paper**
Subsection: Physico-Chemistry of Cellulose. *Registration Code of Publication:* 13-34-6-105
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
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Investigation of the structuring process of cellulose-filled material

© **Sergey V. Soldatov**,[+] **Tatiana A. Eneykina**, **Vladimir A. Hohlov**,* **Vadim N. Chistyuhin**, **Roza F. Gatina**, and **Yuriy M. Mikhailov**[1]

Federal State Enterprise "State Scientific-Research Institute of Chemical Products." Svetlaya St., 1. Kazan, 420033. Tatarstan Republic. Russia. Phone: +7 (843) 544-07-21. E-mail: sternsoldatov@mail.ru

[1] *MIC at the Government of RF.*

*Supervising author; [+]Corresponding author

Keywords: *inert material, physico-mechanical characteristics, cellulose, polyvinyl acetate.*

Abstract

Specific surface areas have been calculated for different types of cellulose: fibers, sawdust of conifers in the form of flakes and sawdust of forest coniferous trees of irregular shape, wood flour. The dependence of the structural and mechanical properties of the material on the type of pulp: shrinkage, tensile strength and elongation have been studied. It is shown that the required tensile strength of the material (16.3-22.5 MPa) is achieved using the fiber form cellulose.

We designed the composition of inert material based on cellulose and polyvinylacetate providing the processing conditions identical with the standard analog by the method of filtration molding and physico-mechanical properties and enabled verification of serviceability of functioning of the equipment.

Thematic Section: Physico-Chemical Research. **Full Paper**
Subsection: Chemistry of Cellulose. *Registration Code of Publication:* 13-34-6-113
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http://butlerov.com/readings/
Contributed: May 22, 2013.

Changing the fine cellulose structure as a result of heterogeneous modification processes

© **Tatiana V. Smotrina**,[1+]* **Marina M. Lezhnina**,[1]* **Roman V. Sergeyev**,[2] and **Peter S. Novikov**[2]
[1] *Department of Physics.* [2] *Department of Forest Selection, Non-Wood Resources and Biotechnology. Volga State Technological University. Lenin St., 3. Yoshkar-Ola, 424000. Mari El Republic. Russia. Phone: +7 (8362) 68-68-04. E-mail: tatyana-smotrina@yandex.ru*

*Supervising author; [+]Corresponding author

Keywords: *cellulose, hemicellulose, structure, modification, mercerization, nuclear magnetic relaxation.*

Abstract

NMR relaxation spectroscopy method was used to analyze the changes of the fine structure of cellulose in the alkali treatment with varying the reactant concentration and the exposure time. It is shown that the spin-lattice relaxation parameter is sensitive both to changes in the degree of crystallinity by mercerizing cellulose and to polymorphic transition of cellulose I to cellulose II. It is suggested that as a result of mercerization a more ordered mesophase is formed in the amorphous regions of cellulose. We demonstrated the relationship between the processes of the spin-spin relaxation of adsorbed water and the depth of the structural changes in the pulp as a result of its stepwise processing by dimethylsulfoxide and alkali solutions.

Full Paper _____ *Thematic Section:* Research into New Materials.
Registration Code of Publication: 13-34-6-118 *Subsection:* Physical Chemistry.
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http://butlerov.com/readings/
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IR optical fibers of nano- and microcrystalline structures for resettable interferometry

© **Alexander S. Korsakov**, **Dmitry S. Wroblewski**, **Liya V. Zhukova**,*+ and **Victor S. Korsakov**
Ural Federal University Named After the First President of Russia B.N. Yeltsin. Mir St., 19. Ekaterinburg, 620002. Russia. Phone: +7 (343) 375-44-45. E-mail: l.v.zhukova@ustu.ru

*Supervising author; +Corresponding author

Keywords: *photonic crystalline IR optical fibers, solid solutions of silver halides, resettable interferometry, middle IR range.*

Abstract

We developed and produced by extrusion IR optical fibers based on the new solid solutions of silver halides and monovalent thallium. Optical fibers are produced in the range from 2.0 to 40.0-45.0 microns depending on the composition and work in one-mode regime at the wavelength 10.6 microns. Their optical properties and fundamental characteristics were measured and calculated. We considered the possibility of using IR-optical fibers as mode filters in interferometry reset to zero when searching for Earth-like planets.

Full Paper _____ *Thematic Section:* Geochemical Research.
Registration Code of Publication: 13-34-6-124 *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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Oil saturation of low permeable rocks of Minnibaevo area of Romashkinskoe oil field (illustrated by well 20355)

© **Igor P. Kosachev**,[1]*+ and **Galina P. Kayukova**[2]
[1] *Technology Laboratory.*[2] *Laboratory of Chemistry and Geochemistry of Oil. A.E. Arbuzov Institute of Organic and Physical Chemistry of Kazan Scientific Center of Russian Academy of Sciences. Arbuzov St., 8. Kazan, 420088. Tatarstan Republic. Russia.*
Phone: +7 (843) 272-73-84. Faxc: +7 (843) 272-73-34. E-mail: kosachev@iopc.ru

*Supervising author; +Corresponding author

Keywords: *low permeable rocks, devonian, extracts, hydrocarbon composition, oil saturation, Minnibaevo area, Romashkinskoye field.*

Abstract

Oil saturation of low permeable rocks of the Upper Devonian Minnibaevo area of Romashkinskoye field in the depth interval of 1486-1522 m, accounting on average 0.13% has been revealed. It is shown that the composition of the extracts, determined by the methods of infrared spectroscopy, gas-liquid chromatography, electron paramagnetic resonance and thermal analysis, is a mixture of high molecular naphthenic and polycyclic aromatic hydrocarbons with a small fraction of normal alkanes and isoprenoids that have been exposed to supergene impact. It is established that the mineral matrix of the samples is an association of carbonate rocks, and the presence of bitumen is due to the migration of oil from the lower strata of Devonian.

Full Paper _____ *Thematic Section:* Physico-Chemical Research.
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Electro-kinetic properties of chlorophyll in aqueous solutions of 1-, 2- and 3-charged cations

© **Ekaterina Yu. Rodionova**,[1+] **Irina B. Dmitrieva**,[2*+] and **Alexander S. Chukhno**
Department of Physical and Colloid Chemistry. St. Petersburg State Chemical-Pharmaceutical Academy. Professor Popov St., 14. St. Petersburg, 197376. Russia. Phone: +7 (812) 234-11-38.
E-mail: rodionova_e_y@mail.ru, irina@dmitriyev.ru, alex-chuhno@yandex.ru

*Supervising author; +Corresponding author

Keywords*: chlorophyll, electro-kinetic properties, microelectrophoresis, isoelectric point.*

Abstract

By the method of microelectrophoresis research into electro-kinetic properties of chlorophyll aqueous dispersions depending on the adsorption duration and the composition of the aqueous phase (pH, the presence of cations of potassium, sodium, magnesium, iron(II) or iron(III)) has been conducted. Their isoelectric point pH_{IEP} = 3.3 ± 0.1 has been defined. It is established that the effect of singly- and doubly-charged cations corresponds to their charge and the position in the lyotropic series. In the aqueous dispersions of chlorophyll in the presence of these cations there is observed an abnormal dependence of electro-kinetic potential of the ionic strength of the solution. Trivalent iron cations cause overcharging of chlorophyll particles and offset of isoelectric point in the alkaline region as compared to the cations of sodium, potassium, magnesium and iron(II).

Thematic Section: Physico-Chemical Research. **Full Paper**
Subsection: Biochemistry. *Registration Code of Publication:* 13-34-6-135
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Electro-kinetic properties of hemoglobin in aqueous solution of 1-, 2- and 3-charged ions

© **Ekaterina Yu. Rodionova**,[1+] **Irina B. Dmitrieva**,[2*+] and **Alexander S. Chukhno**
Department of Physical and Colloid Chemistry. St. Petersburg State Chemical-Pharmaceutical Academy. Professor Popov St., 14. St. Petersburg, 197376. Russia. Phone: +7 (812) 234-11-38. E-mail: rodionova_e_y@mail.ru, irina@dmitriyev.ru, alex-chuhno@yandex.ru

*Supervising author; +Corresponding author

Keywords: *hemoglobin, electro-kinetic properties, microelectrophoresis, isoelectric point.*

Abstract

The influence of singly-, doubly- and triply-charged anions and cations (K^+, Na^+, Ca^{2+}, Mg^{2+}, Fe^{2+}, Fe^{3+}, CO_3^{2-}, HPO_4^{2-}/ $H_2PO_4^-$, Cl^-, SO_4^{2-}, $C_3H_5O(COO)_3^{3-}$) on the electro-kinetic properties of aqueous dispersions of hemoglobin have been studied by the method of microelectrophoresis. It has been found that the values of the electro-kinetic potential of hemoglobin depend on the charge, size of ions and ionic strength of the solution in accordance with the classical theory of electric double layer. It has been shown that the carbonate ions and the cations of iron(II, III) is specifically adsorbed by hemoglobin, while other ions – nonspecifically, because the values of isoelectric point of hemoglobin are not shifted as compared to the potential determining ion H^+ and OH^-.

Thematic Section: Preparative Chemistry. **Brief Communication**
Subsection: Organic Chemistry. *Registration Code of Publication:* 13-34-6-141
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Thematic course: Maleimides and their derivatives. Part 3.

Allyl ester 4-(2,5-dioxo-2,5-dihydro-1*H*- pyrrolyl) of phenylacetic acid

© **Oleg A. Kolyamshin**,*+ **Vladimir A. Danilov**, and **Nikolay I. Kol'tsov**
Department of Physical Chemistry and High Molecular Compounds. I.N. Ul'yanov Chuvash State University. Moskovskiy Pr., 15. Cheboksary, 428015. Chuvash Republic. Russia. Phone: +7 (8352) 45-24-68. E-mail: oleg.kolyamshin@yandex.ru

*Supervising author; +Corresponding author

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

Abstract

Interaction of allyl ester of 4-aminophenylacetic acid with maleic anhydride resulted in obtaining the corresponding monamide of maleic acid by the subsequent cyclization of which we have isolated maleimide – allyl ester 4-(2,5-dioxo-2,5-dihydro-1*H*-pyrrolyl) of phenylacetic acid. Synthesized compounds have been characterized by the data of IR and NMR ^{1}H spectroscopy.

Full Paper _____ *Thematic Section:* Theoretical Research.
Registration Code of Publication: 13-34-6-144 *Subsection:* Thermodynamics.
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Exact solution of a kinetic equation of one-step processes of growth and decay

© Ikhtier H. Umirzakov
The Laboratory of Modeling. Kutateladze Institute of Thermophysics of SB of RAS. Prospect Lavrenteva, 1. Novosibirsk, 630090. Russia. Phone: +7 (383) 354-20-17. E-mail: tepliza@academ.org

Keywords*: kinetic equation, processes of growth and decay, source, run-off.*

Abstract

The exact solution of the kinetic equation of the one step process of growth (birth) in the presence of sources (runs-off) is found for arbitrary dependence of the growth rate on the number of the state (or size). It is shown that the presence of the source leads to the broadening of the state (or size) distribution. It is also shown that the solution obtained can be used for approximate definition of the size distribution of nuclei for the case of large super-saturation of the vapor. The exact solution of the kinetic equation of the one step process of a decay in the presence of sources (runs-off) is found also for arbitrary dependence of the rate of the decay on the number of the state (or size).

Thematic Section: Thermodynamic Research. **Full Paper**
Subsection: Phase Equilibria. *Registration Code of Publication:* 13-34-6-151
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Correlation of the critical parameters of the gas-liquid phase transition and the density of the crystal at zero absolute temperature

© Ikhtier H. Umirzakov
The Laboratory of Modeling. Kutateladze Institute of Thermophysics of SB of RAS. Prospect Lavrenteva, 1. Novosibirsk, 630090. Russia. Phone: +7 (383) 354-20-17. E-mail: tepliza@academ.org

Keywords*: critical temperature, critical volume, critical pressure, critical parameters, equation of state, liquid-gas phase transition.*

Absract

The empirical Timmermann's formula connecting the density of the crystal at zero absolute temperature with the parameters of the critical point of the gas-liquid phase transition is derived theoretically from the Van der Waals equation of state using the conditions of phase equilibrium.

The equations of state $p(T,v) = kT/(v-b) - a/v^{\alpha}$ and $p(T,v) = kT/v + B/v^{\beta+1} - \tilde{N}/v^{\beta}$ with three parameters describing the critical point of any pure substance are considered. The Timmermann's formula is derived approximately from the first equation and exactly from the second one.

Thematic Section: Theoretical Research. **Full Paper**
Subsection: Simulation of Physico-Chemical Processes. *Registration Code of Publication:* 13-34-6-157
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Numerical modeling of physical and chemical processes in the vulcanization of stranded cable products

© **Evgenia V. Ivanova**,[+] and **Pavel A. Strizhak***
National Research Tomsk Polytechnic University. Lenin St., 30. Tomsk, 634050. Russia.
Phone: +7 (3822) 701-777, add. 1910. E-mail: zhenya1@tpu.ru

*Supervising author; [+]Corresponding author

Keywords*: heat and mass transfer, curing, cable product, polymerization, insulating sheath, modeling.*

Abstract

A numerical study of the integral characteristics of vulcanization stranded cable products based on heat and mass transfer model that takes into account a set of basic physical and chemical processes has been carried out. The characteristic times of complete polymerization of the shell of a typical multi-conductor cable have been shown. The influence of the internal structure of the cable on the vulcanization characteristics of its external insulation shell has been established.

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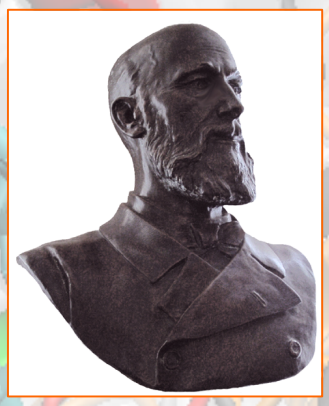

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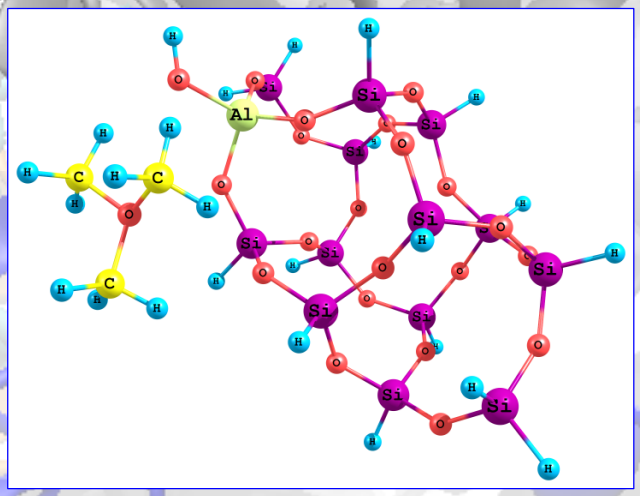

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Evolution of polarization of three spin groups and their contribution to line shape NMR in solids

© **Tatiana P. Kulagina**,[1+] **Grigory E. Karnaukh**,[1] and **Sergey A. Andrianov**[1,2]*
[1] *Institute of Problems of Chemical Physics RAS. Prospect Semenova, 1. Chernogolovka, 142432. Moscow Region. Russia. Phone: +7 (496) 522- 18-79. E-mail: tan@icp.ac.ru*
[2] *Moscow Aviation Institute. Volokolamskoe Shosse, 4. Moscow, 125993. Russia. Phone: +7 (499)158-43-33. Fax: +7 (499) 158-29-77.*

*Supervising author; [+]Corresponding author

Keywords: *antimycotics, proteinase of Candida albicans, metal nanoparticles, hyperbranched polyester polyols.*

Abstract

In this work the kinetic equation of NMR spectra in solids containing selected three-spin groups is obtained. From the equation for density matrix the analytical expression of free induction signal decay for the system of three dipolar-connected spins has been calculated.

Thematic Section: Quantum-Chemical Research. **Full Paper**
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Interaction of human glyceraldehyde-3-phosphate dehydrogenase with cofactor based on molecular docking data

© **Olga N. Makshakova**,[+] and **Elena A. Ermakova***
Kazan Institute of Biochemistry and Biophysics KSC RAS. Lobachevsky St., 2/31. Kazan, 420111. Tatarstan Republic. Russia. Phone: +7 (843) 292-62-88. E-mail: makshakova@gmail.com

*Supervising author; [+]Corresponding author

Keywords*: glyceraldehyde-3-phosphate dehydrogenase, nicotinamide adenine dinucleotide, molecular docking.*

Abstract

The analysis of the interaction of tetrameric glyceraldehyde-3-phosphate dehydrogenase with cofactor NAD was performed by computational methods. Method of molecular docking was used for calculation of interaction energy between molecules of cofactor and the protein. Gaussian network model was used to evaluate the changes in the protein backbone dynamics that took place as a result of the cofactor binding. It has been shown that the cofactor molecules form strong complexes with protein tetramer, wherein the energy of interaction of individual cofactor molecule with different subunits of the protein apo-forms differ insignificantly. At the same time the presence of other NAD molecules in the complex systematically decreased the interaction energy of protein – cofactor complex, this could contribute to negative cooperativity of the cofactor molecule binding to glyceraldehyde-3-phosphate dehydrogenase tetramer.

Full Paper _____ *Thematic Section:* Quantum-Chemical Research.
Registration Code of Publication: 13-35-7-24 *Subsection:* Physical Organic Chemistry.
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Effect of temperature on the mechanism and products of dimethyl ether conversion on the surface of zeolite ZSM-5 catalysts

© **Alexander S. Rodionov**,[+] **Galina N. Bondarenko**,* **Galina N. Shirobokova**,
Natalia V. Kolesnichenko, and **Yury V. Pavluk**
A.V. Topchiev Institute of Petrochemical Synthesis, RAS (TIPS RAS). Leninsky Prospect, 29. Moscow, 119991. Russia. Phone: +7 (495) 955-41-53. E-mail: ASRodionov@ips.ac.ru

*Supervising author; [+]Corresponding author

Keywords: *dimethyl ether, zeolite catalyst, mechanisms of DME conversion, DRIFT.*

Abstract

By means of high-temperature DRIFT spectroscopy *in situ* it has been shown that the mechanism of dimethylether conversion to olefins depends on temperature. At lower temperature there takes place the carbenium mechanism, and at high temperatures – oxonium-ylide.

Full Paper _____ *Thematic Section:* Quantum-Chemical Research.
Registration Code of Publication: 13-35-7-30 *Subsection:* Composite Materials.
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Modeling of nonlinear optical materials on the basis Of composite polymers with binary chromophore groups

© **Alina I. Tuhbatulina**,[+] **Olga D. Fominyh**, and **Marina Yu. Balakina***
Laboratory of Chemistry of Carbon Nanomaterials. A.E.Arbuzov Institute of Organic and Physical Chemistry, KazSC RAS. Acad. Arbuzov St., 8. Kazan, 420088. Tatarstan Republic. Russia.
Phone: +7 (843) 272-73-43. E-mail: april-90@mail.ru

*Supervising author; [+]Corresponding author

Keywords: *nonlinear optical activity, composite materials, molecular modeling, quantum-chemical calculations, oligomers, chromophores.*

Abstract

With the use of molecular modeling we studied the structure of a new type of composite material, wherein the guest chromophores contain tricyanoethenyl electron-acceptor group, and the host polymer matrix is modeled by epoxyamine oligomers with multichromophoric dendritic fragments. Electrical characteristics (dipole moment μ and molecular polarizability α, β) of the researched molecular systems are calculated quantum-chemically at the level of TDHF//AM1. It has been shown that introduction of additional chromophores-guests leads to spatial organization of the chromophore groups and an increase in the quadratic nonlinear-optical activity of molecular systems under investigation. The optimal ratio between the number of additional chromophores attributable to the dendritic segment has been defined.

Full Paper _____ *Thematic Section:* Preparative Chemistry.
Registration Code of Publication: 13-35-7-38 *Subsection:* Composite Materials.
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Olygodimethylsiloxanes containing grafted methoxycarbonyldecyl groups

© **Tatiana A. Pryakhina**,[1]* **Mihail I. Buzin**,[1] **Tatiana V. Strelkova**,[1]
Alexander B. Zachernyuk,[2+] and **Aziz M. Muzafarov**[1,2]
[1] *A.N. Nesmeyanov Institute of Organoelement Compounds. Russian Academy of Sciences. Vavilov St., 28. Moscow, 119991. Russia. Phone: +7 (499) 135-92-23. E-mail: kotov@ineos.ac.ru*
[2] *N.S. Enikolopov Institute of Synthetic Polymer Materials. Russian Academy of Sciences. Profsoyuznaya St.,70. Moscow, 117393. Russia. Phone: +7 (495) 335-90-00. E-mail: a_zacher@mail.ru*

*Supervising author; +Corresponding author

Keywords*: grafted copolymers, hydrosilylation reaction, methyl-10-undecenoate, cohesion strength.*

Abstract

The model oligodimethylsiloxanes with long chain organic side-groups containing the terminally aliphatic carboxylic ester have been obtained. The structure of these olygomers has been confirmed by ^{1}H and ^{29}Si NMR spectra. The influence of the content of substituents on the variation of thermo physical properties has been established by differential scanning calorimetry.

Thematic Section: Preparative Chemistry. **Full Paper**
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Synthesis of new perspective polymer nanocomposite materials for gas separation membranes based on organometallic wireframe compounds

© **Alexander Yu. Alentyev**,[1+] **Vera I. Isaeva**,[2]
Marina I. Barkova,[2] and **Leonid M. Kustov**[2]
[1] *IPChC RAS. Leninsky Prospect, 29. Moscow, 119991. Russia. E-mail: Alentiev1963@mail.ru*
[2] *IOCh RAS. Leninsky Prospect, 47. Moscow, 119991. Russia.*

*Supervising author; +Corresponding author

Keywords*: gas separation membranes, polymer nanocomposite materials, organometallic wireframe compounds.*

Abstract

In this work, nanocomposite materials based on organometallic wireframe compounds were synthesized *in situ* in polymer solutions and characterized. These materials possess high specific surface and good film-forming properties, which makes them promising for membrane gas separation.

Full Paper _____ *Thematic Section:* Preparative Chemistry.
Registration Code of Publication: 13-35-7-50 *Subsection:* Chemistry of Complex Compounds.
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Metal-complex surfaces based on aurophylic terpyridines and their coordination compounds with Rh(III) and Ru(II)

© **Elena K. Beloglazkina**,*+ **Alexander G. Mazhuga**,* **Evgeniy A. Manzheliy**,*
Anna A. Moiseeva, and **Nikolay V. Zyk**
Department of Organic Chemistry. Moscow State University named after M.V. Lomonosov. Faculty of Chemistry. Leninskie Gory, 1, 3. Moscow, 119991. Russia. Phone: +7 (495) 939-40-20.
E-mail: bel@org.chem.msu.ru

*Supervising author; +Corresponding author

Keywords*: terpyridines, coordination compounds, adsorption, gold, rhodium and ruthenium.*

Abstract

Complexing reactions of ligands of terpyridine series, having in their content aurophylic thiol or sulfide moiety, with $RuCl_3$ and $RhCl_3$ have been studied. The possibility of the formation of metal complex surfaces on the basis of coordination compounds on the surface of gold electrodes has been shown. The nature of the aggregation of gold nanoparticles under the influence of solutions of complex compounds aurophylic terpyridines with Ru(II) has been established.

Thematic Section: Preparative Chemistry. **Full Paper**
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Synthesis and nonlinear optical properties of polyether polyols Of azochromophore groups with different structures

© Gulshat N. Nazmieva,[1+] **Tatiana A. Vakhonina**,[1] **Serena M. Sharipova**,[1] **Natalia V. Ivanova**,[1] **Irek P. Nizameev**,[1] **Murad I. Valitov**,[1] **Nikolay N. Smirnov**,[2] **Alexander V. Yakimanskiy**,[2] and **Marina Yu. Balakina**[1]*

[1] *Federal State Institution of Science. A.E.Arbuzov Institute of Organic and Physical Chemistry. KazSC RAS. Arbuzov St., 8. Kazan, 420088. Tatarstan Republic. Russia. Phone: +7 (843) 272-73-43. E-mail: nazmievagn@iopc.ru.*

[2] *Institute of Macromolecular Compounds, Russian Academy of Sciences. Bolshoy Prospect, 31. St. Petersburg, 199004. Russia. Phone: +7 (812) 323-50-25. E-mail: yak@yahoo.com*

*Supervising author; [+]Corresponding author

Keywords: *nonlinear optical polymers, electrical treating, epoxyamine oligomers, azochromophores, dendrite type chromophore.*

Abstract

The work deals with the synthesis and study of nonlinear optical properties of reactive polyether polyols based on the diglycidyl ether of bisphenol-A and *n*-aminobenzoic acid with azochromophores of different structure.

Introduction of azochromophores into the side chain of the oligomer was carried out in the course of the esterification reaction in two ways: one-step or two-step. In the first case, we first prepared aniline-containing oligomer, and then performed azo cross-linking reaction to obtain the oligomer having an azochromophore. In the second case, functionalization of the reactive oligomer was carried out directly by hydroxyl-containing azochromophore. The structure of oligomers is confirmed by physicochemical methods of research. The presence of reactive hydroxyl groups in the chain of synthesized oligomer allows to obtain cross-linked polymers, using diizocyanates as a cross-linking agent.

Using fluid distribution method on rotating thin films were produced with the thickness of 200-300 nm. To obtain a material with quadratic nonlinear optical activity we conducted electrical treating of films in the corona discharge. The method of second harmonic generation was used to measure nonlinear optical coefficients of the synthesized materials.

Full Paper _____ *Thematic Section:* Preparative Chemistry.
Registration Code of Publication: 13-35-7-68 *Subsection:* Polymer Chemistry.
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Solid-state polymerizayion of methylenephthalide

© **Mikhail I. Buzin**,[1]*+ **Galina G. Nikiforova**,[1] **Alexander A. Korlyukov**,[1]
Dmitry E. Arhipov,[1] **Alexander T. Zdvizhgkov**,[2] **Galina I. Timofeeva**,[1]
Sergey N. Salazkin,[1] and **Vladimir S. Papkov**[1]
[1] *A.N. Nesmeyanov Organoelement Compounds Institute. RAS. Vavilov St., 28.*
Moscow, 119991. Russia. Phone: +7 (499) 135-60-50. E-mail: buzin@ineos.ac.ru
[2] *N.D. Zelinskiy Institute of Organic Chemistry. RAS. Leninskiy Prospect, 47.*
Moscow, 119991. Russia.

*Supervising author; +Corresponding author

Keywords*: cardo polymers, solid-state polymerization, X-ray diffraction analysis, differential scanning calorimetry.*

Abstract

The crystal unit cell parameters of poly(3-methylenephthalide) at 100 and 298 K are established by X-ray diffraction analysis. It is shown that the solid state polymerization of methylenephthalide near its melting point, leading to formation of a high molecular polymethylenephthalide with high yield, is in principal possible.

Thematic Section: Biochemical Research. **Full Paper**
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Simulation of plant defensin interaction with phospholipid membrane

© **Bulat I. Khairutdinov**,[+] **Elena A. Ermakova**,* and **Yury F. Zuev**
Kazan Institute of Biochemistry and Biophysics KSC RAS. Lobachevsky St., 2/31.
Kazan, 420111. Tatarstan Republic. Russia. Phone: +7 (843) 292-62-88.
E-mail: khayrutdinov@yahoo.com

*Supervising author; [+]Corresponding author

Keywords*: defensin, phospholipids, molecular docking.*

Abstract

Molecular docking was used for studying plant defensin interaction with phospholipid membrane. Six defensins with different total charges and different charge distributions on the protein surface were used. Comparative analysis of interaction energy between proteins and membrane surfaces shows that defensins slightly interact with membrane surface. Electrostatic interactions and solvatation and hydrophobic effects give a major contribution into interaction energy. Different orientation of proteins relative to membrane surface reveals the specificity of interactions.

Full Paper _____ *Thematic Section:* Biochemical Research.
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Molecular mechanisms of alkylhydroxybenzenes action on serine proteases activity

© **Julia A. Valiullina**,[+] **Elena A. Ermakova**, **Natalia L. Zakhartchenko**, and **Yury F. Zuev***
Kazan Institute of Biochemistry and Biophysics KSC RAS. Lobachevsky St., 2/31.
Kazan, 420111. Tatarstan Republic. Russia. Phone: +7 (843) 292-62-88.
E-mail: valiullina@mail.knc.ru

*Supervising author; [+]Corresponding author

Keywords*: serine proteases, activity, AHB, mechanisms of action.*

Abstract

The influence of chemical analogues of microbial low-molecular weight anabiosis autoinducers (alkylhydroxybenzenes – AHB) on the structure and catalytic activity of serine proteases – trypsin and α-chymotrypsin, was studied. It has been shown that all AHB homologues studied – C7, C12 and C18, with different alkyl group length, inhibit the catalytic activity of trypsin and α-chymotrypsin. The analysis of tryptophan fluorescence spectra of enzymes showed that activity change, induced by AHB addition, is not related to protein destruction. The molecular docking revealed that AHB molecules blocked the different sites of protein surface. However, the most energy preferable protein-ligand complexes involve the residues of active center of enzymes.

Thematic Section: Biochemical Research. **Full Paper**
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Synthesis of Prostatic Acid Phosphatase PAP(248-261), PAP(262-270), PAP(248-286) peptide fragments and their characterization by mass-spectrometry

© **Andrey V. Filippov**,[1]*+ **Sergey A. Kotenkov**,[1] **Stanislav G. Nikulin**,[1] **Elena A. Gerasimova**,[1] **Rezeda R. Valieva**,[1] **Oleg N. Antzutkin**,[2] and **Sergey Afonin**[3]

[1] *Department of Molecular Physics. Institute of Physics. KFU. Kremlevskaya St., 18. Kazan, 420008. Tatarstan Republic. Russia. Phone: +7 (843) 231-51-89. E-mail: Andrey.Filippov@ksu.ru.*

[2] *Interface Chemistry. Luleå University of Technology. Regnbagsallen St., 14. 97187, Luleå, Sweden. Phone: +46920491839. E-mail: Oleg.Antzutkin@ltu.se*

[3] *Institute of Organic Chemistry. Karlsruhe University. Fritz-Haber-Weg 6, D-76131 Karlsruhe, Germany. Phone: +49 721 608-42860. E-mail: Sergiy.Afonin@kit.edu*

*Supervising author; +Corresponding author

Keywords: *Prostatic Acid Phosphatase (PAP), synthesis, Ether Extraction, HPLC purification, mass spectrometry.*

Abstract

In this paper, we describe the synthesis technique of Prostatic Acid Phosphatase (PAP) peptide fragments: PAP(248-261), PAP(262-270), PAP(248-286). Experimentally obtained molecular mass spectra of synthesized peptide fragments by means of mass spectrometry are in good agreement with the theoretical molecular mass spectra determined from the knowledge of the isotopic distribution of those fragments. It is shown that there is no need in additional purification by chromatography for such short fragments as PAP(248-261) and PAP(262-270) after Ether Extraction Procedure. On the contrary, after the synthesis of full length peptide PAP(248-286) post-synthesis mixture has to be purified by chromatography. For hydrophobic segment PAP(262-270) we found that one part molecules of the segment is bound with Na+ ions, one more part is bound with Cl^- ions.

Thematic Section: Biochemical Research. **Short Communication**
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Synthesis of fragments of Prostatic Acid Phosphatase PAP(248-286) peptide and structures of fibrils prepared from this peptide

© **Andrey V. Filippov**,[1]*+ **Maya A. Rudakova**,[1] **Oleg N. Antzutkin**,[2] and **Nils Almqvist**[2]
[1] *Department of Molecular Physics. Institute of Physics. KFU. Kremlevskaya St., 18. Kazan, 420008. Tatarstan Republic. Russia. Phone: +7 (843) 231-51-89. E-mail: Andrey.Filippov@ksu.ru.*
[2] *Interface Chemistry. Luleå University of Technology. Regnbagsallen, 14, 97187 Luleå, Sweden. Phone: +46920491839. E-mail: Oleg.Antzutkin@ltu.se*

*Supervising author; +Corresponding author

Keywords: *Prostatic Acid Phosphatase (PAP), synthesis, fibrillar aggregates, aggregation nucleus, atomic-force microscope (AFM).*

Abstract

We describe detailed protocol of preparation of fibrillar aggregates of Prostatic Acid Phosphatase PAP(248-286) peptide and structural properties of these aggregates studied by atomic-force microscope. We found that PAP aggregates are characterized by filamentous morphology, consisting of fibrils with similar thickness (~ 15 nm in diameter) and various lengths (from 100 nm to 1 μm long). Some fibrils have spherical aggregates. The tendency of fibrils to assemble in high level aggregate was not observed.

Full Paper _____ *Thematic Section:* Biochemical Research.
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Modern approaches to the study of the chemical composition of the genus *Origanum* L. medicinal plants and methods for its standardization

© **Dmitriy O. Bokov**,[1]* **Svetlana L. Morokhina**,[1+]
Natalia V. Pyatigorskaya,[2] and **Dmitriy M. Popov**[2]
[1] *Department of Pharmacognosy. I.M. Sechenov First Moscow State Medical University.*
GSP-1, Trubetskaya St., 8. Moscow, 119991. Russia.
Phone: +7 (925) 358-84-27. E-mail: fmmsu@mail.ru
[2] *Scientific-Research Institute of Pharmacy. I.M. Sechenov First Moscow State Medical University.*
Nahimovskiy Prospect. 45. Moscow, 117418. Russia.
Phone: +7 (916) 123-33-94. E-mail: osipova-mma@list.ru

*Supervising author; [+]Corresponding author

Keywords: *molecular dynamics of heterogeneous systems, Origanum vulgare L., Origanum onites L., water-alcohol extracts from medicinal plant materials, flavonoids, luteolin-7-O-glucoside, cynaroside, condensed tannins.*

Abstract

The study provides data describing the composition of phenolic complex inherent to the genus *Origanum* L. some members using the methods of thin-layer chromatography, titrimetry and UV-spectrophotometry. Qualitative and quantitative compositions of the biologically active compounds of analyzed group were identified. The existing procedures have been modified and a number of new standardized methods have been developed that allow to analyze qualitative and a quantitative composition of phenolic compounds based on experimental data.

Full Paper _____ *Thematic Section:* Biochemical Research.
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Study of acid-base properties of lignin using the method of pK-spectroscopy

© **Vladimir A. Beliy**,*+ **Rais A. Sadykov**, **Valery Yu. Beliaev**, and **Mikhail A. Ryazanov**
Institute of Chemistry. Komi Scientific Center Ural Branch of RAS. Pervomayskaya St., 48. Syktyvkar, 167982. Russia. Phone: +7 (8212) 43-19-77. E-mail: skeyling@yandex.ru

*Supervising author; +Corresponding author

Keywords: *pK- spectrum, dissociation constants, spectrophotometric titration, lignin, phenolic hydroxyl groups.*

Abstract

The acid-base properties of lignin of *Rhodiola rosea* L. and *Serratula coronata* L. using the method of pK-spectroscopy were investigated. The constants of dissociation of acid groups of these lignins were computed. The possibility of differential determination of acidity constants of the phenolic hydroxyl groups of various structural fragments of lignin using a spectrophotometric titration has been shown.

Thematic Section: Biochemical Research. **Full Paper**
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Contributed: July 28, 2013.

Structure and properties of new materials based on fine biopolymers of vegetable origin

© **Larisa A. Kuvshinova**,[+] and **Svetlana V. Frolova***
Institute of Chemistry, Komi Science Center. Pervomayskaya St., 48. Syktyvkar, 167982. The Republic of Komi. Russia. Phone: +7 (8212) 21-99-61. E-mail: fragl74@mail.ru

*Supervising author; [+]Corresponding author

Keywords: *biopolymer composition, fine powder materials, cellulose, titanium tetrachloride, titanium compound modified surface, physico-chemical properties, adsorption, polymerization degree, degree of crystallinity.*

Abstract

Based on biopolymers of vegetable origin compositions there were obtained fine powder materials with surface-modified titanium compounds. On the example of unbleached softwood pulp we studied the dynamics of Ti(IV) adsorption from solutions of Lewis acid. The possibility has been established for using solutions of titanium tetrachloride, allowing in one processing step within a short period of time to obtain the titanium-containing powder materials at relatively low temperatures and concentrations of Lewis acid. It has been shown that the treatment of softwood cellulose with $TiCl_4$ solutions in C_6H_{14} affects the degree of polymerization, degree of crystallinity and crystallographic characteristics of cellulose component of fine powders.

Thematic Section: Biochemical Research. **Full Paper**
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Nanostructure of cellulose microfibrils

© Yury B. Grunin,*+ **Leonid Y. Grunin**, **Vladimir I. Talantsev**, **Darya S. Masas**, **Ekaterina A. Nikolskaya**, and **Osman M. Aslan**
Volga State University of Technology. Lenin Sq., 3. Yoshkar-Ola, 424000. Russia.
Phone: +7 (8362) 68-68-64. E-mail: GruninYB@volgatech.net

*Supervising author; +Corresponding author

Keywords: *biosynthesis, cellulose, microfibril, hydrogen bond, nuclear magnetic resonance.*

Abstract

The analysis of the current ideas about structural organization and nature of the cellulose microfibrils in the formation of its biosynthesis has been carried out. A model of the structure of cellulose microfibrils, providing availability of slit-shaped micropores in its structure has been offered. Basing on experimental studies of sorption processes with the use of proton magnetic relaxation we found that at the cellulose moisture content of 8-10%, its micropores are filled, which is accompanied by increasing their cross-sectional dimension, by increasing surface area and decreasing the degree of crystallinity of the samples.

Full Paper _____ *Thematic Section:* Research into New Materials.
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The effects of small additions of ionic liquids on the process of electrospinning of nonwovens of polypropylene melts with different melt flow index

© **Sergey I. Belousov**,* **Sergey N. Malakhov**,*+
Andrey M. Prazdnichnyi, and **Sergey N. Chvalun**
Laboratory of Polymeric Materials. L. Ya. Karpov Scientific-Research Institute of Physical Chemistry.
Obukha lane, 3-1/12, build. 6. Moscow, 105064. Russia. Phone: +7 (495) 917-43-30.
E-mail: s.malakhov@mail.ru

*Supervising author; +Corresponding author

Keywords: *nonwovens, polypropylene, polymer melts, ionic liquids, electrospinning.*

Abstract

The influence of the addition of ionic liquids on polypropylene melt electrospinning process in the preparation of nonwoven materials is presented in this paper. Nonwoven materials with average fiber diameters 5-23 μm was produced from melts of polypropylenes with different melt flow index. It has been shown that on introducing low molecular weight additives and reducing the polymer molecular weight the diameter of microfibers is reduced due to increasing the conductivity of the polymer.

Thematic Section: Research into New Technologies. **Full Paper**
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Electrospinning of ultrafine fibers from solutions of amino-containing polymers

© **Lina M. Simanenkova**,[+] and **Natalia R. Kildeeva**
Department of Analytical, Physical and Colloid Chemistry. Moscow State University of Design and Technology. Sadovnicheskaya St., 33/1. Moscow, 115035. Russia.
Phone: +7 (495) 955-33-77. E-mail: linasimanenkova@mail.ru

*Supervising author; [+]Corresponding author

Keywords: *electrospinning, amino-containing polymers, Eudragit E, chitosan.*

Abstract

The possibility of obtaining ultrafine fibers by the electrospinning from the amino-containing poly(alkylmethacrylate) esters Eudragit E in organic solvents and in aqueous solutions of acetic acid was shown. The optimization of the electrospinning was carried in installation for spinning Nanospider ™. When electrospinning solutions in binary solvent ethanol – chloroform (60:40) there were obtained fibers with thickness 0.5-1.0 microns. It has been found that the use of aqueous acetic acid resulted in more fine fibers. Nanosized fibers were prepared from 17-22% solutions of Eudragit E in 70% acetic acid. The possibility of spinning chitosan-containing fibers from the mixture of chitosan and Eudragit E was shown.

Full Paper _____ *Thematic Section:* Research into New Materials.
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The material based on carbon nanotubes and polyaniline for potentiometric determination of ascorbic acid in solution

© **Constantine A. Milakin**,*+ **Igor S. Yaremenko**, **Alexey V. Kubarkov**,
Olga A. Pyshkina,* and **Vladimir G. Sergeev**
Department of Macromolecular Compounds. Faculty of Chemistry. Moscow State University named after M.V. Lomonosov. Leninskie Gory St., 1, build. 40. Moscow, 119992. Russia.
Phone: +7 (495) 939-38-77. E-mail: milakin777@yandex.ru

*Supervising author; +Corresponding author

Keywords: *polyaniline, multiwall carbon nanotube, composite material, reactivity, ascorbic acid.*

Abstract

Composite material based on polyaniline (PANI) and multiwalled carbon nanotubes (MWNT) has been synthesized. It has been shown that introduction of MWNT into the composite allows to increase its reactivity in redox reaction with ascorbic acid as compared to the initial PANI. It has been found that the use of PANI-MWNT material allows to increase by an order the sensitivity of the potentiometric determination of ascorbic acid (up to $1 \cdot 10^{-7}$ mol/l).

Full Paper _____ *Thematic Section:* Research into New Materials.
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Synthesis and surface properties of nanomodified substrates, obtained by ionic implantation

© Vitaly V. Goncharov
Department of General Physics and Technical Mechanics. Institute of Chemical Technology (Rubezhnoe). V.Dal' Eastern-ukrainian National University. Lenin St., 31. Rubezhnoe, 93009. Lugansk region. Ukraine. Phone: +7 (06453) 7-11-15. E-mail: gonch_vit@rambler.ru

Keywords*: ionic implantation, composite, substrate, stainless steel.*

Abstract

The study of substrates on the basis of stainless steel produced by the method of ionic implantation has been performed. The technique of the synthesis of samples is described. The synthesized composites were investigated by X-ray photoelectron spectroscopy, scanning electron microscopy, atomic force microscopy and X-ray analysis. Feasibility of using the substrates synthesized by ionic implantation was shown by comparing their data with those of the sample obtained using plasma technique.

Thematic Section: Research into New Technologies. **Full Paper**
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Synthesis and study of mixed-oxide nano-composite photocatalysts used to produce hydrogen

© **Elena D. Fakhrutdinova**,*+ **Anastasiya V. Shabalina**, and **Gennady M. Mokrousov**
Department of Analytical Chemistry. Tomsk State University. Lenin Pr., 36. Tomsk, 634050. Tomsk Region. Russia. Phone: +7 (3822) 42-07-83. E-mail: elenli@sibmail.com

*Supervising author; +Corresponding author

Keywords*: semiconductor photocatalysts, photocatalytic hydrogen production.*

Abstract

In this study we synthesized semiconductor photocatalysts for hydrogen production by decomposition of water and water-organic media under the action of visible light For the preparation of nanostructured mixed oxide materials based on titanium and zinc oxide four methods were used: impregnation method, method of ester precursors (two variants), and chemical deposition method. The structure and optical properties of these materials have been studied. The greatest activity in the process of hydrogen evolution from water-methanol solution was demonstrated by TiO_2, modified by introduction of copper through impregnation – 2600 mkmol/g/h.

Thematic Section: Preparative Chemistry. **Full Paper**
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Oligo(phenylene sulfide)s containing terminal thiol groups

© **Vladimir I. Nedel'kin**,[1]* **Boris A. Zachernyuk**,[1+] **Olga B. Andrianova**,[1]
Ecaterina N. Solov'yeva, **Alexander B. Zachernyuk**,[2] and **Natalia S. Chernova**[1]
[1] *Theoretical Chemistry Division. K.G. Razumovski Moscow State University of Technologies and Management. Zemlyanoy Val St., 73. Moscow, 109044. Russia.*
Phone: +7 (495) 640-54-36. E-mail: zachern@rambler.ru
[2] *Laboratory of Organoelements Polymers. N.S. Enicolopov Institute of Synthetic Polymers Matherials. Profsoyuznaya St., 70. Moscow, 117393. Russia. Phone: +7 (495) 332-58-62. E-mail: a_zacher@mail.ru*

*Supervising author; +Corresponding author

Keywords: *oligo(phenylene sulfide)s, thiol groups, poly(arylene sulfide)s, polycondensation, α,ω-dithiols oligo(phenylene sulfide)s, telehelic oligomers, metallo(sulfide)s-oligo(phenylene sulfide)s.*

Abstract

Chemical modification of oligo(phenylene sulfide)s by introduction of terminal thiol groups was performed. Telehelic α,ω-dithiols oligo(phenylene sulfide)s were synthesized through the reaction between isomeric oligo(phenylene sulfide)s and sodium hydrosulfide. The reactivity of the thiol groups was investigated in the reaction with metal(II) salts. Thermostable metallo(sulfide)s-oligo(phenylene sulfide)s, having at the chain C-metal bond, were obtained by polycondensation between α,ω-dithiols oligo(phenylene sulfide)s and Pb or Cd acetates.

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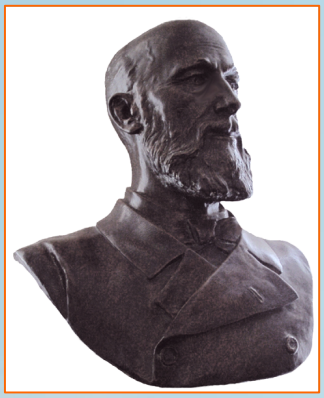

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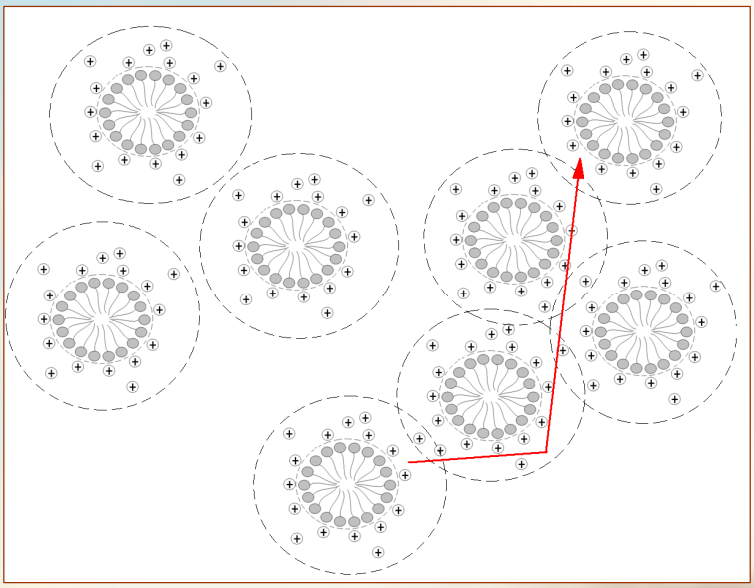

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Phylloquinone. Excited electronic states and intersystem conversion.

© **Svetlana N. Tseplina**,[+] **Evgeny E. Tseplin**,* and **Olga G. Khvostenko**
Institute of Molecular and Crystal Physics. Ufa Research Centre of Russian Academy of Sciences.
Octyabrskiy Prospect, 151. Ufa, 450075. Russia. Phone: +7 (347) 292-14-17. E-mail: sn_tseplina@mail.ru

*Supervising author; [+]Corresponding author

Keywords: *singlet-triplet intersystem conversion, phylloquinone, excited states.*

Abstract

The optical absorption, emission and excitation spectra of phylloquinone (Vitamin K1) were recorded. On the basis of TDDFT B3LYP/6-31+G(d,p) calculations we carried out the assignment of the absorption bands to specific singlet transitions. It has been revealed that two different excitation spectra are registered in phylloquinone depending on the registration length wave where one of the spectra is related to fluorescence and the other corresponds to phosphorescence, also in agreement with the appropriate attribution of the luminescence bands. On the basis of the complex analysis of absorption, luminescence and excitation spectra in accordance with the selection rule, it has been shown that the intersystem crossing mainly occurs between S_1 and T_2 states.

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Quartet states of tetracyanoquinodimethane (TCNQ) negative molecular ions

© Olga G. Khvostenko,*+ **Laysan Z. Khatymova**, **Vladimir G. Lukin**, **Evgeny E. Tseplin**, and **Georgy M. Tuimedov**
Institute of Molecular and Crystal Physics, Ufa Research Center of Russian Academy of Sciences. Octyabrskiy Prospect, 151. Ufa, 450075. Bashkortostan Republic. Russia.
Phone: +7 (347) 292-14-17. E-mail: khv@mail.ru

*Supervising author; +Corresponding author

Keywords: *resonance electron capture by molecules, long-lived negative ions, tetracyanoquinodimethane.*

Abstract

In this paper, anomalously long-lived (ms) negative molecular ions of tetracyanoquinodimethane (TCNQ) were registered by means of the negative ion mass-spectrometry of the resonance electron capture. The ions are formed at several resonance states of the molecule plus electron system as a result of the electron capture by TCNQ molecule in the gas phase, when the electrons attached have nonzero energy. It is shown that the anomalously high life time of the ions is caused by the ions-quartets formation from the ions-doublets via the intersystem crossing. The results obtained can be useful for understanding TCNQ behavior in the devices of single molecule electronics and the negative differential resistance effect which governs, as it is well-known, the work of such devices.

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Effect of chiral dopant on the particular orientation of transitions in the drops nematocholesteric

© **Yulay I. Timirov**,[+] **Oleg A. Skaldin**,* **Elena R. Gareeva** and **Ildar Kayumov**
Institute of Molecular and Crystal Physics, Ufa Research Center of Russian Academy of Sciences.
Octyabrskiy Prospect, 151. Ufa, 450075. Russia. E-mail: scala@anrb.ru

*Supervising author; [+]Corresponding author

Keywords: *chiral dopant nematocholesteric liquid crystals, orientation structures, defects.*

Abstract

We have studied the orientation quasi-static transformations in drops of nematic cholesteric liquid crystal in the isotropic environment with changing concentration of the cholesteric dopant and under the influence of an external electric field. The case where the droplet radius (R) is less than or of the order of the equilibrium helical pitch (P) induced by the dopant has been considered. It is shown that there exists a critical concentration of the chiral dopant, above which the boundary between the liquid crystal in isotropic phase with the decrease in P initiates the growth of the deformation field with correlation length depending on P. In the case of an electric field, it has been shown that the process of transformation of the initial homeotropic orientation of the liquid crystal molecules of the considered drops has non-threshold character. Such behavior of the boundary "liquid crystal - isotropic phase" is due to the presence of small additions of cholesteric leading with the increase in voltage to the continuous growth of the effective size of the deformation field from the interface of liquid crystal - isotropic phase.

Full Paper _____ *Thematic Section:* Physico-Chemical Research.
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Peculiarities of stable multi-walled carbon nanotubes dispersions formation in the presence of polycarbonic acids

© Olga A. Pyshkina,[+]* **Zhanna A. Boeva**,
Nadezhda S. Volosova, and **Vladimir G. Sergeyev**
Polymer Department. Chemistry Department. M.V. Lomonosov Moscow State University.
Leninskie Gory St., 1/40. Moscow, 119992. Russia.
Phone: +7 (495) 939-38-77. E-mail: pyshkina@genebee.msu.su

*Supervising author; [+]Corresponding author

Keywords: *multi-walled carbon nanotubes, polycarbonic acids, stable dispersions.*

Abstract

It was shown that multi-walled carbon nanotubes dispersing in the aqueous solutions of polycarbonic acids with different molecular masses leads to breaking their aggregates and formation of their stable dispersions. The poly-carbonic acid molecular mass increase leads to the increase of multi-walled carbon nanotubes amount transferred to the dispersion. The mechanism of multi-walled carbon nanotubes solubilization by poly-acids was suggested.

Thematic Section: Physico-Chemical Research **Full Paper**
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Study of the reduced graphene oxide suspension and the behavior of its particles on the surface of water sub-phase

© **Evgeny P. Mironov**,[1a+] **Anatoly N. Baranov**,[1b] **Larisa D. Kvacheva**,[3] **Alexander M. Saletsky**,[1c] **Gennady S. Plotnikov**,[1d] **Semyon P. Chervonobrodov**,[4e] and **Tatiana V. Bukreeva**[2f]*

[1 a)] *Department of General Physics and Molecular Electronics*. [b)] *Department of General Physics. M.V. Lomonosov Moscow State University. Leninskiye Gory., 1 block.2. Moscow, 119991. Russia.* [a)] *Phone: +7 (499) 135-40-20. E-mail: qvantus@mail.ru.* [b)] *Phone: +7 (495) 939-26-36. E-mail: barnov@physics.msu.ru.* [c)] *Phone: +7 (495) 939-36-32. E-mail: salzky@rambler.ru.* [d)] *Phone: +7 (495) 939-30-27. E-mail: plot@vega.phys.msu.ru*

[2] *A.V. Shubnikov Institute of Crystallography. RAS. Leninskiy Prospect, 59. Moscow, 119333. Russia.* [f)] *Phone: +7 (499) 135-60-10. E-mail: bukreeva@ns.crys.ras.ru*

[3] *A.N. Nesmeyanov Institute of Organometallic Compounds.RAS. Vavilov St., 28. Moscow, 119991. Russia.*

[4] *JSC «Karbonlait». Institute Lane, 9. Dolgoprudny, 141700. Russia. Moscow oblast.* [e)] *Phone: +7 (905) 582-08-25. E-mail: chervon@mail.ru*

*Supervising author; [+]Corresponding author

Keywords: *reduced graphene oxide, Langmuir–Blodgett trough, correlation spectroscopy of scattered light, atomic-force microscope.*

Abstract

The particles of the reduced graphene oxide (RGO) were obtained from natural and synthetic graphite using the chemical reduction method. These particles have been investigated by atomic-force microscopy. The suspensions of the particles in CCL_4 were studied using correlation spectroscopy of scattered light that allowed to obtain size distribution before and after sonication. We obtained isotherms of RGO for various amounts of material applied on the surface of the water sub-phase in the Langmuir–Blodgett trough. Layers of RGO could be transferred by the Langmuir-Blodgett method on silicon substrates.

Thematic Section: Physico-Chemical Research. **Full Paper**
Subsection: Polymer Chemistry. *Registration Code of Publication:* 13-35-8-31
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Dielectric spectroscopy as a method for studying curing processes of polymer composits based on epoxy oligomes

© **Dmitry L. Rodin**,[1+] **Alexandr V. Solopchenko**,
Alexey V. Kepman, **Sergey U. Stefanovich**, and **Marina U. Yablokova**[2]*
[1] *Department of Chemical Technology and New Materials. Chemical Faculty. MSU. Leninskie gori, b.1/11. Moscow, 119991. Phone: +7 (916) 461-17-68. E-mail: robinhood89@yandex.ru*
[2] *Department of Chemical Technology and New Materials. Chemical Faculty. MSU. Leninskie gori, b.1/11. Moscow, 119991. Phone: +7 (495) 939-33-16. E-mail: marapfel@yandex.ru*

*Supervising author; [+]Corresponding author

Keywords: *dielectric spectroscopy, epoxy, polysulphone, degree of conversion, curing.*

Abstract

Relaxation processes, electric conductivity and dielectric permittivity in the curable compositions based on the epoxy oligomer, hardener and modifier were investigated by dielectric spectroscopy. This technique allowed to conduct real-time evaluation of conversion degree, gel and vitrification times, the beginning of phase separation in curing processes. Results of this method were proved by DSC and rheological investigations. There were measured physical and chemical parameters, as well as morphology of polymer system was studied.

Full Paper _____ *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 13-35-8-42 *Subsection:* Polymer Chemistry.
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Thematic course: Control over physical and chemical properties of polymers by direct synthesis. Part 1.

Influence of the nature of the co-monomer on the thermal behavior of acrylonitrile co-polymers

© **Artem A. Baskakov**,[1] **Julia V. Kostina**,[1]*+ and **Elena V. Chernikova**[2]*
[1] *Institution of the Russian Academy of Sciences. A.V. Topchiev Institute of Petrochemical Synthesis of RAS. Leningradskiy Pr., 29. Moscow, 119991. Russia. Phone: +7 (495) 955-41-35. E-mail: julia@ips.ac.ru*
[2]*M.V. Lomonosov Moscow State University. Chemical Faculty. Leninskiye gory. Moscow, 119991. Russia. Phone: +7 (495) 939-54-09. E-mail: chernikova_elena@mail.ru*

*Supervising author; +Corresponding author

Keywords: *polyacrylonitrile, polyconjugated system, pseudoliving radical polymerization, IR-spectroscopy, IR- pyrolysis.*

Abstract

We studied the laws of the formation of actylonitrile co-polymers in the presence of small additions of co-monomers – styrene and *tret*-butylacrylate – in pseudoliving radical polymerization under the action of agents of reversible chain-transfer. The influence of the nature of co-monomer on the rate of formation and the structure of polyconjugated system under the thermal effect on the synthesized co-polymers have been studied.

Thematic Section: Physico-Chemical Research. **Full Paper**
Subsection: Composite Materials. *Registration Code of Publication:* 13-35-8-51
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Formation of Fe-containing functional materials and their activity in the process of photochemical hydrogen production

© **Valentina N. Batalova**,[+] **Gennady M. Mokrousov**,*
Lidia N. Skvortsova, and **Lyudmila B. Naumova**
Analytical Chemistry Department. National Research Tomsk State University. Lenina St.,36. Tomsk, 634050. Russia. Phone: +7 (3822) 42-10-41. E-mail: batvn@sibmail.com

*Supervising author; [+]Corresponding author

Keywords: *photocatalysis, destruction of organic pollutants, hydrogen production, silicon nitride, boron nitride, peat, zeolites.*

Abstract

The possibility of hydrogen production simultaneously with the destruction of organic pollutants of water using natural sorbents: peat and zeolites modified with iron and synthesized silicon nitride, boron nitride with phase of iron was investigated. H_2-production rates (mL/h) and the performance of the investigated composites for hydrogen evolution (mkmol/h·g) were estimated under irradiation of aqueous solutions of carboxylic acids, hydrazine, phenolic compounds. It is shown that there is a principal possibility of using peat and zeolites modified with iron for the generation of hydrogen simultaneously with the destruction of organic toxicants in water, but the process efficiency is not high and requires further optimization. In the case of synthetic boron and silicon nitrides hydrogen evolution was more efficient. It has been found that production of hydrogen is the most effective in the aqueous solutions of formic acid and hydrazine with boron nitride.

Thematic Section: Physico-Chemical Studies. **Full Paper**
Subsection: Physical Chemistry. *Registration Code of Publication:* 13-35-8-59
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Titanium(IV) citrates in aqueous-chloride solutions

© **Sergey G. Bezryadin**,[1]*+ **Vladimir V. Chevela**,[2]* **Olga P. Ajsuvakova**,[1]
and **Valentina Yu. Ivanova**[2]
[1] *Department of Chemistry. Orenburg State Agrarian University. Chelyuskintsev St., 18. Orenburg, 460014. Orenburgskaya region. Russia. Phone: +7 (3532) 77-95-06. E-mail: sergbezryadin@mail.ru*
[2] *Department of Inorganic Chemistry. A.M. Butlerov Institute of Chemistry of Kazan (Volga Region) Federal University. Kremlevskaya St., 18. Kazan, 420008. The Republic of Tatarstan. Russia. Phone: +7 (843) 231-54-16.*

*Supervising author; +Corresponding author

Keywords: *titanium(IV) citrate, complex formation, potentiometric titration, mathematical simulation.*

Abstract

The titanium(IV) – citric acid system was studied by the method of potentiometric titration in conjunction with mathematical simulation for the ratios of metal-to-ligand 1:1, 2:3, 1:2 and 1:3. The composition, stability and quantity of accumulation of citrate titanium(IV) in aqueous solution were calculated. It was found that for the equimolar ratio of the reactants di-, tri- and tetranuclear particles are formed, while for the excess of ligand the mononuclear complex forms $[Ti(H_{4-n}Cit)_3]^{4-3n}$ (n = 2-4) at pH ≤ 8 and $[Ti(OH)_2(Cit)_2]^{6-}$ at pH ≥ 8 are dominant.

Thematic Section: Physico-Chemical Research. **Full Paper**
Subsection: Physical Chemistry. *Registration Code of Publication:* 13-35-8-67
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Heteronuclear titanium(IV) and dysprosium(III) citrates in aqueous solutions

© **Sergei G. Bezryadin**,[1]*+ **Vladimir V. Chevela**,[2]*
Olga P. Ajsuvakova,[1] and **Valentina Yu. Ivanova**[2]
[1] *Department of Chemistry. Orenburg State Agrarian University. Chelyuskintsev St., 18. Orenburg, 460014. Orenburgskaya region. Russia. Phone: +7 (3532) 77-95-06. E-mail: sergbezryadin@mail.ru*
[2] *Department of Inorganic Chemistry. AM Butlerov Institute of Chemistry of Kazan (Volga Region) Federal University. Kremlevskaya St., 18. Kazan, 420008. The Republic of Tatarstan. Russia. Phone: +7 (843) 231-54-16.*

*Supervising author; +Corresponding author

Keywords: *Heteronuclear titanium(IV) and dysprosium(III) citrates, complex formation, nuclear magnetic relaxation, mathematical simulation.*

Abstract

The titanium(IV) – citric acid system was studied by the method of nuclear magnetic relaxation in conjunction with mathematical simulation in the molar reactant ratios 1:1:4 and 1:1:6. The composition, stability and the quantity of accumulation of heteronuclear titanium(IV) and dysprosium(III) complexes with citric acid in aqueous solution were calculated. The formation forms of 1:1:2, 1:1:3, 1:1:4, 2:2:8, 1:1:6 were determined.

Full Paper _____ *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 13-35-8-74 *Subsection:* Physical Chemistry.
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http://butlerov.com/readings/
Contributed: June 12, 2013.

The structure and solubilization properties of aqueous solutions of lithium and sodium dodecyl sulfates

© **Lilia R. Bogdanova**,[1+] **Nadezhda N. Benevolenskaya**,[2] **Anastasia O. Borovskaya**,[2] **Ellina A. Sharipova**,[2] **Olga S. Zueva**,[2] and **Yury F. Zuev**[1]*
[1] *Kazan Institute of Biochemistry and Biophysics. Kazan Scientific Center of the Russian Academy of Science Lobachevsky St., 2/31. Kazan, 420111. Russia.*
[2] *Kazan State Energy University. Krasnoselskaya St., 51. Kazan, 420066. Russia.*
Phone: +7 (843) 292-62-88. E-mail:bogdanova.lilly@gmail.com

*Supervising author; [+]Corresponding author

Keywords: *surfactant, counterions, micelles. structure, properties.*

Abstract

Micellization of lithium and sodium dodecyl sulfates (LDS and SDS respectively) was studied in aqueous solutions by conductometry. Besides the CMC inflection point the other one was observed on electrolytic conductivity plots. Phenomenological explanation of this event was proposed basing on overlapping the diffusion regions of electrical double layers. Solubilization properties of SDS and LDS solutions were determined before and after micelle formation.

Thematic Section: Physico-Chemical Research. **Full Paper**
Subsection: Physical Chemistry. *Registration Code of Publication:* 13-35-8-81
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Correlations of contact angles of liquids on the surface of polymer films with the transport properties of amorphous polymers

© **Yulia G. Bogdanova**,[+]* and **Valentina D. Dolzhikova**
Moscow Lomonosov State University. Chemistry Department.
Leninskie Gory, 1/3. Moscow, 119991. Russia.
Phone: +7 (495) 939-32-18. E-mail: yulibogd@yandex.ru

*Supervising author; [+]Corresponding author

Keywords: *wetting, surface energy, films of amorphous polymers, fractional free volume, gas permeability, nanofiltration.*

Abstract

The specific surface free energy of the films of amorphous polymers of different classes was determined using contact angle method. Interrelation between the dispersive component of surface energy values, the free volume and gas permeability of polymers was demonstrated. The possibilities of using wetting isotherms to determine the alcohol concentration corresponding to the beginning of its sorption in nanofiltration of water-ethanol mixtures through solid polymer membrane were shown.

Full Paper _____ *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 13-35-8-88 *Subsection:* Physical Chemistry.
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Behavior of comb-shaped liquid crystalline stereoregular cyclolinear methylsiloxane copolymers with chiral mesogenic groups at the air/water interface

© **Julia N. Malakhova**,[1,2+] **Andrew V. Taldrik**,[3] **Natalia N. Makarova**,[3]*
and **Alexander I. Buzin**[1]

[1] *Laboratory of Functional Polymeric Structures. N.S.Enikolopov Institute of Synthetic Polymer Materials, Russian Academy of Sciences. Profsoyuznaya St., 70. Moscow. 117393. Russia. Phone: +7 (495)332-58-20. E-mail: j.malakhova@mail.ru*

[2] *Laboratory of Polymeric Materials. National Research Centre "Kurchatov Institute". Pl. Akademik Kurchatov, 1. Moscow, 123098. Russia.*

[3] *A.N. Nesmeyanov Institute of Organo-Element Compounds, Russian Academy of Sciences. Vavilov St., 28. Moscow. 119334. Russia.*

*Supervising author; +Corresponding author

Keywords: *liquid crystal copolymers, Langmuir monolayer.*

Abstract

Surface pressure isotherms, surface potential isotherms and morphology directly at the air-water interface of a series of comb-shaped liquid crystalline stereoregular cyclolinear methylsiloxane copolymers with chiral mesogenic groups of two types were investigated. The effects of the chemical structure of the mesogenic groups, stereoregularity of the copolymer, the temperature of the sub-phase on the thermodynamic and electrical properties of the surface layer were assessed.

Full Paper _____ *Thematic Section:* Physico-Chemical Research.
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The study of physical and chemical properties aqueous dispersion of enterosorbent Polysorb MP

© **Alyona S. Shklyaeva**,* **Oxana V. Vasilieva**,+ and **Vera I. Kucuk**
Saint-Petersburg Chemical-Pharmaceutical Academy. Professor Popov St.,14, lit. A.
Saint-Petersburg, 197101. Russia. Phone: 8-981-760-99-61.
E-mail: Oxana.Vasilieva@pharminnotech.com

*Supervising author; +Corresponding author

Keywords: *Polysorb MP, adsorption, photocolorimeter, viscometer, adsorbate.*

Abstract

We investigated a number of physico-chemical (viscosity, electrical conductivity, electrical mobility, adsorption capacity) characteristics of enterosorbent Polysorb MP. It has been shown that the adsorption activity of this preparation in relation to a series of substances of organic and inorganic origin is high enough. We estimated the number of adsorption centers on Polysorb surface, considered the mechanism of adsorption process.

Full Paper _____ *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 13-35-8-100 *Subsection:* Physical Chemistry.
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Dependence of transverse relaxation time T_2 on the flow rate of fluid in porous medium

© Valentin V. Loskutov
Department of Theoretical Physics and Teaching Methods in Physics.
Mari State University. Lenin Sq. 1., Yoshkar-Ola, 424000. Russia.
Phone: +7 (8362) 41-22-50. E-mail: val_losk@rambler.ru

Keywords: *NMR, porous media, relaxation, flow.*

Abstract

To study the structure of porous media and various processes in these porous media there is commonly used the method of nuclear magnetic resonance (NMR). If the external pressure gradient is applied to the porous sample then in the sample there occurs the movement of the fluid filling the medium, which leads to an additional contribution to the decay of the NMR signal and changing the relaxation time distribution T_2. In this paper, an expression has been obtained that defines the dependence of the transverse relaxation time of liquid contained in a porous medium on the flow rate. The experimental verification of this expression was performed. It is shown that at low flow rates the transverse relaxation rate is proportional to the flow rate of the liquid.

Thematic Section: Theoretical Research. **Full Paper**
Subsection: Physical Chemistry. *Registration Code of Publication:* 13-35-8-105
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Topological structure and self-diffusion in linear flexible polymers

© **Tatiana P. Kulagina**, **Grigory E. Karnauksh**,*+ **Varvara A. Varakina**, **Lev P. Smirnov**, and **Anastasiya N. Kuzina**
Institute of Problems of Chemical Physics RAS. Prospect Semenova,1. Chernogolovka, 142432. Moscow region. Russia. Phone: +7 (496) 522- 18-79. E-mail: tan@icp.ac.ru

*Supervising author; +Corresponding author

Keywords: *nuclear magnetic resonance, linear flexible polymers, free induction decay, physical network of entanglement, stimulated echo, self-diffusion.*

Abstract

In this work the theory of free induction decay in linear flexible polymers with various average lengths of polymeric chain in a wide temperature range is developed. It is shown that with the growth of mean molecular weight of cross-site chains M_w topological structure of linear polymers changes, and at $M_w > 10^5$ the physical network of entanglements is formed. The correlation function of molecular motion is obtained which is applied for calculating the diffusion attenuation of spin echo.

The general approach to calculation of diffusion attenuation spin echo signals and its application to determination of self-diffusion coefficient in linear polymers with different topological structure is offered. It allowed to explain the observed experimentally anomalous diffusion.

Full Paper _____ *Thematic Section:* Physico-Chemical Research.
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The study of complexing reactions in the system erbium(III) – citric acid in aqueous solution

© **Valentina Yu. Ivanova**,[1]*+ **Vladimir V. Chevela**,[1]*
Julia V. Efremova,[1] and **Sergey G. Bezryadin**[2]
[1] *Inorganic Chemistry Division. A.M. Butlerov Institute of Chemistry. KFU.*
Kremlevskaya St., 18. Kazan, 420008. Tatarstan Republic. Russia.
Phone: +7 (843) 233-72-01. E-mail: Valja331@rambler.ru
[2] *Chemistry Division. A.E. Orenburg State Agrarian University.*
Chelyuskintsev St., 18. Orenburg, 460014. Orenburg region. Russia.
E-mail: sergbezryadin@mail.ru

*Supervising author; +Corresponding author

Keywords: *mono-and poly-nuclear citrates of erbium(III), pH – metric titration, nuclear magnetic relaxation, mathematical simulation, stoichiometry, stability of complexes.*

Abstract

The complex formation of erbium(III) with citric acid was investigated by pH-metric, proton magnetic relaxation and mathematical simulation methods in the pH range 2-10 at 25 °C. The stoichiometry and stability of the erbium(III) citrates were determined. The system erbium(III) – citric acid is characterized by mononuclear and binuclear citrates with varying degrees of protonation. The formation of highly polymerized citrates of erbium(III) was not found. With the three-fold excess of ligand, binuclear complexes are not formed, and throughout the pH range mononuclear forms of 1:3 composition dominate.

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Evaluation of the hyperfine interaction constants and the spin density distribution in the region of copper nuclei in cubanite

© **Alexander I. Pogoreltsev**,[1]* **Vadim L. Matukhin**,[1]*
Barys V. Korzun,[2] and **Andrey N. Gavrilenko**[1+]
[1] *Department of Physics. Kazan State Power University. Krasnoselskaya St.,51. Kazan, 420066. Tatarstan Republic. Russia. Phone: +7 (917) 930-42-46. E-mail: ang_2000@mail.ru;*
[2] *Scientific-Practical Materials Research Centre, National Academy of Sciences of Belarus. P. Brovki St., 19. Minsk, 220072. Belarus. E-mail: korzun@physics.by*

*Supervising author; [+]Corresponding author

Keywords: *resonance spectroscopy, NMR in the internal magnetic field, electric field gradient, the quadrupole parameters, ab initio electronic structure calculations, electron density distribution, hyperfine interactions, spin density distribution*

Abstract

The resonance NMR spectra of ^{63,65}Cu have been studied experimentally in a local field. Using cluster approach, ab initio evaluation of the electric field gradient at the nuclei of copper in cubanite $CuFe_2S_3$ have been made. Calculations have been carried out in the framework of the self-consistent restricted method of Hartree-Fock with open shells (SCF-LCAO-ROHF). The largest cluster for which the calculations have been carried out has a formula $Cu_7Fe_{14}S_{29}^n$ (R ~ 6Å, 50 atoms), where *n* is a cluster charge. The best fitting of values of the quadrupole parameters (quadrupole frequency ν_Q and the asymmetry parameter of the electric field gradient tensor η), determined experimentally ($\nu_Q \approx 7.3$ MHz and $\eta \approx 0.82$) and by calculation ($\nu_Q \sim 7.38$ MHz and $\eta \sim 0.87$), has been obtained for a cluster $Cu_7Fe_{14}S_{29}^{10}$. For the cluster $Cu_7Fe_{14}S_{29}^{10}$, maps of the electron density distribution in the neighborhood of quadrupole nucleus of copper have been built. Based on the analysis of the resulting electron density distribution, it is suggested that the bond in cubanite is not covalent. Evaluations of the hyperfine interaction constants have been made and maps of spin density distribution in the neighborhood of quadrupole nucleus of copper have been built. Energy level diagram calculated in the high-spin approximation ROHF, defines cubanite as semiconductor with a very narrow gap LUMO-HOMO rather well and is consistent with the notion of cubanite as semiconductor.

Thematic Section: Physico-Chemical Research. **Full Paper**
Subsection: Colloidal Chemistry. *Registration Code of Publication:* 13-35-8-133
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Interaction of glycine with cations of Fe(III) and Ni(II) in water solutions and on surfaces of their oxides

© **Irina B. Dmitriyeva**,∗ **Alexander S. Chukhno**,[+] and **Roman V. Novichkov**
Department of Physical and Colloidal Chemistry. Saint-Petersburg State Chemical-Pharmaceutical Academy. http://www.spcpa.ru Professor Popov St., 14. Saint-Petersburg, 197376. Russia.
Phone: +7 (812) 234-11-38. E-mail: irina@dmitriyev.ru , alex-chuhno@yandex.ru

*Supervising author; [+]Corresponding author

Keywords: *glycine, electrokinetic properties, microelectrophoresis, isoelectrical point, adsorption, oxides of Fe(III) and Ni(II).*

Abstract

Electrosurface properties (electrokinetic potential, isoelectric point, adsorption) of NiO and Fe_2O_3 oxides in water solutions of glycine depending on its concentration, pH of solutions, and time of adsorption have been investigated. It has been established that glycine in all systems is adsorbed specifically while anion is the factor determining the specific adsorption on Fe_2O_3, and cations – on NiO. It has been shown that specific adsorption of determining anion takes place with the formation of donor-acceptor bond on $-NH_2$ group, and determining cation on –COOH group. It has been discovered that glycine is adsorbed on NiO more intensively than on Fe_2O_3 due to stronger interaction of Fe cation with OH^- ions.

Full Paper _____ *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 13-35-8-138 *Subsection:* Colloidal Chemistry.
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Micelle formation in aqueous solutions of cationic surfactants with bicyclic head group. Data of IGMP-NMR.

© **Nail K. Gaisin**,[1+] **Oleg I. Gnezdilov**,[2] **Ferid I. Bashirov**,[1] **Elena P. Zhiltsova**,[3] **Lucia Ya. Zakharova**,[3]* **Tatiana N. Pashirova**,[3] and **Svetlana S. Lukashenko**[3]
[1] *Department of Physics. Kazan National Research Technological University. K.Marx St., 68. Kazan, 420015. Tatarstan Republic. Russia. E-mail: NailGaisin@yandex.ru*
[2] *E.K. Zavoiskiy Kazan Physico-technical Institute. Sibirskiy Tract, 10/7. Kazan, 420029. Russia.*
[3] *A.E. Arbuzov Institute of Organic and Physical Chemistry. Arbuzov St., Kazan, 420088. Russia. E-mail: lucia@iopc.ru*

*Supervising author; [+]Corresponding author

Keywords: *dicationic surface-active substance, micelle formation, micelle radius, aggregation number, NMR-spectroscopy.*

Abstract

With NMR-IGMP method we studied micelle formation process in dicationic surfactant with the head group of bicyclic structure of 4-ethyl-1-tetradecyl-1,4-diazo-niabicyclo [2.2.2] octane dibromide in heavy water. The critical micelle concentration was defined, the radii of the micelles were established as well as their aggregation numbers. A comparison of the data with the characteristics of micelle mono-cation 4-aza-1-tetradecyl-1-azoniabicyclo [2.2.2] bromide octane was carried out.

Thematic Section: Physico-Chemical Research. **Full Paper**
Subsection: Phase Equilibria. *Registration Code of Publication:* 13-35-8-141
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Phase equilibrium and interdiffusion in the polystyrene-polysiloxane system

© **Arkady A. Poteryaev**,[1] **Anatoly E. Chalyh**,[1] **Ekaterine V. Surovyatkina**,[1]
Nikita Yu. Budylin,[1] **Victor M. Kopylov**,[2] and **Denis I. Sharagin**[3]
[1] *Laboratory of Structural and Morphological Studies. A.N. Frumkin Institute of Physical Chemistry and Electrochemistry. Russian Academy of Sciences. Lenin Prospect, 31, build. 4. Moscow, 119071. Russia. Phone: +7 (495) 955-46-01.*
[2] *State Scientific-Research Institute of Chemistry and Technology of Organometallic Compounds.*
[3] *Laboratory of Organometallic Polymers. N.S. Enikolopov Institute of Synthetic Polymer Materials. RAS. Shosse Entuziastov, 38. Moscow, 111123. Russia. Phone: +7 (495) 673-49-53.*

*Supervising author; [+]Corresponding author

Keywords: *phase equilibria, diffusion, phase diagrams, polystyrene, polydimethylsiloxane.*

Abstract

Using optical interferometry we studied the diffusion zone, phase equilibrium and translational mobility of macromolecules in mixtures of polystyrene-polymethylsiloxane over a wide temperature, molecular weight and concentration ranges. The diagrams of phase states were built, mutual diffusion coefficients, the activation energy of translational motion and the thermodynamic parameters of mixing the components were calculated.

Full Paper _____ *Thematic Section:* Spectral Research.
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Microwave spectrum and hindered pseudorotation of tetrahydrofuran

© **Marat G. Fayzullin**,[+] **Rustem V. Galeev**, and **Ayrat H. Mamleev***
Laboratory of Microwave Spectroscopy. Institute of Molecular and Crystal Physics.
Prospect Oktyabrya, 151. Ufa, 450075. Bashkortostan Republic.
Phone: +7 (347) 235-95-22. E-mail: mwsm@anrb.ru, fayzullinmg@gmail.com

*Supervising author; [+]Corresponding author

Keywords: *tetrahydrofuran, hindered pseudorotation, microwave spectrum, rotation-vibration transitions.*

Abstract

Pseudorotation-rotational transitions between pseudorotational states v = 4, 5 of tetrahydrofuran have been observed in the 11-52 GHz frequency range. The joint analysis of pseudorotation-rotational and rotational transitions of three pseudorotational states v = 4, 5, 6 has been carried out. The types of symmetry of these states were established and energy intervals ΔE_{45} , ΔE_{56} were determined. By the data of ΔE_{45} , ΔE_{56}, the reported earlier ΔE_{01}, ΔE_{02}, ΔE_{23}, ΔE_{78} and a set of pseudorotational transitions from the far IR-field spectroscopy there was determined the potential function of hindered pseudorotation of the molecule.

Short Communication _____ *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 13-35-8-158 *Subsection:* Physical Chemistry.
The article is published on the materials of speech at the XX All-Russian Conference
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Sorption of iron(III) on synthetic cation exchangers in aqueous solutions

© **Larisa G. Smirnova**,* **Alexander K. Smirnov**,+
Svetlana V. Al Ansari, **Ekaterina S. Starodubtseva**, and **Andrey K. Vasiliev**
Department of General Chemistry. Mari State University. Lenin St., 1. Yoshkar-Ola, 424000. Mary El Republic. Russia. Phone: +7 (8362) 42-55-94. E-mail: aksmi@yandex.ru

*Supervising author; +Corresponding author

Keywords: *sorption kinetics, temperature dependence, activation energy of sorption constants.*

Abstract

The processes of sorption of iron(III) from aqueous solutions of chloride salts in weakly acidic cation exchanger KB-4 and strongly acidic cation exchangers KU-1, KU-2, KU-2-8 have been studied. We have carried out the research into the kinetics of sorption, determined the temperature dependences, calculated the activation energy of sorption processes. The constants of adsorption of ions Fe^{3+}, Gibbs energies of sorption processes were defined.

Thematic Section: Physico-Chemical Research. **Short Communication**
Subsection: Physical Chemistry. *Registration Code of Publication:* 13-35-8-161
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Optimization of photometric determination of iron in water

© **Anastasia V. Apakaeva**, **Svetlana V. Al Ansari**,
Larisa G. Smirnova, and **Alexander K. Smirnov**
Department of General Chemistry. Mari State University. Lenin St., 1. Yoshar-Ola, 424000. Mary El Republic. Russia. Phone: +7 (8362) 42-55-94. E-mail: aksmi@yandex.ru

*Supervising author; +Corresponding author

Keywords: *analysis, extraction, concentration.*

Abstract

The results of the research showed that acetylacetone could be recommended as photometric reagent for various objects including iron. Higher sensitivity of acetylacetone method for determining Fe(III) as compared to sulfosalicylate method recommended in standards has been revealed.

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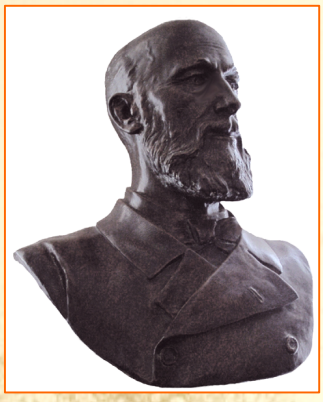

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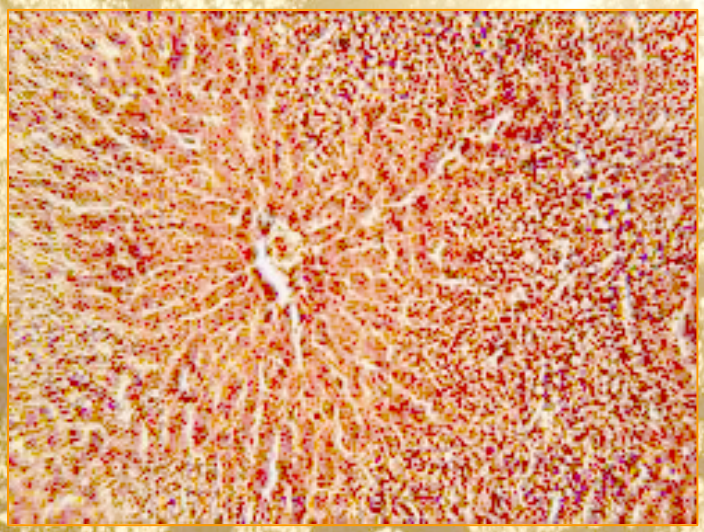

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http://butlerov.com/readings/
Contributed: June 5, 2013.

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

Quantum chemical simulation of the mechanism of benzoyl chloride and benzenesulphonyl chloride interactions with amino compounds of different classes

© **Ludmila B. Kochetova**,[1] **Maria G. Paikova**,[1]
Natalia V. Kalinina,[2] and **Tatiana P. Kustova**[1]*[+]
[1] *Department of Organic and Physical Chemistry. Ivanovo State University.*
Ermak St., 39. Ivanovo, 153025. Russia. Phone: +7 (4932) 37-37-03. E-mail: kustova_t@mail.ru
[2] *Department of Inorganic and Analytical Chemistry. Ivanovo State University.*
Ermak St., 39. Ivanovo, 153025. Russia. Phone: +7 (4932) 37-37-03.

*Supervising author; [+]Corresponding author

Keywords: *acylation, amino compounds,benzoyl chloride, benzenesulfonyl chloride, quantum chemical calculations, reaction mechanism, potential energy surface.*

Abstract

Potential energy surfaces are calculated for reactions of ammonia and a number of amino compounds with benzoyl chloride and benzenesulfonyl chloride in gas phase, as well as for ammonia interaction with benzoyl chloride in water by using the polarized continuum model. It is shown that all the reactions proceed by the concerted mechanism, and benzoylation occurs by the pathway with frontal nucleophilic attack, when whereas arensulfonylation – by the pathway with varying attack angle. Non-specific solvation by water decreases activation energy of ammonia acylation as compared to gas phase reaction**.**

Thematic Section: Investigation of Reactivity. **Full Paper**
Subsection: Organic Chemistry. *Registration Code of Publication:* 13-35-9-9
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 influence of solvent nature on the mechanism of the reaction of anionic macroinitiators and aromatic isocyanates

© **Ruslan S. Davletbaev**,[1]* **Alsu I. Akhmetshina**,[2+]
Askhat M. Gumerov,[2] **Rafael R. Sharifullin**,[3] and **Ilsia M. Davletbaeva**[2]
[1] *Department of Materials Science, Welding and Structure-Forming Technology. Kazan National Research Technical University n.a. A.N. Tupolev. K. Marx St., 10. Kazan, 420111. The Republic of Tatarstan. Russia. Phone: +7 (432) 31-00-27. E-mail: darus@rambler.ru*
[2] *Department of Synthetic Rubber. Kazan National Research Technical University. K. Marx St., 68. Kazan, 420015. The Republic of Tatarstan. Russia. Phone: +7 (927) 42-27-99. E-mail: aai-89@mail.ru*
[3] *Research & Technology Center JSC "Nizhnekamskneftekhim". Nizhnekamsk, 423570. Tthe Republic of Tatarstan. Russia. Phone: +7 (8555) 37-97-72. E-mail: Rafael_Sharif@mail.ru*

*Supervising author; [+]Corresponding author

Keywords: *anionic macroinitiators, 2,4-toluene diisocyanate, infrared spectroscopy, polyisocyanates, solvent.*

Abstract

The mechanism of polyaddition of 2,4-toluene diisocyanate to a anionic macroinitiator in solvents of various chemical character was studied by infrared spectroscopy. Both isocyanate blocks and polyisocyanate blocks of acetal nature are the products of interaction. Solvent nature influences considerably on the possibility of a reaction going in one direction or the other.

Thematic Section: Preparative Chemistry. **Full Paper**
Subsection: Chemistry of Complex Compounds. *Registration Code of Publication:* 13-35-9-14
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http://butlerov.com/readings/
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Thiosemicarbasidehidoroxyethylidenediphosphonic complex and its inhibitor characteristics

© **Michail A. Yershov**,[1+] **Eugeny V. Kamayev**,[1] and **Vikenty G. Skvortsov**[2]*
[1] *Department of Chemistry. Chuvash State Agricultural Academy. K. Marx St, 29. Cheboksary, 428003. Chuvash Republic. Russia. Phone: +7 (352) 62-02-26.E-mail: ema11@mail.ru*
[2] *Department of Chemistry and Biosynthesis. I. Y. Yakovlev Chuvash State Pedagogical University. K. Marx St. 38. Cheboksary.428000. Chuvash Republic. Russia. Phone: +7 (352) 58-67-66; +7 (352) 58-68-45.*

*Supervising author; [+]Corresponding author

Keywords: *phosphorus- and nitrogen organic complexes, physical and chemical, X-ray phase, X-ray structural, IR-spectroscopic analysis, gravimetrical, corrosion-electrochemical researches, fatigue, corrosion-fatigue tests.*

Abstract

During the isothermal evaporation (25 °C) of water solution that contains 1-hydroxyethane-1,1-diphosphone acid and tiocemicarbaside the authors could get a new complex combination of monohydrate [1-hydroxyethane-1,1-diphosphonato(2-)]ditiocemicarbaside (tiosemikarbasidehydroxiethylenediphosphonic complex – TOC). Its structure and inhibitor characteristics were studied.

Thematic Section: Preparative Chemistry. **Full Paper**
Subsection: Organic Chemistry. *Registration Code of Publication:* 13-35-9-21
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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Stereospecific synthesis of insect pheromones of *E*- alkene series based on isopropyl 3*E*,8-nonadienoates – the product of catalytic telomerization of butadiene or carbon oxide

© **Gumer Yu. Ishmuratov**,* **Valentina A. Vydrina**, **Marina P. Yakovleva**,+
Gulshat V. Nasibullina, **Rinat R. Muslukhov**, and **Nailya M. Ishmuratova**
Institute of Organic Chemistry. Ufa Scientific Center, RAS. Octyabr Prospect, 71. Ufa, 450054. Bashkortostan Republic. Russia. Fax: +7 (3472) 35-60-66. E-mail: insect@anrb.ru Phone: +7 +7 (352) 58-67-66; +7 (352) 58-68-45.

*Supervising author; +Corresponding author

Keywords: *isopryl 3E,8-nonadienoate, E-monoenic pheromone, synthesis.*

Abstract

We have implemented stereospecific synthesis series *E*-mono-olefin components of reproductive insects pheromones of the order *Lepidoptera* [6*E*-nonen-1-ola and its acetate – Mediterranean fruit fly pheromones *Ceratitis capitata* and melon butterfly *Dacus cucurbitae*, as well as 11*E*-tetra-decene-1-ola and its acetoxyderivative – pheromones of fruit leaf *Archips argyrospilus* and webworm *Loxostege sticticalis* respectively] from the available product catalyzed by complex compounds of palladium, catalyzed by palladium complex of codimerization of butadiene and carbon oxide – isopryl-3*E*,8-nonadienoate – with the use at key stages of the reactions of hydride reduction of the ester derivatives, thermal hydroaluminizing – oxidation and cross-coupling of dialkyl lithium cuprate reagent with *para*-toluenesulfonate derivative.

Full Paper _____ *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 13-35-9-32 *Subsection:* Physical Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: July 12, 2013.

Experimental study of integral characteristics of ignition of air mixture with typical liquid fuel vapor by a fixed heated metal rod

© **Roman S. Volkov**, **Dmitry O. Glushkov**,[+]
Valery V. Medvedev, and **Pavel A. Strizhak***
National Research Tomsk Polytechnic University. Lenin St., 30. Tomsk, 634050. Russia.
Phone: +7 (3822) 70-17-77 , 1957. E-mail: dmitriyog@tpu.ru

*Supervising author; [+]Corresponding author

Keywords: *ignition, heat and mass transfer, evaporation, oxidation, liquid fuel, warmed rod, ignition time delay.*

Abstract

Experimental study of vapors ignition of typical liquid fuel – gasoline by a local heating source is conducted. Conditions of interaction of combustible substance evaporation products with the fixed metal rod warmed to high temperatures are considered at direct contact of the condensed substance with a power source and at its arrangement in some distance from evaporation border. The value of the main integrated characteristic of the process – ignition time delay is determined. Value of the limiting (minimum) temperature of the local source at which the ignition in the system "metal rod – combustible liquid – steam-gas mix" ignition is happening has been determined. Dependence of ignition time delay for a mix of air with vapors of gasoline on the distance between the steel rod and the surface of evaporating fuel is obtained. Comparison of experimental results with well-known consequences of numerical researches is carried out.

Full Paper _____ *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 13-35-9-38 *Subsection:* Physical Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: June 17, 2013.

Experimental research of evaporation regularities for pulverized water moving through high-temperature combustion products

© **Roman S. Volkov**,[+] **Olga V. Vysokomornaya**, **Geny V. Kuznetsov**, and **Pavel A. Strizhak***
National Research Tomsk Polytechnic University. Lenin St., 30. Tomsk, 634050. Russia.
Phone: +7 (3822) 70-17-77 , 1957. E-mail: romanvolkov@tpu.ru

*Supervising author; [+]Corresponding author

Keywords: *evaporation, heat-and-mass transfer, combustion products, flame, drops, sprayed water, field of velocities.*

Abstract

An experimental research of evaporation integrated characteristics for pulverized water moving through high-temperature combustion products is performed. Scales of the velocity, weight and the characteristic sizes changes of water drops moving through the flame of fixed height are determined. The parameters of water dispersion at which completeness of evaporation is provided are established.

Thematic Section: Physico-Chemical Research. **Full Paper**
Subsection: Analytical Chemistry. *Registration Code of Publication:* 13-35-9-47
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
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Assesment of efficiency of internal standardization for iron ores and slags analysis by inductively coupled plasma atomic emission spectroscopy

© **Anna V. Mayorova**,* **Nadegda V. Pechishcheva**,+
Ksenia A. Vorontsova, and **Anatoly A. Shchepetkin**
Laboratory of Analytical Chemistry. UB RAS Institute of Metallurgy. Amundsena St., 101. Russia. Yekaterinburg, 620016. Phone: +7 (343) 267-89-36. E-mail: k_shun@mail.ru

*Supervising author; +Corresponding author

Keywords: *thermodynamic modeling, inductively coupled plasma atomic emission spectrometry, internal standardization*.

Abstract

The efficiency of internal standardization for correction of instrumental drift during determining the concentration of iron ores, concentrates and slags of main components by inductively coupled plasma atomic emission spectrometry have been shown using thermodynamic modeling (by «TERRA» software). Basing on modeling results, analytical procedure have been developed, its experimental testing on certified reference materials showed decreasing of the analysis error with scandium as internal standard in the analytes concentration range 0.1-48 wt. %.

Thematic Section: Biochemical Research. **Full Paper**
Subsection: Biochemistry of Lipids. *Registration Code of Publication:* 13-35-9-55
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: July 16, 2013.

Molecular chemiluminescence of lipids

© **Rostislav F. Vasiliev**, **Timur L. Veprintsev**, **Vladimir V. Naumov**, and **Aleksey V. Trofimov***
Emanuel Institute of Biochemical Physics, Russian Academy of Sciences. Kosygina St., 4. Moscow, 119334. Russia. Phone: +7 (8495) 939-73-58. E-mail: avt_2003@mail.ru

*Supervising author; +Corresponding author

Keywords: *antioxidants, chemiluminescence, oxidation, kinetics, lipids.*

Abstract

We studied the influence of lipid extracts from sea-fish tissues on the chemiluminescence kinetics in model system of the initiated free-radical oxidation of ethylbenzene. The character of the concentration dependences of chemiluminescence emission upon introduction of lipid portions substantially differs from that in the presence of individual antioxidants. To rationalize the experimental results, a kinetic scheme has been proposed, which involves the stage of non-radical (molecular) chemiluminescence derived from thermal decomposition of oxidation products contained in lipids.

Thematic Section: Biochemical Research. **Full Paper**
Subsection: Analytical Chemistry. *Registration Code of Publication:* 13-35-9-61
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
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Application of solid phase extraction for co-extraction of zolpidem and its metabolites from urine

© **Elena A. Krylova**,[1+] **Sergey S. Kataev**,[1] **Oksana N. Dvorskaya**,[2]* **Yury A. Khomov**[3]
[1] *Forensic-Chemical Department. State Healthcare Establishment of Special Type "Perm Regional Bureau of Forensic-Medical Expertise". Startseva St., 61. Perm, 614077. Perm Region. Russia. Phone: +7 (342) 210-67-83. E-mail: forenschemist@narod.ru*
[2] *Department of Toxicological Chemistry. Perm State Pharmaceutical Academy of the Ministry of Health of the Russian Federation. Polevaya St., 2. Perm, 614990. Perm Region. Russia. Phone: +7 (342) 282-58-64. E-mail: kaftox@mail.ru*
[3] *Department of Pharmaceutical Chemistry. Perm State Pharmaceutical Academy of the Ministry of Health of the Russian Federation. Polevaya St., 2. Perm, 614990. Perm Region. Russia. Phone: +7 (342) 233-51-10. E-mail: homov@pfa.ru*

*Supervising author; [+]Corresponding author

Keywords: *zolpidem, solid phase extraction, modeling of Box-Behnken designs, gas chromatography – mass spectrometry.*

Abstract

The application of the method of solid phase extraction (SPE) is described for co-extraction of zolpidem and urine metabolites, different physical-chemical properties for their further determination by gas chromatography – mass spectrometry (GC-MS). The optimization step of SPE was carried by modeling of Box-Behnken designs, wherein the effect on the extraction efficiency of such factors as the pH of buffer solution and solvents used for washing the sorbent and volume of eluents, and its composition was investigated. Using the optimized method allows to extract from the urine of hydrophilic metabolites of zolpidem. The limits of detection and quantification in urine zolpidem were 13.2 ng/ml and 40 ng/ml, respectively. Precision was proved in terms of repeatability method (coefficient of variation 2.6-5.7%; n = 9) and intermediate precision (CV – 5.8-11.4%; n = 15) at three concentration levels of zolpidem – 50, 150 and 400 ng/ml. Yield of zolpidem from urine was 98.6-108.4%.

Thematic Section: Biochemical Research. **Full Paper**
Subsection: Biochemistry of Yeast Culture. *Registration Code of Publication:* 13-35-9-71
Publication is available for discussion in the framework of the on-line Internet conference
"*The chemical basis for the rational use of renewable natural resources*".
http://butlerov.com/natural_resources/
Contributed: July 15, 2013.

Influence of the composition of the nutrient medium on the biosynthesis of lipase by yeasts *Yarrowia lipolytica*

© **Valentina S. Gamayurova**,* **Maria E. Zinovyeva**,*+
Tran Thi Thu Huong, and **Anna V. Vasileva**
Department of Food Biotechnology. Kazan National Research Technological University (KNRTU).
K. Marx St., 6. Kazan, 420015. Tatarstan Republic. Russia.
Phone: +7 (843) 231-41-65. E-mail: gamaur@kstu.ru.

*Supervising author; +Corresponding author

Keywords: *yeast Yarrowia lipolytica*, *sources of nitrogen, tween-20, lipase activity.*

Abstract

Conditions for biosynthesis of lipase by yeasts *Yarrowia lipolytica Y-3153* were studied. It is established that inorganic sources of nitrogen are not used by the culture for growth and lipase production. It was determined that good sources of nitrogen to the crop are peptone, untrimmed and defatted soy flour. The optimal concentration of sources of nitrogen was obtained. It was demonstrated that the introduction of tween-20 in the composition of the culture medium increases the lipase activity of the culture. It is established that the maximum activity of the enzyme appeared on the following nutrient medium: olive oil – 1%; glucose – 5 g/l; yeast extract – 5 ml/l; defatted soy-bean flour – 40 g/l; tween-20 – 0.001 mg/ml. cultivation temperature being 30°C and biosynthesis duration – 24 hours.

Full Paper _____ *Thematic Section:* Biochemical Research.
Registration Code of Publication: 13-35-9-78 *Subsection:* Agricultural Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*The chemical basis for the rational use of renewable natural resources* ".
http://butlerov.com/natural_resources/
Contributed: July 12, 2013.

The drug-phytoregulators "Novosil" and its impact on protein-proteinase complex of malting barley

© **Gennady P. Karpilenko**,[1] **Sergey L. Belopukhov**,[2*+] **Irina S. Vitol**,[1] **Olga V. Gavrilina**,[1] and **Tatiana I. Shatilova**,[3] and **Vladimir T. Semko**[2]

[1] *Department of Organic, Food and Biochemistry. Moscow State University of Food Production. Volokolamskoe. Sh., 11. Moscow, 123080. Russia. Phone: +7 (499) 158-71-33. E-mail: vitolis@yandex.ru*

[2] *Department of Physical and Organic Chemistry. RGAU-MSHA named after K.A. Timiryazev. Timiryazevskaya St., 49. Moscow, 127550. Russia. Phone: +7 (499) 976-32-16. E-mail: belopuhov@mail.ru*

[3] *Department of Agronomic and Biological Chemistry. RGAU-MSHA named after K.A. Timiryazev. Timiryazevskaya St., 49. Moscow, 127550. Russia. Phone: +7 (499) 976-29-71.*

*Supervising author; +Corresponding author

Keywords: *barley, barley malt, regulators of metabolism, protein-proteinases complex.*

Abstract

The influence of the preparation «Novosil» on protein-proteinase complex of malting barley. It is established that the processing of the product of vegetating plants of barley leads to the change in the fractional composition of barley proteins and the malt obtained from it, as well as increases catalytic activity of neutral and acid proteinases. Gel-chromatography method has shown that the processing of the preparation «Novosil» increases the degree and depth of hydrolysis of spare proteins in germinated barley seeds and provides the necessary degree of hydrolysis of endosperm proteins – an important indicator of the finished malt.

Full Paper _____ *Thematic Section:* Biochemical Research.
Registration Code of Publication: 13-35-9-84 *Subsection:* Properties of Natural Compounds.
Publication is available for discussion in the framework of the on-line Internet conference "*The chemical basis for the rational use of renewable natural resources*".
http://butlerov.com/natural_resources/
Contributed: July 8, 2013.

Hepatoprotective activity of chaga melanins

© **Guzel A. Ivanova**,[1+] **Maria A. Sysoeva**,[1]* and **Vladimir V. Zobov**[2]
[1] *Department of Food Biotechnology. Kazan National Research Technological University. K. Marx St., 68. Kazan, 420015. Tatarstan Republic. Russia. Phone: +7 (843) 231-41-73. E-mail: guziva@rambler.ru*
[2] *Department of Biologically Active Compounds. Laboratory of Chemical-Biological Research. A.E. Arbuzov Institute of Organic and Physical Chemistry. Akad. Arbuzov St., 8. Kazan, 420088. Tatarstan Republic. Russia. Phone: +7 (843) 273-93-64. E-mail: zobov@iopc.knc.ru*

*Supervising author; [+]Corresponding author

Keywords: *melanin, chaga, hyperbranched polymer, antioxidant activity, hepatoprotective activity, carbon tetrachloride.*

Abstract

The hepatoprotective properties of chaga melanins were studied on the model of rats acute toxic hepatitis induced by carbon tetrachloride. Hepatoprotective activity analysis was based on the content of experimental animals serum indices such as alanineaminotransferase, aspartateaminotransferase, alkaline phosphatase, total protein, bilirubin, cholesterol, urea, and liver slices. It was shown that the highest antioxidant properties of melanin provides its highest hepatoprotective activity.

Full Paper _____ *Thematic Section:* Biochemical Research.
Registration Code of Publication: 13-35-9-90 *Subsection:* Physico-Chemical Treatment of Seeds.
Publication is available for discussion in the framework of the on-line Internet conference "*The chemical basis for the rational use of renewable natural resources*".
http://butlerov.com/natural_resources/
Contributed: June 1, 2013.

Determination of the specific activity of peroxidase of common barley (*Hordeum vulgare*) and common millet (*Panicum miliaceum*) when exposed to ozone and constant magnetic field

© **Pyotr P. Purygin**,[+] **Denis A. Tsaplev**, **Ekaterina V. Tsapleva**, and **Yury P. Zarubin***
Department of Organic, Bioorganic and Medicinal Chemistry. Samara State University.
Akad. Pavlov St., 1. Samara, 443011. Samara Region. Russia.
Phone: +7 (846) 334-54-59. E-mail: puryginpp2002@mail.ru.

*Supervising author; [+]Corresponding author

Keywords: *peroxidase, barley, millet, ozone generator, magnetic field.*

Abstract

An effective and environmentally safe method of crops treatment with ozone and constant magnetic field is proposed. When conducting the experimental study of the level of peroxidase of common barley and millet exposed to constant magnetic field and ozone there was established higher concentration of the enzyme under investigation as compared to the control data. This method of plant treatment can be used in various branches of agriculture.

Full Paper _____ *Thematic Section:* Chemical and Technological Research.
Registration Code of Publication: 13-35-9-94 *Subsection:* Applied Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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Processing the iron dust metallurgical wastes into the pigment for coloring construction materials

© **Viktor B. Fedoseev**,[1]* **Arkady D. Zorin**,[2] **Elena N. Fedoseeva**,[2+]
Valentina F. Zanozina,[2]* and **Evgeny V. Zhebryakov**[2]
[1] *KDepartment of Material Science. Physical Faculty. N.I. Lobachevskiy Nizhny Novgorod State University. Gagarin Prospect, 23, bl.3. Nizhny Novgorod, 603950. Russia.*
Phone: +7 (831) 465-81-66. E-mail: vbfedoseev@yandex.ru
[2] *Laboratory of Applied Chemistry and Ecology. Scientific-Research Institute of Chemistry. N.I. Lobachevsky Nizhny Novgorod State University. Gagarin Prospect, 23, bl.5. Nizhny Novgorod, 603950. Russia.*
Phone: +7 (831) 465-81-66. E-mail: enfedoseeva@front.ru

*Supervising author; [+]Corresponding author

Keywords: *iron oxide, iron-containing dust, sand-lime brick, coloring.*

Abstract

A comparative analysis of the composition of waste iron and steel industries of the Nizhny Novgorod region was performed. The fundamentals of the technology of manufacturing iron oxide pigment from waste iron-containing dusts, used as a raw material. Strength properties of sand-lime brick, colored by the obtained pigment were investigated. It is shown that by the strength characteristics the colored bricks conform to the silicate materials. Показано, что по прочностным характеристикам окрашенные кирпичи удовлетворяют requirements of standards on silicate materials.

Thematic Section: Chemical and Technological Research. **Full Paper**
Subsection: Technological Modeling. *Registration Code of Publication:* 13-35-9-103
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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Modelling of mixing process into a volumetric type reactor of formation

© **Andrey A. Permyakov**, **Tatiana A. Eneikina**, **Marsel I. Gainutdinov**,*+
Alexey I. Hatsrinov, and **Yury M. Mihailov**
The Federal State Enterprise "The State Scientific Research Institute of Chemical Products".
Svetlaya St., 1. Kazan, 420033. Tatarstan Republic. Russia. Phone: +7 (843) 544-07-21.

*Supervising author; +Corresponding author

Keywords: *modelling, mixing, a reactor, a stream, a mixer.*

Abstract

The results of calculation of water mixing process into a volumetric type reactor with two-level and three-level blade mixer on ANSYS program are submitted in this work. It is showed, that circular velocities of a stream at walls of a reactor are on 19-37% less by using of a two-level mixer, and velocity of an ascending stream is half as large in comparison with a three-level mixer. The three-level blade mixer is recommended and installed in a 45 litre reactor.

Thematic Section: Research into New Materials. **Full Paper**
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http://butlerov.com/readings/
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Revealing the possibilities for applying highly fluorinated polymers as eluent modifiers in thin-layer chromatography

© **Svaytoslav V. Nayden**,[1]*+ **Ludmila A. Kartsova**,[1] **Daria V. Dzema**,[1]
and **Gennady A. Emelyanov**[2]
[1] *Chemical Faculty, Department of Organic Chemistry. St.-Petersburg State University. Universitetskiy Prospect, 26. Petrodvorets. St.-Petersburg, 198504. Phone: +7 (812) 428-67-33. Email: sv.nayden@gmail.com*
[2] *FGUP "NIISK". Gapsalskaya St., 1, St.-Petersburg, 198035. Phone: +7 (812) 251-40-28.*

*Supervising author; +Corresponding author

Keywords: *thin-layer chromatography, fluoropolymer, eluent modifier, vitamin B, amino acids.*

Abstract

Two water-soluble high fluorinated polymers (FS-141m and AE FS-101m) were synthesized and the possibility of their application as eluent modifiers in thin-layer chromatography was studied. Application of both polymers stimulates the efficiency increase in amino acids (*glycine, lysine, tryptophan, glutamic acid*) and vitamins B (B_1 thiamine, B_6 pyridoxine, B_{12} cyanocarbalamine), as it is shown by our work.

Full Paper _____ *Thematic Section:* Research into New Materials.
Registration Code of Publication: 13-35-9-116 *Subsection:* Applied Chemistry.
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http://butlerov.com/readings/
Contributed: May 6, 2013.

Laser radiation impact on the polyelectrolyte microcapsules modified with fluorescein isothiocyanate

© **Irina V. Marchenko**,[1,2] **Gennady S. Plotnikov**,[3] **Anatoly N. Baranov**,[3] **Alexander M. Saletsky**,[3] and **Tatiana V. Bukreeva**[1,2]

[1] *A.V. Shubnikov Institute of Crystallography, RAS. Leninsky prospekt, 59. Moscow, 119333. Russia. E-mail: iramarchenko85@mail.ru*

[2] *SRC «Kurchatov Institute». Academician Kurchatov Sq., 1. Moscow, 123182. Russia.*

[3] *Physical faculty of Lomonosov Moscow State University. Leninskie Gory, 1, bl.2. Moscow, 119991. Russia.*

*Supervising author; +Corresponding author

Keywords: *polyelectrolyte microcapsules, dyes, laser radiation.*

Abstract

Polyelectrolyte capsules become promising technological object due to their monodispersity with a wide range of variation of size, ease of controlling the permeability, ease of changes and a wide choice of material for shells. To create systems for the specific delivery of drugs we need to perform the remote control of permeability of shells. One of the ways of shell destruction is laser radiation. In this study, there were obtained polyelectrolyte capsule shells with the inclusion in the molecules of fluorescein isothiocyanate. Inclusion of dye molecules into the capsule shell enables the possibility of photosensitized destruction of such structures. We investigated the dependence of the temperature of capsule size. We investigated the dependence of capsule size on temperature. On heating the suspensions of capsules there was observed irreversible decrease in the mean radius of the capsules.

Thematic Section: Research into New Materials. **Full Paper**
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http://butlerov.com/readings/
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Organic-inorganic gels on the basis of thermodynamically incompatible oligomers

© **Ruslan S. Davletbaev**,[1] **Olesya R. Gumerova**,[2] and **Ilsia M. Davletbaeva**[3+]*
[1] *Materials Science & Technology. Kazan National Research Technical University.*
K. Marx St., 10. Kazan, 420111. Tatarstan Republic. Russia. Phone: +7 (843) 238-44-10.
E-mail: Darus@rambler.ru
[2] *Graphic Arts and Photography Technology Department. Kazan National Research Technological University.*
K. Marx St., 68. Kazan, 420015. Tatarstan Republic. Russia.
Phone: +7 (843) 231-41-68. E-mail: olese4ka85@mail.ru
[3] *Technology of Synthetic Rubber Department. Kazan National Research Technological University.*
K. Marx St., 68. Kazan, 420015. Tatarstan Republic. Russia.
Phone: +7 (843) 231-95-88. E-mail: davletbaeva09@mail.ru

*Supervising author; [+]Corresponding author

Keywords: *organic-inorganic gel, sol-gel method, silica, structural modification of polymers.*

Abstract

On the basis of tetraethoxysilane and thermodynamically incompatible oligomers, such as oligooxyethyleneglycol and oligodimethylsiloxane, organic-inorganic gels were developed. It was shown that as a result of the hydrolysis of tetraethoxysilane and subsequent polycondensation process clusters of silica are formed in the volume of oligomeric matrix, forming associates of potassium siloxanolate groups at the interface of thermodynamically incompatible oligomers. Due to the lability of association bonds organic-inorganic gel is able to dissolve in the polymers melt or reactive oligomers.

Thematic Section: Research into New Materials. **Full Paper**
Subsection: Applied Chemistry. *Registration Code of Publication:* 13-35-9-125
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http://butlerov.com/readings/
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Development of new adhesive compositions based on filled polymers for metal-based products

© **Alexander V. Pestov**,[1]* **Igor S. Puzyrev**,[1+] **Alexander V. Mekhaev**,[1]
Tatiana I. Gorbunova,[1] **Alexander Ya. Zapevalov**,[1] **Denis N. Bazhin**,[1]
Viktor I. Vichyzhanin,[2] and **Sergey V. Smirnov**[2]

[1] *I.Ya. Postovsky Institute of Organic Sinthesys of the Ural Branch of the Russian Academy of Sciences. S. Kovalevskaya St., 22. Ekaterinburg, 620990. Russia. Phone: +7 (343) 362-34-39. E-mail: pestov@ios.uran.ru*

[2] *Institute of Engineering Science of the Ural Branch of the Russian Academy of Sciences. Komsomolskaya St., 34. Ekaterinburg, 620990. Russia. Phone: +7 (343) 362-34-39. E-mail: ges@imach.uran.ru*

*Supervising author; [+]Corresponding author

Keywords: *adhesives for metals, filled polymers.*

Abstract

The adhesive compositions based on polymers filled with inorganic and organic compounds were characterized by the degree of swelling, yield strength of the bond under shear in the cured state. The effect of composition on the rate of uniform corrosion of the metal was evaluated on model surfaces exposed to corrosion. Roughing and chromium-containing steel and aluminum based alloys are used as structural metals. Adhesion of the coating compositions depends both on the metal and the type of filler. Uniform corrosion rate of reduced metal surface in the presence of previously developed fluorinated quaternary ammonium salts practically does not change in many cases.

Thematic Section: Research into New Materials. **Letter to the Editor**
Subsection: Applied Chemistry. *Registration Code of Publication:* 13-35-9-129
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Covering for protection of metals against corrosion

© **Svetlana I. Tumenceva**,* and **Svetlana N. Parfyonova**[+]
Department of General and Inorganic Chemistry.
Samara State Technical University. Molodogvardeyskaya St., 244.
Samara, 443100. Samara region. Russia. Phone: +7 (846) 278-44-77.
E-mail: parfy-svetlana@yandex.ru

*Supervising author; [+]Corresponding author

Keywords: *removable coverings, temporary coverings, adhesion, power of cohesion, composition, structure.*

Abstract

For inter-operational protection of details from ferrous and non-ferrous metals, as well as for the protection of finished products against corrosion, mechanical damages during the warehousing and transportation there are widely used temporary removable coverings. This way of protection of metals is based on isolation from environment by means of thin film coverings in case of penetration of aggressive reagents to metal interfere with development of corrosion process.

Removable film coverings are a type of protective materials at which powers of cohesion are much higher than forces of adhesion of a film to a substrate that makes possible their mechanical removal – deleting by "stocking".

In the work, the structure on the basis of perchlorovinyl pitch with addition to it ionol is presented.

Thematic Section: Physics and Chemistry of Radicals. **Full Paper**
Subsection: Toxological Chemistry. *Registration Code of Publication:* 13-35-9-131
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 metabolites of cannabimimetics AB-PINACA in urine by GC-MS

© **Sergey S. Kataev**,[1+] **Nadezhda B. Zelenina**,[1] and **Oksana N. Dvorskaya**[2]*
[1] *Forensic-Chemical Department. State Healthcare Establishment of Special Type "Perm Regional Bureau of Forensic-Medical Expertise". Startseva St., 61. Perm, 614077. Perm Region. Russia. Phone: +7 (342) 210-67-83. E-mail: forenschemist@narod.ru*
[2] *Department of Toxicological Chemistry. Perm State Pharmaceutical Academy of the Ministry of Health of the Russian Federation. Polevaya St., 2. Perm, 614990. Perm Region. Russia. Phone: +7 (342) 282-58-64. E-mail: kaftox@mail.ru*

*Supervising author; [+]Corresponding author

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

Abstract

The data's for determine the fact of usage of cannabimimetic *N*-[1-(aminocarbonyl)-2-methylpropyl]-1-pentyl-1*H*-indazole-3-carboxamide (AB-PINACA) in course of screening of urine using the methods of solid phase extraction and gas chromatography – mass spectrometry methods are presented. Identification of metabolites AB-PINACA in urine of consumers of smoking mixtures was performed. The data of gas chromatography and mass spectrometry for some derivatives of metabolites AB-PINACA were obtained, the latter can be used in the practice of forensic chemical and chemical-toxicological analysis.

Thematic Section: Physics and Chemistry of Explosives. **Full Paper**
Subsection: Physics and Chemistry of Radicals. *Registration Code of Publication:* 13-35-9-139
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Ring strain energy and its influence on dissociation energy of C–H-bond in cycloalkanes, cycloalkenes, cycloaromatic hydrocarbons and O-H-bond in cyclocarboxylic acids

© **Vladimir E. Tumanov**,[+] and **Evgeny T. Denisov***
Institute of Problems of Chemical Physics RAS. Chernogolovka, 142432.
Moscow Region. Russia. Fax: +7 (496) 522-35-07. E-mail: tve@icp.ac.ru

*Supervising author; [+]Corresponding author

Keywords: *bond dissociation energy, ring strain energy, cycloalkanes, cycloalkenes, cycloaromatic compounds, cyclocarboxylic acids, electronegativity, linear correlations.*

Abstract

Empirical research of influence of ring stain energy (E_{rsc}) on dissociation energy of C–H-bond ($D_{C–H}$) in cycloalkanes, cycloalkenes and cycloaromatic hydrocarbons (indane, tetraline) is conducted. It is shown that for all cyclic compounds, except cyclopropane, the simple relation is carried out: $D_{C–H} = D_{C–H}(\Delta E_{rsc} = 0) + \Delta E_{rsc}$, где ΔE_{rsc} represents a difference of energies of ring strain energy of the formed radical and an initial molecule. Values $D_{C–H}(\Delta E_{rsc} = 0)$ are close to $D_{C–H}$ of linear hydrocarbons (paraffins, olefins). For cyclocarboxylic acids linear correlation between dissociation energy of O–H-bond and its electronegativity is established.

Full Paper _____ *Thematic Section:* Physico-Chemical Research.
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Influence of processes of a cocristallization on rheological and mechanical characteristics of mixes on the basis of hexanitrohexaazaisowurtzitane (HNIW)

© **Vladimir N. Popok**,*+ **Viktor I. Desyatykh**, and **Nikolay I. Popok**
Open Joint Stock Company «Federal Research and Production Center "ALTAY".
Sotsialisticheskaya St., 1. Biysk, 659322. Altai Region. Russia.
Phone: +7 (3854) 30-19-37. E-mail: vnpopok@mail.ru

*Supervising author; +Corresponding author

Keywords: *cocrystals, softeners, polymers, mixed energy materials, physical and mechanical properties, spreadability.*

Abstract

Results of researches of mechanical and rheological characteristics of HNIW mixes are presented in the article with softeners and binders. Influence of the processes of cocrystals formation on the level of these characteristics is investigated. The effect of additional mixing and thermal treatment is estimated. The possibility of occurrence in mixtures of co-crystallization processes of HNIW with components of softeners without presence of auxiliary deleted solvents is shown.

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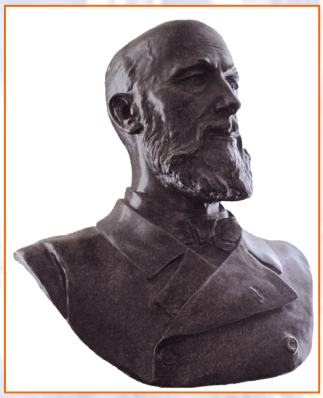

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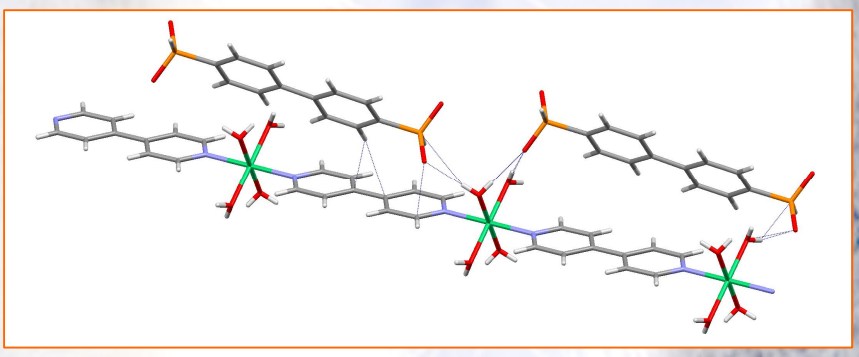

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New confirmation for white phosphorus biodegradation

© **Anton Z. Mindubaev**,[1]*+ **Farida K. Alimova**,[2] **Serge C. Ahossiyenagbe**,[2]
Salima T. Minzanova,[1] **Lubov G. Mironova**,[1] and **Dmitry G. Yahvarov***[1]
[1] *Institution of RAS. 62 A.E. Arbuzov Institute of Organic and Physical Chemistry of KazSC RAS. Arbuzov St., 8. Kazan, 420088. Tatarstan Republic. Russia. E-mail: mindubaev@iopc.ru*
[2] *Department of Biochemistry. Kazan (Volga Region) Federal University. Universitetskaya St., 18. Kazan, 420008. Tatarstan Republic. Russia.*

*Supervising author; +Corresponding author

Abstract

In the previous works, we have demonstrated for the first time the possibility of white phosphorus (dangerous industrial pollutant) biodegradation by the wastewater sludge from waste disposal plant. This discovery can form the basis for the creation of new more efficient methods for preventing this substance ingress in the environment. The fact of biodegradation was initially assumed – the population of microorganisms in the municipal sewerage participates in the process of P_4 degradation. However there were no direct evidences of biodegradation – white phosphorus, being a chemically active substance, can transform even under the effect of abiotic factors. In this work, there are reported the results of experiments, in which microflora was activated non-simultaneously in three parallel tests. 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.

Thematic Section: Biochemical Research. **Full Paper**
Subsection: Physical Chemistry of Allergens. *Registration Code of Publication:* 13-36-10-13
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http://butlerov.com/natural_resources/
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Actual aspects and specificity of birch pollen allergen extract standardization, in particular, as biological drug the production of which is based on native raw materials

© **Dmitry O. Bokov**,[1]*+ **Valery V. Smirnov**,[1] **Svetlana L. Morohina**,[2] and **Alexander N. Luferov**[3]
[1] *Department of Pharmaceutical and Toxicological Chemistry. I.M. Sechenov First Moscow State Medical University. Nikitinsky Boulevard, 13. Moscow, 119019. Russia. Phone: +7 (925) 358-84-27. E-mail: fmmsu@mail.ru.*
[2] *Department of Pharmacognosy. I.M. Sechenov First Moscow State Medical University. Nahimovskiy St., 45. Moscow, 117418. Russia. Phone: +7 (916) 150-60-58. E-mail: morohinas@mail.ru.*

*Supervising author; +Corresponding author

Keywords: *standardization, allergenic extracts, pollen, silver birch, Betula pendula Roth., Betv1, LC-MS.*

Abstract

Species of birch *Betula* L., (Fam. Birch – *Betulaceace* L.) are among the most popular medicinal plants which are widely used in medical practice. Currently, a number of effective medications based on the birch (*Betula pendula* Roth.) raw medicinal plant materials have been received. Allergen extract has been similarly prepared from birch pollen – a biological preparation used for allergen-specific immunotherapy. At the moment the question of unbiased assessment of qualitative and quantitative characteristics of the biological drug and natural raw materials from which it is made, is still not fully resolved. In this paper we detail the methodological techniques that help to find a solution to this problem.

Thematic Section: Biochemical Research. **Full Paper**
Subsection: Physiogenic Biominerals. *Registration Code of Publication:* 13-36-10-21
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Crystallization of calcium phosphates from prototypes of biological fluids on bone samples

© **Ekaterina A. Malovskaya**,[1+] **Olga A. Golovanova**,[1]*
Tatiana V. Panova,[2] **Svetlana A. Gerk**,[1] and **Vasily A. Osintsev**[2]
[1] *Department of Inorganic Chemistry. F.M. Dostoevsky Omsk State University.*
Mira Pr., 55a. Omsk, 644077. Omsk Region. Russia. Phone: +7 (3812) 64-27-00. E-mail: katovi@mail.ru
[2] *Department of Applied and Medical Physics. F.M. Dostoevsky Omsk State University.*
Mira Pr., 55a. Omsk, 644077. Omsk Region. Russia. Phone: +7 (3812) 64-27-00.
E-mail: golovanoa2000@mail.ru

*Supervising author; [+]Corresponding author

Keywords: *crystallization of calcium phosphates in biological fluids prototypes bone samples.*

Abstract

With the increasing number of bone diseases, greater attention is paid to the creation of bio-composite materials. There are large perspectives of experimental and clinical application for synthetic materials based on calcium phosphates, possessing high biocompatibility with respect to the human bone tissue and the ability to perform, by virtue of its inertia, the matrix function along which the neo-formation of bone structures take place. An important direction is the study of the crystallization process of the prototypes of biological fluids. In the work, the composition of bone tissue is determined: a primary crystalline phase is poorly crystallized carbonate-containing hydroxyapatite. It is shown that the crystallization of calcium phosphate on bone samples from the prototypes of bioliquids is possible, wherein carbonate-hydroxyapatite is produced in the interstitial fluid, and in synovial – octacalcium phosphate and hydroxyapatite.

Thematic Section: Biochemical Research. **Full Paper**
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Identification of PB-22 cannabimimetic metabolites in urine

© **Sergey S. Kataev**,[1+] **Aleksey B. Melentyev**,[2] and **Oksana N. Dvorskaya**[3]*
[1] *Forensic-Chemical Department. State Healthcare Establishment of Special Type "Perm Regional Bureau of Forensic-Medical Expertise". Startseva St., 61. Perm, 614077. Perm Region. Russia.*
Pone: +7 (342) 210-67-83. E-mail: forenschemist@narod.ru
[2] *Forensic-Chemical Department. State Healthcare "Chelyabinsk Regional Bureau of Forensic-Medical Expertise". Varnenskaya St., 4-b. Chelyabinsk, 454076. Chelyabinsk region. Russia.*
Phone: +7 (351) 232-80-58. E-mail: amelentyev@sme74.ru
[3] *Chair of Toxicological Chemistry. Perm State Pharmaceutical Academy of the Ministry of Health of the Russian Federation. Polevaya St., 2. Perm, 614990. Perm Region. Russia.*
Phone: +7 (342) 282-58-64. E-mail: kaftox@mail.ru

*Supervising author; +Corresponding author

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

Abstract

Facts enabling to identify administration of *N*-[1-(aminocarbonyl)-2-methylpropyl]-1-pentyl-1*H*-indazole-3-carboxamide (AB-PINACA) cannabimimetics in the process of urine screening by solid-phase extraction technique and gas chromatography and mass spectrometry are described herein. AB-PINACA metabolites in the urine of smoking mixtures users are identified. Gas chromatography and mass spectrometry characteristics of some AB-PINACA metabolite derivatives that can be used both in chemico-forensic and chemico-toxicological analyses are obtained.

Thematic Section: Preparative Chemistry. **Full Paper**
Subsection: Supramolecular Chemistry. *Registration Code of Publication:* 13-36-10-37
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http://butlerov.com/readings/
Contributed: September 16, 2013.

Synthesis of polycarboxylic dendrimers based on *p-tert*-butylthiacalix[4]arene in *1,3-alternate* conformation

© **Andrey V. Galukhin**,[1] **Roman V. Nosov**,[1] **Olga A. Mostovaya**,[1] and **Ivan I. Stoikov**[1,2]
[1] *Kazan Federal University. A.M. Butlerov Chemical Institute, Russian Federation.*
Kremlevskaya St., 18. Kazan, 420008. Fax: +7 (843) 233-74-16. E-mail: Ivan.Stoikov@ mail.ru
[2] *Kazan Institute of Biochemistry and Biophysics. Russian Academy of Science. Russian Federation.*
Lobachevskogo St., 2/31. Kazan, 420111.

*Supervising author; +Corresponding author

Keywords: *thiacalixarene, dendrimer, contrast agents, Magnetic Resonance Tomography.*

Abstract

The series of polycarboxylic derivatives of *p-tert*-butylthiacalix[4]arene in *1,3-alternate* conformation which can be used as a potential contrast agents for Magnetic Resonance Tomography was synthesized. Structure of synthesized compounds was characterized by a complex of physical methods. It was shown that the Michael reaction is more preferable for obtaining high-generation dendrimers as compared to the Gabriel reaction.

Thematic Section: Preparative Chemistry. **Full Paper**
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Synthesis and structure of coordination polymer based on biphenylene-4,4'-diphosphonous acid

© **Anna V. Kraiushkina**, **Ruslan P. Shekurov**, **Artem I. Tufatullin**, **Kiril E. Metlushka**, **Kristina A. Nikitina**, **Diana F. Saifina**, **Olga N. Kataeva**,*+ **Vladimir A. Alfonsov**, **Vasily A. Milukov**, and **Oleg G. Sinyashin**
A.E. Arbuzov Institute of Organic and Physical Chemistry of the Kazan Scientific Center of RAS. Arbuzov St., 8. Kazan, 420088. Russia. Phone: +7 (843) 273-93-44.

*Supervising author; +Corresponding author

Keywords: *phosphonous acid, coordination polymers, nickel ions, synthesis, structure.*

Abstract

Coordination polymer based on biphenylene-4,4'-diphosphonous acid was synthesized and structurally characterized. According to X-ray single crystal diffraction the building block of coordination polymer consists of cationic part, represented by nickel ions, solvated water molecules, and associated molecules of 4,4'-bipyridyl, and anionic part, containing the biphenylene-4,4'-diphosphonous acid ion.

Full Paper _____ *Thematic Section:* Preparative Chemistry.
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http://butlerov.com/synthesys/
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Synthesis polimagniyfenilsiloksanes with different ratios of magnesium to silicon

© **Nikolay P. Shapkin**,[1]*+ **Lev B. Leontyev**,[2] **Leonid N. Alekseiko**,
Konstantin V. Pobozhev,[1] and **Sergey V. Gardionov**[1]
[1] *Department General, Inorganic and Organometallic Chemistry. The Far Eastern Federal University. Sukhanov St., 8. Vladivostok, 690600. Russia. Phone: +7 (423) 245-76-69. E-mail: npshapkin@gmail.com*
[2] *Department of Welding. The Far Eastern Federal University. Sukhanov, St., 8. Vladivostok, 690600. Russia. Phone: +7 (423) 245-76-69.*

*Supervising author; +Corresponding author

Keywords: *polymagniyphenilsiloksanes, fenilsilantriol, modification vermiculite geomodifiers friction pairs.*

Abstract

A study of the interaction of magnesium salts with sodium salts of fenilsilantriola has been carried out. The composition of the polymers obtained by IR, XRF spectroscopy and elemental analysis has been studied. The possibility of using the polymers as modifiers vermiculite was studied.

Full Paper _____ *Thematic Section:* Preparative Chemistry.
Registration Code of Publication: 13-36-10-52 *Subsection:* Organoelemental Chemistry.
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Synthesis and structure of *μ*-oxo-*bis*[triphenyl(2,6-dichlorophenoxy)antimony] and *μ*-oxo-*bis*[triphenyl(2,6-dibromo-4- nitrophenoxy)antimony]

© **Vladimir V. Sharutin**,[+]* **Olga K. Sharutina**, **Vladislav S. Senchurin**,
and **Olga V. Shepeleva**
Department of Chemistry. National Research South Ural State University. Lenin St., 76. Chelyabinsk, 454080. Russia. Phone: +7 (351) 267-95-70. E-mail: vvsharutin@rambler.ru

*Supervising author; [+]Corresponding author

Keywords: *synthesis, structure, compounds, $(Ph_3SbOAr)_2O$.*

Abstract

As a result of the reaction of triphenylantimony with 2,6-dichlorophenol and 2,6-dibromo-4-nitrophenol in the presence of hydrogen peroxide in water-ether solution there were prepared *μ*-oxo-*bis*[triphenyl(2,6-dichlorophenoxy)antimony] (**I**) and μ-oxo-*bis*[triphenyl(2,6-dibromo-4-nitrophenoxy)antimony] (**II**) with the yield up to 92%. In **I** and **II** SbOSb angles make up 142.7(6)° and 147.6(6)°. Antimony atoms have a distorted trigonal-bipyramidal coordination. Atomic bonds of antimony with the bridging oxygen atom [1.969(2), 1.973(2) Å (**I**) and 1.950(10), 1.968(9) Å (**II**)] are shorter than with the oxygen atoms of Ar-groups [2.135(2), 2.156(2) Å (**I**) and 2.204(11), 2.223(12) Å (**II**)].

Thematic Section: Preparative Chemistry. **Brief Communication**
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Methanolysis of bis(germatrane-1-yl)oxane

© **Le Nhat Thuy Giang**,[1] **Victor P. Baryshok**,[1+] and **Mikhail G. Voronkov**[2]*
[1] *Department of Chemical Technology. Irkutsk State Technical University. Lermontov St., 83. Irkutsk, 664074. Russia. Phone: +7 (3952) 40-55-13. E-mail: baryvik@yandex.ru*
[2] *Laboratory of Organometal Compounds. A.E. Favorsky Irkutsk Institute of Chemistry, Siberian Branch of the Russian Academy of Sciences. Academician Favorsky St., 1. Irkutsk, 664033. Russia. Phone/Fax: +7 (3952) 42-64-00.*

*Supervising author; [+]Corresponding author

Keywords: *reaction of fission, 1-methoxygermatrane, bis(germatrane-1-yl)oxane, acid catalysis.*

Abstract

Methanolysis of bis(germatrane-1-yl)oxane in xylene medium by consecutive transformations leads to the formation of 1-methoxygermatrane with the yield of 83.9%. In the presence of *p*-toluenesulfonic acid these transformations are accelerated and the output of 1-methoxygermatrane increases up to 90.2%.

Full Paper _____ *Thematic Section:* Preparative Chemistry.
Registration Code of Publication: 13-36-10-60 *Subsection:* Organic Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: September 3, 2013.

Synthesis of 2,6-di(3,3',5,5'-di-*tert*-buthyl-4,4'-oxybenzul)-cyclohexan-1-one and its effectiveness in PVC stabilization

© **Svetlana Sh. Saygitbatalova**,[1+] **Elena N. Cherezova**,[1]* **Faina B. Balabanova**,[1]
Alexander G. Liakumovich,[1] **Rinat M. Ahmethanov**,[2] and **Dinara S. Salimgareeva**[2]
[1] *Department of Synthetic Rubber Technology. Kazan National Research Technological University. Karl Marx St., 72. Kazan, 420015. The Republic of Tatarstan. Russia.*
Phone: +7 (843) 231-42-14. E-mail: saygitbatalova@mail.ru
[2] *Department of Macromolecular Compounds and General Chemical Technology. Bashkir State University. Zaki Validi St., 32. Ufa, 450076. Republic of Bashkortostan. Russia.*
Phone: +7 (347) 229-97-07. E-mail: rimasufa@rambler.ru

*Supervising author; [+]Corresponding author

Keywords: *stabilizer, sterically hindered phenol, antioxidative properties, polyvinylchloride.*

Abstract

In the reaction of 3,5-di-*tert*-buthyl-4-oxy-*N,N*-dimethylbenzylamine and cyclohexanone the 2,6-di(3,3',5,5'-di-*tert*-buthyl-4,4'-oxybenzul)-cyclohexan-1-one was obtained. Its effectiveness in stabilization of polyvinylchloride was studied.

Thematic Section: Preparative Chemistry. **Full Paper**
Subsection: Organic Chemistry. *Registration Code of Publication:* 13-36-10-65
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: August 9, 2013.

Acid-catalyzed cyclocondensation of chromone-3-carboxaldehydes with indole: a convenient synthesis of chromone-containing indolo[3,2-*b*]carbazoles

© **Anton Yu. Teslenko**,[1] **Pavel A. Slepukhin**,[1] **Roman A. Irgashev**,[1+]
Gennady L. Rusinov,[1,2]* and **Valery N. Charushin**[1,2]*
[1] *I. Postovsky Institute of Organic Synthesis. Ural Division, Russian Academy of Sciences. S. Kovalevskoy St., 22. Ekaterinburg, 620041, Russia. Phone/fax: +7 (343) 374-11-89. E-mail: Irgashev@ios.uran.ru*
[2] *Ural Federal University Named After the First President of Russia B. Eltsin. Mira St., 19. Ekaterinburg, 620002. Russia.*

*Supervising author; [+]Corresponding author

Keywords: *indole, indolo[3,2-b]carbazoles, chromones, chromone-3-carboxaldehydes, cyclocondensation, triflic acid.*

Abstract

The interaction of the chromone-3-carboxaldehydes with indole under acid catalysis was studied. It has been found that this reaction proceeds rapidly under mild conditions and leads to the formation of 3,3'-(5,6,11,12-tetrahydroindolo[3,2-*b*]carbazole-6,12-diyl)bis(4*H*-chromen-4-ones), representatives of the chromone-substituted indolo[3,2-*b*]carbazole ring system. Best yields of these indolo[3,2-*b*]carbazoles were obtained when triflic acid was used as a catalyst for the cyclocondensation.

Thematic Section: Preparative Chemistry. **Full Paper**
Subsection: Organic Chemistry. *Registration Code of Publication:* 13-36-10-69
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: September 16, 2013.

(*R*)-4-Menthen-3-one in the synthesis of (*S*)-(+)-hydroprene

© **Gumer Yu. Ishmuratov**,[1,2]*+ **Vadim S. Tukhvatshin**,[2+] and **Rifkat F. Talipov**[2]
[1] *Laboratory of Insect Bioregulators. Federal State Budget Establishment of Science Institute of Organic Chemistry. Ufa Sientific Centre of the Russian Academy of Sciences. Prospekt Octyabrya, 71. Ufa, 450054. E-mail: insect@anrb.ru*
[2] *Department of Organic and Bioorganic Chemistry. Bashkir State University. Zaki Validi St., 32. Ufa, 450074. E-mail: vadimtukhvatshin@yandex.ru*

*Supervising author; +Corresponding author

Keywords: *(R)-4-Menthen-3-one, methyl (3S)-3,7-dimethyl-5-oksooctanoat, (3S)-3,7-dimetiloctanoic acid, (3S) -3,7-dimethyloctanal, (S)-(+)-hydroprene.*

Abstract

A new scheme for the synthesis of optically pure (*S*)-(+)-hydroprene (insect juvenile hormone analogue with incomplete conversion cycle) from (*R*)-4-menthen-3-one has been presented. (2*E*,4*E*)-Isomer of (*S*)-(+)-hydroprene has been isolated.

Thematic Section: Study of Reactivity. **Full Paper**
Subsection: Organic Chemistry. *Registration Code of Publication:* 13-36-10-73
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: August 30, 2013.

Comparison of reactivity of fluoro- and chlorosubstituents of ethylene with ozone

© Eldar A. Mamin,[2+]* **Boris E. Krisyuk**,[1] and **Alexey V. Maiorov**[2]
[1] *Laboratory for the Kinetics of of Heterophase Processes. Institute of Problems of Chemical Physics of RAS. Akademik Semenov Prospect, 1. Chernogolovka, 142432. Moscow Region. Russia.*
[3] *Department of Chemistry and Physics. G.V. Plekhanov Russian University of Economics. Stremyanny Per., 36. Moscow, 117997. Russia. Phone: 8 905 503 6933. E-mail: bkris@mail.ru*
[2] *Laboratory of Physical Chemistry of the Compositions of Synthetic and Natural Polymers. N.M. Emanuel Institute of Biochemical Physics of RAS. Kosygin St., 4. Moscow, 119334. Russia. Phone: +7 (915) 018-05-71, +7 (910) 455-89-31. E-mail: yeldar443@mail.ru , hruk@list.ru*

*Supervising author; [+]Corresponding author

Keywords: *quantum chemical calculation, ozone, substituents of ethylene, activation energy, rate constant.*

Abstract

DFT B2PLYP, *ab initio* CASSCF, MRMP2, coupled-cluster CCSD calculations were applied to reactivity of C=C bound of 1-monofluorethylene, 1-monochloroethylene, 1,1-difluorethylene, 1,1-dichloro-ethylene in reaction with ozone, aug-cc-pVDZ basis sets. Concerted and nonconcerted additions were investigated. It was shown that CCSD is better for modeling of reaction characteristics, MRMP2 results do not correspond to experiment in each case due to partial optimization. Once polar substituent is present, the role of nonconcerted mechanism becomes greater – about 50% in 1,1-difluorethylene, 98% in 1,1-dichloroethylene.

Thematic Section: Physicochemical Research. **Full Paper**
Subsection: Physical Chemistry. *Registration Code of Publication:* 13-36-10-81
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: September 19, 2013.

Effect of dispersed solid particles with modified surface on the intensity of oxygen mass transfer in gas-liquid system

© **Dmitry A. Kazakov**,[+] **Vladimir V. Volkhin**,* **Irina S. Borovkova**, and **Natalia P. Popova**
Department of Chemistry and Biotechnology. Perm National Research Polytechnic University.
Komsomolsky St., 29. Perm, 614990. Permskiy krai. Russia.
Phone/fax: +7 (342) 239-15-11. E-mail: kazakovbiotech@mail.ru

*Supervising author; [+]Corresponding author

Keywords: *gas-liquid system, mass transfer activators, dispersed solid particles, surface modification, mass transfer, oxygen.*

Abstract

Fine particles of quartz and titanium dioxide modified by thin films of polymers (polyvinyl chloride, polystyrene, polymethyl methacrylate) were obtained. Influence of these particles on the rate of oxygen mass transfer in gas (air) – liquid (water) system was studied. It was shown that the ability of modified particles to oxygen mass transfer enhancement was increased with decreasing of surface wettability, size and density of the particles. It was found that maximum oxygen mass transfer enhancement factor was observed in the presence of quartz particles coated with polyvinyl chloride (SiO_2/PVC). The effect of SiO_2/PVC particles concentration on the oxygen mass transfer was investigated. Hydrodynamic conditions for the maximum effect of SiO_2/PVC particles on oxygen mass transfer were determined.

Full Paper _____ *Thematic Section:* Physicochemical Research.
Registration Code of Publication: 13-36-10-90 *Subsection:* Physical Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: September 19, 2013.

Effect of stearic acid on the phase equilibrium in the system triacylglycerides-ethanol-stearic acid

© **Irina A. Permyakova**,[+] **Vladimir V. Volkhin**,* **Elizaveta A. Suhoplecheva**, **Ivan Yu. Zorichev**, **Natalia S. Voronina**, and **Dmitry A. Kazakov**
Department of Chemistry and Biotechnology. Perm National Research Polytechnic University. Komsomolsky St., 29. Perm, 614990. Perm Krai. Russia. Phone/Fax: +7 (342) 239-15-11. E-mail: vvv@purec.pstu.ac.ru, zernina88@mail.ru

*Supervising author; [+]Corresponding author

Keywords: *triacylglycerides, wastesunflower oil, stearic acid, oleic acid, ethanol, phase diagram, phase equilibria, biodiesel.*

Abstract

The paper presents the results of the study of phase composition of two-component systems TAG – StA and EtOH – StA at the temperatures from 30 to 72 ºC and phase composition of ternary system TAG – StA – EtOH at the temperatures from 50 to 70 ºC, where TAG – triacylglycerides(sunflower oil), OlA – oleic acid, EtOH – ethanol, StA – stearic acid. The role of StA ascosolvent of the mixture TAG – EtOH was investigated. The relative ability of StA and OlA for homogenization of the system was determined. For the separation region of system TAG – StA – EtOHat 70 ºC nodes were built, critical point of the system was determined, the distribution coefficients of StA between phases TAG and EtOH at 70 ºC and different compositions of the system were found. Ability of StA and OlA for homogenization of the TAG-EtOH mixture was analyzed with GSP model which took into account molecular interact ions of the components of systems with the participation of functional groups of their molecules.

Full Paper _____ *Thematic Section:* Physicochemical Research.
Registration Code of Publication: 13-36-10-98 *Subsection:* Inorganic Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: September 11, 2013.

Theme: Physico-chemical studies of aluminum hydroxides. Part 1.

The effect of hydrargillite phase transitions on the mechanical properties of floccules

© **Svetlana R. Egorova**,*+ **Giyaz E. Bekmukhamedov**, and **Alexandr A. Lamberov**
Departament of Physiacal Chemistry. Kazan (Volga Region) Federal University.
Kremlin, St., 18. Kazan, 420008. Tatarstan Republic. Russia.
Phone: +7 (843) 231-53-46. E-mail: Segorova@rambler.ru

*Supervising author; +Corresponding author

Keywords: *hydrargillite, boehmite, aluminum oxide, floccule, phase transition.*

Abstract

The factors, which cause the decrease in the mechanical strength of hydrargillite floccules under heating from 250 ºC to 500 ºC in air, were investigated. The formation of two boehmite fractions with crystallites varying in size was detected. Turning hydrargillite into boehmite and χ-Al_2O_3 contributes to minimum decrease in floccule mechanical strength. Dehydration of boehmite into γ-Al_2O_3 leads to a considerable decrease in the mechanical strength of the floccules because of their shrinkage resulting from the displacement of γ-Al_2O_3 microblocks in the bulk of the crystal.

Thematic Section: Physicochemical Research. **Full Paper**
Subsection: Phase Equilibria. *Registration Code of Publication:* 13-36-10-107
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: August 9, 2013.

Miscibility, diffusion and hardening in epoxy oligomer – diaminodiphenyl sulfone system

© **Nikita Yu. Budylin**,[+] **Aleksey V. Shapagin**, **Ramil R. Khasbiullin**, and **Anatoly E. Chalykh***
Laboratory of Structure and Morphological Investigations. A.N. Frumkin Institute of Physical Chemistry and Electrochemistry of RAS. Leninskiy pr., 31, korp. 4. Moscow, 119071. Russian Federation.
Phone: +7 (495) 955-46-53. E-mail: budylin_nikita@mail.ru

*Supervising author; [+]Corresponding author

Keywords: *epoxy resin, diaminodiphenyl sulfone, phase equilibrium, diffusion.*

Abstract

Solution kinetics of diaminodiphenyl sulfone particles in epoxy oligomer was studied for the first time. Temperature region of the diffusion stage of solution without chemical reaction was determined, and the changes in the structure of the diffusion zone were estimated during chemical hardening. By the diffusion section, the diffusion constants and their changes were determined, and the effective activation energy of diffusion was calculated. It was shown that diaminodiphenyl sulfone solution in epoxy resin media takes place without chemical interactions within fixed temperature region, which is lower than the curing agent melting point.

Thematic Section: Physicochemical Research. **Brief Communication**
Subsection: Organometallic Compounds. *Registration Code of Publication:* 13-36-10-111
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: September 18, 2013.

Structural features of triarylbismuth compounds

© **Vladimir V. Sharutin**,*+ and **Olga K. Sharutina**
Department of Chemistry. National Research South Ural State University. Avenue Lenin, 76. Chelyabinsk, 454080. Russia. Phone: +7 (351) 267-95-70. E-mail: vvsharutin@rambler.ru

*Supervising author; +Corresponding author

Keywords*: aryl bismuth compounds, tris(3-methylphenyl)bismuth, structure.*

Abstract

According to X-ray analysis, bismuth atoms in the molecules of *tris*(3-methylphenyl)bismuth have tetragonal coordination with the carbon atoms and unshared electron pair at the vertices of a tetrahedron. Lengths Bi-C bonds and CBiC angles are 2.216(8), 2.222(8), 2.293(9) Å and 93.8(3)°, 95.3(3)°, 96.7(3)°, respectively. Geometric characteristics of molecules of triarylbismuth compounds were analyzed, and the factors that influence the value of Bi-C bond lengths and CBiC bond angles were identified.

Full Paper _____ *Thematic Section:* Study of the Properties of Compounds.
Registration Code of Publication: 13-36-10-114 *Subsection:* Problem of Corrosion.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: August 12, 2013.

Comparative study of anticorrosion characteristics of aminoborates

© **Vikenty G. Skvortsov**,[1]* **Michail A. Yershov**,[2+]
Eugeny V. Kamajev,[2] and **Anna U. Chiplenkova**[1]
[1] *Department of Chemistry and Biosynthesis. I.Y. Yakovlev Chuvash State Pedagogical University. K. Marx St., 38. Cheboksary, 428000. Chuvash Republic. Russia. Phone: +7 (352) 58-67-66; +7 (352) 58-68-45.*
[2] *Department of Chemistry. Chuvash State Agricultural Academy. K. Marx St., 29. Cheboksary, 428003. Chuvash Republic. Russia. Phone: +7 (352) 62-02-26. E-mail: ema11@mail.ru*

*Supervising author; [+]Corresponding author

Keywords: *aliphatic amines, aminoalcohols, orthoboric acid, aminoborate complexes, gravimetrical, corrosion-electrochemical investigations, fatigue, corrosion-fatigue tests.*

Abstract

Inhibitor properties of new integrated combinations on the base of ortoboric acid, aliphatic amines and aminoalcohols were investigated by gravimetrical method, corrosion-electrochemical, corrosion fatigue behaviour methods. It has been revealed that aminoborate complexes have bigger inhibitory ability than the appropriate aliphatic amines. Increased inhibitory ability of St.10 steel corrosion by aminoborate complexes is explained by the formation of a better ferrohydroxoaminoborate protective film on the metal surface produced by means of the donor-acceptor bond with the unshared pairs of electrons of nitrogen atoms, OH-groups and chemisorption of borate ions.

Thematic Section: Thermodynamic Research. **Full Paper**
Subsection: Physical Chemistry of Isotopes. *Registration Code of Publication:* 13-36-10-123
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: August 12, 2013.

Kinetic and thermodynamic reasons for fractionation of chlorine isotopes in the process of halite sedimentation

© **Andrey V. Bochkarev**,[1] **Sergey L. Belopukhov**,[2]*+
Aleksey V. Zhevnerov,[1] and **Artem A. Ovod**[3]
[1] *K.A.Timiryazev Russian State Agrarian University.*
[2] *Department of Inorganic and Analytical Chemistry.* [2] *Department of Physical and Organic Chemistry.*
[3] *Laboratory for agroecological monitoring, modeling and forecasting ecosystems.*
Timiryazevskaya St., 49. Moscow, 127550. Russia. Phone: [1)] *+7 (499) 976-16-28,* [2)] *+7 (499) 976-32-16,*
[3)] *+7 (499) 977-04-86. E-mail: belopuhov@mail.ru*

*Supervising author; +Corresponding author

Keywords: *chlorine isotopes, isotope separation, rock salt, halite.*

Abstract

Previously obtained

The data previously obtained with the use of *ab initio* quantum chemical methods in relation to the given statistical sums on the states of isotopic forms (β-factors) for the hydrated chloride ion and crystalline halite have been used for theoretical modeling of the process of fractionation chlorine isotopes during sedimentation of NaCl from saturated solution. It has been shown that during precipitation of halite in the process of evaporation of natural water reservoirs, appreciable separation of isotopes of chlorine may take place, wherein the thermodynamic component of isotope effect being dominant.

Full Paper _____ *Thematic Section:* Thermodynamic Research.
Registration Code of Publication: 13-36-10-134 *Subsection:* Phase Equilibrium.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: September 9, 2013.

The effect of temperature fluctuations of the nucleus on the nucleation rate of the new phase

© Ihtiyor H. Umirzakov
Laboratory of Modeling. Kutateladze Institute of Thermophysics of SB of RAS.
Lavrentev Pr., 1. Novosibirsk, 630090. Russia.
Phone: +7 (383) 354-20-17. E-mail: tepliza@academ.org

Keywords: *first order phase transition, kinetic equation, fluctuations of temperature, nucleus of new phase, droplet, cluster.*

Abstract

The formula has been derived for the stationary nucleation rate (nucleation) with the account of temperature fluctuations in the of new phase nuclei.

It is shown that the germ temperature fluctuations results in decreasing the nucleation rate by several orders of magnitude and therefore they must be taken into account when calculating the nucleation rate.

Thematic Section: Research of the New Materials. **Full Paper**
Subsection: Inorganic Chemistry. *Registration Code of Publication:* 13-36-10-141
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: September 26, 2013.

Dedicated to the memory of Yuriy Grigor'evich Yatluk

Template synthesis and sorption of water vapor by porous silica gels with a high specific surface area

© **Igor S. Puzyrev**,[1]*+ **Egor P. Sobina**,[2] and **Sergey V. Medvedevskih**[2]
[1] *I.Ya. Posyovsky Institute of Organic Synthesis, UB of RAS. Kovalevskaya St., 22. Ekaterinburg, 620990. Russia. Phone: +7 (343) 362-34-39. E-mail: igor.puzyrev@mail.ru*
[2] *Urals Scientific Research Institute of Metrology. Krasnoarmeyskaya St., 4. Ekaterinburg, 620000. Russia. Phone: +7 (343) 350-26-18. E-mail: sobina_egor@uniim.ru*

*Supervising author; +Corresponding author

Keywords: *silica gels, micropores, mesopores, adsorption of water.*

Abstract

With mixed surfactants of primary distilled alkylamines as template agents and tetraethylorthosilicate as a silica source, micro- and mesoporous silica gels were synthesized in basic medium. Characteristics of porous silica gel were studied by the low-temperature nitrogen adsorption-desorption. Specific surface areas of microporous silica gels are 1055 or 1392 m^2/g depending on calcination conditions, mesoporous silica – 887 m^2/g, and the pore volumes are 0.82, 0.68 и 0.81 cm^3/g, respectively. SEM images exhibited lamellar structure of microporous, and spherical shape of mesoporous silica gels. The adsorption isotherms of the water vapour on the silica gels were investigated. The larger specific area of microporous silica gel provides the greater adsorption value.

Full Paper _____ *Thematic Section:* Research of the New Technologies.
Registration Code of Publication: 13-36-10-146 *Subsection:* Polymer Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: August 2, 2013.

Increasing the compatibility of a mixture of low density polyethylene with polyamide-6

© **Min' Thi Thao**,[1] **Regina R. Spiridonova**,[1+] **Thi Thu Loan Doan**,[2]*
Anna V. Sheremet'eva,[1] and **Alexander M. Kochnev**[1]
[1] *Department of TSR. Kazan National Research Technological University.*
K. Marx St., 72. Kazan, 420015. E-mail: minhthao1985t@yahoo.com.
[2] *Department of Chemistry and Materials Science. Danang Technological University.*
Danang. Vietnam. E-mail: dttloan2001@yahoo.com

*Supervising author; [+]Corresponding author

Keywords: *low density polyethylene, polyamide-6, ethylene copolymer with vinyl acetate, modification.*

Abstract

The effect of an ethylene copolymer with vinyl acetate on the performance properties of low density polyethylene and its mixtures with polyamide-6 has been investigated. It is shown that the introduction of ethylene copolymer with vinyl acetate improves the physical and mechanical properties as well as the value of flow index of melt compositions.

Full Paper _____ *Thematic Section:* Theoretical Research.
Registration Code of Publication: 13-36-10-150 *Subsection:* Ecology.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
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Effect of time of year on the formation of acid rain sedimentation in the location area of thermal power plants

© **Dmitry V. Gvozdyakov**,*+ and **Vladimir E. Gubin**
National Research Tomsk Polytechnic University. Lenin St., 30. Tomsk, 634050. Russia.
Phone: +7 (3822) 70-17-77 , 1626. E-mail: dim2003@tpu.ru

*Supervising author; +Corresponding author

Keywords: *mathematical modelling, thermal power plant, smoke gases, pollution, sulfuric anhydride, condensation, particle, sulfuric acid, time of year.*

Abstract

The results of numerical simulations of the formation of sulfuric acid droplets in the airspace for different times of the year and the corresponding typical parameters of thermal power stations are presented. Time intervals, characteristic for fulfilling the conditions of anthropogenic substance dispersion in the air space, adjoining to the source, are considered. There are defined geometrical parameters of condensation nucleus, on which surface drops of the acid are formed, which are capable to drop out on the surface of the Earth in the process of sedimentation.

Thematic Section: Preparative Chemistry. **Brief Communication**
Subsection: Organic Chemistry. *Registration Code of Publication:* 13-36-10-157
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: October 3, 2013.

Imines in reactions with 1,3-dioxolane

© **Lidia P. Yunnikova**,*+ **Nadezhda N. Yaganova**, and **Irina D. Yakimova**
Acad. D.N. Pryanishnikov Perm State Agricultural Academy.
Petropavlovskaya St., 23. Perm, 614990. Russian Federation.
Phone: +7 (342) 212-95-68. E-mail: yunnikova@yahoo.com

*Supervising author; +Corresponding author

Keywords: *imines, 1,3-dioxolane, 4,4[1]-bis(arylmethyleneamino)diphenylmethanes.*

Abstract

Interaction of 1,3-dioxolane with *N*-benzylidene-4-nitroaniline in the presence of zinc chloride and concentrated hydrochloric acid is accompanied by the formation of *N*-benzyl-4-nitroaniline. However, 1,3-dioxolane is a condensing agent for *para*-substituted *N*-arylmethyleneanilines in a medium of trifluoroacetic acid and benzene. Reaction of the said compounds results in the formation of 4,4'-bis(arylmethyleneamino)diphenylmethanes.

Full Paper _____ *Thematic Section:* Study of Preparative Methods.
Registration Code of Publication: 13-36-10-160 *Subsection:* Polymer Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: October 20, 2013.

Investigation of microwave assisted reaction of ethylene carbonate with *p-tert*-butylphenol

© **Sofia R. Kleshnina**,[1+] **Nguyen Phi Long**,[2] **Svetlana E. Solovieva**,[1]* and **Igor S. Antipin**[1,2]*
[1] *A.E. Arbuzov Institute of Organic and Physical Chemistry. Akad. Arbuzova St., 8. Kazan, 420088. Republic of Tatarstan. Russia. Phone: +7 (843) 273-22-83. E-mail: skleshni@iopc.ru*
[2] *Department of Organic Chemistry. A.M. Butlerov Institute of Chemistry. Kazan Federal University. Kremlevskaya St., 18. Kazan, 420008. Republic of Tatarstan. Russia. Phone: +7 (843) 231-42-30. E-mail: igor.antipin@ksu.ru*

*Supervising author; [+]Corresponding author

Keywords: *phenol, ethylene carbonate, oligomerization, basic catalyst*

Abstract

Oligoethers have been prepared based on the reaction of *p-tert*-buthylphenol with ethylene carbonate in the presence of potassium and cesium carbonates using microwave irradiation. It has been established that during the reaction of *p-tert*-buthylphenol with ethylene carbonate under microwave irradiation the products were formed with the higher degree of oligomerization than those at conventional heating, the reaction proceeds at a higher rate, and ethylene carbonate fragments appear in addition to ethylene oxide fragments in reaction products.

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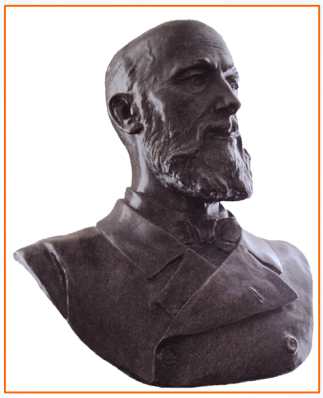

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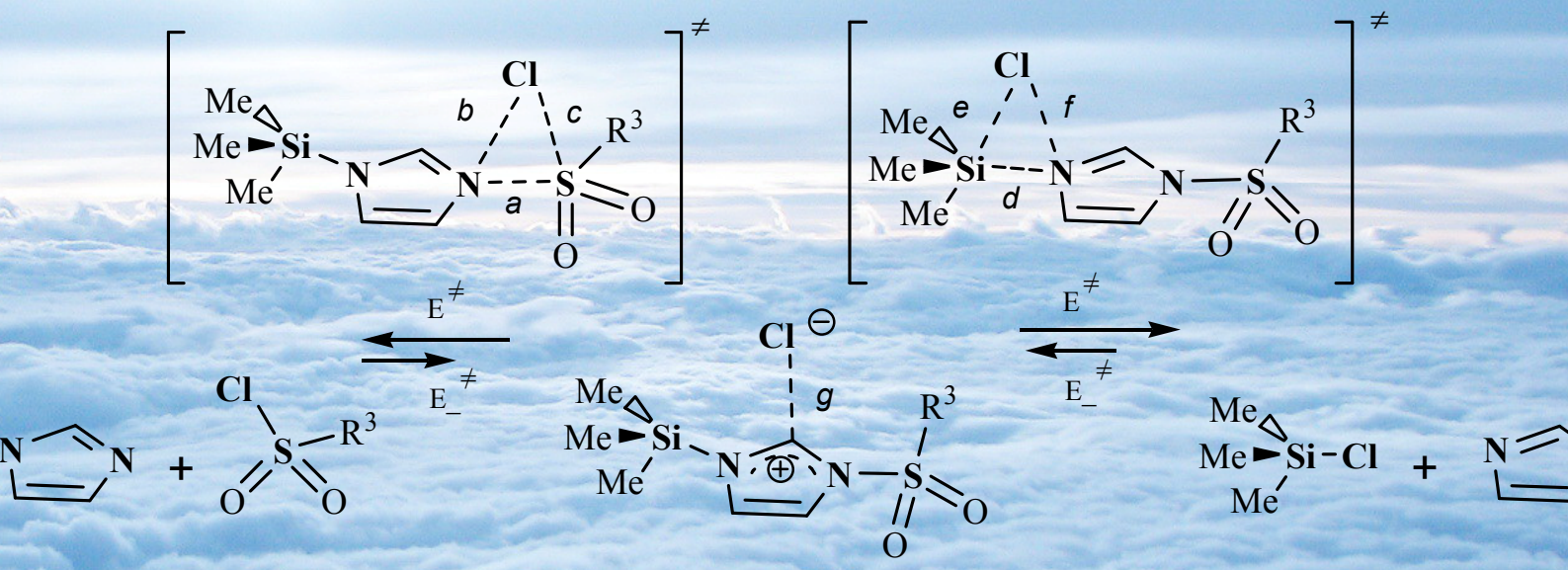

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5-Methoxy-3,4-di[(4-methylphenyl)sulfanyl]-2(5*H*)-furanone in the reactions with nitrogen-containing nucleophiles

© **Lilia S. Kosolapova**,[1] **Almira R. Kurbangalieva**,*[+1] **Denis A. Kozyakov**,[1] **Olga A. Lodochnikova**,[2] **Evgeny A. Berdnikov**,[1] and **Galina A. Chmutova**[1]

[1] *Department of Organic Chemistry. A.M. Butlerov Chemical Institute. Kazan Federal University. Kremlevskaya St., 18. Kazan, 420008. Russian Federation. Phone: +7 (843) 233-74-62. E-mail: Almira.Kurbangalieva@ksu.ru*

[2] *Diffraction Methods Laboratory. A.E. Arbuzov Institute of Organic and Physical Chemistry. Kazan Scientific Center of the Russian Academy of Sciences. Akad. Arbuzova St., 8. Kazan, 420088. Russian Federation. Phone: +7 (843) 231-91-68. E-mail: olga@iopc.ru*

*Supervising author; [+]Corresponding author

Keywords: *heterocycles, 1,5-dihydro-2H-pyrrol-2-ones, 3-pyrrolin-2-ones, 2(5H)-furanones, thioethers, nitrogen-containing nucleophiles, X-ray diffraction analysis.*

Abstract

The chemical behavior of 5-methoxy-3,4-di[(4-methylphenyl)sulfanyl]-2(5*H*)-furanone in the reactions with nitrogen-containing nucleophiles was characterized. Depending on the reagents and the reaction conditions used, the nucleophilic attack can be directed both at the carbonyl carbon atom and at C^4 carbon atom of the lactone ring. Novel sulfur-containing derivatives of 3-pyrrolin-2-one, 2(5*H*)-furanone and pyridazin-3(2*H*)-one are obtained by interaction of 5-methoxy-3,4-di[(4-methylphenyl)sulfanyl]-2(5*H*)-furanone with ammonia, benzylamine and hydrazine. The structure of all synthesized compounds was confirmed by IR, ^{1}H and ^{13}C NMR spectroscopy; the molecular and crystal structure of three new heterocycles were characterized by single crystal X-ray diffraction.

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Quantum-chemical study of the elementary reactions acts of 2-phthalimidoethanesulfonylhalides with *N*-trimethylsilylimidazole

© **Alexandre I. Kourdioukov**,[1]*+ **Tatiana S. Yudakhina**,[2+]
Yury P. Zarubin,[2] **Peter P. Purygin**,[2]* and **Evgeny N. Ofitserov**[3]
[1] *Center of New Information Technologies. Kazan National Research Technological University. K. Marx St., 68. Kazan, 420015. Tatarstan Republic. Russia.*
Phone: +7 (843) 231-42-30. E-mail: butlerov@mail.ru
[2] *Department of Organic, Bioorganic and Medicinal Chemistry. Samara State University. Akad. Pavlov St.,1. Samara, 443011. Russia.*
Phone: +7 (846) 334-54-59. E-mail: utschem-2007@mail.ru
[3] *Dtpartment of Chemistry and Technology of Biomedical Preparations. Faculty of Technology of Organic Substances and Chemical-Pharmaceutical Products. D.I. Mendeleyev Russian Chemical Technological University. Miusskaya Sq., 9. Moscow, 125047. Russia.*
Phone: +7 (495) 978-32-61. E-mail: ofitser@mail.ru

*Supervising author; +Corresponding author

Keywords: *2-aminoethanesulfonic acid, taurine, 2-phthalimidoethanesulfonic acid, imidazolides, synthesis, reaction mechanism, elementary acts, quantum-chemical modeling, DFT method.*

Abstract

Quantum-chemical method DFT with density functional PBE in the basis 3z (similar to basis set cc-pVTZ) in the gas phase and supramolecular approximation was used to study the reactions of 2-phthalimidoethanesulfonylhalides with *N*-trimethylsilylimidazol, where Hal = F, Cl. We discussed in detail the specificity of the reaction systems in the geometric and energy context depending on the nature of the halide and the specific solvation with chloroform.

It is shown that for the studied reaction systems various synchronous one-step reaction mechanisms are not implemented, and a two-step mechanism holds true. The first stage is nucleophilic attack by unsaturated nitrogen center of *N*-trimethylsilylimidazol on sulfur atom of the corresponding sulfonylhalide with simultaneous bond cleavage S-Cl and the formation of middleware intermediate, which is a tight ion pair of galogenaniona and cation-delocalized disubstituted imidazole heterocycle with the preserved N-Si bond and the newly formed covalent bond N-S. The second stage of the reaction is the migration of galogenanion with the position in tight ion pair on the silicon center with simultaneous cleavage of the bond N-Si (that can be classified as ipso-substituted) and the formation of desired products – trimethylsilylсилилhalide and imidazolide 2-phthalimidoethanesulfonic acid.

The conclusion is made on the need to further clarify the mechanism of the reaction by using a high-precision quantum chemical methods and modeling various promoter effects facilitating the activation barrier of the forward direction of the first reaction step.

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Analysis of silver four-atom cluster interaction with the surface of silicon dioxide by density functional theory

© **Tatiana I. Isaak**,[1]* **Daria O. Martinova**,[1] and **Oleg Kh. Poleshchuk**[2+]
[1] *National Research Tomsk State University. Lenin Pr., 36. Tomsk, 634050. Russia.*
Phone: +7 (909) 546-63-06. E-mail: taina_i@mail.ru
[2] *National Research Tomsk State University. Lenin Pr., 30. Tomsk, 634050. Russia.*
Phone: +7 (913) 829-14-54. E-mail: poleshch@tspu.edu.ru

*Supervising author; +Corresponding author

Keywords: *density functional theory, DGDZVP, silicon dioxide, metallic silver, natural bond orbitals.*

Abstract

The calculations were carried out of some silver and silicon-containing molecules in the gas phase with the use of density functional theory using the all-electron basis set DGDZVP in the software package GAUSSIAN'03 and TZ2P+ of the Amsterdam density functional program. It is shown that silicon oxide with a high probability can be reacted with silver cluster. The calculated ESCA levels and the natural bond orbitals indicate the significant interaction between the virtual orbitals of silver atoms.

Full Paper _____ *Thematic Section:* Physicochemical Research.
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New principles of the research into imperfect crystallographic forms of colloidal chemical clusters

© **Yury I. Sucharev**,*+ **Boris A. Markov**, and **Oksana M. Shanina**
Department of Solid Body Chemistry and Nanoprocesses. Chelyabinsk State University.
Br. Kashirins St., 129. Chelyabinsk, 454000. Russia. Phone: +7 (9634) 60-27-75.
E-mail: Yuri_Sucharev@mail.ru.

*Supervising author; +Corresponding author

Keywords: *Lagrangian mappings, oxyhydrate gel systems, colloid clusters, spontaneous pulsation current, spike surge, diffuse double electric layer, bi-particle interactions, topologic 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, which we have presented on our website (http//:oxyhydrate-gel.ru), as well as in our major works.

We consider these properties to be connected with colloid systems symmetry and their wave oscillations in time. In this work, we prove our point that is based upon experimental data of current diagrams and their study.

Full Paper _____ *Thematic Section:* Research Into new Technologies.
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Purification, modification and application of carbon nanotubes in low-temperature oxidation of cumene

© **Alexey S. Orlov**,[1] **Natalia S. Kobotaeva**,[1] **Oleg Kh. Poleshchuk**,[2]
Tatiana S. Skorohodova,[1] **Dmitry A. Afanasyev**,[2] and **Alexey G. Zherlitsyn**[3]
[1] *Federal State Institution of Science, Institute of Petroleum Chemistry,*
Siberian Branch of the Russian Academy of Sciences. Akademicheskiy Pr., 4. Tomsk, 634021. Russia.
Phone: +7 (9234) 20-71-39. E-mail: orlov_alex1984@mail.ru
[2] *National Research Tomsk Polytechnical University. Lenin Pr., 30. Tomsk, 634050. Russia.*
[3] *Physico-Technical Institute of the National Research Tomsk Polytechnic University.*
Lenin Pr., 2a. Tomsk, 634000. Russia

*Supervising author; [+]Corresponding author

Keywords: *carbon nanotubes, amorphous carbon, catalysis, cumene, cumene hydroperoxide.*

Abstract

The paper describes two different methods of purification of carbon nanotubes from amorphous carbon. Purification samples were characterizaed by XRD, IR spectroscopy, TGA, ESR, and tested their catalytic activity in the oxidation of cumene to cumene hydroperoxide at the temperature of 60 °C. During the reaction, the conversion was achieved equal to 8.9% and the selectivity on cumene hydroperoxide by 90.3%.

Full Paper _____ *Thematic Section:* Technological Research.
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http://butlerov.com/readings/
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Reconstruction of the vacuum creation system of rectification column K-3 TPP "Kogalym Neftegas" (OAO "LUKOIL - Western Siberia)

© **Eduard V. Osipov**,[1+] **Hanpasha S. Shoipov**,[2] and **Eduard Sh. Telyaykov**[1]*
[1] *Department of Mechanical Engineering for Chemical Industry.*
Kazan National Research Technological University.
Karl Marx St., 68. Kazan, 420015. Tatarstan Republic. Russia.
Phone: +7 (843) 231-42-41. E-mail: mahp_kstu@mail.ru
[2] *OOO "Lukoil-NizhegorodNIInefteproekt". Maxim Gorky St., 147a. Nizhny Novgorod, 603006.*
Russia. Phone: +7 (831) 421-05-11. E-mail: nnp@nnp.lukoil.com

*Supervising author; [+]Corresponding author

Keywords: *vacuum creation systems, vacuum rectification of fuel oil, liquid ring vacuum pump.*

Abstract

This paper describes the technological inspection of vacuum rectification column of fuel oil K-3 (atmospheric-vacuum distillation unit of *TPP "Kogalym Neftegas"*), which was held in August 2013. Inspection data have been integrated into computational models. According to the results of calculations the recommendations were developed for the reconstruction of vacuum creation system (VCS) of the column and selection of the liquid ring vacuum pump (LRVP).

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Research into the burning of perchlorate metallized composites containing the salts of dinitramide

© **Vladimir N. Popok**,*+ **Vandel A. Pavlovich**, and **Alexey Yu. Kolesnikov**
Open Joint Stock Company «Federal Research and Production Center «Altay».
Sotsialisticheskaya St., 1. Biisk, 659322. Altai territory, Russia.
Phone: +7 (3854) 30-19-37. E-mails: vnpopok@mail.ru

*Supervising author; +Corresponding author

Keywords: *salts of dinitramide, binder, burning speed, thermal decomposition.*

Abstract

In the article, the analysis results are presented on the effect of the guanilurea content and guanidinium salts of dinitramide in the metallized compositions on the basis of inert combustible binders and ammonium perchlorate on the burning rate. It is shown that the use of these salts allows to regulate in a wide range the level of the burning rate of compositions at rather low values of an exponent in the law of burning rate (~0.5), to minimize the content of adverse products of burning at insignificant decrease in power mass characteristics in comparison with basic compositions.

Thematic Section: Theoretical Research. **Full Paper**
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Calculation of the concentration of autocomplexes in halide melts of bivalent metals

© **Ksenia G. Peshkina**[1], **Nikolay K. Tkachev**[1+] and **Anatoly Ya. Fishman**[2]
[1] *Laboratory of interphase phenomena. Institute of High Temperature Electrochemistry, Ural Branch of RAS. Kovalevskaya St., 22. Ekaterinburg, 620219. Russia. Phone: (343) 362-31-35. E-mail: n.tkachev@ihte.uran.ru*
[2] *Laboratory for statics and kinetics of processes. Institute of Metallurgy, Ural Branch of RAS. Amundsen St., 101. Ekaterinburg, 620016. Russia. Phone: +7 (343) 267-94-72. E-mail: fishman@uran.ru*

*Supervising author; +Corresponding author

Keywords: *chemical equilibrium in nonideal systems, dissociation of complexes in ionic liquids.*

Abstract

Model calculation of chemical equilibrium of the reaction $M^{2+} + 4X^{-} = (MX_4)^{2-}$ in halide melts of bivalent metals has been presented. It was found that the concentration of autocomplex anions is strongly reduced by the effects of the electrostatically screened interaction between ions in the reaction mixture. It is shown that the shift of the chemical equilibrium state with the largest possible number of autocomplexes to their complete dissociation occurs within a rather narrow temperature range and accompanies the maximum atomic density.

Thematic Section: Physicochemical Research. **Short Communication**
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Investigation of phase equilibria in Ga–InBi system

© **Vladimir V. Filippov**,[1,2+] **Viktor A. Bykov**,[1] **Konstantin Yu. Shunyaev**,[1]*
and **Alexey B. Shubin**[1]
[1] *Institute of Metallurgy UB RAS. Amundsena St., 101.*
Ekaterinburg, 620016. Sverdlovsk Region. Russia. Phone: +7 (8343) 232-91-69. E-mail: vvfilippov@mail.ru
[2] *Ural Federal University Named after the First President of Russia B.N. Yeltsin. Mira St., 19.*
Ekaterinburg, 620002. Sverdlovsk Region. Russia.

*Supervising author; +Corresponding author

Keywords: *system Ga-InBi, phase equilibria, DSC, SEM.*

Abstract

Phase equilibria in the Ga-InBi system is investigated by DSC and scanning electron microscopy. It is established that the section on the Ga-Bi-InBi phase diagram is non-quasibinary. We found two of invariant equilibria: eutectic $L \leftrightarrow$ (Ga) + (Bi) + InBi at 24.3 ± 0.5 °C and monotectic $L'' \leftrightarrow L'$ + (Bi) + InBi at 98.4 ± 0.5 °C. The position of the liquid phase separation boundary in the Ga-InBi system is defined more exactly.

Letter to the Editor _____ *Thematic Section:* Physicochemical Research.
Registration Code of Publication: 13-36-11-76 *Subsection:* Phase Equilibria.
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Investigation of a two-component system of K//Br, CrO_4

© **Irina I. Salnikova**,[+] and **Igor M. Kondratuk***
Department of General and Inorganic Chemistry. Samara State Technical University.
Molodogvardeyskaya St., 244. Samara, 443100. Russia.
Phone: +7 (846) 278-44-77. E-mail: isechka24@yandex.ru, kondratuk2@mail.ru

*Supervising author; [+]Corresponding author

Keywords: *differential thermal analysis, phase equilibria, eutectic.*

Abstract

By differential thermal analysis two-component system K//Br, CrO_4 was investigated, T-X diagram was presented, melting point and composition of eutectic point were defined. On the basis of the studied state diagram, we can make a conclusion about the absence of oxidation-reduction reaction in these molten salts up to 900 ^oC.

Full Paper _____ *Thematic Section:* Preparative Research.
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Synthesis and structure of bismuth complexes $[Bu_4P]^+_2[Bi_2I_8 \cdot 2Me_2S=O]^{2-}$, $[(Me_2S=O)_8Bi]^{3+}[Bi_2I_9]^{3-}$

© **Vladimir V. Sharutin**,*+ **Olga K. Sharutina**,
Vladislav S. Senchurin, and **Radmir M. Hisamov**
Department of Organic Chemistry. Chemistry Faculty. South Ural State University.
Lenin Pr., 76. Chelyabinsk, 454080. Russia. Phone: +7 (351) 267-95-70.
E-mail: vvsharutin@rambler.ru

*Supervising author; +Corresponding author

Keywords: *synthesis, structure, complex, bismuth, iodine.*

Abstract

By the reaction of tetrabutylphosphonium iodide with bismuth triiodide (2:1, 1:1, 1:2 mol) we synthesized the complex $[Bu_4P]^+_2[Bi_2I_8(Me_2S=O)_2]^{2-}$ (**I**) in dimethylsulfoxide. The second reaction product is the complex $[(Me_2S=O)_8Bi]^{3+}[Bi_2I_9]^{3-}$ (**II**) (tetrabutylphosphonium iodide, bismuth triiodide: 1:2 mol.) In cationic complexes **I** P atoms have distorted tetrahedral coordination (CPC angles are 104.1(1)°-112.6 (1)°). In dinuclear centrosymmetric anions complex **I** hexacoordinative bismuth atoms linked by two bridging iodine atoms (Bi-Ibr 3.260(1) and 3.315(1) Å), the terminal iodine atoms atom form stronger bonds bismuth (Bi-Iterm 2.926(1)-3.031(1) Å), the bond length Bi-O 2.436(1) Å. In the cation complex **II** eight molecules of dimethyl sulfoxide on the bismuth atom is coordinated via oxygen atoms (angles OBiO 69.9(2)°-98.9(3)°, the length of the Bi-O bonds constitute 2.381(4)-2.476(4) Å). In the anion +[Bi2I9]3- of complex **II** Bi atoms have octahedral coordination; BiI3 groups linked to each other through a three bridging atoms of iodine (Bi-Ibr 3.156(1)-3.343(1) Å, Bi-Iterm 2.910(1)- 3.021(1) Å).

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Synthesis and structure of μ-oxo-bis-[(trifluoroacetato)-(tri-*m*-tolyl)antimony][$(C_6H_4Me\text{-}3)_3SbOC(O)CF_3)]_2O$

© **Vladimir V. Sharutin**,*+ **Olga K. Sharutina**, and **Vladislav S. Senchurin**
Department of Organic Chemistry. Chemistry Faculty. South Ural State University. Pr. Lenin, 76. Chelyabinsk, 454080. Russia. Phone: +7 (351) 267-95-70. E-mail: vvsharutin@rambler.ru

*Supervising author; +Corresponding author

Keywords: *synthesis, structure, [(C6H4Me-3)3SbOC(O)CF3)]2O.*

Abstract

By reaction of (tri-*m*-tolyl)antimony with trifluoroacetic acid in the presence of hydrogen peroxide in aqueous-ether solution we obtained μ-oxo-bis-[(trifluoroacetate)(tri-*m*-tolyl)antimony] (**I**) with the yield of 91%. In the dinuclear molecule **I** SbOSb angle is 146.0(5)°. Antimony atoms have a distorted trigonal-bipyramidal coordination. Distances Sb-C vary in the range 2.086(7)-2.118(7) Å. Bonds of the antimony atom with bridging oxygen atom [1.962(6), 1.957(6) Å] are shorter than with oxygen atoms of trifluoroacetate groups [2.209(5), 2.209(5) Å].

Thematic Section: Preparative Research. **Full Paper**
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http://butlerov.com/synthesys/
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Synthesis and structure of 2-bromo-4-formylphenoxytetraphenylantimony

© **Vladimir V. Sharutin**,*+ **Olga K. Sharutina**, **Vladislav S. Senchurin**, and **Artem O. Shhelokov**
Department of Organic Chemistry. Chemistry Faculty. South Ural State University. Pr. Lenin, 76. Chelyabinsk, 454080. Russia. Phone: +7 (351) 267-95-70. E-mail: vvsharutin@rambler.ru

*Supervising author; +Corresponding author

Keywords: *synthesis, structure, aroxyd, tetraphenylantimony.*

Abstract

By the reaction of pentaphenylantimony with 2-bromo-4-formylphenol in toluene there were obtained by heating 2-bromo-4-metoxyphenoxytetraphenylantimony and 2-bromo-4-formylphenoxytetraphenylantimony with the yield of 97%. According to X-ray analysis the antimony atom in the molecule of 2-bromo-4-formylphenoxyfntimony has distorted trigonal bipyramidal configuration, bond lengths Sb-O and Sb-C are equal to 2.257(3) and 2.166(4), 2.113(4), 2.127(4), 2.122(4) Å, respectively, axial angle OSbC and equatorial angles CSbC are 176.8(1)° and 116.0(1)°, 118.7(1)°, 121.1(1)°.

Thematic Section: Preparative Research. **Full Paper**
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Synthesis and structure of *bis*(salisylaldoximato)triphenylantimony

© **Vladimir V. Sharutin**,*+ **Olga K. Sharutina**, and **Vladislav S. Senchurin**
Department of Organic Chemistry. Chemistry Faculty. South Ural State University.
Pr., Lenin, 76. Chelyabinsk, 454080. Russia. Phone: +7 (351) 267-95-70.
E-mail: vvsharutin@rambler.ru

*Supervising author; +Corresponding author

Keywords: *synthesis, structure, bis(salisylaldoximato)triphenylantimony.*

Abstract

By the reaction of triphenylantimony with *t*-butylhydroperoxide and salisylaldoxime (1:2:1 mol.) in heptane we obtained bis(salisylaldoximate)triphenylantimony (**I**), which structure was established by X-ray diffraction. Sb atoms in a centrosymmetric molecule **I** (inversion center – antimony atom) have a distorted trigonal-bipyramidal coordination with the oxime groups in axial positions. Bond lengths Sb-C and Sb-O are 2.103(3), 2.103(3), 2.112(2) and 2.073(2) Å, intramolecular contacts Sb···N constitute 2.884(2) Å.

Thematic Section: Preparative Research. _____ **Short Communication**
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Synthesis and structure of 4-methyl-benzenesulfonate tetraphenylbismuth

© **Vladimir V. Sharutin**,*+ and **Olga K. Sharutina**
Department of Organic Chemistry. Chemistry Faculty. South Ural State University. Pr., Lenin, 76. Chelyabinsk, 454080. Russia. Phone: +7 (351) 267-95-70. E-mail: vvsharutin@rambler.ru

*Supervising author; +Corresponding author

Keywords: *synthesis, structure, $Ph_4BiOC_6H_4Me$-4.*

Abstract

By interaction of pentaphenylbismuth with 4-methylbenzenesulfonate diphenylbismuth we obtained 4-methylbenzenesulfonate tetraphenylbismuth which structure was established by X-ray. Bi atom in the compound has a distorted trigonal-bipyramidal coordination with tosylate substituent in the axial position. Bond lengths of Bi-C are equal to 2.192(2)-2.225(2) Å, Bi-O distance and the magnitude of the axial angle CBiO constitute 2.759(2) Å and 171.6(1)° respectively.

Letter to the Editor _____ *Thematic Section:* Preparative Research.
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Interaction of diphenylacetylene with platinum diiodide in dimethyl sulfoxide in the presence of oxygen

© **Vladimir V. Sharutin**,*+ **Olga K. Sharutina**, and **Vladislav S. Senchurin**
Department of Organic Chemistry. Chemistry Faculty. South Ural State University. Pr. Lenin, 76. Chelyabinsk, 454080. Russia. Phone: +7 (351) 267-95-70. E-mail: vvsharutin@rambler.ru

*Supervising author; +Corresponding author

Keywords: *oxidation, diphenylacetylene, platinum diiodide, dimethylsulfoxide, diphenylethanedion-1,2.*

Abstract

Diphenylacetylene in dimethylsulphoxide in the presence of atmospheric air and platinum diiodide is oxidized to diphenylethanedion-1, 2 with the yield of 91%. In the absence of platinum diiodide in the reaction mixture the formation of diphenyletandion-1,2 did not take place.

Full Paper _____ *Thematic Section:* Physicochemical Research.
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Study of the effect of copolymer composition with glycolic and lactic acids on their solubility

© **Olga K. Kuchina**, **Olga V. Babkina**,* **Kira V. Alekseenko**,+ and **Anna L. Nemoykina**
Tomsk Regional Common use center. Tomsk State University. Lenin Pr., 36. Tomsk, 634050. Russia.
Phone: +7 (3822) 53-48-45. E-mail: ckp@mail.tsu.ru

*Supervising author; +Corresponding author

Keywords: *Biopolymer, Glycolid, Lactid, polyglicolidlactide.*

Abstract

In this paper, the effect of structure and molecular weight on solubility of polymers based on glycolic and lactic acids in organic solvents such as dimethylsulfoxide, tetrahydrofuran, methylene chloride, chloroform and hexafluoroisopropanol has been studied. The solubility data are used for setting the method of molecular weight studying by the gel permeation chromatography techniques and for testing the method of antimicrobial coating on the surface of the biodegradable filaments made of glycolic and lactic acids copolymers.

Full Paper _____ *Thematic Section:* Biochemical Research.
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Crystallization of calcium phosphates from solutions simulating the composition of human blood plasma

© **Olga A. Golovanova*** and **Anna A. Solodyankina**[+]
Department of Inorganic Chemistry. F.M. Dostoevsky Omsk State University.
Prospekt Mira, 55-A. Omsk, 644077. Russia. Phone: +7 (3812) 26-81-99.
E-mail: golovanoa2000@mail.ru, solodyankina.a @ gmail.com

*Supervising author; [+]Corresponding author

Keywords: *crystallization, supersaturation, calcium phosphate, blood plasma, kinetics.*

Abstract

This paper presents the results of studies on the kinetics of nucleation and crystal growth in solutions simulating the composition of human blood plasma. The results of X-ray phase analysis and optical microscopy are presented. It has been found that when supersaturation changes the composition of the deposit varies – oktocalcium phosphate is transferred into hydroxyapatite. The effect of some inorganic (magnesium ion) and organic (alanine and glucose) additives on the crystallization kinetics has been shown.

Thematic Section: Biochemical Research. **Full Paper**
Subsection: Analytical Chemistry. *Registration Code of Publication:* 13-36-11-111
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Contributed: October 30, 2013.

Identification of AB-FUBINACA markers in urine by GCh-MS method

© **Aleksey B. Melent'ev**,[1+] **Sergey S. Kataev**[2] **Oksana N. Dvorskaya**,[3]* and **Andrey V. Labutin**[4]
[1] *Forensic-Chemical Department. State Healthcare Establishment of Special Type "Perm Regional Bureau of Forensic-Medical Expertise". Startseva St., 61. Perm, 614077. Perm Region. Russia.*
Phone: +7 (342) 210-67-83. E-mail: forenschemist@narod.ru
[2] *Forensic-Chemical Department. State Healthcare "Chelyabinsk Regional Bureau of Forensic-Medical Expertise". Varnenskaya St., 4-b. Chelyabinsk, 454076. Chelyabinsk Region. Russia.*
Phone: +7 (351) 232-80-58. E-mail: amelentyev@sme74.ru
[3] *Department of Toxicological Chemistry. Perm State Pharmaceutical Academy of the Ministry of Health of the Russian Federation. Polevaya St., 2. Perm, 614990. Perm Region. Russia.*
Phone: +7 (342) 282-58-64. E-mail: kaftox@mail.ru
[4] *Forensic Center UMVD, Tomsk region. Elizarovs St., 48/10. Tomsk, 634012. Tomsk region. Russia.*

*Supervising author; [+]Corresponding author

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

Abstract

The markers are described which allow to establish the fact of AB-FUBINACA cannabimimetic being used in the procedure of screening urine on narcotic and medicinal substances applying the methods of solid-phase extraction and a gas chromatography with mass spectrometry. Identification of the main metabolites of AB-FUBINACA in urine of consumers of smoking mixes was performed. It is established that the metabolism of AB-FUBINACA 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 of main metabolites which can be useful in practice of the forensic-chemical and chemical-toxicological analysis are obtained.

Thematic Section: Biochemical Research. **Full Paper**
Subsection: Composition of Plants. *Registration Code of Publication:* 13-36-11-119
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Weight parameters of hawthorn fruits and trace element content

© **Svetlana V. Muhametova**,[1+]* and **Vladimir I. Talantsev**[2]*
[1] *Botanical Garden-Institute. Volga State University of Technology. Mira St., 2B. Yoshkar-Ola, 424030. Mari El Republic. Russia. Phone: +7 (8362) 64-75-60. E-mail: MuhametovaSV@volgatech.net.*
[2] *Chemistry Division. Volga State University of Technology. Lenin Sq., 3. Yoshkar-Ola, 424000. Республика Mari El Republic. Russia. Phone: +7 (8362) 68-68-04. E-mail: TalancevVI@volgatech.net*

*Supervising author; [+]Corresponding author

Keywords*: hawthorn, Crataegus, officinal plants, fruits, weight, moisture, ash, trace element.*

Abstract

In this paper, the results of the study weight parameters of 13 hawthorn taxa fruits of the VSUT Botanical Garden-Institute collection are presented: 100 fruits weight, moisture content, ash content and the percent yield of dry material. The studied taxa are divided into small- and large-fruited ones. The analysis of 8 trace elements content in fruits is given; the taxa with high, medium and low metal content are identified. The correlations between the accumulations of certain elements are found.

Full Paper _____ *Thematic Section:* Biochemical Research.
Registration Code of Publication: 13-36-11-128 *Subsection:* Composition of Plants.
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http://butlerov.com/natural_resources/
Contributed: October 3, 2013.

Bioelemental composition of some strains of medicinal plants of Araliaceae family (*Araliaceae*)

© **Larisa I. Slepyan**,[1]* **Nadezhda V. Kirillova**,[1+] **Irina E. Kauhova**,[1] **Alexey L. Marchenko**,[1] **Olesya N. Gromova**,[1] **Maria A. Vlasenko**,[3] **Maria V. Yakovleva**,[2] and **Igor I. Shantyr**[2]

[1] *Department of Industrial Technology of Drugs and Biochemistry. St. Petersburg State Chemical-Pharmaceutical Academy. Prof.Popov St., 14.St.Petersburg, 1977376. Russia. Phone: +7 (812) 234-90-33. Fax: +7 (812) 234-60-44. E-mail: larisa.slepyan@pharminnotech.com, nadezhda.kirillova@mail.ru*

[2] *A.M. Nikiforov Russian Center of Emergency and Radiation Medicine of Russian Ministry of Emergency Situations. St. Petersburg. Russia.*

[3] *Department of Biophysics. St. Petersburg State University. Biology and Soil Faculty. St. Petersburg. Russia.*

*Supervising author; [+]Corresponding author

Keywords: *tissue culture of medicinal plants, macroelements, microelements.*

Abstract

By mass spectrometry with inductively coupled plasma (ICP-MS) we studied macro- and microelement composition in tissue cultures of different strains of the families *Araliaceae* (*Panax ginseng C.A.Mey, Panax quinquefolius L.* and *Polyscias filicifolia (Moore ex Fournier) Bailey*. The presence of all vital elements in the investigated objects was established. Analysis of the data showed that despite the same composition of the culture medium used for the cultivation of biomass in cultured cells of the studied strains there were observed large differences in the content of macro-and microelements.

Full Paper _____ *Thematic Section:* Biochemical Research.
Registration Code of Publication: 13-36-11-134 *Subsection:* Composition of Plants.
Publication is available for discussion in the framework of the on-line Internet conference "*Chemical basis for the rational use of renewable natural resources*".
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Identification of alkaloids in Greater Celandine grass and Macleaya heart leaves by HPLC

© Dmitry V. Moiseev
Department of Standardization of Drugs. Vitebsk State Medical University. Frunze St., 27. Vitebsk, 210023. The Republic of Belarus. Phone: +375212370006. E-mail: ussr80@yandex.ru

Keywords: *alkaloids, HPLC, Greater Celandine, Macleaya Heart.*

Abstract

The universal chromatography system for identification of alkaloids in medicinal plants is offered. As a mobile phase it is offered to use 0.005M solution of lauryl sulfate sodium and acetonytrile in the ratio 60:40 (in volume) at the temperature of the column 30 °C. Capacity factors were calculated for 14 alkaloids in chromatographic columns of 250·4.6 mm with sorbents Phenyl, C-18, C-8, the size of particles was 5 microns. The obtained database was used at identification of alkaloids in Macleaya heart leaves and in Greater Celandine grass, collected in the conditions of continental climate of Belarus Republic.

Thematic Section: Biochemical Research. **Full Paper**
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Research into the properties of labile organic matter formed during bioremediation in the coal stockpile

© **Lyudmila B. Naumova**,[1]* **Tatiana P. Alekseeva**,[2] **Nina M. Trunova**,[2]
Lidya A. Egorova,[1] and **Aleksey G. Zarubin**[1+]
[1] *Department of Chemistry. Tomsk State University. Lenin Pr., 36. Tomsk, 634050. Russia. Phone: +7 (3822) 42-10-41. E-mail: zagtsuru@gmail.com, NaumovaLB@mail.ru*
[2] *Laboratory for Physical and Chemical Research. GNU SibNII of agriculture and peat at SB RAAS. Gagarin St., 3 (PO Box 1668). Tomsk, 634050. Russia. Phone: +7 (3822) 53-33-90.*

*Supervising author; [+]Corresponding author

Keywords: *recultivation of soil, labile organic matter, peat.*

Abstract

The influence of biologically active additives obtained on the basis of peat on recultivation of Kemerovo region soils disturbed by mining by methods of potentiometry, photocolorimetry, infrared spectroscopy and simultaneous thermal analysis is investigated. It is shown that the addition of peat products contributes to the formation of labile organic matter on the surface of degraded soil, which provides accelerated soil-forming process and the creation of sustainable phytocenoses.

Full Paper _____ *Thematic Section:* Physicochemical Research.
Registration Code of Publication: 13-36-11-146 *Subsection:* Organic Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: December 30, 2013.

Physical and chemical systems of dicarboxylic acids, aminoalcohol and water at 25 °C

© Anna Yu. Tsyplenkova,[1] **Olga V. Koltsova**,[1] **Nikolay N. Lobanov**,[2]
Mikhail A. Yershov,[3+] and **Vikenty G. Skvortsov**[1]*
[1] *Department of Chemistry and Biosynthesis. FSBEI HPE «The Chuvash State Pedagogical University Named after I.Y. Yakovlev». K. Marx St., 38. Cheboksary, 428000. The Chuvash Republic. Russia. Phone: +7 (835) 258-67-66.*
[2] *Department of Inorganic Chemistry. FSBEI HPE «The Russian University of Peoples' Friendship». Ordzhonikidze St., 3. Moscow, Russia.*
[3] *Department of Chemistry. FSBEI HPE «The Chuvash State Agricultural Academy». K. Marx St., 29. Cheboksary, 428003. The Chuvash Republic. Russia. Phone: +7 (835) 262-02-26. E-mail: ema11@mail.ru*

*Supervising author; +Corresponding author

Keywords: *dicarboxylic acids, monoethanol amine, isothermal solubility*, *X-ray diffraction spectrums, physiological activity, growth stimulants, biocides.*

Abstract

Methods of physical and chemical analysis were applied to study the interaction of dicarboxylic acids – oxalic, malonic, succinic with monoethanolamine in an aqueous medium at 25 °C. Complex compounds having the composition: $H_2C_2O_4 \cdot NH_2C_2H_4OH$, $CH_2(COOH)_2 \cdot NH_2C_2H_4OH$, $C_2H_4(COOH)_2 \cdot NH_2C_2H_4OH$ were prepared. Their structures and biogenic properties were investigated. It has been established that the obtained complexes have a wholesome effect on the growth and development of cereal crops.

Full Paper _____ *Thematic Section:* Physicochemical Research.
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Study of the oxygen partial pressure effect on the melting point of ultrafine copper powder

© **Vladislav M. Kozin**, **Larisa B. Vedmid**, and **Olga M. Fedorova**
Laboratory of Statics and Kinetics of the Processes.
Institute of Metallurgy, Ural Branch of RAS. Amundsen St., 101. Ekaterinburg, 620016.
Sverdlovsk region. Russia. Phone: +7 (343) 267-91-86. E-mail: vlad.kozin@mail.ru

*Supervising author; +Corresponding author

Keywords: *copper, powder, nano, melting temperature, partial pressure of oxygen.*

Abstract

Dimensional characteristics of the copper powder produced by the method of electric conductor were studied. The content of oxygen was established in it. The melting temperatures of the powder at various oxygen partial pressures were studied. It has been established that with decreasing the oxygen partial pressure the melting point of copper nanopowder increases, and at the value of $lgPo_2$ = -19.5 within the experimental error equals the melting point of monolithic copper (1083.6 ºC).

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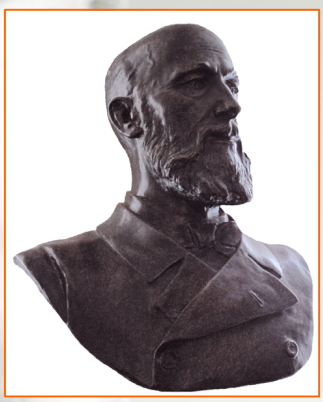

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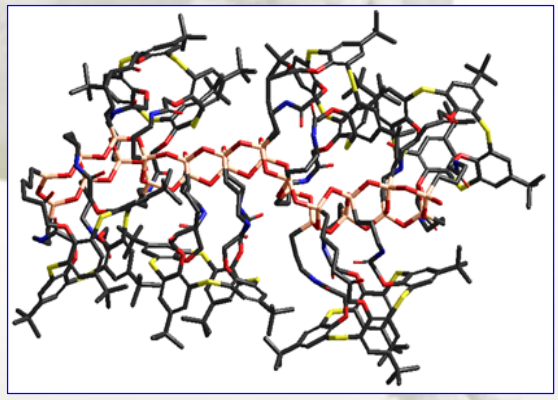

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Thematic Course: Kinetics and mechanism of acyl transfer reactions. Part 5.

Dipeptides and amino acids reactivity in sulfamide bond formation processes

© **Ludmila B. Kochetova**,[1] **Natalia V. Kalinina**,[2]
Tatiana P. Kustova,[1]*[+] and **Lev V. Kuritsyn**[2]
[1] *Department of Organic and Physical Chemistry. Ivanovo State University.*
Ermak St., 39. Ivanovo, 153025. Russia. Phone: +7 (84932) 37-37-03. E-mail: kustova_t@mail.ru
[2] *Department of Inorganic and Analytical Chemistry. Ivanovo State University.*
Ermak St., 39. Ivanovo, 153025. Russia. Phone: +7 (84932) 37-37-03.

*Supervising author; [+]Corresponding author

Keywords: *kinetics, arensulfonylation, aliphatic amino acids, dipeptides, water – 1,4-dioxane, amino groups basicity.*

Abstract

The kinetics of reactions of α- and β-alanine, dipeptides on their basis, glycile-glycine, *L*-proline and L-asparagine with chlorides of benzenesulfonic, 3-nitro benzenesulfonic and 4-methyl benzenesulfonic acids is studied in the solvent water-1,4-dioxane. Correlations are established between amino acids and dipeptides arensulfonylation rate constants and rate constants of their interaction with carbonyl compounds: benzoyl chloride and picryl benzoate, pointing out the amino acids and dipeptides amino groups basicity as the main factor which determine their nucleophilic reactivity.

Full Paper _____ *Thematic Section:* Biochemical Research.
Registration Code of Publication: 13-36-12-8 *Subsection:* Physical Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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Investigation of bacterial luminescence under the action of electromagnetic radiation of millimeter and infrared ranges

© **Denis B. Kuznecov**,[1]*+ **Tatiana F. Odegova**,[1]* **Valery A. Neschislyaev**,[2]*
Vladimir L. Gein,[1] **Igor V. Lunegov**,[3] and **Igor L. Volhin**[3]

[1] *Perm State Pharmaceutical Academy of Russian Ministry of Health. Polevaya St., 2. Perm, 614990. Perm region. Russia. Phone: +7 (342) 233-55-01. E-mail:denis.pfa@gmail.com*

[2] *Filial branch FSUE "NPO"Microgen" of the Russian Ministry of Health,"Perm NGO "Biomed". Bratskaya St., 177. Perm, 614089. Perm Krai. Russia. Phone: (342) 262-32-14. E-mail: neschislayew@gmail.com*

[3] *Perm State National Research University. Bukirev St., 15, Perm, 614068. Perm Krai. Russia. Phone: (342) 239-65-15.*

*Supervising author; +Corresponding author

Keywords: *bioluminescence, microwave radiation, infrared radiation, multilayer adsorption, water.*

Abstract

It is shown that exposure to electromagnetic radiation of millimeter and infrared ranges causes both stimulatory and inhibitory effect on bioluminescence strain *Escherichia coli lum*$^+$. A comparative study of different modes of action of electromagnetic radiation on the reaction of bacterial luminescence has been performed. High sensitivity of biosensor to radiation has been revealed. Optimal modes of radiation to activate bioluminescence of test strain were established.

Thematic Section: Biochemical Research. **Full Paper**
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Identification of FUB-PB-22 cannabimimetic metabolites in urine by GC-MC

© **Sergey S. Kataev**,[1+] and **Oksana N. Dvorskaya**[2]*
[1] *Forensic-Chemical Department. State Healthcare Establishment of Special type "Perm Regional Bureau of Forensic-Medical Expertise". Startsev St., 61. Perm, 614077. Perm region. Russia.*
Phone: +7 (342) 210-67-83. E-mail: forenschemist@narod.ru
[2] *Department of Toxicological Chemistry. Perm State Pharmaceutical Academy of the Ministry of Health of the Russian Federation. Polevaya St., 2. Perm, 614990. Perm region. Russia.*
Phone: +7 (342) 282-58-64. E-mail: kaftox@mail.ru

*Supervising author; [+]Corresponding author

Keywords: *FUB-PB-22, cannabimimetics, metabolism, enzymic hydrolysis, solid-phase extraction, gas chromatography – mass spectrometry.*

Abstract

The metabolism of quinolin-8-yl-1-[(4-fluorophenyl)methyl]-1*H*-indole-3-carboxylate (FUB-PB-22) cannabimimetics is considered. The identification of FUB-PB-22 metabolites in the urine of smoking mixtures consumers was performed. Gas chromatographic and mass spectrometric characteristics of some FUB-PB-22 metabolite derivatives are described. A conclusion is made about analytical significance of metabolites FUB-PB-22, having a value in the expert practice.

Full Paper _____ *Thematic Section:* Preparative Research.
Registration Code of Publication: 13-36-12-22 *Subsection:* Organic Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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Non-template production of 5,7,7,12,14,14-hexamethyl-1,4,8,11-tetraazacyclotetradec-4,11-diene and its analogues

© **Nadezhda A. Anisimova**, **Ekaterina N. Gomzyakova**,
Roza R. Kondrateva, and **Yury G. Trishin***[+]
St. Petersburg State Technological University of Plant Polymers.
Ivan Chernykh St., 4. St. Petersburg, 198095. Russia.
Fax: +7 (812) 786-66-57. E-mail: trish@YT4470.spb.edu

*Supervising author; [+]Corresponding author

Keywords: *ethylenediamine, acetone, ethyl methyl ketone, substituted 1,4,8,11-tetraazacyclotetradeca-4,11-dienes, nitrogen containing macrocycles, complexes of copper (II) and nikel(II).*

Abstract

5,7,7,12,14,14-Hexamethyl-1,4,8,11-*tetraazacyclotetradeca*-4,11-diene and its 5,7,12,14-tetraethyl analogue were first obtained by non-template method by condensation of ethylenediamine with acetone, and ethyl methyl ketone, respectively. Synthesized nitrogen containing macrocyclic compounds are intended for use as molecules-«hosts» when creating supramolecular systems.

Thematic Section: Biochemical Research. **Full Paper**
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Identification of AB-FUBINACA markers in urine by GC-MS method

© **Sergey S. Kataev**,[1+] and **Oksana N. Dvorskaya**[2]*
[1] *Forensic-Chemical Department. State Healthcare Establishment of Special type "Perm Regional Bureau of Forensic-Medical Expertise". Startsev St., 61. Perm, 614077. Perm region. Russia.*
Phone: +7 (342) 210-67-83. E-mail: forenschemist@narod.ru
[2] *Department of Toxicological Chemistry. Perm State Pharmaceutical Academy of the Ministry of Health of the Russian Federation. Polevaya St., 2. Perm, 614990. Perm region. Russia.*
Phone: +7 (342) 282-58-64. E-mail: kaftox@mail.ru

*Supervising author; [+]Corresponding author

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

Abstract

The markers are described, allowing to establish the fact ща uшtп cannabimimetic AB-FUBINACA in the procedure of urine screening on narcotic and medicinal substances with application of methods of solid-phase extraction and a gas chromatography with mass spectrometry. Identification of the main metabolites of AB-FUBINACA in urine of consumers of smoking mixes was performed. It is established that the metabolism of AB-FUBINACA 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 main metabolite derivative which can be useful in practice of the forensic-chemical and chemical-toxicological analysis are obtained.

Analytical Review _____ *Thematic Section:* Biochemical Research.
Registration Code of Publication: 13-36-12-34 *Subsection:* Laws of Metabolism.
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Microbial metabolism of white phosphorus

© **Anton Z. Mindubaev**,[1]*+ **Farida K. Alimova**,[2] **Serge Codjo Ahossiyenagbe**,[2] **Chuluun Bolormaa**,[2] **Alexandra D. Voloshina**,[1] **Natalia V. Kulik**,[1] **Salima T. Minzanova**,[1] **Lubov G. Mironova**,[1] and **Dmitry G. Yahvarov**[1]*

[1] *A.E. Arbuzov Institute of Organic and Physical Chemistry, KazSC RAS. Arbuzov St., 8. Kazan, 420088. Tatarstan Republic.Russia. E-mail: mindubaev@iopc.ru*

[2] *Kazan (Volga Region) Federal University. Kremlevskaya St., 18. Kazan, 420008. Tatarstan Republic. Russia.*

*Supervising author; +Corresponding author

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

Abstract

In the previous works we have for the first time demonstrated the biodegradation of industrial pollutant - white phosphorus - by the wastewater sewage of the treatment facilities. We have also obtained the cultures of microorganisms, developed resistance to the white phosphorus. There are no references to the works of the kind in literature. However biodegradation assumes metabolic pathway of the substance, which is also unknown in the case of white phosphorus. In the present work for the first time the research work devoted to the search for the white phosphorus metabolites is described, and the probable way of the phosphorus metabolism is proposed. Besides, significant attention is paid to the literature sources, devoted to the study of oxidative-reductive metabolism of phosphorus and confirming our hypothesis.

Thematic Section: Biochemical Research. **Full Paper**
Subsection: Biochemistry of Cell Cultures. *Registration Code of Publication:* 13-36-12-53
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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Research into surface modifications of *E. coli lum* + under the influence of microwave radiation of millimeter range

© **Denis B. Kuznecov**,[1]*+ **Igor V. Lunegov**,[2] **Igor L. Volhin**,[2]
Vladimir L. Gein,[1] **Valery A. Neschislyaev**,[1] and **Anna A. Shirokih**[1]
[1] *Perm State Pharmaceutical Academy of Russian Ministry of Health. Polevaya Sr., 2. Perm, 614990. Perm Krai. Russia. Phone: +7 (342) 233-55-01. E-mail: denis.pfa @ gmail.com*
[2] *Perm State National Research University. Bukireva, St., 15. Perm, 614068. Perm Krai. Russia. Phone: +7 (342) 239-65-15. E-mail: neschislayew@gmail.com*

*Supervising author; +Corresponding author

Keywords: *atomic force microscopy, microwave radiation, adhesion, multilayer adsorption, water, cell.*

Abstract

It is shown that the adhesion strength at the surface of the bacterial cells depends on the time of exposure to electromagnetic radiation of the millimeter range. The value of the adhesion force shows how the thickness of layers of water molecules adsorbed on the surface of bacterial cells change. Rightfulness of the use of modern phase theory in interpreting the experimental data obtained in studies of changes in the properties of microorganisms irradiated millimeter microwave radiation has been demonstrated.

Thematic Section: Biochemical Research. **Full Paper**
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Divinyl ethers – bioactive products of linoleic acid metabolism

© Faimya K. Mukhitova,* **Anna V. Ogorodnikova**,*+ and **Alexandr N. Grechkin***
Kazan Institute of Biochemistry and Biophysics of Kazan Scientific Centre, RAS.
Lobachevsky St., 2/31. Kazan, 420111. The Republic of Tatarstan. Russia.
Phone: +7 (843) 231-90-40. E-mail: anyuta_ogorodnik@mail.ru

*Supervising author; +Corresponding author

Keywords: *linoleic acid, oxylipins, divinyl ether synthase (DES), divinyl ethers, colneleic acid, etheroleic acid.*

Abstract

The divinylethersynthase (DES) activity and divinyl ethers have been detected in the species of Asparagales: iris (*Iris germanika* L.*)*, gladiolus (*Gladiolus comunis* L.), crocus **(***Crocus vernus* L.) and hyacinth **(***Hyacinthus orientalis* L.). Exogenous linoleic acid was metabolized by roots and bulbs of the species predominantly into the divinyl ethers – etheroleic and colneleic acids. The products in the form of methyl esters of trimethylsilyl derivatives (Me TMS) were analyzed by gas chromatography–mass spectrometry. Testing the etheroleic acid on antiaggregatory activity showed hight effect on the platelets.

Full Paper _____ *Thematic Section:* Biochemical Research.
Registration Code of Publication: 13-36-12-66 *Subsection:* Organic Chemistry.
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http://butlerov.com/natural_resources/
Contributed: December 24, 2013.

Quantitative analysis of phenolic compounds in marigold flowers (*Calendula officinalis* L.) using microcolumn HPLC

© **Nina I. Kashchenko**, and **Daniil N. Olennikov**[+]*
Laboratory of Medical and Biological Research. Institute of General and Experimental Biology. Siberian Division. Russian Academy of Science. Sakh'yanovoy St., 6. Ulan-Ude, 670047. Russian Federation. Phone: +7 (3012) 43-47-43. E-mail: oldaniil@rambler.ru. Fax: +7 (3012) 43-47-43

*Supervising author; [+]Corresponding author

Keywords: *Calendula officinalis, Asteraceae, phenylpropanoids, flavonoids, microcolumn HPLC-UV.*

Abstract

The method of microcolumn reversed-phase HPLC with two wavelengths detection (330, 360 nm) was developed for quantitative analysis of 14 phenolic compounds using *ProntoSIL-120-5-C18* (2×75 mm) column and gradient eluent system [0.2 M $LiClO_4$ in 0.006 M $HClO_4$ – 0.01 M sodium dodecylsulphate in water (1:1)]-acetonitrile. The method was used for the analysis of marigold flowers (*Calendula officinalis* L.) and some drugs (tincture, liquid extract, dry extract, infusion, decoction). A comparative study of quantitative indicators of the mentioned drugs was performed.

Thematic Section: Preparative Research. **Full Paper**
Subsection: Supramolecular Chemistry. *Registration Code of Publication:* 13-36-12-75
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Contributed: December 6, 2013.

Synthesis of polysilsesquioxanes utilizing organosilicon derivatives of *p-tert*-butyl thiacalix[4]arene in cone conformation using base catalyst

© **Ludmila S. Yakimova**,[1] **Ramilya V. Ziatdinova**,[1] **Vladimir V. Gorbachuk**,[1] **Alena A. Vavilova**,[1] and **Ivan I. Stoikov**[1,2]*[+]

[1] *Department of Organic Chemistry. A.M. Butlerov Chemical Institute. Kazan Federal University. Kremlevskaya St., 18. Kazan, 420008. Russia. Phone: +7 (843) 233-74-62. E-mail: ivan.stoikov@mail.ru*
[2] *Kazan Institute of Biochemistry and Biophysics of Kazan Scientific Center of RAS. Lobachevsky St., 2/31. Kazan, 420111. Russia.*

*Supervising author; [+]Corresponding author

Keywords: *thiacalixarene, colloid particles, silsesquioxanes, IR-spectroscopy.*

Abstract

Using base-catalysis, colloidal particles on the basis of tetrasubstituted organosilicon derivatives of *p-tert*-butyl thiacalix[4]arene in *cone* conformation were synthesized. Colloid systems were characterized by ^{1}H NMR, IR spectroscopy and dynamic light scattering method. The particles with hydrodynamic diameter of about 2.2 μm were obtained. IR-spectrometry was used for characterization of polycondensation products. It is shown that the obtained product exists in the ladder structure containing more than five cyclotetrasiloxane fragments.

Short Communication _____ *Thematic Section:* Preparative Research.
Registration Code of Publication: 13-36-12-82 *Subsection:* Inorganic Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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Synthesis and investigation of polychromiumphenilsiloksanes, containing chromium atoms in oxidation state of +6

© **Svetlana G. Krasitskaya**,[+] **Alexander V. Alikovskiy**,*
Alexander A. Morontsev, **Mikhail I. Balanov**, and **Viktoria V. Vasileva**
Department of General, Inorganic and Elementoorganic Chemistry. School of Natural Sciences.
Far Eastern Federal University. Sukhanov St., 8. Vladivostok, 690950. Russia.
Phone: +7 (423) 248-83-80. E-mail: krasitskayasg@gmail.com

*Supervising author; [+]Corresponding author

Keywords: *synthesis, heterosiloxane, polychromiumphenilsiloxane, siloxane bond.*

Abstract

The article shows the possibility of synthesis of polychromiumphenilsiloxanes containing chromium atoms in highest oxidation state by phenyltrichlorosilane interaction with potassium chromate. The ratio of silicon to chromium can be increased by changing the stoichiometric ratio of the starting reagents. To obtain a positive result it is needed to introduce potassium carbonate into the reaction system in the amount considerably greater than stoichiometric. The resulting polymers were explored by elemental analysis, IR spectroscopy, X-ray diffraction analysis. Interplanar distances of polychromiumphenilsiloxanes with high chromium content are higher as compared to poliphenilsilseskvioxane.

Thematic Section: Chemical and Technological Research._____ **Full Paper**
Subsection: Organic Chemistry. *Registration Code of Publication:* 13-36-12-97
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: December 4, 2013.

Topic: Kinetics and mechanism of acyl transfer reactions. Part 6.

Quantum chemical interpretation of dipeptides and aminoacids reactivity in processes of acids amides and sulfamides formation

© **Ludmila B. Kochetova**,[1] **Natalia V. Kalinina**,[2] **Tatiana P. Kustova**,[1]*[+] and **Lev V. Kuritsyn**[2]
[1] *Department of Organic and Physical Chemistry. Ivanovo State University. Ermak St., 39. Ivanovo, 153025. Russia. Phone: +7 (84932) 37-37-03. E-mail: kustova_t@mail.ru*
[2] *Department of Inorganic and Analytical Chemistry. Ivanovo State University. Ermak St., 39. Ivanovo, 153025. Russia. Phone: +7 (84932) 37-37-03.*

*Supervising author; [+]Corresponding author

Keywords: *acylation, aminoacids, dipeptides, benzoyl chloride, sulfonyl chlorides, benzoic acid esters, quantum chemical calculation, reaction mechanism, potential energy surface.*

Abstract

Quantum chemical simulation of aminoacids and dipeptides anions, as well as chloroanhydrides of benzoic, sulfobenzoic, 3-nitro-, 4-methylsulfobenzoic acids and nitro substituted phenyl esters of benzoic acids is carried out by ab initio methods. It is established that values of nitrogen atoms charges can be used as reactivity indexes of nucleophiles in *N*-acylation; acylation agents reactivity is connected with LUMO energies of their molecules. PES of glycine reaction with 4-methylbenzene sulfonyl chloride in gaseous phase is calculated, it is shown that the reaction occurs by S_N2 mechanism.

Thematic Section: Study of Reactivity. **Full Paper**
Subsection: Supramolecular Chemistry. *Registration Code of Publication:* 13-36-12-105
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: December 6, 2013.

Thematic Course: Solid phase nanoreactor. Part IV.

Hydrogenation of *p*-nitrobenzoic acid esters in nanoreactors on the basis of sulfonated polymers

© **Heinrich N. Altshuler**,* **Galina Yu. Shkurenko**,+ and **Alexey A. Gorlov**
Institute of Coal Chemisry and Material Science, Siberian Branch of Russian Academy of Sciences.
Sovetskaya St., 18. Kemerovo, 650000. Russia. Phone: +7 (384-2) 36-80-22. E-mail: altshulerh@gmail.com

*Supervising author; +Corresponding author

Keywords: *nanoreactor, cross-linked polymers, p-nitrobenzoic acid esters, hydrogenation.*

Abstract

Hydrogenation of aromatic nitro compounds in the nanoreactors based on sulfonated cross-linked polymers containing nanoparticles of palladium have been studied. The kinetic characteristics of the hydrogenation of nitrobenzene, *p*-nitrobenzoic acid, methyl, ethyl and propyl esters of the *p*-nitrobenzoic acid were calculated.

Full Paper _____ *Thematic Section:* Study of Reactivity.
Registration Code of Publication: 13-36-12-110 *Subsection:* Chemistry of Complex Compounds.
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Contributed: December 19, 2013.

Ions of oxovanadium(IV) in the reactions of formation of heterometallic dtpa-complexes with cations of chromium(III)

© Tatiana V. Popova,[1]* **Natalia V. Scheglova**,[2]
Tatiana V. Smotrina,[3+] and **Ekaterina V. Motovilova**[2]
[1] *Department of Pharmacology and Pharmaceutical Sciences. Moscow Region State Institute of Humamities (MGOGI). Zelenaya St., 22. Orekhovo-Zuevo, 142611. Russian Federation. Phone: +7 (965) 328-23-58. E-mail: tvpopova45@yandex.ru*
[2] *Department of Chemistry. Mari State University. Lenin Sq., 1. Yoshkar-Ola, 424000. Mari El Republic. Russian Federation. Phone: +7 (8362) 42-55-94. E-mail: ecoanalit@marsu.ru*
[3] *Department of Physics. Volga State Technological University. Lenin Sq., 3. Yoshkar-Ola, 424000. Mari El Republic. Russia. Phone: +7 (8362) 68-68-04. E-mail: tatyana-smotrina@yandex.ru*

*Supervising author; +Corresponding author

Keywords: *spectrophotometric method, diethylenetriaminepentaacetic acid, heterobinuclear complexes of oxovanadium(IV) with cations of chromium (III).*

Abstract

The reactions of formation of heterometallic diethylenetriaminepentaacetates of oxovanadium(IV) with cations of chromium(III) in aqueous solution have been studied by the spectrophotometric method. The accelerating effect of oxovanadium(IV) cations on the process of coordination of chromium(III) cations by anions of carboxylate ligand in heterometallic complex has been established.

Thematic Section: Investigation of Properties of Substances._____ **Full Paper**
Subsection: Chemistry of Dyes. *Registration Code of Publication:* 13-36-12-115
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: November 20, 2013.

Assessment of the impact of the structure of heterocyclic radical on the properties of the hetarylcontaining azo dyes

© **Alexander I. Ryndin**,[1] **Dmitry N. Kuznetsov**,[1]*+ **Konstantin I. Kobrakov**,[1] **Olga V. Kovalchukova**,[2] and **Maria B. Dmitrieva**[3]

[1] *Department of Organic Chemistry. Moscow State University of Design and Technology. Sadovnichesky St., 33. Moscow, 117997. Russia. Phone: +7 (495) 955-35-58. E-mail: occd@mail.ru*

[2] *Department of General Chemistry. Russian University of Peoples' Friendship. Maclay St., 6. Moscow, 117198. Russia. Phone: +7 (495) 955-08-60. E-mail okovalchukova@mail.ru*

[3] *Center for Biological Control Laboratory Microfilming and Document Restoration. Russian State Archive of Scientific and Technical Documentation. Profsoyuznaya St., 82. Moscow, 117393. Russia. Phone: +7 (495) 335-00-95. E-mail: biorest.maria@gmail.com*

*Supervising author; +Corresponding author

Keywords: *heterocyclic hetaryl-containing azo dyes, dyeing polyamide fabric, fungicidal activity, analysis of the relationship "structure-property".*

Abstract

In this paper, synthesized series of structurally similar aryl(hetaryl)containing azo dyes are described. The influence of the nature of the heterocyclic radical on the spectral, operational and biocidal properties of the dyes was analyzed.

Full Paper _____ *Thematic Section:* Study of Materials Modifications.
Registration Code of Publication: 13-36-12-124 *Subsection:* Inorganic 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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Transformations on the surface of indium arsenide in nitric acid

© **Oksana N. Zarubina**,[+] **Liubov V. Maliy**, and **Gennady M. Mokrousov***
Department of Chemistry. Tomsk State University.
Lenin Pr., 36. Tomsk, 634050. Russia. Phone: +7 (3822) 42-07-83.
*E-mail: zagtsuru@gmail.com[+], NaumovaLB@mail.ru**

*Supervising author; [+]Corresponding author

Keywords*: indium arsenide, interphase transformations, surface, etching, diagram of potential – pH.*

Abstract

The conditions of formation of dense phase layer consisting mainly of arsenic and small amount of its oxide on the *n*-InAs surface in concentrated nitric acid are founded. With the use of thermodynamic concepts (diagram potential of InAs – pH) the possible mechanism of reactions at the interface and the formation of arsenic phase was considered. Phase and elemental composition, morphology of formed surfaces are investigated by Raman spectroscopy, solid-state voltammetry, scanning electron microscopy, X-ray diffraction and EDX analysis.

Full Paper _____ *Thematic Section:* Technological Study.
Registration Code of Publication: 13-36-12-128 *Subsection:* Petrochemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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Effect of activation conditions of high modulus silicate systems and raw materials volumetric feed rate on conversions of *n*-hexane

© **Raisa I. Kuzmina**, **Sergey V. Ignatyev**, and **Anton Yu. Pilipenko**
Department of Petrochemicals and Technological Security. Institute of Chemistry. N.G. Chernyshevsky Saratov State University. Astrakhanskaya St., 83, block 1. Saratov, 410012. Russia.
Phone: +7 (8452) 52-50-07. E-mail: kuzminaraisa@mail.ru

*Supervising author; +Corresponding author

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

Abstract

Conversion of *n*-hexane in the temperature range 250-500 °C has been investigated. It has been established that the conversion process of *n*-hexane involves the cracking reaction, isomerization and aromatization. Direction of chemical reactions depends on the activation parameters and process conditions.

Thematic Section: Technological Research. **Brief Communication**
Subsection: Composite Materials. *Registration Code of Publication:* 13-36-12-137
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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Contributed: November 12, 2013.

Development of composite materials for the construction of motorways on the basis of oil slime and drilling mud residue

© **Dina K. Mendalieva**,[2] **Zaripa Ha. Kunasheva**,[2] **Jamila B. Yakupova**,[2]
Raisa I. Kuzmina,[1] and **Ilya P. Shirokov**[1]
[1] *Department of Petrochemicals and Technological Security. Institute of Chemistry, Saratov State University. Astrakhanskaya St., 83. Saratov, 410012. Russia. Phone: +7 (8452) 52-50-07.*
E-mail: kuzminaraisa@mail.ru, shirokov_ip@mail.ru
[2] *Department of Chemistry. West-Kazakhstan State University. Dostyk Pr., 162. Uralsk, 090006. Kazakhstan.*

*Supervising author; +Corresponding author

Keywords*: bitumen, composite material, drilling mud, oil slime.*

Abstract

The phase and elemental composition of the solid residue of the drilling mud was studied. Physical and mechanical parameters of oil slime were evaluated. A series of test samples of composite materials was developed and their physicochemical characteristics were studied. The physicochemical characteristics of the resulting material comply with the requirements and can be used in motorway construction.

Full Paper _____ *Thematic Section:* Research Into New Technologies.
Registration Code of Publication: 13-36-12-140 *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/
Contributed: December 19, 2013.

Researches on determination of an optimal dispersing component during production of a disk like powder

© **Aigul R. Ignat'eva**,*+ **Elena I. Staroverova**, **Sufiya M. Abdulkayumova**, **Andrey S. Arutyunian**, **Rosa F. Gatina**, **Alexey I. Khatsrinov**, and **Yury M. Mikhailov**
"State Research Institute of Chemical Products" Federal State Enterprise.
Svetlaya St., 1. Kazan, 420033. Russia. Phone: +7 (843) 544-07-21. E-mail: gniihp@bancorp.ru

*Supervising author; +Corresponding author

Keywords: *dispersing component, surface active substance (SAS), water dispersing process, emulsion, dispersion, sedimentation stability, disk like powder.*

Abstract

The results of experiments on choosing a dispersing component (SAS) during the production of a disk like powder are presented. The possibility of obtaining disk like powder granules by means of changing hydrodynamical parameters of dispersion and using of dispersing component with more than 7°E viscosity during the procedure has been shown.

Thematic Section: Physicochemical Research. **Full Paper**
Subsection: Physical Chemistry of Explosives. *Registration Code of Publication:* 13-36-12-147
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Research of burning of mixed compositions on the basis of ammonium nitrate, containing dinitramide salts

© **Vladimir N. Popok**,*+ **Valentina S. Loginova**, and **Alexey Yu. Kolesnikov**
Open Joint Stock Company «Federal Research and Production Center «Altay».
Sotsialisticheskaya St., 1. Biysk, 659322. Altay territory. Russia.
Phone: +7 (3854) 30-19-37. E-mails: vnpopok@mail.ru

*Supervising author; +Corresponding author

Keywords: *salts of dinitramide, ammonium nitrate, powders of aluminum, combustible-binding, burning speed, thermal decomposition.*

Abstract

In the article, the results of researches of guanylurea and guanidinium salts of dinitramide effects on the parameters of burning and thermal decomposition of compositions on the basis of ammonium nitrate and combustible-binding with nitramino-nitrotriazole softener are presented. The metallic and metal-free compositions are considered. For comparison, the results are given of the compositions containing HMX and HNIW. It is shown that at introduction of the considered salts of dinitramide into the structure of compositions the realized level of speed of burning corresponds to the level for systems with nitramines, thus burning temperature sharply decreases.

Full Paper _____ *Thematic Section:* Physicochemical Research.
Registration Code of Publication: 13-36-12-156 *Subsection:* Physical Chemistry of Cellulose.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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Contributed: November 29, 2013.

Influence of deuterium exchange on the processes of proton magnetic relaxation in polysaccharides

© **Tatiana V. Smotrina**,*+ and **Leonid Yu. Grunin**
Department of Physics. Volga State Technological University. Lenin Sq., 3. Yoshkar-Ola, 424000. Mari El Republic. Russia. Phone: +7 (8362) 68-68-04. E-mail: tatyana-smotrina@yandex.ru

*Supervising author; +Corresponding author

Keywords: *celulose, chitosan, deuterium exchange, nuclear magnetic resonance.*

Abstract

Method of relaxation spectroscopy of proton magnetic resonance (PMR) using the technique of deuterium exchange was applied to analyze free induction decay signals obtained from dried and wet polysaccharides. Free induction decay signals were approximated by the function of three exponents sum, each of them describing the magnetization decay in areas with different degree of orderliness. Cellulose and chitosan were used as samples. It was found that if the isotope exchange reaction is carried out with an excess of liquid D_2O, protons are involved to reaction not only from amorphous areas, but also from some parts of the ordered areas. It is shown that the influence of the plasticizing action of sorbate molecules increases the mobility of each component of the whole system, accompanied by changes of the proton density in the areas with different orderliness.

Thematic Section: Thermodynamic Research. **Full Paper**
Subsection: Inorganic Chemistry. *Registration Code of Publication:* 13-36-12-163
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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Phase equilibria involving oxide-fluoride melts of sodium and aluminium

© **Svetlana E. Pratskova**,[+] and **Aleksandr G. Tyurin***
Department of Analytical and Physical Chemistry. Chelyabinsk State University. Br. Kachirinych St., 129. Chelyabinsk, 454136. Russia. Phone: +7 (351) 799-70-69. E-mail:se_pratskova@mail.ru.

*Supervising author; [+]Corresponding author

Keywords: *oxide-fluoride melts, generalized model of "regular" ionic solutions, active component, energy parameters of theory, kvazibinary.*

Abstract

In this paper, within the frameworks of the generalized model of "regular" ionic solutions there are described thermodynamic properties of oxide-fluoride melts NaF – Na_2O – Al_2O_3 – AlF_3 in the temperature range 1270-2300 K. Standard Gibbs energies of the formation reactions of the intermediates of fluorides and oxides of sodium and aluminum have been calculated. Qvazibinars of the system studied have been built. Thermodynamic properties are made consistent with thermodynamic melting characteristics of pure oxides and fluorides, Gibbs energy of the exchange reaction and phase diagrams.