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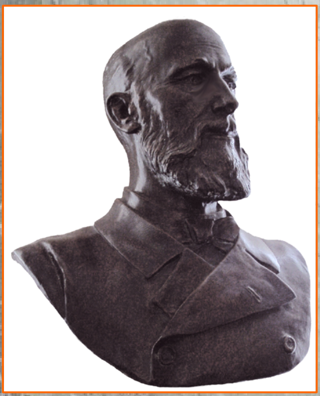

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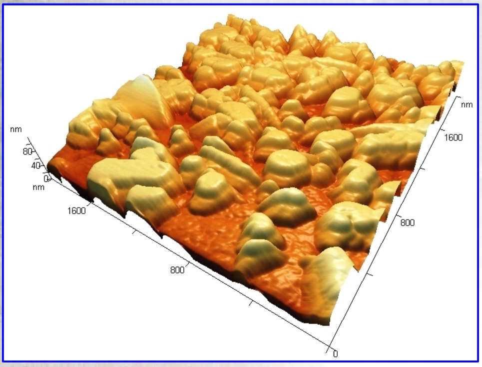

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Thematic Section: Study of New Processes. **Full Paper**
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Selective oxidation of CO in H_2 stream on nano Au catalyst supported on $CuO-CeO_2$

© **Der-Shing Lee**, and **Yu-Wen Chen***⁺
Department of Chemical Engineering. National central University.
Jhong-Li, 32001. Taiwan. Phone: +886 3 4227151. E-mail: ywchen@ncu.edu.tw

*Supervising author; ⁺Corresponding author

Keywords: selective oxidation, carbon monoxide, hydrogen stream, catalysts, deposition-precipitation method.

Abstract

Nanoscaled gold particle supported on CeO_2 and modified by CuO was used for selective oxidation of carbon monoxide in hydrogen stream (PROX). CuO-modified CeO_2 support was prepared by co-precipitaion method. Gold was loaded on the support by deposition-precipitation method. These catalysts were characterized by X-ray diffraction, N_2-sorption, TEM, HR-TEM, and XPS to gain the structural information. The PROX reaction was carried out in a fixed bed continuous flow reactor with a feed of CO: O_2: H_2: He = 1.33: 1.33: 65.33: 32.01 in volume ratios. CO/O_2 ratio was fixed at 1. The recation was caried out between ambient temperature and 100 ^oC with GHSV of 30.000 h^{-1}. The particle size of gold was around 2-5 nm and Au particles were dispersed well on the support. The results showed that the catalyst with specific Cu content and calcination temperature could reach 100% of CO conversion at the PEM fuel cells operating temperature (65 ^oC-100 ^oC) even as the gold content was reduced from 1 wt. % to 0.5 wt. %. The incorporation of copper ion into ceria lattice promoted the oxygen storage capacity of ceria support and enhanced the activity of catalysts. The higher calcinations temperature for the support resulted higher crystallinity of CeO_2, leading to the higher activity. The CO selectivity increased with increasing copper content. The catalyst with CuO content of 20% demonstrated the highest activity and selctivity for CO oxidation and suppress H_2 oxidation at 100 ^oC.

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Thematic course: Hydrochemical synthesis of metal chalcogenide films. Part 25.

Hydrochemical deposition features of metal sulfide and selenide films

© **Vyacheslav F. Markov**,[1,2]* **Larisa N. Maskaeva**,[1,2+] and **Tatiana A. Alekseeva**[1]
[1] *Chair Physical and Colloidal Chemistry. The Ural Federal University of a Name of 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@ural.ru*
[2] *Chair of Chemistry and Burning Processes. Ural Institute GPS of the Ministry of Emergency Measures of Russia. Mira St., 22. Ekaterinburg, 620022. Russia. Phone: +7 (343) 360-81-68.*

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*Supervising author; [+]Corresponding author

Keywords: chemical bath deposition, thin films, metal sulfides, metal selenides, fractality.

Abstract

The features of the chalcogenizator nature, the reaction solution composition and temperature prehistory at hydrochemical deposition described. It is offered to expand idea of the chalcogenizator activation by joining various strength nucleophils. The reaction solution anions play a role of nucleophil. It is shown the role of anionic component of cadmium salt in the solid solution formation $Cd_xPb_{1-x}S$. Influence of a cationic component of the entered salt on morphology, texture and properties of sulfide films is established. Mixed effect of temperature prehistory of water solution components of reactionary mixture is revealed on the architecture, composition and photoelectrical properties of the thin films. The fractal regularities are calculated for deposition of thin sulfide and selenide films. It is concluded that the cluster - cluster aggregation of particles is the basis of chemical bath deposition.

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Thematic course: Hydrochemical synthesis of metal chalcogenide films. Part 26.

Effect of complexing agent on the morphological features of the CdS thin films formation by the chemical bath deposition

© **Natalia A. Forostyanaya**,[1] **Larisa N. Maskaeva**,[1,2] **Vyatcheslav F. Markov**,[1,2]*
Danila V. Leontiev,[3] and **Lev V. Shaidarov**[1]

[1] *Physical and Colloid Chemistry Department. Ural Federal University Named After the first President of Russia B.N. Yeltsin. St. Mira, 28. Yekaterinburg, 620002.*
Russia. Phone: +7 (343) 375-93-67. E-mail: natal-ku8@yandex.ru
[2] *Ural Institute of State Fire Service Russian Emergencies Ministry. St. Mira, 22. Yekaterinburg, 620062.*
Russia. Phone: (343) 378-38-75. E-mail: mln@ural.ru
[3] *Immunochemistry Department . Ural Federal University Named after the first President of Russia B.N. Yeltsin. St. Mira, 28. Yekaterinburg, 620002.*
Russia. Phone: +7 (343) 375-93-18. E-mail: Donshinigami1@mail.ru

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*Supervising author; +Corresponding author

***Keywords**:* chemical bath deposition, complexing agents, degree of supersaturation, thin films, cadmium sulfide, morphology, scanning electron microscopy, atomic force microscopy.

Abstract

Equity concentration of prevailing complex compounds were defined by analyzing of the ionic equilibria in the system «Cd^{2+} – L – N_2H_4CS», where (L – NH_3, $H_2NCH_2CH_2NH_2$, $C_6H_5O_7^{3-}$, (NH_3+$C_6H_5O_7^{3-}$). It was found that the maximum degree of supersaturation in the reaction mixture is matches to system containing the citrate ions and the minimum when ethylenediamine was used. The regularities of the surface topography of cadmium sulfide thin films synthesized from aqueous solutions with different ligands were identified. Connection between the surface development and set of ligand, which inputs into solution was established by scanning electron and atomic force microscopy.

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Theoretical and experimental estimation of tungsten and iron separation effectiveness for further arsenic and antimony determination in ferrotungsten by ICP-AES

© **Anna V. Maiorova,**[1]*+ **Anastasia A. Belozerova,**[1] **Nadezda V. Pechishcheva,**[1]
Natalia G. Boyarnikova,[2] and **Konstantin Yu. Shunyaev**[1]
[1] *Institute of Metallurgy UB RAS. Amundsena St., 101. Yekaterinburg, 620016. Russia.*
Phone: +7 (343) 267-89-36. E-mail: imeturoran@mail.ru
[2] *Ural Federal University. Mira St., 19. Yekaterinburg, 620002. Russia.*

*Supervising author; +Corresponding author

Keywords: tungsten, arsenic and antimony determination, thermodynamic modeling, inductively coupled plasma atomic emission spectrometry.

Abstract

Thermodynamic modeling with «HSC» software was used to choose a composition of the reagents mixture for ferrotungsten samples sintering before determining arsenic and antimony by inductively coupled plasma atomic emission (Na_2CO_3:K_2CO_3:S mixture). The sintering allows separating analytes from the main part of interfering tungsten matrix. Missing data for modeling, namely, thermochemical properties of some sodium and potassium antimonates and antimonites, tungsten, arsenic and antimony thiosalts were calculated by group contribution method. Further experiments showed that leaching of the cake by solution containing $Ba(CH_3COO)_2$ can additionally separate analytes from matrix components and improve the analysis results. Analysis of ferrotungsten certified reference materials showed the effectiveness of the proposed method of sample preparation.

Thematic Section: Study of New Processes. **Full Paper**
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Kinetics of the joint recovery of nickel and hydrogen in the diffusion mode

© **Andrey V. Patrushev**, **Tatiana N. Ostanina**,
Valentin M. Rudoy, and **Anna Borisovna Darintseva**
Department of Electrochemical Production Technology. Ural Federal University
named after the first President of Russia Boris Yeltsin. St. Mira, 28. Ekaterinburg, 620002.
Sverdlovsk region. Russia. Phone: +7 (343) 375-44-63. E-mail: patrushev.xs666@mail.ru

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*Supervising author; +Corresponding author

***Keywords**:* recovery, nickel ions, hydrogen, kinetic parameters, diffusion regime.

Abstract

On the basis of polarization measurements to determine the kinetic parameters of the discharge of nickel ions and hydrogen. Discharge of hydrogen has no significant effect on the kinetics of recovery of nickel ions, but affects the diffusion parameters of the near-electrode space due to the mixing of gas bubbles. Given the current efficiency and the real surface area of the electrode evaluated currents partial recovery of nickel and hydrogen under conditions of high diffusion limitations for delivery of metal ions to the interface dendritic crystallization and precipitation. It has been shown that the apparent heterogeneous rate constant discharge hydrogen at the joint with the recovery of nickel ions is substantially less than in the background solution.

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Studying of possibility of division of compounds of cobalt and molybdenum in the fulfilled catalysts

© **Yulia A. Khatsrinova**,[1] **Alexey I. Khatsrinov**,[2] and **Alsy Z. Sylejmanova**[3]
[1] *Kafedra Technologies of Inorganic Substances and Materials. Kazan National Research Technological University. St. Siberian path, 12 buildings E. Kazan, 420029. Republic of Tatarstan. Russia.*
Phone: +7 (843) 231-40-13. Email: Khatsrinova12@mail.ru
[2] *Kafedra Technologies of Inorganic Substances and Materials. Kazan National Research Technological University. St. Siberian path, 12 buildings E. Kazan, 420029. Republic of Tatarstan. Russia.*
Phone: +7 (843) 231-40-13.
[3] *Kafedra Technologies of Inorganic Substances and Materials. Kazan National Research Technological University. St. Siberian path, 12 buildings E. Kazan, 420029. Republic of Tatarstan. Russia.*
Phone: +7 (843) 231-40-13.

*Supervising author; +Corresponding author

Keywords: molybdenum, cobalt, catalyst, utilization, alloy, extraction method.

Abstract

Article is devoted to a scientific problem of division of compounds of cobalt and molybdenum in the fulfilled catalysts. It will provide utilization and processing. The technology of division on the basis of alloyage of the fulfilled catalyst with sodium hydroxide is offered. The schematic diagram of division of compounds of cobalt and molybdenum for the catalysts fulfilled the kobaltomolibdenovykh is offered.

Thematic Section: Study of New Processes. **Full Paper**
Subsection: Inorganic Chemistry. *Registration Code of Publication:* 15-41-1-53
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Research of possibility of utilization molibdensoderzhashchikh of catalysts

© **Yulia A. Khatsrinova**,[1] **Alexey I. Khatsrinov**,[2] and **Alsy Z. Sylejmanova**[3]
[1] *Kafedra Technologies of Inorganic Substances and Materials. Kazan National Research Technological University. St. Siberian path, 12 buildings E. Kazan, 420029. Republic of Tatarstan. Russia. Phone: +7 (843) 231-40-13. Email: Khatsrinova12@mail.ru*
[2] *Kafedra Technologies of Inorganic Substances and Materials. Kazan National Research Technological University. St. Siberian path, 12 buildings E. Kazan, 420029. Republic of Tatarstan. Russia. Phone: +7 (843) 231-40-13.*
[3] *Kafedra Technologies of Inorganic Substances and Materials. Kazan National Research Technological University. St. Siberian path, 12 buildings E. Kazan, 420029. Republic of Tatarstan. Russia. Phone: +7 (843) 231-40-13.*

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*Supervising author; +Corresponding author

Keywords: utilization, molibdensoderzhashchy catalysts, technology of division.

Abstract

Article is devoted to development of a technique of division of cobalt and molybdenum in the kobaltomolibdenovykh catalysts. The method of alloyage of the fulfilled catalyst with sodium hydroxide was used. For joint extraction acetone was offered. It will allow to reduce quantity of waste and to improve ecology of industrial regions.

Full Paper ____ *Thematic Section:* Study of New Processes.
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The article is published on materials of the report on "International Scientific Forum
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Submitted on March 12, 2015.

Thermophysical bases of catalytic and non-catalytic transesterification of rapeseed oil in ethanol under supercritical fluid conditions

© **Sergey V. Mazanov,**[1*+] **Rustem A. Usmanov,**[1] **Ilgiz R. Gabitov,**[1]
Farid M. Gumerov,[1] **Zufar I. Zaripov,**[1] and **Rashid Z. Musin**[2]
[1] *Heat Engineering Department. Kazan National Research Technological University.*
K. Marx St., 68. Kazan, 420015. The Republic of Tatarstan. Russia.
Phone: +7 (843) 231-42-11. E-mail: serg989@yandex.ru
[2] *The Laboratory of Physical and Chemical Analysis. A.E. Arbuzov Institute of Organic and Physical Chemistry. Kazan Scientific Center of Russian Academy of Sciences. Arbuzov St., 8. Kazan, 420088.*
The Republic of Tatarstan. Russia. Phone: +7 (917) 289-31-75. E-mail: musin@iopc.ru

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*Supervising author; +Corresponding author

Keywords: transesterification, biodiesel fuel, heterogenic catalysis, ethyl ethers of fatty acids, thermal degradation, heat capacity.

Abstract

Catalytic and non-catalytic transesterification reactions of rapeseed oil in ethanol medium have been experimentally investigated under SCF condition with ultrasonic exposure on the reactive environment. The temperature range from 623 K to 653 K, pressures up to 30 MPa and molar ratio of "ethyl alcohol - rapeseed oil" from 6: 1 to 20:1. Heterogeneous catalysts have been used (Al_2O_3, ZnO/Al_2O_3, MgO/Al_2O_3, SrO/Al_2O_3). New data have been obtained on the isobaric heat capacity of the ternary system "ethanol - rapeseed oil - catalyst" with a molar ratio from 6:1 to 30:1 in the temperature range of 303-563 K and pressures of 9.8 - 29.4 MPa.

Thematic Section: Study of New Processes. **Full Paper**
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Effect of oxygen-containing surface functional groups of carbon electrodes on the self-discharge of supercapacitors

© **Svetlana V. Stakhanova,**[+] **Mikhail V. Astakhov,*** **Anastasia A. Klimont**, **Ilya S. Krechetov**,
Anatoly T. Kalashnik, **Ruslan R. Galymzyanov**, **Olesya V. Zaytseva**,
and **Natalia V. Sviridenkova**
Physical Chemistry Division. National University of Science and Technology MISiS.
Leninsky Prospekt, 6. Moscow, 119049. Russia.
Phone: +7 (495) 638-46-64. E-mail:svladlen@rambler.ru

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*Supervising author; [+]Corresponding author

Keywords: supercapacitor, carbon fiber, carbon cloth, carbon felt, sodium borohydride.

Abstract

The mechanism of self-discharge of supercapacitors due to redox reactions of oxygen-containing surface functional groups of the carbon electrode material is discussed. It has been shown that treatment of the carbon material with sodium borohydride or ammonia modification can significantly reduce the self-discharge without loss or with some increase in capacitance characteristics.

Full Paper ____ *Thematic Section:* Study of New Processes.
Registration Code of Publication: 15-41-1-74 *Subsection:* Physical Chemistry.
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Physical and chemical properties of the modified vermiculite

© **Irina G. Khalchenko,**[+] **Nikolay P. Shapkin,*** **Irina V. Svistunova**,
and **Edward Anatolyevich Tokar**
The Department of General. Inorganic and Organoelemental Chemistry of the School of Natural Sciences.
Far Eastern Federal University. Octyabrskaya St., 27. Vladivostok, 690000. Russia.
Phone: +7 (8423) 245-76-69. E-mail: npshapkin@gmail.com

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*Supervising author; [+]Corresponding author

***Keywords**:* modified vermiculite, chitosan, composition and structure of the modified silicate, adsorption characteristics, specific surface area, internal pore volume.

Abstract

Vermiculite from Kovdorskiy (Karelia), modified be acid, chitosan, were investigated by positron annihilation spectroscopy, density measurement, dye adsorption, the nitrogen adsorption BET and porosimetry.

It was shown that the density of vermiculites after acid treatment varies compared to the density of the initial samples, depending on the concentration of acid. The density increases with the increasing acid concentration. Internal volume of the micropores and the value of maximum adsorption of brilliant green change is directly proportional to the density of modified vermiculite.

Thematic Section: Study of New Processes. **Full Paper**
Subsection: Physical Chemistry. *Registration Code of Publication:* 15-41-1-83
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The influence of asparagine on electrokinetic and adsorption properties of the iron(III) and nickel(II) oxides

© **Irina B. Dmitrieva**,* **Alexander S. Chukhno**,$^+$ and **Ekaterina Yu. Rodionova**
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: irina@dmitriyev.ru, alex-chuhno@yandex.ru

*Supervising author; $^+$Corresponding author

Keywords: asparagine, electrokinetic properties microelectrophoresis, isoelectric point, the adsorption of oxides, iron(III) and nickel(II).

Abstract

Electrosurface properties of NiO and Fe_2O_3 oxides have been investigated in water solutions of asparagine depending on its concentration, pH of solutions and time of adsorption. It has been found that asparagine is specifically adsorbed on the surface of Fe_2O_3 and NiO. It has been demonstrated that the adsorption of anionic forms asparagine at Fe_2O_3 and cationic forms at NiO predominates.

Full Paper *Thematic Section:* Study of New Processes.
Registration Code of Publication: 15-41-1-90 *Subsection:* Organic Chemistry.
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Influence of the benzyl-substitution in porphyrin macrocycles on its ability to extra-ligand axial coordination

© **Galina M. Mamardashvili,***+ **Olga V. Maltceva**, and **Natalya V. Chizhova**
G.A. Krestov Institute of Solution Chemistry of the Russian Academy of Sciences. Akademicheskaya St., 1. Ivanovo, 153045. Russia.Phone: +7 (4932) 33-69-90. E-mail: gmm@isc-ras.ru

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*Supervising author; +Corresponding author

Keywords: zinc tetrabenzoporphyrin complexes, axial ligands, nitro-substitution, spectrophotometric titration.

Abstract

Axial coordination processes of the extra-ligands (pyridine and 1-methilmidasol) with zinc(II) tetrabenzoporphyrin and its tetra-nitrosubstituted analogue were investigated in toluene by the spectrophotometric titration and computer simulating methods. It was established, that the expansion of the aromatic π-system by addition of additional cycles results in the increasing of the porphyrinic macrocycle binding ability with axial ligands, in comparison with zinc(II) aryl- and alkyl-substuted porphyrins. The coordination process is accompanied by the red shifts of the absorption bands in the UV-Vis spectra of the reactionary system. It was shown, that the influence of the nito-substitution in tetrabenzoporphyrinic macrocycle on the axial coordination processes is less as compared with the influence of similar substitution in the octaethylporphirin.

Full Paper *Thematic Section:* Study of New Processes.
Registration Code of Publication: 15-41-1-96 *Subsection:* Polymer Chemistry.
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Studying the process of foaming of epoxy resin in the presence of new polyaminoalkylphenols acting as a blowing agent and hardener

© **Ksenia A. Medvedeva**,[+] **Dmitry G. Miloslavskiy**[+] **Elena N. Cherezova**,* and **Elena M. Gotlib***
Department of Synthetic Rubber Technology. Institute of Polymers. Kazan National Research Technological University. Karl Marx St., 72. Kazan, 420015. Tatarstan Republic. Russia.
Phone: +7 (843) 231-42-14. E-mail: ksmedvedeva@rambler.ru

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*Supervising author; [+]Corresponding author

***Keywords**:* epoxy foam, poliaminoalkilphenols, blowing agent, surface active agents.

Abstract

Process of foaming of epoxy resin ED-20 in the presence of new poliaminoalkilfenol (PAPh) received by interaction of phenol (Ph), an etilenbisamin (EBA) and a paraformaldehyde (P) at a different order of input of ingredients and their ratio is studied. It is shown that the technology of its preparation, namely an order of input of reagents has impact on efficiency of PAPh as a blowing agent. For further development of work it is offered to use PAPh-1 received at 45 °C by option 1 and the ratio Ph:P:EBA = 1:2:2.

Thematic Section: Research of the New Processes. **Full Paper**
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Modification of vulcanizates based on styrene-butadiene rubber (SBR-1705 HI-AR) by lignocellulosic additives

© **Elena N. Cherezova**,[1] **Elena V. Udoratina**,[2] **Evgeny G. Shakhmatov**,[2] and **Yulia S. Karaseva**[1]
[1] *Technology of Synthetic Rubber Department. Kazan National Research Technological University. Karl Marx St., 68. Kazan, 420015. Tatarstan. Russia. E-mail: cherezove@rambler.ru*
[2] *Laboratory of Plant Polymers. Komi Scientific Center of UB RAS. Institute of Chemistry. Pervomaiskaya St., 48. Syktyvkar, 167982. Komi Republic. Russia.*

*Supervising author; +Corresponding author

Keywords: lignocellulosic powders, modifier, rubber.

Abstract

Lignocellulosic additives-modifiers for polymers were obtained by thermomechanical processing of wood pulp and its further modification by Lewis acids and by processing of microcrystalline cellulose with organic amines. The influence of the additives on vulcanization kinetics of compounds and complex of physico-mechanical properties of vulcanizates based on styrene-butadiene rubber (SBR-1705 HI-AR) was examined.

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Generation of sulfur aerosol by pyrotechnic compositions

© **Anastasia V. Strelkova**,[1] **Aleksander M. Pyzhov**,[1]*+ **Vladimir A. Rekshinskiy**,[1]
Ivan K. Kukushkin,[1] and **Pyotr P. Purygin**[2]
[1] *Chair of Chemistry and Technology of Organic Nitrogen Compounds. Samara State Technical University. Molodogvardeyskaya St., 244. Samara, 443100. Samara region. Russia. Phone: +7 (846) 337-08-89. E-mail: argel33@mail.ru*
[2] *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: puryginpp2002@mail.ru*

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*Supervising author; +Corresponding author

***Keywords**:* sulfur aerosol, a pyrotechnic composition, ammonium nitrate, activated carbon, sulfur aerosol generators, ignition system, industrial tests.

Abstract

This article presents results of research on the development of pyrotechnic composition and device for the generation of sulfur aerosol in combustion mode. The main tasks that it was decided, was to increase the safety of the manufacture and application of sulfur aerosol generator, simplification and cheapening of the process of its manufacture while maintaining a high efficiency of its application, as well as in the development of system of ignition of his pyrotechnic composition. The main difference pyrotechnic composition for generating sulfur aerosol, developed by the authors from the currently existing in Russia and abroad is that the composition does not contain nitrocellulose and processed products is scarce and sensitive to external influences components. As oxidant, as one of the components of the thermal fundamentals of aerosol composition was used ammonium nitrate and fuel – activated carbon. It was shown that only in this case it was possible to achieve stable low-temperature combustion process composition containing about 40% active ingredient is sulfur. As a result of long research was the design of a generator of sulfur aerosol and its ignition system with enhanced safety of manufacture and use, simplicity and low cost and with high efficiency.

Full Paper _______________________________ *Thematic Section:* Study of New Processes.
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Coprocessing organochlorine and TNT productions

© **Aleksander M. Pyzhov**,[1+] **Ivan K. Kukushkin**,[1]* **Yaroslav A. Yakovlev**,[1]
and **Pyotr Petrovich Purygin**[2]
[1] *Chair of Chemistry and Technology of Organic Nitrogen Compounds. Samara State Technical University. Molodogvardeyskaya St., 244. Samara, 443100. Samara region. Russia.*
Phone: +7 (846) 337-08-89. E-mail: argel33@mail.ru
[2] *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: puryginpp2002@mail.ru*

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*Supervising author; [+]Corresponding author

***Keywords**:* industrial waste, organochlorine production bleach sludge, TNT production, sulphite liquor, sulfate ash, co-processing, gypsum, bleaching compositions, silicate glass.

Abstract

This article presents results of research on the development of an efficient method for the recovery and recycling joint waste organochlorine and TNT productions in the manufacture of silica glass and bleaching compositions like "Belizna". Existing methods of co-processing of wastes of these industries had flaws that were or low quality target product, or need to use up to 80% of scarce natural resources. The proposed method of disposal of organochlorine and TNT productions based on the replacement of natural calcium and sulfate-containing components of the original glass batch on the waste mentioned industries in the manufacture of silica glass. It is shown that the quality of the silicate glass and the whitening composition matches the quality of industrial materials.

Thematic Section: Study of New Processes. **Full Paper**
Subsection: Physical Chemistry of Explosives. *Registration Code of Publication:* 15-41-1-117
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Assessment of opportunities waste of TNT different retention periods

© **Aleksander M. Pyzhov,**[1+] **Ivan K. Kukushkin,**[1]*
Evgeniy E. Romashin[1] and **Pyotr P. Purygin**[2]
[1] *Chair of Chemistry and Technology of Organic Nitrogen Compounds. Samara State Technical University. Molodogvardeyskaya St., 244. Samara, 443100. Samara region. Russia. Phone: +7 (846) 337-08-89. E-mail: argel33@mail.ru*
[2] *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: puryginpp2002@mail.ru*

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*Supervising author; [+]Corresponding author

***Keywords**:* waste of TNT, sulfite lye, sulfate ash, current waste, a ten-year shelf life, chemical analysis, method of disposal, silicate glass, assessment opportunities.

Abstract

This article presents the results of studies to assess the feasibility of using sulfate as waste production of TNT ten-year period of storage in the manufacture of silicate glass. In this regard, we have analyzed the composition of the current industrial waste production of TNT and waste ten-year shelf life. It was shown that the storage of waste under the open sky did not increase the content of nitro-derivatives of toluene. The content of TNT in them remained at the level of trace. Expect significant relative increase in the content of TNT and organic compounds - explosive derivatives of TNT in the ash was not confirmed. It was found that the coincidence time is a relative decrease in the content of water-soluble components of the waste. However, the content of the main component of waste – sodium sulfate over time has increased, although it remained within normal limits in accordance with TU 3.75 10103-13-90. The relative content of components such as sodium carbonate, decreased by 4 times, the sodium chloride is 28 times that of the sodium sulfide - 6 times, and the content of water-insoluble precipitate is increased almost in 2 times. As it turned out, the quality of samples of glass, made on the basis of glass batch using a ten-year waste differs slightly from the samples produced on the basis of the glass batch of the current waste.

Full Paper _Thematic Section:_ Research into New Materials.
Registration Code of Publication: 15-41-1-122 _Subsection:_ Composite Materials.
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Polycomposite coatings on chromiummatrix base

© **Svetlana V. Vodopi'yanova,**[+] **Renat S. Sayfullin**,* and **Anastasia S. Fakhrutdinova**
Department Technology of Inorganic Substances and Materials. Kazan National Research Technological University. Ul. K. Marx St., 68. Kazan, 420015. The Republic of Tatarstan. Russia.
Tel.: +7 (843) 231-40-64. E-mail: vod-sveta@yandex.ru

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*Supervising author; [+]Corresponding author

Keywords: composite electrochemical coatings (CEC), chromium, dispersed phase (DP), aluminum oxide, silicon oxide, electrolyte slurry, viscosity, density, thickness, the output current of chromium, x-ray analysis, heat treatment, strength, ductility and hardness polycomposite coatings.

Abstract

Some peculiarities of polycomposite chromaticy coating formation with dispersed phase of nanoparticles of aluminum oxide and silicon oxide are reviewed. The influence of nanoparticles on the properties of suspensions, the process of electrodeposition of chromium and some performance properties of the coatings are studied. The obtained polycomposite coatings Cr-Al_2O_3-SiO_2 possess improved properties in comparison with control and monocomposite coatings. For the evaluation of coating thickness and chemical composition the X-ray-phase analysis is used. The influence of heat treatment on properties chromaticy coatings is studied.

Full Paper *Thematic Section:* Research into New Materials.
Registration Code of Publication: 15-41-1-130 *Subsection:* Composite Materials.
The article is published on materials of the report on "International Scientific Forum
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Containing polyaniline composites based on porous fibrous carbon materials for supercapacitor electrode structures

© **Svetlana V. Stakhanova**,[+] **Mikhail V. Astakhov**,* **Anastasia A. Klimont**, **Ilya S. Krechetov**,
Anatoly T. Kalashnik, **Ruslan R. Galymzyanov** and **Kirill A. Semushin**
Physical Chemistry Division. National University of Science and Technology MISiS. Leninsky Prospekt, 6.
Moscow, 119049. Russia. Phone: +7 (495) 638-46-64. E-mail:svladlen@rambler.ru

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*Supervising author; [+]Corresponding author

Keywords: supercapacitor, specific capacitance, polyaniline, carbon fiber, carbon cloth, carbon felt, conducting polymer.

Abstract

Polyaniline (PANI) based composites have been prepared with various porous carbon materials – cloth and fabric - by chemical polymerization of aniline in an acidic medium. Carbon cloth /PANI composites demonstrate significant capacitance enhancement in compared to carbon materials up to 250 F/g^{-1} and 7.5 F/cm^{-2} for Busofit T-040 /PANI composite. The coulombic efficiency of composites has been measured to be about 97-99%. The potential for using these carbon materials/polyaniline composites as supercapacitor electrodes has been explored by cyclic voltammetry and galvanostatic charge/discharge tests.

Full Paper *Thematic Section:* Research into New Materials.
Registration Code of Publication: 15-41-1-138 *Subsection:* Polymer Composition.
The article is published on materials of the report on “International Scientific Forum Butlerov Heritage – 2015”. http://foundation.butlerov.com/bh-2015/ *(English Preprint)*
Submitted on March 31, 2015.

Creation of high strength composite materials which show a biodegradation in the conditions of deposition

© **Alsu N. Dautova,**[+] **Vladislav V. Yanov**, **Lyubov A. Zenitova**,* and **Olga A. Nikolaeva**
Department of Technology of Synthetic Rubber. Kazan National Research Technological University.
Karl Marx St., 68. Kazan, 420015. Republic of Tatarstan. Russian Federation. Phone: +7 (843) 231-42-51.
E-mail: alsu_5572@mail.ru, zenit@kstu.ru

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*Supervising author; [+]Corresponding author

Keywords: polymer compositions, polyamide, natural rubber, biodegradation.

Abstract

The work presents researches of polymer compositions based on polyamide filled with fiberglass in an amount of 30 wt% and 50 wt% by PA6-210KS and PA NE 50-1 brands correspondingly. As a biodegradable components were used crude natural rubber (NR-C) and natural rubber that has undergone of purification (NR-P) introduced into the polymer composition in an amount of 5 and 10%.

The results of physical and mechanical tests of samples of polymer compositions had been evaluated. Determined that with growth of quantity of entered NR strength characteristics are falling independently of its degree of purification. With increasing amount of injected NR-C indices largely decreased: for samples with NR-C they are from 6 to 34%, with NR-P they are from 9 to 37%.

The test for the aerobic biodegradation in soil during 6 months showed that to the greatest exposure the samples with NR-C content were subjected. The greatest weight loss – 5.8% was showed of the sample that contents 10% by weight of NR-C.

Full Paper ____ *Thematic Section:* Research into New Materials.
Registration Code of Publication: 15-41-1-142 *Subsection:* Composite Materials.
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Composite nickel layers with a carbon phase

© **Venera Sh. Haybieva**,[+] **Raisa E. Fomina**,* and **Gulfia G. Mingazova**
The Department of Inorganic Substances and Materials. Kazan National Research Technological
University. Karl Marx St., 68. Kazan, 420015. Tatarstan Republic. Russia.
Phone: +7 (843) 231-41-31. E-mail: 3_venerka_3@mail.ru

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*Supervising author; [+]Corresponding author

Keywords: CEC with a matrix of Nickel, ammonia electrolyte Nickel plating, dispersed phase, technical carbon, corrosion resistance, polarization curves, microhardness.

Abstract

Electrochemical coating composition (CEC) are obtained with a matrix of nickel containing the particles of carbon phase. Studied the influence of the concentration of carbon particles on the composition of the CEC and soluble additives NaF at quality coatings. It is shown that the particle of carbon phase accelerate the discharge ions of the main metal. Found increasing corrosion resistance CEC of nickel-carbon compared with a control coating of nickel. The morphology of the surface of the nickel coatings and their microhardness are studied.

Thematic Section: Research into New Materials. **Full Paper**
Subsection: Physical-Chemistry of Polymers. *Registration Code of Publication:* 15-41-1-147
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The influence of fillers on process of formation and structure of the polyurethane coatings based on polyethers

© **Elena A. Kiyanenko**,*[+] **Lyubov A. Zenitova**, **Nail Z. Mingaleev**, and **Olga A. Nikolayeva**
Department of Synthetic Rubber. Kazan National Research Technological University.
Karl Marx St., 72. Kazan, 420015. Republic of Tatarstan. Russia. E-mail: kiyanenko.lena@yandex.ru

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*Supervising author; [+]Corresponding author

Keywords: polyethers, polyurethane, fillers.

Abstract

Polyurethane coatings based on polyethers filled with natural mineral shungite and solid particulate inorganic chemical production waste - wasted and sub-standard dryers: aluminum oxide, silica gel, zeolite was synthesized. The influence of fillers on process of formation and structure of polyurethane coatings by IR spectroscopy is studied. It is shown that the amount of of fillers has an effect on the rate of polyurethane coatings curing. Optimum amounts for filling compositions with silica gel and aluminum oxide is 30 wt.%, with zeolite is 40 wt%, with shungite 50wt%.

Full Paper ____ *Thematic Section:* Research into New Materials.
Registration Code of Publication: 15-41-1-152 *Subsection:* Physical Chemistry.
The article is published on materials of the report on "International Scientific Forum
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Acid-base properties of the surface of fluorescent compounds on base of sulfides calcium and strontium

© **Sergey A. Seleznev**,[1,2] **Anatoly F. Golota**[1], and **Svetlana P. Pivneva**[1]
[1] *«North-Caucasus Federal University». Institute of Living Systems. Pushkin St. 1. Stavropol, 355009.*
Russia. Phone: +7 (8652) 95-68-08. E-mail: info@ncfu.ru
[2] *"Luminophor" CJSC RPF. Kulakov St., 8. Stavropol, 355044. Russia. Phone: +7 (8652) 56-02-70.*
E-mail: lumin@mail.stv.ru

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*Supervising author; +Corresponding author

Keywords: Sulfides of alkaline earth metals, phosphor, hydrolysis, acid-base indicators, pH-metry, IR-spectrum.

Abstract

Conducted research to identify the kinetics of hydrolysis processes on the surface of the crystals of alkaline earth metal sulfides. Found influence of additives of rare earth elements on a stability Sr(Ca)S to hydrolytic processes. Proved the effect of increasing the stability of the synthesized phosphors activation recent rare earth elements, due to the formation phase of the "difficult" double sulphides of $(Sr_{0.95}Sm_{0.05})S_{0.983}$ and $EuSrS_2$.

Thematic Section: Research into New Materials. **Full Paper**
Subsection: Physical Chemistry. *Registration Code of Publication:* 15-41-1-159
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Magnetic characteristics of mesoporous materials $0.1NiO\text{-}1SiO_2$ as influenced upon by introduction of trialkoxysilane additives during synthesis

© **Natalia B. Kondrashova**,[1]* **Viktor A. Valtsifer**,[1] **Vladimir N. Strelnikov**,[1]
Valentin Ya. Mitrofanov,[2] and **Sergey A. Uporov**[2]
[1] *Institute of Technical Chemistry of Ural Branch of the RAS. Academician Korolev St., 3. Perm, 614013. Russia. Phone: +7 (342) 237-82-72. Email: itch-ura-ran@yandex.ru*
[2] *Institute of Metallurgy of Ural Branch of the RAS. Amundsen St., 101. 620016, Ekaterinburg. Russia. Phone: +7 (343) 267-91-24. Email: imet.uran@gmail.com*

*Supervising author; [+]Corresponding author

Keywords: template hydrothermal synthesis, organo-substituted trialkoxysilanes, magnetization of saturation, blockage temperature.

Abstract

Mesoporous silicate compositions $0.1NiO\text{-}1SiO_2$ were obtained with use of the oxide co-condensation method in the presence of template (cetyltrimethylammonium bromide) and of organo-substituted trialkoxysilanes, namely (2-cyanoethyl)triethoxysilane and tris(trimethylsiloxy)silane, under conditions of hydrothermal synthesis. Magnetic properties of these materials were investigated. The specimens were shown to manifest typical super-paramagnetic behavior with the maximum corresponding to blockage temperature $T_b = 15$ K. The presence of organo-substituted trialkoxysilanes – as temperature progresses – most efficiently influences values and variations (non-uniformly directed) of the coercive force.

Thematic Section: Research into New Technologies. **Information Report**
Subsection: Chemical Industries. *Registration Code of Publication:* 15-41-1-163
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New technologies and devices to solve environmental problems in the production of energy-materials

© **Alexey F. Mahotkin**,* **Vladimir I. Petrov**,+ **Rifkat A. Khalitov**, and **Igor A. Mahotkin**
The Department "Equipment of Chemical Plants". Engineering Institute of Chemical Technology.
Kazan National Research Technological University. K. Marx St., 68. Kazan, 420015.
The Republic of Tatarstan. Russia. Phone: +7 (843) 231-40-98. E-mail: oxzkstu@rambler.ru.

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*Supervising author; +Corresponding author

Keywords: exhaust gas cleaning, energy-saturated materials, swirling apparatus, catalysis.

Abstract

This work presents the results of research and introduction into production of new vortex apparatus for intensification of mass transfer processes in the production of energy-materials. Presents a comparison of the effectiveness of vortical absorbers with known apparatus for the purification of exhaust gases from vapour and mist of nitric acid and nitrogen oxides. Developed and implemented catalytic purification of waste gases from nitrogen oxides. Developed and implemented a new vortex ferrosilicone column concentration of spent sulfuric acid that helps to reduce the consumption of materials technology 50 times compared with the known processes.

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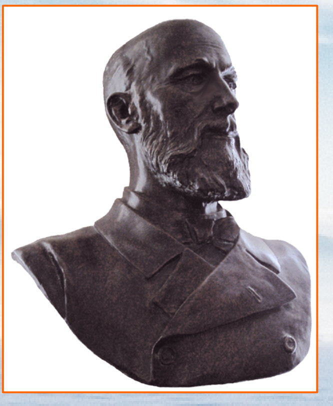

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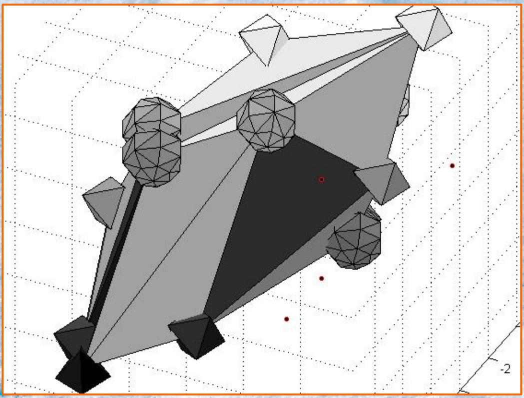

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Fundamental bases of the structure of substance

© **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

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*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**
Subsection: Physical Chemistry. *Registration Code of Publication:* 15-41-2-47
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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.
Registration Code of Publication: 15-41-2-56 *Subsection:* Physical Chemistry.
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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.
Registration Code of Publication: 15-41-2-76 *Subsection:* Computer Modeling of Gas Purification.
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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

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*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.
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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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*

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*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.

Full Paper ______________________________________ *Thematic Section:* Quantum-Chemical Research.
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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

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*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**
Subsection: Organic Chemistry. *Registration Code of Publication:* 15-41-2-103
The article is published on materials of the report on "International Scientific Forum
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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 ($3\cdot10^3$) and previous computational results.

Thematic Section: Quantum-Chemical Research. **Full Paper**
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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.

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*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*

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*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.
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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

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*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

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*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**
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Quantum-chemical мodeling 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**
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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

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*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**
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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**
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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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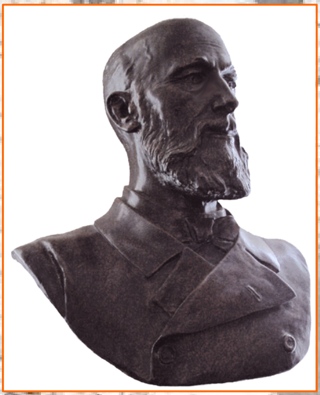

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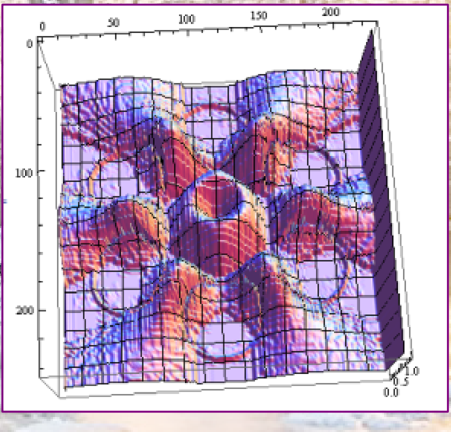

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Ионообменные свойства гидратированных фосфатов титана(IV)

© **Иваненко***+ **Владимир Иванович**, **Корнейков Роман Иванович**,
Аксенова Светлана Владимировна и **Локшин Эфроим Пинхусович**
Федеральное государственное бюджетное учреждение науки Институт химии и технологии редких элементов и минерального сырья им. И.В.Тананаева Кольского научного центра Российской Академии наук (ИХТРЭМС КНЦ РАН). Академгородок 26а. г. Апатиты, Мурманская область, 184209. Россия. Тел.: (8155) 57-92-40. E-mail: ivanenko@chemy.kolasc.net.ru

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*Ведущий направление; +Поддерживающий переписку

Ключевые слова: фосфаты титана(IV), неорганические сорбенты, катионы токсичных металлов, ионный обмен.

Аннотация

На основе изучения процессов комплексообразования определены условия существования гидратированных акваоксогодроксогидрофосфатов Ti(IV) в водных средах. Поляризация ацидолиганда в поле атома титана приводит к повышению подвижности протона в гидрофосфате Ti(IV) и способности к катионному обмену. Изучено влияние природы катионов сорбируемых металлов на процесс замещения протонов гидрофосфата Ti(IV). Значения константы катионного замещения зависят от степени гидратации катионов металла. В высоко гидратированных образцах возможно достижение статической обменной емкости, близкой к теоретической и равной содержанию HPO_4-групп в сорбенте. Разработаны способы модификации титано-фосфатного сорбента катионами Fe(III), Zr(IV) и Nb(V). Модифицирование основано на образовании гетерополиядерных ассоциатов при взаимодействии оксогидроксоацидокомплеков переходных металлов, имеющих различие в кислотно-основных свойствах. Легирование увеличивает константу сорбции, что позволяет использовать сорбенты для извлечения катионных примесей из более кислых растворов. Термическая обработка отработанных сорбентов обеспечивает надежную иммобилизацию сорбированных катионов в виде нерастворимых в водной среде кристаллических соединений. Разработанные сорбенты могут быть эффективно использованы для очистки от радионуклидов жидких радиоактивных отходов с высоким содержанием солей нерадиоактивных элементов, а также для извлечения из технологических стоков катионов токсичных металлов. Гидрофосфат титанила $TiOHPO_4 \cdot aq$ может быть использован в качестве прекурсора при синтезе соединений группы титанилфосфата калия в водных растворах.

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УДК 544.478-03. Поступила в редакцию 9 апреля 2015 г.

Минерализация 4-нитрофенола под действием озона в присутствии магнитосепарируемого композиционного катализатора на основе диоксида титана и магнетита

© **Казаков**$^{+}$ **Дмитрий Александрович**, **Вольхин* Владимир Васильевич**,
Гуленова Юлия Олеговна, **Обирина Марина Николаевна**
и **Рожина Дарья Андреевна**
Кафедра химии и биотехнологии. Пермский национальный исследовательский политехнический университет. Комсомольский пр., 29. г. Пермь, 614990. Пермский край. Россия.
Тел./Факс: (342) 239-15-11. E-mail: kazakovbiotech@mail.ru

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*Ведущий направление; $^{+}$Поддерживающий переписку

Ключевые слова: 4-нитрофенол, минерализация, озон, магнитосепарируемый композиционный катализатор, диоксид титана, магнетит.

Аннотация

Приведены результаты изучения процесса минерализации 4-нитрофенола при озонировании в присутствии образцов диоксида титана с различной структурой. Установлено, что наиболее высокая скорость минерализации 4-нитрофенола наблюдается в присутствии аморфного диоксида титана. Показано, что магнетит не влияет на скорость минерализации 4-нитрофенола. Предложена методика синтеза магнитосепарируемого композиционного катализатора, включающего фазу магнетита и аморфного диоксида титана. Определена зависимость каталитической активности композиционного катализатора при минерализации 4-нитрофенола в ходе озонирования от содержания в нём магнетита. Установлено, что при введении в фазу аморфного диоксида титана фазы магнетита до 30 % масс. каталитическая активность полученных образцов композиционного катализатора повышается, при дальнейшем увеличении доли магнетита в составе катализатора до 50 % масс. происходит снижение его активности. Более высокая каталитическая активность композиционного катализатора по сравнению с аморфным диоксидом титана объяснена более высокой удельной поверхностью и развитым объёмом пор полученного композита. Обнаружено, что в образце композиционного катализатора, содержащем 30 % масс. магнетита и проявившем наиболее высокую каталитическую активность, неактивная фаза магнетита находятся внутри частиц, а каталитически активная фаза диоксида титана – на их поверхности.

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форуме “*Бутлеровское наследие-2015*”. http://foundation.butlerov.com/bh-2015/
УДК 678.01:54+678.84. Поступила в редакцию 31 марта 2015 г.

Синтез полиалюмо- и полигаллийфенилсилоксанов в условиях механохимической активации

© **Либанов Виталий Викторович**, **Капустина**[+] **Алевтина Анатольевна**,
Шапкин* **Николай Павлович** и **Касприк Анна Эдуардовна**
Кафедра общей, неорганической и элементоорганической химии. Дальневосточный федеральный университет. Ул. Октябрьская, 27. г. Владивосток, 690090. Россия.
Тел.: (8423) 245-76-09. E-mail: kapustina.aa@dvfu.ru

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*Ведущий направление; [+]Поддерживающий переписку

Ключевые слова: полиалюмофенилсилоксан, полигаллийфенилсилоксан, полифенилсилсесквиоксан, механохимическая активация.

Аннотация

Изучено взаимодействие полифенилсилоксана с оксидами алюминия и галлия в условиях механохимической активации. Получены растворимые полиалюмофенилсилоксаны (ПАФС) с выходом от 68.2% до 69.3%. Показано, что получаемое в ПАФС соотношение Si/Al не зависит от его исходной величины. Показано, что расщепление силоксановой связи под действием оксида галлия при проведении взаимодействия в планетарной мельнице не происходит. Состав полученных продуктов исследован методами элементного, рентгенофазового анализов, ИК-спектроскопии и гель-хроматографии.

Полная исследовательская публикация *Тематический раздел:* Исследование новых материалов.
Регистрационный код публикации: 15-41-3-22 *Подраздел:* Фотонные ИК-световоды.
Статья публикуется по материалам доклада на Международном научном
форуме "*Бутлеровское наследие-2015*". http://foundation.butlerov.com/bh-2015/
УДК 548.5. Поступила в редакцию 10 апреля 2015 г.

Научные основы получения новых кристаллов и фотонных ИК-световодов на их основе

© **Корсаков Александр Сергеевич** и **Жукова***⁺ **Лия Васильевна**
Кафедра физической и коллоидной химии. Уральский федеральный университет им. первого
Президента России Б.Н. Ельцина. Ул. Мира, 19. г. Екатеринбург, 620002. Россия.
Тел.: (343) 375-44-45. E-mail: l.v.zhukova@urfu.ru

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*Ведущий направление; ⁺Поддерживающий переписку

Ключевые слова: исследование диаграмм; фотостойкие кристаллы, твердые растворы галогенидов серебра и таллия, моделирование структуры, фотонные ИК-световоды.

Аннотация

Разработаны фотостойкие и прозрачные в спектральном диапазоне от 0.4 до 45.0 мкм новые кристаллы $Ag_{1-x}Tl_xBr_{1-x}I_x$; $Ag_{1-x}Tl_xBr_{1-0.54x}I_{0.54x}$. Усовершенствована технология их получения, включающая нетрадиционный синтез многокомпонентной (однофазной) шихты и выращивание кристаллов на новых установках *КПЧ-01* и *КПЧ-02*. Методом ДТА исследованы диаграммы фазовых равновесий систем AgBr – TlI и AgBr – ($TlBr_{0.46}I_{0.54}$) и установлены области существования гомогенных твердых растворов. Для первой системы максимальное содержание TlI в твердом растворе составляет 25 % масс.; для второй системы содержание $TlBr_{0.46}I_{0.54}$ в твердом растворе составляет 50 % масс. Фотонные ИК-световоды нанокристаллической структуры получают методом экструзии из новых кристаллов. Размер зерен в ИК-световоде – от 60 до 90 нм.

Полная исследовательская публикация *Тематический раздел:* Исследование новых материалов.
Регистрационный код публикации: 15-41-3-36 *Подраздел:* Биосенсоры.
Статья публикуется по материалам доклада на Международном научном
форуме "*Бутлеровское наследие-2015*". http://foundation.butlerov.com/bh-2015/
УДК 543.866. Поступила в редакцию 17 декабря 2014 г.

Моноаминоксидазные биосенсоры на основе наночастиц серебра и оксида графена для определения лекарственных веществ с антидепрессивным действием

© **Медянцева**[1]*[+] **Эльвина Павловна**, **Брусницын**[1] **Даниил Владимирович**,
Варламова[1] **Регина Марковна**, **Максимов**[1] **Александр Александрович**,
Коновалова[2] **Ольга Анатольевна** и **Будников**[1] **Герман Константинович**
[1] *Кафедра аналитической химии. Химический институт им. А.М. Бутлерова;* [2] *Кафедра оптики и нанофотоники. Институт физики. Казанский (Приволжский) федеральный университет*
Ул. Кремлевская, 18. г. Казань, 420008. Республика Татарстан. Россия. Тел.: (843) 233-77-93.
E-mail: Elvina.Medyantseva@kpfu.ru

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*Ведущий направление; [+]Поддерживающий переписку

Ключевые слова: биосенсор, моноаминоксидаза, углеродные нанотрубки, наночастицы серебра, оксид графена, антидепрессанты.

Аннотация

Разработаны амперометрические моноаминоксидазные биосенсоры на основе графитовых печатных электродов, модифицированных многостенными углеродными нанотрубками, наночастицами серебра или оксидом графена для определения лекарственных веществ имипрамина, афобазола и моклобемида. Показана возможность использования биосенсоров для контроля качества лекарственных веществ при определении основного лекарственного вещества в лекарственных формах. Нижняя граница определяемых содержаний при использовании в качестве субстрата адреналина для моклобемида, имипрамина и афобазола $2 \cdot 10^{-9}$, $6 \cdot 10^{-9}$, $8 \cdot 10^{-9}$ моль/л соответственно.

Полная исследовательская публикация *Тематический раздел:* Исследование новых материалов.
Регистрационный код публикации: 15-41-3-44 *Подраздел:* Биохимия.
Статья публикуется по материалам доклада на Международном научном
форуме "*Бутлеровское наследие-2015*". http://foundation.butlerov.com/bh-2015/
УДК 547.458:[541.64+544.015.4+617]. Поступила в редакцию 31 марта 2015 г.

Особенности получения микротрубок хитозана межфазной реакцией полимераналогичного превращения

© **Гегель**[1]* **Наталья Олеговна**, **Бабичева**[1, 2] **Татьяна Сергеевна**
и **Шиповская**[1,2] **Анна Борисовна**
[1] *Образовательно-научный институт Наноструктур и биосистем. Саратовский государственный университет имени Н.Г. Чернышевского. Ул. Астраханская, 83. г. Саратов, 410012. Россия. Тел.: (8452) 21-07-59. E-mail: GegelNO@yandex.ru*
[2] *Базовая кафедра полимеров. Саратовский государственный университет имени Н.Г. Чернышевского. Ул. Астраханская, 83. г. Саратов, 410012. Россия. Тел.: (8452) 51-69-57. E-mail: ShipovskayaAB@rambler.ru*

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*Ведущий направление; [+]Поддерживающий переписку

Ключевые слова: хитозан, микротрубки, формование, полимераналогичные превращения, высаливатель, биодеградируемые протезы кровеносных сосудов.

Аннотация

Описан процесс получения и свойства новых материалов на основе хитозана в форме полых бесшовных структур (микротрубок) межфазной реакцией полимераналогичного превращения полимера из растворимой формы полисоли в нерастворимую в воде форму полиоснования или ПАВ–полиэлектролитного комплекса. Проведена оценка влияния химической природы высаливателя на механизм химической реакции. Оценены морфология, физико-механические характеристики, упруго-деформационные и биохимические свойства микротрубок хитозана. Выявлена высокая адгезия и пролиферирующая активность культуры эпителиоподобных клеток MA-104 на поверхности микротрубчатых субстратов в модельных опытах *in vitro*.

Полная исследовательская публикация *Тематический раздел:* Биохимические исследования.
Регистрационный код публикации: 15-41-3-54 *Подраздел:* Метаболические пути.
Статья публикуется по материалам доклада на Международном научном
форуме “*Бутлеровское наследие-2015*”. http://foundation.butlerov.com/bh-2015/
УДК 579.695; 546.85; 502.55; 661.63. Поступила в редакцию 10 апреля 2015 г.

Включение белого фосфора в природный круговорот веществ. Культивирование устойчивой микрофлоры.

© **Миндубаев**[1]*[+] **Антон Зуфарович**, **Волошина**[1] **Александра Дмитриевна**,
Горбачук[2] **Елена Валерьевна**, **Кулик**[1] **Наталья Владимировна**, **Алимова**[2] **Фарида Кашифовна**, **Минзанова**[1] **Салима Тахиятулловна**, **Миронова**[1] **Любовь Геннадьевна**,
Сапармырадов[2] **Керемли Ашырмухаммедович**, **Хаяров**[2] **Хасан Рафаэлевич**
и **Яхваров**[1]***Дмитрий Григорьевич**

[1] *Институт органической и физической химии им. А.Е. Арбузова Казанского научного центра Российской академии наук. Ул. Арбузова, 8. г. Казань, 420088. Республика Татарстан. Россия.*
E-mail: mindubaev@iopc.ru
[2] *Казанский (Приволжский) федеральный университет. Ул. Университетская, 18.*
г. Казань, 420008. Республика Татарстан. Россия.

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*Ведущий направление; [+]Поддерживающий переписку

Ключевые слова: детоксикация, белый фосфор, осадки сточных вод, анаэробные условия, метаболический путь, метаболиты, ядерный магнитный резонанс, *Bacillus, Streptomyces sp.*, *Aspergillus niger*, *Trichoderma asperellum F-1087*, культуральные среды, химическое равновесие, селекция.

Аннотация

Впервые произведены посевы микроорганизмов различных таксономических групп (грибов, стрептомицетов и бактерий) на синтетические культуральные среды, содержащие белый фосфор в качестве единственного источника фосфора. На данных средах микроорганизмы росли и не испытывали фосфорное голодание. Это первый в мире пример включения белого фосфора в биосферный круговорот элемента фосфора. Показано, что устойчивость культур микроорганизмов к белому фосфору зависит от их таксономической принадлежности – грибы из рода *Trichoderma* адаптируются к нему лучше, чем аспергиллы, аспергиллы лучше чем стрептомицеты, а стрептомицеты лучше, чем бактерии рода *Pseudomonas*. Сравнивая две культуры стрептомицетов, мы показали, что устойчивость к белому фосфору – признак, который может усиливаться или ослабляться в зависимости от условий культивирования. По всей видимости, микроорганизмы потребляют растворенные продукты окисления белого фосфора (фосфат, фосфит и гипофосфит) и, тем самым, смещают химическое равновесие в сторону его дальнейшего окисления. Это заметно ускоряет процесс детоксикации белого фосфора. Характер и состав продуктов окисления белого фосфора исследовался нами методом ^{31}P ЯМР. Самая высокая концентрация соответствует превышению ПДК белого фосфора в сточных водах в 5000 раз, а в питевой воде – в 100000000 раз!

Полная исследовательская публикация *Тематический раздел:* Биохимические исследования.
Регистрационный код публикации: 15-41-3-82 *Подраздел:* Антимикробные препараты.
Статья публикуется по материалам доклада на Международном научном
форуме “*Бутлеровское наследие-2015*”. http://foundation.butlerov.com/bh-2015/
УДК 547.458:[54-148+541.65/654+615.281.9]. Поступила в редакцию 31 марта 2015 г.

Новые антимикробные препараты на основе комплексной соли хитозана с хиральным органическим лигандом

© **Шиповская**[1, 2]*+ **Анна Борисовна**, **Зудина**[2] **Ирина Витальевна**,
Фомина[2] **Валентина Ивановна** и **Малинкина**[1, 2] **Ольга Николаевна**
[1] *Базовая кафедра полимеров. Институт химии. Саратовский государственный университет имени Н.Г. Чернышевского. Ул. Астраханская, 83. г. Саратов, 410012. Россия. Тел.: (8452) 51-69-57.*
E-mail: ShipovskayaAB@rambler.ru
[2] *Отдел высокомолекулярных соединений. Образовательно-научный институт наноструктур и биосистем. Саратовский государственный университет имени Н.Г. Чернышевского.*
Ул. Астраханская, 83. г. Саратов, 410012. Россия. Тел.: (8452) 21-07-59.
E-mail: Olga-Malinkina@yandex.ru

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*Ведущий направление; +Поддерживающий переписку

Ключевые слова: хитозан, комплексная соль, неорганический и хиральный органический лиганд, гидрогель, антимикробный препарат, пародонтит, цитокины.

Аннотация

Методами элементного анализа, потенциометрического титрования, спектрополяриметрии, ИК- и ЯМР-спектроскопии исследованы процессы соле- и гелеобразования в системе гидрохлорид хитозана+аскорбиновая кислота+вода. Установлено, что взаимодействие данных компонентов в водной среде сопровождается образованием гидрогеля комплексной соли хитозана с неорганическим (хлорид) и хиральным органическим лигандом (аскорбат). Изучены вискозиметрические и реологические свойства водных растворов гидрохлорид-аскорбат хитозана. В разбавленных растворах макромолекулы полисоли проявляют полиэлектролитный эффект, в концентрированных – реализуется типичный для неньютоновских жидкостей характер течения. Отмечено существенное влияние на эти свойства энантиомерной формы аскорбиновой кислоты, температуры и времени хранения растворов. На основании проведённых исследований высказано предположение, что узлы сетки гидрогеля бинарной соли хитозана образованы системой сложных ион-ионных и водородных контактов между макромолекулами полимера и молекулами органической кислоты. Методами *in vitro* и *in vivo* установлена способность гидрогелей гидрохлорид-аскорбат хитозана оказывать антибактериальное действие в отношении условно-патогенных бактерий. Изучена динамика изменения содержания цитокинов ФНО-α и ИЛ-1β в жидкости зубодесневых карманов у пациентов с воспалительными заболеваниями тканей пародонта на фоне обработки десны гидрогелем комплексной соли хитозана. Установлено, что препарат проявляет ярко выраженную противовоспалительную активность, по всей видимости, за счет регуляции уровня цитокинов в очаге воспаления. Выявленные закономерности показывают, что лечебный эффект гидрогелей обусловлен не только пролонгированной санацией зубодесневых карманов, но и иммунотропным действием на эффекторы врожденного иммунитета. Механизм воздействия комплексной соли хитозана с хиральным органическим лигандом на живые клетки, по всей видимости, тот же, что и у поликатионных антимикробных белков, прежде всего, дефензинов β.

Тематический раздел: Биохимические исследования. **Полная исследовательская публикация**
Подраздел: Состав растительного сырья. *Регистрационный код публикации:* 15-41-3-95
Статья публикуется по материалам доклада на Международном научном форуме "*Бутлеровское наследие-2015*". http://foundation.butlerov.com/bh-2015/
Поступила в редакцию 11 апреля 2015 г. УДК 577.114:535.243.2:582.573.21:615.322

Качественное и количественное определение углеводов в сырье и настойках матричных гомеопатических подснежника Воронова, белоснежного методами тонкослойной хроматографии и УФ-спектрофотометрии

© **Боков**[1]*+ **Дмитрий Олегович**, **Самылина**[1] **Ирина Александровна** и **Попов**[2] **Дмитрий Матвеевич**

[1] *Кафедра фармакогнозии. Первый Московский государственный медицинский университет имени И.М. Сеченова. ГСП-1. Ул. Трубецкая, 8. г. Москва, 119991. Россия. Тел.: (925) 358-84-27. E-mail: fmmsu@mail.ru*

[2] *Научно-исследовательский институт фармации. Первый Московский государственный медицинский университет имени И.М. Сеченова. Нахимовский проспект, 45. г. Москва, 117418. Россия.*

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*Ведущий направление; +Поддерживающий переписку

Ключевые слова: углеводы, подснежник Воронова (*Galanthus woronowii Losinsk*), подснежник белоснежный (*Galanthus nivalis* L.), настойка матричная гомеопатическая, глюкоза, фруктоза.

Аннотация

Изучен качественный состав и количественное содержание углеводов в гомеопатическом лекарственном растительном сырье и настойках матричных гомеопатических подснежника Воронова и подснежника белоснежного. Подобраны оптимальные условия проведения ТСХ-анализа, экстракции сырья, разработаны спектрофотометрические методики определения количественного содержания углеводов в пересчёте на фруктозу и на глюкозу.

Тематический раздел: Биохимические исследования. **Полная исследовательская публикация**
Подраздел: Химический состав растений. *Регистрационный код публикации:* 15-41-3-103
Статья публикуется как материал заочного участия в Международном научном форуме “*Бутлеровское наследие-2015*”. http://foundation.butlerov.com/bh-2015/
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Оценка содержания фитоменадиона в надземной части растений семейства гречишные флоры Сибири

© **Лукша**[1]*+ **Елена Александровна**, **Погодин**[1] **Илья Сергеевич**
и **Иванова**[2]* **Евгения Викторовна**

[1] *Кафедра фармацевтической, аналитической и токсикологической химии.* [2] *Кафедра фармацевтической технологии с курсом биотехнологии. ГБОУ ВПО «Омский государственный медицинский университет» Минздрава РФ. Ул. Ленина, 12. г. Омск, 644099. Омская область. Россия. Тел.: (381-2) 370-360. E-mail: chem68@mail.ru*

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*Ведущий направление; +Поддерживающий переписку

Ключевые слова: *Polygonaceae*, фитоменадион, филлохинон, витамин К$_1$, рабочий стандартный образец, ВЭЖХ.

Аннотация

В статье приведены результаты определения содержания фитоменадиона (витамина К$_1$) в надземной части некоторых растений семейства гречишные сибирской флоры. Показано, что фитоменадион не обнаруживается в растениях семейства после двух лет хранения сырья. Установлено, что фитоменадион присутствует во всех 15 исследуемых образцах, срок хранения которых составляет менее двух лет. Наибольшее содержание фитоменадиона отмечено для представителей рода *Persicaria* (горец), *Polygonum* (спорыш), *Rumex* (щавель). Полученные результаты позволяют сформулировать рекомендации по хранению и оптимальному использованию растительного сырья на основе представителей семейства гречишные в качестве источника витамина К$_1$. Количественная оценка содержания фитоменадиона в растениях семейства гречишные флоры Сибири проведена впервые.

Тематический раздел: Биохимические исследования. **Полная исследовательская публикация**
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Особенности биосинтеза оксилипинов в плаунке семейства *Selaginellaceae*

© **Огородникова***[+] **Анна Владимировна**, **Мухитова*** **Фаимя Киямовна**
и **Гречкин*** **Александр Николаевич**
Федеральное государственное бюджетное учреждение науки Казанский институт биохимии
и биофизики Казанского научного центра Российской академии наук.
Ул. Лобачевского, 2/31. г. Казань, 420111. А/я 30. Республика Татарстан. Россия.
Тел.: (843) 231-90-40. E-mail: anyuta_ogorodnik@mail.ru

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*Ведущий направление; [+]Поддерживающий переписку

Ключевые слова: *Selaginella martensii* Spring, липоксигеназный путь, оксилипины, дивиниловые эфиры, 12-оксофитодиеновая кислота.

Аннотация

Изучен профиль оксилипинов в зеленых тканях плаунка *Selaginella martensii* Spring. Большинство из них является продуктами метаболизма ненасыщенных жирных кислот (линолевой и α-линоленовой), опосредованного действием ферментов 13-липоксигеназы и дивинилэфирсинтазы (ДЭС) или алленоксидсинтазы (АОС). Алленоксидсинтазные продукты представлены изомерами 12-оксофитодиеновой кислоты (12-оксоФДК), среди которых преобладает 12-oxo-9(13), 15-ФДК, Это соединение нехарактерно для цветковых растений. Дивиниловые эфиры обнаружены у нецветковых наземных растений впервые. Впервые описан липоксигеназный метаболизм жирных кислот в плаунках (Lycopodiophyta).

Тематический раздел: Биохимические исследования. **Полная исследовательская публикация**
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Новые подходы к стандартизации травы душицы

© Хазиев[1+]* Рамиль Шамилевич, **Петрова[1] Диляра Наильевна**
и **Ситенков[2] Александр Юрьевич**
[1] *Кафедра фармакологии фармацевтического факультета с курсами фармакогнозии и ботаники.*
[2] *Кафедра фармацевтической химии с курсами аналитической и токсикологической химии*
Казанский государственный медицинский университет. Пр. Амирхана, 16. г. Казань, 420016.
Республика Татарстан. Россия. Тел.: (843) 521-27-88. E-mail: xaziev@inbox.ru

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*Ведущий направление; [+]Поддерживающий переписку

Ключевые слова: *Origanum vulgare*, флавоноиды, дифференциальная спектрофотометрия, количественный анализ.

Аннотация

Целью исследования была разработка быстрого метода количественного определения действующих веществ в траве душицы. Испытания проводились на траве душицы обыкновенной, заготовленной в республиках Татарстан и Башкортостан. В результате проведенных экспериментов были подобраны условия экстракции флавоноидов – одной из основных групп действующих веществ данного сырья, при которых в течение 10 минут извлекалось 94% этих соединений. Расчет истинного содержания их в растительном сырье проводился с использованием коэффициента на неполноту экстракции. Методом высокоэффективной жидкостной хроматографии было показано, что доминирующим флавоноидом этого сырья является цинарозид, удельный показатель которого в комплексе с хлоридом алюминия предлагается использовать для расчетов. Достоверность методики была проверена статистически, ошибка метода не превышает 2.48%.

Тематический раздел: Биохимические исследования. **Полная исследовательская публикация**
Подраздел: Органическая химия. *Регистрационный код публикации:* 15-41-3-119
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Изучение токсичности некоторых производных бензимидазола

© **Васин* Антон Евгеньевич**, **Белоусова**[+] **Зоя Петровна**,
Зарубин Юрий Павлович и **Пурыгин Петр Петрович**
Кафедра органической, биоорганической и медицинской химии. Самарский государственный университет. Ул. Акад. Павлова, 1. г. Самара, 443011. Самарская область. Россия.
Тел.: (846) 334-54-59. E-mail: zbelousova@mail.ru

*Ведущий направление; [+]Поддерживающий переписку

Ключевые слова: бензимидазол, 2-метилбензимидазол, 2-бензилбензимидазол, 1,2-дибензилбензимидазол, токсичность, мутагенность, *Paramecium caudatum*, *Allium cepa*.

Аннотация

Изучена токсичность бензимидазола, 2-метилбензимидазола, 2-бензилбензимидазола и 1,2-дибензилбензимидазола (**I-IV**) в водных растворах для *Paramecium caudatum* и *Allium cepa и* мутагенность для *Allium cepa*. Рассчитанные физико-химические параметры изученных соединений свидетельствуют о том, что токсичность и мутагенность **I–IV** коррелируют с липофильностью и объемом их молекул. Вероятно, что возрастание липофильности от **I** к **IV** приводит к соответст-вующему увеличению степени их мутагенности, так как большее количество молекул **I-IV** может связываться с ДНК по механизму интеркаляции. Токсичность и мутагенность **I-IV** для *Paramecium caudatum* и *Allium cepa* носят дозозависимый характер. Рассчитанные физико-химические параметры изученных соединений свидетельствуют о том, что токсичность и мутагенность коррелируют с липофильностью и объемом их молекул.

Полная исследовательская публикация *Тематический раздел:* Биохимические исследования.
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форуме “*Бутлеровское наследие-2015*”. http://foundation.butlerov.com/bh-2015/
УДК 556.541.32. Поступила в редакцию 28 апреля 2015 г.

Сравнительный анализ химико-биологических показателей молоди рыб разных участков Волжского отрога Куйбышевского водохранилиаще в условиях антропогенного воздействия

© **Гордеева Мария Эдуардовна**, **Лапин***+ **Анатолий Андреевич**
и **Карусева Александра Юрьевна**
Кафедра “Водные биоресурсы и аквакультура”. Казанский государственный энергетический университет. Ул. Красносельская, 51. г. Казань, 420066. Республика Татарстан. Россия.
Тел.: (843) 519-43-53. E-mail: Maria.Galeeva@gmail.com

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*Ведущий направление; +Поддерживающий переписку

Ключевые слова: ихтиофауна, молодь рыб, Куйбышевское водохранилище, размерный состав, видовой состав, возрастной состав, коэффициент упитанности, атиоксидантная активность крови, антропогенное воздействие.

Аннотация

При анализе данных, предоставленных ФГУ «Средневолжрыбводом» было установлено, что преобладающими видами молоди рыб Волжского отрога Куйбышевского водохранилища при разной степени антропогенной воздействия является уклея, лещ и окунь. В работе проведен сравнительный анализ таких биологических показателей молоди рыб как длина тела, масса тела, возраст, упитанность, атиоксидантная активность крови в условиях разной степени антропогенной нагрузки. Были разработаны размерно-весовые модели уклеи, леща и окуня, которые позволят спрогнозировать промысловую массу рыб при разрешенных размерах вылова при условии стабильной кормовой базы на уровне 2013 года и улучшения качества воды. Помимо исследования биологических показателей был проанализирован и один из современных новаторских химических показателей – суммарная антиоксидантная активность крови рыб.

Полная исследовательская публикация *Тематический раздел:* Биохимические исследования.
Регистрационный код публикации: 15-41-3-132 *Подраздел:* Аналитическая химия.
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форуме “*Бутлеровское наследие-2015*”. http://foundation.butlerov.com/bh-2015/
УДК 544.08+543.08. Поступила в редакцию 31 марта 2015 г.

Идентификация органических соединений различных классов в волосах человека методом ГХ-МС/МС

© **Кислякова***+ **Яна Юрьевна**, **Шешко Татьяна Федоровна**
и **Серов Юрий Михайлович**
Кафедра физической и коллоидной химии. Российский университет дружбы народов.
Ул. Миклухо-Маклая, 6. г. Москва, 117198. Россия. Тел.: (495) 955-07-66. E-mail: rupf@mail.ru

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*Ведущий направление; +Поддерживающий переписку

Ключевые слова: химико-токсикологический анализ, волосы, 3-нафтоилиндолы, индазол-3-карбоксамиды, ГХ-МС/МС.

Аннотация

Проведена классификация синтетических каннабиноидов на основе их химического строения. Определены масс-спектрометрические и хроматографические характеристики исследуемых соединений. Подобраны условия исследования внешней поверхности волос на наличие компонентов курительных смесей. Разработана методика анализа внутренней области волос. Проведена процедура валидации данной методики.

Тематический раздел: Биохимические исследования. **Полная исследовательская публикация**
Подраздел: Физическая химия. *Регистрационный код публикации:* 15-41-3-141
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Определение констант диссоциации карбоксильных и аминогрупп на альбумине методом потенциометрического титрования

© **Дмитриева*** **Ирина Борисовна**, **Кергенцев Антон Андреевич**
и **Чухно**$^+$ **Александр Сергеевич**
*Кафедра физической и коллоидной химии. Санкт-Петербургская государственная
химико-фармацевтическая академия. Ул. Профессора Попова, 14, лит. А. г. Санкт-Петербург,
197376. Россия. Тел.: (812) 234-11-38. E-mail: irina@dmitriyev.ru_*

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*Ведущий направление; $^+$Поддерживающий переписку

Ключевые слова: альбумин, сорбция, потенциометрическое титрование, точка нулевого заряда, константы диссоциации.

Аннотация

Методом потенциометрического титрования исследовано влияние pH и хлорида калия на сорбцию ионов водорода и гидроксид-ионов на альбумине. Установлено, что количества сорбированных ионов H^+ и OH^- на альбумине зависит от pH и ионной силы растворов. Определена точка нулевого заряда альбумина. На основе сорбционных данных вычислено количество функциональных групп альбумина, участвующих в обмене протонами и гидроксид-ионами, рассчитаны средние константы диссоциации этих групп.

Тематический раздел: Биохимические исследования. **Полная исследовательская публикация**
Подраздел: Моделирование биосинтеза. *Регистрационный код публикации:* 15-41-3-147
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Теоретическое и экспериментальное моделирование биосинтеза лигнина

© **Карманов**[1]*+ **Анатолий Петрович**, **Полещиков**[2] **Сергей Михайлович**
и **Кочева**[3] **Людмила Сергеевна**

[1] *Лаборатория биохимии и биотехнологии. Федеральное государственное бюджетное учреждение науки Институт биологии Коми научного центра УрО РАН. Ул. Коммунистическая, 28. г. Сыктывкар, 167982. Республика Коми. Россия. Тел.: (909) 120-81-63. E-mail: apk0948@ib.komisc.ru*
[2] *Кафедра высшей математики. Сыктывкарский лесной институт (филиал) федерального государственного бюджетного образовательного учреждения высшего профессионального образования «Санкт-Петербургский государственный лесотехнический университет имени С.М. Кирова». Ул. Ленина, 39. г. Сыктывкар, 167982. Республика Коми. Россия. Тел.: (922) 581-04-57. E-mail: polsm@list.ru*
[3] *Лаборатория химии минерального сырья. Федеральное государственное бюджетное учреждение науки Институт геологии Коми научного центра УрО РАН. Ул. Первомайская, 54. г. Сыктывкар, 167982. Республика Коми. Россия. Тел.: (8212) 24-54-16. E-mail: lskocheva@geo.komisc.ru*

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*Ведущий направление; +Поддерживающий переписку

Ключевые слова: лигнин, биосинтез, математическое моделирование.

Аннотация

Приведены результаты экспериментального моделирования биосинтеза *in vitro* в системе пероксидаза–пероксид водорода–конифериловый спирт. Выявлено сложное поведение системы в ходе дегидрополимеризации монолигнола и предложена математическая модель процесса в виде системы дифференциальных уравнений. Рассмотрены особенности этих уравнений. Приведены результаты численного интегрирования, выполненного методом Рунге-Кутты-Фельберга восьмого порядка.

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УДК 543.064; 663.952. Поступила в редакцию 01 апреля 2015 г.

Антиоксидантная активность кефира

© **Сагдеева Камила Ринатовна**, **Азизова Альфия Ильфатовна**,
Мухаметзянова Лейсан Рифкатовна, **Девятко Валерия Сергеевна**,
Захаров Вадим Валерьевия, **Щербакова**[+] **Юлия Владимировна**
и **Ахмадуллина* Фарида Юнусовна**
Кафедра промышленной биотехнологии. Казанский национальный исследовательский технологический университет. Ул. К. Маркса, 68. г. Казань, 420015. Республика Татарстан. Россия.
Тел.: (843) 231-43-28. E-mail: balakirevajulia3@mail.ru

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*Ведущий направление; [+]Поддерживающий переписку

Ключевые слова: антиоксидантная активность, кефир.

Аннотация

В работе приведены данные исследований интегральной антиоксидантной активности кефира различных торговых марок методом кулонометрического титрования. Было выявлено влияние жирности кефира на данный показатель. Наибольшей антиоксидантной активностью обладал кефир, выпускаемый *ОАО «Зеленодольским молочноперербатывающим комбинатом».*

Полная исследовательская публикация *Тематический раздел:* Биохимические исследования.
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Метод биотестирования – альтернативный метод оценки изменения качества молока при его термообработке

© **Зиганшина Гульназ Атласовна**, **Баданова Екатерина Григорьевна**,
Гарипова Энджe Рузалевна, **Азизова Альфия Ильфатовна**,
Щербакова[+] **Юлия Владимировна** и **Ахмадуллина*** **Фарида Юнусовна**
Кафедра промышленной биотехнологии. Казанский национальный исследовательский технологический университет. Ул. К. Маркса, 68. г. Казань, 420015. Республика Татарстан. Россия.
Тел.: (843) 2314328. E-mail: balakirevajulia3@mail.ru

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*Ведущий направление; [+]Поддерживающий переписку

Ключевые слова: биотестирование, молоко, дрожжи *Saccharomyces cerevisiae*.

Аннотация

В работе предложена и проведена начальная апробация для оценки качества термообработанного молока система биоконтроля, базирующаяся на дрожжах *Saccharomyces cerevisiae*. Козье молоко, обработанное при режимах пастеризации 76 °С 5 мин (преимущественно) и 90 °С 20 с, обладало более высокой биологической активностью и рост стимулирующими свойствами по сравнению с другими изученными режимами пастеризации (65 ^{o}С, 30 мин и 95 ^{o}С, 5 мин).

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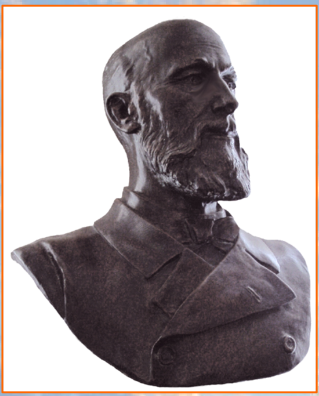

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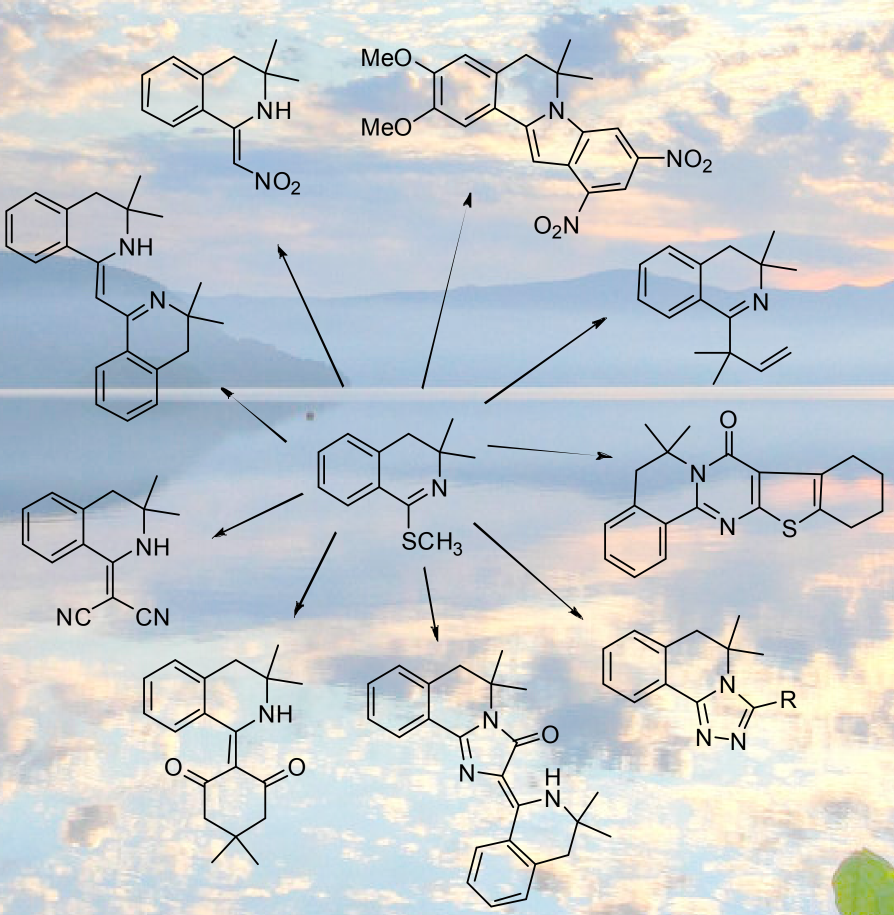

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Synthesis of partially hydrogenated nitrogen heterocycles. How does the heterocyclization on Ritter proceed?

© **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

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*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.

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*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

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*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

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*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, ^1H NMR and $^{13}C\ \{^1H\}$.

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

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*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**
Subsection: Organic Chemistry. *Registration Code of Publication:* 15-42-4-55
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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*

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*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**
Subsection: Organic Chemistry. *Registration Code of Publication:* 15-42-4-61
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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.
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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

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*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

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*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.

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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

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*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.

Full Paper ____ *Thematic Section:* Preparative Research.
Registration Code of Publication: 15-42-4-86 *Subsection:* Organic Chemistry.
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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

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*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.
Registration Code of Publication: 15-42-4-100 *Subsection:* Organic Chemistry.
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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*

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*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.

Full Paper ____ *Thematic Section:* Preparative Research.
Registration Code of Publication: 15-42-4-104 *Subsection:* Organic Chemistry.
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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

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*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.

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Registration Code of Publication: 15-42-4-108 *Subsection:* Organic Chemistry.
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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

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*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.
The article is published as a material of correspondence participation in International Scientific Forum "Butlerov Heritage-2015". http://foundation.butlerov.com/bh-2015/ *(English Preprint)*
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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.
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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

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*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.

Thematic Section: Preparative Research. **Full Paper**
Subsection: Inorganic Chemistry. *Registration Code of Publication:* 15-42-4-119
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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.

Full Paper ____ *Thematic Section:* Preparative Research.
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

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*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.
The article is published as a material of correspondence participation in International Scientific Forum "Butlerov Heritage-2015". http://foundation.butlerov.com/bh-2015/ *(English Preprint)*
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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

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*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'-{(ethoxycarbonylmethyl)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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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

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*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.

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Registration Code of Publication: 15-42-4-158 *Subsection:* Physical Chemistry of Cellulose.
The article is published as a material of correspondence participation in International Scientific
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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

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*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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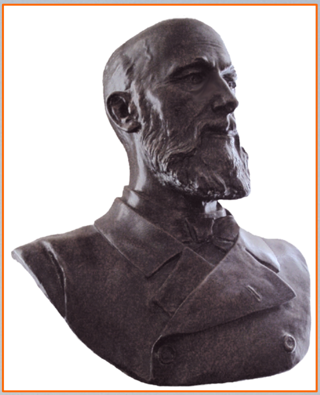

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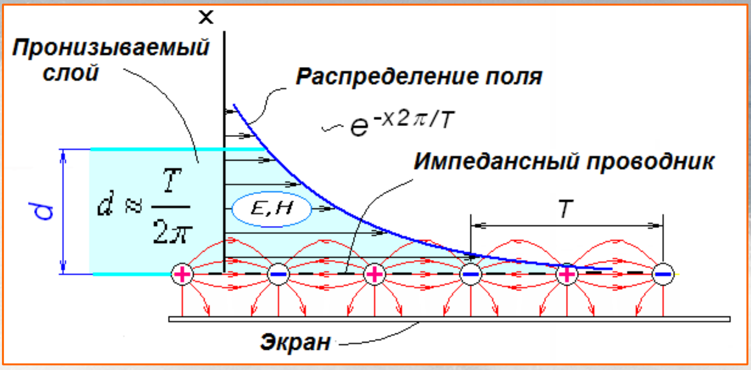

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The use of sensitive elements on the spiral slow to control processes in liquid media

© **Mikhail V. Astakhov**,[1+] **Andrey A. Yelizarov**,[2*] and **Alexey O. Rodin**[1]
[1] *Department of Physical Chemistry. Institute for New Materials and Nanotechnologies. National Research Technological University "MISA" NUST "MISA". Leninskiy Prospect St., 4. Moscow, 119991. Russia. Phone: (495) 236-87-38. E-mail: astahov@misis.ru*
[2] *Department Electronic Engineering. Moscow Institute of Electronics Mathematics and the National Research University "Higher School of Economics" (MIEM HSE) Russia. E-mail: yelizarov@list.ru*

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*Supervising author; [+]Corresponding author

Keywords: electromagnetic radiation, slowing down the system, micelles, colloidal systems.

Abstract

Currently, electronic devices and devices based on the use of slow-wave systems and excited in their electromagnetic waves are widely used in microwave electronics, chemistry, biology and medicine as sensing elements for the study of the processes occurring in liquids.

The features of the control of the formation of solid phases diethyl zinc and copper in electrolyte solutions, the formation and dissolution of crystals of Rochelle salt and nickel sulfate from a supersaturated solution, micellar structures on the example of sodium oleate with sensitive elements based on spiral slow.

Full Paper ________________________________ *Thematic Section:* Research into the Effects of Physical Fields.
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Influence of highly diluted aqueous solutions and weak physical fields on behavior of aquatic organisms

© **Nina E. Lebedeva,**[1]* **Yulia V. Kiseleva,**[2+] **Svetlana Yu. Sergeeva,**[2]
Sergey A. Ryzhkin,[3,4] **Irina S. Ryzhkina,**[2+] and **Alexander I. Konovalov**[2]
[1] *Faculty of Biology. Lomonosov Moscow State University. Leninskie Gory, 1-12. Moscow, 119991. Russia.*
Phone: +7 (495) 939-27-76. E-mail: lebedeva1502@yandex.ru
[2] *Laboratory of Chemistry and Physics of Supramolecules . A.E. Arbuzov Institute of Organic and Physical Chemistry KSC RAS. Arbuzov, 8. Kazan, 420088. Tatarstan Republic. Russia.*
Phone: +7 (843) 273-22-53. E-mail: ryzhkina@iopc.ru, kiseleva@iopc.ru
[3] *Kazan State Medical University. Butlerov, 49. Kazan, 420012, Tatarstan Republic. Russia.*
Phone: +7 (843) 236-06-13. E-mail: rsa777@inbox.ru.
[4] *Department of General Physics. Kazan Federal University. Kremlyovskaya, 16a.*
Kazan. Tatarstan Republic. Russia. Phone: +7 (843) 292-76-33.

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*Supervising author; [+]Corresponding author

Keywords: highly diluted aqueous solutions, external electromagnetic fields, potassium phenosan salt, *Spirostomum ambiguum*, behavior activity, nanoassociates, self-organization, physicochemical properties.

Abstract

In the work it is discusses experimental results on the effect of highly diluted solutions of synthetic broad-spectrum drug potassium phenozan salt (PPh) on the behavioral activity of aquatic organisms associated with self-organization of PPh solutions. The formation of nanoassociates in highly diluted PPh solutions causes the emergence of nonmonotonic concentration dependences of the physicochemical properties of solutions and correlated with their biological effects. It was studied the effect of weak physical fields as natural background radiation and certain types of electromagnetic fields and ionizing radiation on the physiological status of aquatic organisms and the physicochemical parameters of water.

Thematic Section: Research into the Effects of Physical Fields. **Full Paper**
Subsection: Biochemistry. *Registration Code of Publication:* 15-42-5-19
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The influence of the water activated by plasma-solution sistems on phytogenous objects

© **Irina K. Naumova**,[1+] **Irina N. Subbotkina**,[1*]
Sergey Vladimirovich Silkin,[2*] and **Tatiana A. Shapovalova**[1]
[1] *Chemistry Department. Ivanovo State Agricultural Academy named after academician D.K. Belyaev. Sovetskaya St., 45. Ivanovo, 153012. Russia. E-mail: irinauma@mail.ru*
[2] *Agrochemistry and Agriculture Department. Ivanovo State Agricultural Academy named after academician D.K. Belyaev. Sovetskaya St., 45. Ivanovo, 153012. Russia. E-mail:ssv-bunker@rambler.ru*

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*Supervising author; +Corresponding author

Keywords: plasma-solution treatment, face discharge, GDA, sowing potatoes, sprouting seeds.

Abstract

During the investigations we found that gas-discharge water treatment resulting in it decontamination, removal the organic admixtures and heavy metals ions intensifyes the plants prime growth (germinating capacity, rootage growth). The raising the level crop yield and quality treated crops are observed by plasma treated water application for root preparation.

Thematic Section: Research into the Effects of Physical Fields. ____________ **Short Communication**
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The study of the level of carotenoids, chlorophyll *a* and *b* in seedlings of common barley (*Hordeum vulgare*) after treatment of seeds constant magnetic field and UV radiation in the presence of ozone

© **Pyotr P. Purygin**,[1]* **Denis A. Tsaplev**,[1] **Vitaly A. Purygin**,[1]
Yury P. Zarubin,[1+] and **Tatiana I. Vasil'yeva**[2]
[1] *Chair of Organic, Bioorganic and Medicinal Chemistry. Samara State University. Akad. Pavlova St., 1. Samara, 443011. Samara region. Russia. Phone: +7 (846) 334-54-59. E-mail: puryginpp2002@mail.ru*
[2] *Chair of Biological Chemistry. Samara State University. Akad. Pavlova St., 1. Samara, 443011. Samara region. Russia. Phone: +7 (846) 334-54-42. E-mail: biofak@samsu.ru.*

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*Supervising author; +Corresponding author

Keywords: chlorophyll a and b, constant magnetic field, UV radiation, ozone.

Abstract

An efficient and environmentally friendly way of handling crops ozone, UV radiation and a constant magnetic field. This method of processing plants can be applied in various branches of agriculture.

Analytical Review ________________________ *Thematic Section:* Research into the Effects of Physical Fields.
Registration Code of Publication: 15-42-5-26 *Subsection:* Physico-Chemistry of Polymers.
The article is published on materials of the report on "International Scientific Forum
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The use of microwaves in the production of monomers

© **Rustem R. Daminev**,* and **Oleg Kh. Karimov** +
Division of General Chemical Technology. Ufa State Petroleum Technological University, Branch of USPTU
in Sterlitamak. Pr. Oktyabrya, 2. Sterlitamak, 453118. Bashkortostan Republic. Russia.
Phone: +7 (3473) 24-25-12. E-mail: karimov.oleg@gmail.com

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*Supervising author; +Corresponding author

Keywords: microwave radiation, monomers, isoprene, dehydrogenation, chromia-alumina catalyst, isobutylene, methylbutane.

Abstract

The results of studies on the use of electromagnetic microwave radiation to enhance the process of synthesis of monomers to production of synthetic rubber. Application of microwave discussed as an example of technology synthesis of butadiene and isoprene by two-step dehydrogenation of paraffins and a synthesis of isoprene from isobutylene and formaldehyde. In the two-step method of dehydrogenation of butane and pentane application of microwave energy is possible at both stages. In the first stage dehydrogenation of paraffins to olefins technology is proposed synthesis alumina-chromium catalysts under the influence of electromagnetic radiation at various stages of its preparation. Exposure to the microwave field in the steps of impregnation of an alumina support, and drying the catalyst allows to obtain a catalyst with a high catalytic properties, the olefin yield is increased by 4.3%, the selectivity increases by 3.8%. The catalyst has high strength and is supposed to work period. Is improved technological scheme of the process of dehydrogenation of paraffins on this catalyst. In the second step the dehydrogenation of olefins to diolefins is proposed to use the energy of the electromagnetic radiation directly to the activation reaction on the iron-potassium catalysts operating in the industry. Dehydrogenation of olefins under the action of microwave radiation can reduce the energy consumption of the process without reducing yield of diolefins. Exposure to microwave radiation in the process of synthesis of isoprene from isobutylene and formaldehyde, also allows to obtain a high yield. The highest catalytic properties in the electromagnetic field has a catalyst based on cationite of KU-2.

Thematic Section: Research into the Effects of Physical Fields. **Full Paper**
Subsection: Physical-Chemistry Polymers. *Registration Code of Publication:* 15-42-5-31
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A study on the effect of microwave radiation on the operational characteristics of insulating materials based on polyvinyl chloride

© **Nikolay S. Shulaev**,*+ **Damir F. Suleymanov**, and **Elena M. Abutalipova**
Ufa State Petroleum Technical University, branch FGBOU VPO USPTU in Sterlitamak.
October ave., 2. Sterlitamak, 453100. Republic of Bashkortostan. Russia.
Phone: +7 (3473) 24-25-12. E-mail: suldf@yandex.ru

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*Supervising author; +Corresponding author

Keywords: microwave radiation, polyvinyl chloride, breaking load, water absorption, electrical resistance

Abstract

In the present paper presents the results of experimental studies of changes in the properties of polyvinyl chloride at relatively low (not leading to a significant temperature increase) doses absorbed energy of ultra high frequency electromagnetic radiation (RF EMR). The relevance of such studies is due on the one hand, extensive use of this polymer in the manufacture of various products, in particular for large-scale production of insulating coatings of pipeline systems and the relatively high (compared with other polymers) the rate of absorption of radiation in the microwave range. From experimental studies it follows that the specific absorbed energy of less than 10 kJ/kg, there was a slight increase in strength properties, and at a dose of more than 30 kJ/kg reduction compared to the unmodified sample. In the energy interval from 15 to 20 kJ/kg the increase, the actual breaking load of more than 1.5 times. In addition, it was found that in the range indicated doses of microwave AMY volumetric electrical resistivity, determined by the presence in the polymer of free carriers and their mobility, takes the maximum value. With the increase of electrical resistivity, the decrease of the free charges, due to the formation of additional bonds and conformational changes of macromolecules, resulting in increased tensile strength. Determined that in the range of radiation doses of 10-20 kJ/kg, a decrease of water absorption in two times. The reduction of moisture absorption can be explained by the increase in the density of a three-dimensional network of macromolecules of the polymer due to the formation of cross-links. The rate of swelling is reduced, indicating the occurrence of a more rigid structure of the modified polymer. Experimentally proved the possibility of using microwave radiation for targeted modification of the structure of the polar polymer that provides an improvement in their physical and mechanical properties. Estimations show that the proposed method improve the performance of less energy intensive and more environmentally friendly compared to traditional way of hardening of PVC products.

Full Paper _______________________________________ *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 15-42-5-36 *Subsection:* Organic Chemistry.
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Kinetics and mechanism of UV-phototransformations new synthetic antioxidants series of N-substituted amides of salicylic acid

© **Nadezhda P. Medyanik**,[1] **Nadezhda M. Storozhok**,[1]*
Ivan P. Pozdnyakov,[2] and **Sergey A. Krekov**[3]
[1] *HPE «Tyumen State Medical University" Ministry zdrvoohraneniya Russia.*
Odessa St., 54. Tyumen, 625023. Russia. Fax: +7 (3452) 20-74-21. E-mail: nadinstor@mail.ru
[2] *Institute of Chemical Kinetics and Combustion. Siberian Branch of the Russian Academy*
of Sciences. Institutskaya St. 3. Novosibirsk, 630090. Russia.
Fax: +7 (3832) 30-73-50. E-mail: pozdnyak@ns.kinetics.nsc.ru
[3] *HPE «Tyumen State University" Ministry of Education of Russia. Semakova St., 10. Tyumen, 625003.*
Russia. Phone: +7 (3452) 25-15-94. E-mail: nadinstor@mail.ru

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*Supervising author; [+]Corresponding author

Keywords: salicylic acid amide, photolysis, phenoxy radical recombination, IR, UV spectroscopy, hydrogen bonding, deuteration.

Abstract

The photolysis products of *N*-substituted amides salicylate-Cretaceous acid: 1-(*N*-4′-hydroxyphenyl-3,3′,5′-)tri-*tert*-butyl-5-ethyl salitsilovoy acid (**I**) and 1-acid (*N*-4′-hydroxyphenylpropyl-3′,5′-di-*tert*-butyl) salicylic acid (**II**) in heptane have been investigated by optical spectroscopy, stationary and nanosecond laser flash photolysis (Nd: YAG laser, 355 nm). The method of partial-foot deuteration of the molecules of amides **I**, **II** shows that they are in a free state, and in the form of complexes with intra- and intermolecular hydrogen bonds. Photolysis subjected to free phenolic groups of amides **I**, **II**, which leads to the triplet state and the formation of phenoxy radicals $RO^{\bullet}$ allegedly as a result of the absorption of a quantum of light of the second excited singlet state. The main channel of the triplet states, the death of the $RO^{\bullet}$ radicals and a triplet-triplet (TT) annihilation and recombination (k rek $\approx 2.3 \cdot 10^{8}$ $L \cdot mol^{-1} \cdot s^{-1}$), respectively. Upon UV irradiation of the compounds **I**, **II** are excited amide groups established by the formation of radical products due to ionization of NH-bond.

Thematic Section: Physico-Chemical Research. **Full Paper**
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Influens of the protein microenvironment on the spectral properties of prodigiosin

© **Irina N. Andreyeva**,*+ **Tatiana I. Ogorodnikova**, and **Natalia L. Zaharchenko**
Kazan Institute of Biochemistry and Biophsics, Kazan Science Center of Russian Academy of Sciense.
Lobachevsky St., 2/31. Kazan, 420111. Russia. Phone: +7 (843) 292-72-22. E-mail: irinanikandr@gmail.ru

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*Supervising author; +Corresponding author

Keywords: prodigiosin; absorption; flourescensce; protein environment.

Abstract

The linear tripyrrole prodigiosin is produced by *Serratia marcescens* and give character red colouring to culture. Prodigiosin is dissolved in polar and non-polar organic solvent and is water-insoluble but transfer to water fase as protein-pigment complex by biomass treatment with detergents (SDS and Triton X-100). There are two spectral form of prodigiosin accoding to pH: red with maximal absorbance at 535 nm and yellow with maximal absorbance at 460-470 nm. Growing *S.marcescens* accumulate both pigment forms. Absorbance curve of cellular suspension covers absorbance area of both pigment forms and this is the new absorbance peak at 500 nm. The absorption curve of native pigment-protein complex coincides with that of intact pigmented cells. Absorption at 500 nanometers is characteristic for prodigiosin associated with native protein and denote that pigment-protein relations is similar to that into bacterial cells. Effect of denaturated agents leads to disappearance of this maximum at absorbance spectrum of prodigiosine-pigment complex. Both prodigiosin forms fluoresce at 560-580 nanometers (depending on concentration), both as ethanol solutione and as pigment-protein complex. *In vitro* disruption of a pigment – proteine interaction leads to prodigiosin absorption increase and fluorescence decrease. In cellular suspension fluorescence of the red form of a pigment (E_{535}) is more expressed and fluorescence of yellow ($E_{460-470}$) and novel, E_{500}, are smaller. There is the fact that may point out functional differences of this prodigiosine forms at *S.marcescens* methabolism.

Full Paper ____________________________________ *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 15-42-5-56 *Subsection:* Biochemistry.
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Application of electrode modified with carbon nanofibers and cationic surfactant for simultaneous voltammetric determination of syringaldehyde and vanillin

© **Guzel K. Ziyatdinova**,[+] **Ekaterina V. Kozlova**,
Endzhe R. Ziganshina, and **Herman C. Budnikov**
Analytical Chemistry Department. A.M. Butlerov Institute of Chemistry. Kazan Federal University.
Kremlevskaya St., 18. Kazan, 420008. Republic of Tatarstan. Russia.
Phone: +7 (843) 233-77-36. E-mail: Ziyatdinovag@mail.ru

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*Supervising author; [+]Corresponding author

***Keywords**:* differential pulse voltammetry, chemically modified electrodes, carbon nanofibers, surfactants, phenolic antioxidants.

Abstract

Syringaldehyde and vanillin are oxidized at 0.77 and 0.88 V, respectively, on the glassy carbon electrode modified with carbon nanofibers and cationic surfactant cetylpyridinium bromide in Britton-Robinson buffer pH 2.0. Two-fold increase of oxidation currents and cathodic shift of oxidation potentials on 10-20 mV as well as improvement of voltammograms shapes have been observed in comparison to bare electrode. Analytes peaks potential separation of 110 mV allows to perform their simultaneous determination. Variation of one component concentration at fixed concentration of the second one has shown that oxidation of syringaldehyde and vanillin runs independently. Voltammetric method for simultaneous determination of syringaldehyde and vanillin has been developed. The linear dynamic range is 2.5-30 and 5.0-40 μM for syringaldehyde and vanillin, respectively with detection limits of 0.53 and 1.17 μM.

Full Paper *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 15-42-5-64 *Subsection:* Biochemistry.
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Kinetics of thermal injury of bioobjects

© **Rustyam Sh. Enaleev,**[1]* **Gulnara I. Amerkhanova,**[2+]
Edward Sh. Telyakov,[3] and **Vyacheslav S. Gasilov**[4]
[1] *Departament of Chemical Cybernetics;* [2] *Department Technology of Inorganic Substances and Materials;*
[3] *Departament of Mechanical Engineering for Chemical Industry;* [4] *Departament of Industrial Safety.*
Kazan State Technological University. K. Marx St., 68. Kazan, 420015. Republic of Tatarstan. Russia.
Phone: +7 (843) 231-40-13. E-mail: Amerkhanova-g-i@rambler..ru

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*Supervising author; [+]Corresponding author

***Keywords*:** fire, thermal injury, threshold impulse, skin models.

Abstract

The analysis of foreign methods on criteria of thermal injury of bioobjects in emergencies is conducted. The algorithm of experimental data processing is offered by determination of kinetic parameters of bioobjects' skin thermal injuries for contact burns and thermal radiation. New approach in predicting of probabilities for thermal burns of varying severity under various boundary conditions of heat transfer is justified.

Thematic Section: Physico-Chemical Research. **Full Paper**
Subsection: Biochemistry. *Registration Code of Publication:* 15-42-5-71
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Spectrophotometry in the analysis of two snowdrop species (*Galanthus* L.)

© **Dmitriy O. Bokov**,[1]*+ **Irina A. Samylina**,[1] and **Dmitry M. Popov**[2]

[1] *Division 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] *Research Institute of Pharmacy. I.M. Sechenov First Moscow State Medical University. Nahimovskiy ave., 45. Moscow, 117418. Russia.*

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*Supervising author; +Corresponding author

Keywords: spectrophotometry, *Galanthus woronowii* Losinsk, *Galanthus nivalis*, homeopathic mother tincture, alkaloids, flavonoids.

Abstract

We studied the electronic UV absorption spectra of homeopathic mother tinctures prepared from medicinal plant material of two snowdrop species – *Galanthus woronowii* Losinsk and *Galanthus nivalis* L. In the present study, data were obtained characterizing the composition of the main biologically active compounds of the genus *Galanthus* L. by UV spectrophotometry, we received their "spectrophotometric profiles." It is shown that this method can be used to assess the quality of homeopathic mother tinctures dilutions, serve to prove their identity.

Full Paper ____ *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 15-42-5-78 *Subsection:* Medical Products.
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The role of detergents used in sanitary-and-hygienic treatment of stopper in the contamination of drugs

© **Svetlana V. Guzhova**,[1+] **Natalia K. Romanova**,[3] **Nadezhda N. Simonova**,[2]
Elena N. Cherezova,[1] **Yury N. Khakimullin**,[2*] and **Rafinat S. Yarullin**[1]
[1] *Department of Technology of Synthetic Rubber.* [2] *Department of Chemistry and Processing Technology of Elastomers.* [3] *Department of food Production Technology. Kazan National Research Technological University. K. Marx St., 68. Kazan, 420015. Republic of Tatarstan. Russia. Phone:+7 (843) 231-42-87.*

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*Supervising author; +Corresponding author

Keywords: infusion and injection pharmaceuticals, rubber stoppers, sterilization, disinfection, detergents, migration, destruction.

Abstract

The role of detergents used for washing of stopper in the contamination of drugs was studied. Detergents and modes of washing, disinfection and sterilization have a destructive effect on the stoppers. The method of atomic emission spectrometry showed that the chemical elements of the compounds included in the composition of detergents can diffuse into the stoppers and then into the drugs.

Full Paper *Thematic Section:* Physicochemical Research.
Registration Code of Publication: 15-42-5-84 *Subsection:* Medical Products.
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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Methods for evaluating the flowability of powdered drug substance

© **Aleksander M. Pyzhov**,[1+] **Ivan K. Kukushkin**,[1]* **Artyom S. Anisimov**,[1]
Aleksey G. Usenko,[1] and **Pyotr P. Purygin**[2]
[1] *Chair of Chemistry and Technology of Organic Nitrogen Compounds. Samara State Technical University. Molodogvardeyskaya St., 244. Samara, 443100. Samara region. Russia.*
Phone: +7 (846) 337-08-89. E-mail: argel33@mail.ru
[2] *Chair of Organic, Bioorganic and Medicinal Chemistry. Samara State University. Akad. Pavlova St., 1. Samara, 443011. Samara region. Russia. Phone: +7 (846) 334-54-59. E-mail: puryginpp2002@mail.ru*

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*Supervising author; $^{+}$Corresponding author

***Keywords**:* dosage forms, tablets, tablet machines, evaluation of flowability medicinal materials, new method and apparatus.

Abstract

This article presents the results of research on the development of a new method for evaluating the flow properties of powdered drugs, which is based on sequential dosing of the test substance in the container of the same volume and the subsequent definition of the standard deviation portions dosed substances, so-called, "the relative scatter sample" of the substance, which is a measure of the flow properties of the substance. The estimation accuracy of the dosing substances is a few tenths of a milligram. To assess the flowability by the novel process developed effective device that mimics real conditions in the tablet dosing machine capable of accurately and in a short time to evaluate the flowability of substances taken in small quantities.

Thematic Section: Physico-Chemical Research. **Full Paper**
Subsection: Colloidal Chemistry. *Registration Code of Publication:* 15-42-5-89
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Influence of the emulsion parameters on the size of nanoparticles of Fe_3O_4 under heterophase synthesis

© **Anton I. Nechayev**, **Victor A. Valtsifer** and **Vladimir N. Strelnikov**
Institute of Technical Chemistry, Ural Branch of the Russian Academy of Sciences. Academician Korolev St., 3. Perm, 614013. Russia. Phone: +7 (342) 237-82-90. E-mail:toxambj@mail.ru

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*Supervising author; [+]Corresponding author

Keywords: magnetic nanoparticles, magnetite, organosol, heterophase synthesis, emulsion, HLB.

Abstract

In this paper, the technique of heterophasic one step synthesis of nonpolar organosol of nanoscale Fe_3O_4 has been worked out. The synthesized samples of nanoparticles Fe_3O_4 were investigated by infrared Fourier transform spectroscopy (FT-IR), X-ray diffraction (XRD), dynamic light scattering (DLS), and transmission electron microscopy of high resolution (HRTEM). The boundary conditions were defined for the synthesis of Fe_3O_4 nanoparticles by the developed method. The effect of the emulsion type, the phase relationship, the hydrodynamic parameters of emulsification, the ratio of stabilizer/Fe_3O_4, HLB the surfactants entered into the system at an average hydrodynamic size of particles and their size distribution in the organosol have been investigated. It has been shown that the surface area of the phase boundary has a decisive influence on the size of nanoparticles. It was established that this method is applicable for the synthesis of monodisperse nanoparticles Fe_3O_4 with the size up to 1 nm having an affinity to non-polar liquid media.

Full Paper ____ *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 15-42-5-98 *Subsection:* Colloidal Chemistry.
The article is published on materials of the report on "International Scientific Forum
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Colloidal properties of aqueous dispersions of dextran

© **Irina B. Dmitriyeva**,* **Alexander S. Chukhno**,+ **Ekaterina Yu. Rodionova**,
and **Albina R. Nazipova**
Department of Physical and Colloidal Chemistry. St. Petersburg State Chemical-Pharmaceutical Academy.
Professor Popov St., 14. St. Petersburg, 197376. Russia.
Phone: +7 (905) 214-59-73. E-mail: alex-chuhno@yandex.ru

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*Supervising author; +Corresponding author

Keywords: dextran, microelectrophoresis, sorption, potentiometric titration, the isoelectric point, point of zero charge, coagulation.

Abstract

The colloidal properties of aqueous dispersions of dextran have been investigated in this paper. The study of the rheological properties by viscometric method has allowed to establish that its aqueous dispersion is a Newtonian liquid at all studied concentrations of dextran. The zeta potential of dextran particles has been determined by electrophoresis depending on the composition of the dispersion medium (pH, nature and concentration of electrolyte). The influence of various electrolytes and pH on the sorption of hydrogen ions and hydroxide ions has been investigated. The isoelectric point ($pH_{IET} = 5$) and the point of zero charge of dextran have been determined. The point of zero charge varies in the range $pH_{PZC} = 4.3$-4.8. The difference of the isoelectric point and the point of zero charge is related to the specific sorption of ions. It is found that dextran coagulation at $pH > pH_{IET}$ occurs by concentration mechanism.

Full Paper _______________________________________ *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 15-42-5-104 *Subsection:* Physical Chemistry of Cellulose.
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Structure and properties of modified cellulose

© **Zimfira T. Valishina,*** **Guzel N. Galiullina,**$^+$ and **Anatoly V. Kostochko***
Department of Chemistry and Technology of Macromolecular Compounds. Kazan National Research Technological University. Karl Marx St., 68. Kazan, 420015. Respublic of Tatarstan. Russia.
Phone: +7 (843) 231-40-95. E-mail: zimval1@yandex.ru

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*Supervising author; $^+$Corresponding author

Keywords: modified cellulose, viscosity, molecular structure, X-ray analysis, modeling.

Abstract

Complex investigations of molecular, supramolecular, viscosity, morphological properties of modified cellulose were made. The correlation between the viscosity characteristics of cellulose solutions with the parameters of molecular and supramolecular structure was founded, which is necessary for the creation of new polymer materials based on high purity cellulose with the desired combination of physical and chemical properties.

A mathematical model of acid hydrolysis process for various kinds of cellulose was developed, which allows to predict the viscometric properties depending on the concentration, temperature, nature of acid and forecast the properties of the new compositions.

Full Paper ______________________________________ *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 15-42-5-112 *Subsection:* Composite Materials.
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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The chemical analysis of the silicone polymers and materials on their basis, applied in micro- and nanoelectronics

© **Olga V. Neyelova**,*+ and **Rimma A. Gazzaeva**
Chemistry-Technological Faculty. North Ossetian State University after K.L. Khetagurov.
Vatutina St., 44-46. Vladikavkaz, 362025. RSO-Alanija. Russia.
Phone: +7 (867) 254-44-22. E-mail: o.neelova2011@yandex.ru

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*Supervising author; +Corresponding author

Keywords: silicone polymers, composite materials, the maintenance of ionic impurity, microelectronics and nanotechnologies.

Abstract

The method of the atomic emission spectral analysis is developed at 100-fold enrichment, allowing to supervise 15 elements of impurity of metals in high-purity silicone materials. The method is based on concentration of the impurity on a coal collector after burning of the sample and removal of a basic element of silicon in a kind tetrafluoride or extraction by deionization water of soluble impurity from the insoluble rest. The concentrate of impurity on a collector is raised in plasma of an arch of an alternating current. The developed technique allows to spend definition of impurity K, Na, Li, Ba, Sr, Ca, Mg, Al, Fe, Ti, Mn, Cr, Cu, Zn, Pb in silicone rubbers, pitches and the unfilled and filled compositions at their maintenance of 10^{-2}-10^{-6}%.

Thematic Section: Physico-Chemical Research. **Full Paper**
Subsection: Analytical Chemistry. *Registration Code of Publication:* 15-42-5-119
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Separation of manganese(II), iron(III), copper(II) and nickel(II) ions on the strongly acidic cation exchangers for subsequent determination of the water-soluble inorganic forms of arsenic by stripping voltammetry

© **Anastasia V. Te**,[1+] **Lidia N. Skvortsova**,[2]* and **Elza A. Zakharova**[3]*
[1] *Student, Chemical Faculty. National Research Tomsk State University. Lenin St., 36. Tomsk, 634050. Russia. Phone: +7 (952) 891-46-66. E-mail: injurious_girl@mail.ru*
[2] *Ph.D. (Chemistry). Associate Professor of Analytical Chemistry Department. National Research Tomsk State University. Chemical Faculty. Lenin St., 36. Tomsk, 634050. Russia. Phone: +7 (913) 887-55-39. E-mail: lnskvorcova@inbox.ru*
[3] *Ph.D. (Chemistry). Senior Research Scientist of Physical and Analytical Chemistry Department. National Research Tomsk Polytechnic University Limited. Lenin St., 30. Tomsk, 634050. Russia. Phone: +7 (3822) 56-37-22. E-mail: elaz38@mail.ru*

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*Supervising author; +Corresponding author

Keywords: ion exchange, interfering ions, arsenic speciation, stripping voltammetry, water.

Abstract

The possibility of using the method of ion exchange to separate the ions Mn(II), Fe(III), Cu(II) and Ni(II) of arsenite and arsenate ions with the cartridge *IC-H Hypersep* (Switzerland) and sulfonated cationite resin (*КУ-2-8*, Russia), *Pirolite C100* (UK). The conditions to remove interfering cations by ion exchange procedure during As speciation in water samples by stripping voltammetry (SV) method were chosen. It was found that the proposed method of water preparation with domestic cartridges based on КУ-2-8 resin may be used. The developed method of analysis used to determine the inorganic forms of arsenic in drinking water. The validity of the analysis was proved by standard addition method.

Full Paper ____ *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 15-42-5-128 *Subsection:* Spectroscopy.
The article is published on materials of the report on “International Scientific Forum
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Submitted on April 15, 2015.

Influence of topological structure and molecular motion on the signal of stimulated echo NMR in polymer networks

© **Tatiana P. Kulagina**,[1] **Grigory E. Karnauksh**,[1] **Oleg M. Vyaselev**,[2] and **Aisa S. Sarmutkina**[1,3]
[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] *Institute of Solid State Physics RAS. Academician Ossipyan St., 2. Chernogolovka, 142432.*
Moscow region. Russia. Phone: +7 (496) 522-19-82. E-mail: vyasel@issp.ac.ru
[3] *Lomonosov Moscow State University. Leninskie Gory1, bild. 51. Moscow, 119991. Russia.*
Phone: +7 (495) 939-01-75. E-mail: ice1992.2011@mail.ru

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*Supervising author; +Corresponding author

Keywords: nuclear magnetic resonance, polymer networks, free induction decay, physical network of entanglement, stimulated echo, correlation function of molecular motion.

Abstract

The theory of stimulated echoes for different sequences of three RF pulses is represented. The methods of determination of correlation function of molecular motion of polymer chains from NMR experiments directly (free induction decay (FID) and stimulated echo) is developed on the base of the theory. The modeling of FID and stimulated echo in polymer networks is carried out, the type of correlation function at different average length of a polymeric chain N_0 between knots is defined. Strong influence of the molecular-weight distribution (MWD) on the type of correlation function in polymer melts is established.

Thematic Section: Physico-Chemical Research. **Full Paper**
Subsection: Thermophysical Properties. *Registration Code of Publication:* 15-42-5-133
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Modified Fogel-Fulcher-Tamman viscosity equation for mixtures of monoethylene glycol – diethylene glycol – triethylene glycol taking into consideration their composition

© **Damir I. Sagdeev**,[1]*+ **Marina G. Fomina**,[1] **Evgeny S. Vorobiev**,[2]
Gabdlnur Kh. Mukhamedzyanov,[1] and **Ilmutdin M. Abdulagatov**[3]
[1] *Department of Vacuum Engineering.* [2] *Department of General Chemical Technology.*
[3] *Department of Heat Engineering. Kazan National Research Technological University.*
Karl Marx St., 68. Kazan, 420015. Russia. Phone: +7 (843) 231-42-70. E-mail: sagdeev@mail.ru.

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*Supervising author; +Corresponding author

Keywords: polyethylene glycols, mixtures, Fogel-Fulcher-Tamman viscosity equation; simplex lattice method.

Abstract

To know physicochemical and thermal properties of pure polyethylene glycols and their mixtures is necessary for accurate technological calculations. Relationships obtained by simplex lattice method with the help of computer simulation (changing component concentration, temperature and pressure) make it possible to get optimal conditions for process technology meeting the requirements of output parameters.

Simplex lattice design has the advantage in predicting a property of a mixture with arbitrary composition if the experimental results for pure materials, their binary and one ternary mixtures were obtained (as in our case).

A relationship is developed on the basis of Fogel-Fulcher-Tamman equation with coefficients depending on pressure which can be used for representing viscosity-temperature dependence of mixtures of MEG, DEG and TEG with the help of simplex lattice method in a wide range of temperatures, pressures and concentrations.

This relationship is used for viscosity calculation of mixtures of monoethylene glycol – diethylene glycol – triethylene glycol taking into consideration their composition in the temperature range from 298 to 473 K and pressures up to 245 Pa.

Thematic Section: Physico-Chemical Research. **Full Paper**
Subsection: Physical Chemistry of Explosives. *Registration Code of Publication:* 15-42-5-139
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Intensification of the fine grinding process of ammonium nitrate

© **Alina R. Krivosheeva**,[+] **Zalimhan K. Omarov**, **Roza F. Gatina**, and **Yury M. Mihaylov***
Federal State Enterprise “State Scientific Research Institute of Chemical Products”.
Svetlaya St., 1. Kazan, 420033. Republic of Tatarstan. Russia.
Phone: +7 (843) 541-76-02. E-mail: aneco_ic@mail.ru

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*Supervising author; [+]Corresponding author

Keywords: ammonium nitrate, surface-active substances, modification, intensification the grinding process, sodium stearate.

Abstract

Intensification of the fine grinding process of ammonium nitrate using surface-active substances in water-resistant ammonium nitrate technology have been investigated.

The investigations of the kinetics and mechanism of grinding ammonium nitrate in the presence of stearic and palmitic acids and their simple salts have been performed. The addition of ammonium nitrate to the majority of the investigated surfactants in the amount of 1.0% by weight leads to intensification of the process of fine salt grinding. It has been revealed that on increasing the content of additives from 1.0 to 5.0% by weight does not increase the degree of crushing of ammonium nitrate.

Thematic Section: Physico-Chemical Research. **Full Paper**
Subsection: Physical Chemistry of Explosives. *Registration Code of Publication:* 15-42-5-147
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Submitted on April 21, 2015.

Physical and mechanical properties of binary compounds polyvinyl butyral – RDX

© **Tatiana A. Eneykina**,* **Diana B. Zinatullina**,+ **Nadezhda A. Romanko**, **Sergey G. Volyanyuk**, **Rosa F. Gatina** and **Yury M. Mikhailov**
State Scientific-Research Institute of Chemical Products. Svetlaya St., 1. Kazan, 420033. Tatarstan Republic. Russia. Phone: (843) 560-20-42. E-mail: diana.zinatullina89@mail.ru

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*Supervising author; +Corresponding author

Keywords: gas-generating composition, polyvinyl butyral, RDX, intermolecular interaction, IR spectroscopy.

Abstract

IR spectroscopic method was used to investigate the intermolecular interaction components in the polyvinyl butyral – hexogen compositions with a ratio 1:1, 1:3 и 1:6. Physical and mechanical tests of compositions were conducted on the universal testing complex *Instron*. It has been defined that at the ratio of polyvinyl butyral and RDX equal to 1: 3 there is observed a maximum level of their interaction.

Full Paper _____________________________________ *Thematic Section:* Quantum-Chemical Research.
Registration Code of Publication: 15-42-5-152 *Subsection:* Organic Chemistry.
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Quantum-chemical study of the molecular structure and vibrational spectra of methyl nitrate and ethyl nitrate

© **Ravia M. Shaikhullina,**[1+] **Gregory M. Hrapkovsky,**[2*] and **Elena Evgenievna Zvereva**[3]
[1] *Department of Physics. Naberezhnye Chelny Institute (branch) of Kazan Volga Federal University.*
Pr. World, 68/19. Naberezhnye Chelny, 423810. Republic of Tatarstan. Russia.
Phone: +7 (855) 258-95-36. E-mail: raviya1@yandex.ru
[2] *Department of Catalysis. Kazan State Technological University. K. Marx St., 68. Kazan, 420015.*
The Republic of Tatarstan. Russia. Phone: +7 (843) 231-42-53.
[3] *Institute of Organic and Physical Chemistry. A.E. Arbuzov of the Kazan scientific centre of RAS.*
Acad. Arbuzova St., 8. Kazan, 420088. Republic of Tatarstan. Russia. Phone: +7 (843) 273-18-92.

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*Supervising author; [+]Corresponding author

Keywords: methyl nitrate, ethyl nitrate, quantum chemistry, molecular structure, conformation, vibrational spectra.

Abstract

The data presented theoretical analysis of the vibrational spectra of methyl nitrate, *trans* - and *gauche* - conformations of ethyl nitrate obtained using the methods of the density functional theory *(B3LYP/6-31G(d))*. Installed most energetically favorable structure of methyl nitrate and ethyl nitrate calculated corresponding to these structures, frequencies and forms of normal vibrations. Identified spectral features conformational state of methyl-, ethyl nitrate, and the effects of the formation of intramolecular hydrogen bonds.

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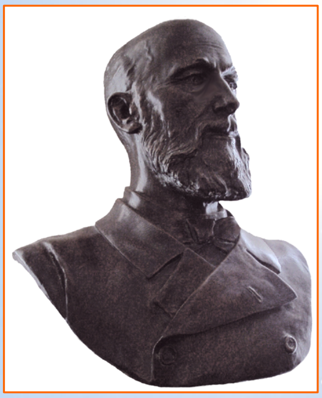

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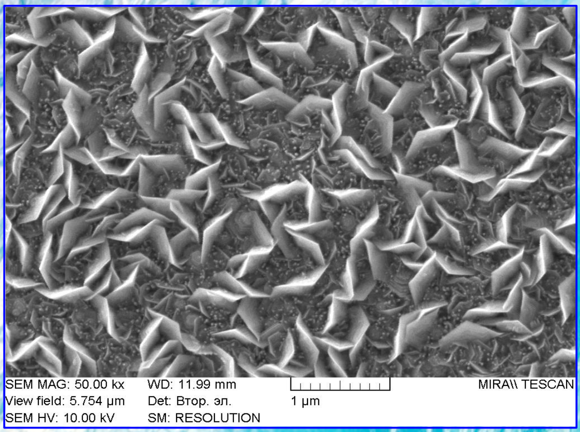

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Subsection: Composite Materials. *Registration Code of Publication:* 15-42-6-1
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Sorption and biocidal properties of the composite based on glauconite Saratov region and copper nanoparticles

© **Elena M. Soldatenko**, **Sergey Yu. Doronin**,$^+$ **Rimma K. Chernova**, **Sergey B. Venig**,*
Viktor G. Serzhantov, **Olga G. Shapoval**, and **Andrey M. Zaharevich**
Saratov State University namely after N.G. Chernyshevsky. Astrakhanskaya St., 18/3. Saratov, 410012. Russia.
Phone: +7 (8452) 26-45-53. E-mail: Doroninsu@mail.ru

*Supervising author; $^+$Corresponding author

Keywords: inorganic sorbents, glauconite, copper nanoparticles, sorption, composites.

Abstract

Copper nanoparticle based glauconite composite has been synthesized by in situ reduction of a copper ammonium complex ion and characterized by different analytical instruments. The copper nanoparticles were both intercalated and adsorbed. The sorption properties of the glauconite and composite basis on it in relation to iron ions(III) have been studied, the sorption isotherms were obtained. Antimicrobial activity of the composite was observed on Escherichia coli, Staphylococcus aureus. In the present form the glauconite composite shows good promise use for applications in medical practice.

Thematic Section: Physico-Chemical Research. **Full Paper**
Subsection: Composite Materials. *Registration Code of Publication:* 15-42-6-7
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Technology sulfides silicates and composite materials with application of activators of aluminum chloride

© **Rezida T. Akhmetova**, **Alsu A. Yusupova**,*
Linara R. Baraeva,$^+$ and **Aleksey I. Khatsrinov**
Technology of Inorganic Substances and Materials Division. Institute of Petroleum,
Chemistry and Nanotechnologies. Kazan National Research Technological University.
K. Marx St., 68. Kazan, 420015. Republic of Tatarstan. Russia.
Phone: +7 (843) 238-56-94. E-mail: office@kstu.ru, baraeva.linara@yandex.ru

*Supervising author; $^+$Corresponding author

Keywords: sulfides silicates, aluminum chloride, composite materials.

Abstract

The efficiency of technology of inorganic substances on the basis of silicates in the preparation of sulfides sulfur composites. High mechanical properties obtained are due to the chemical interaction of the samples with sulfur chloride, aluminum fixed on the surface of silica-containing material. The results of quantum-chemical studies were confirmed by the study of physical and mechanical properties of the materials and methods of physicochemical analysis (IR spectroscopy, thermogravimetry, X-ray, by electron paramagnetic resonance and petrography). The materials developed can be used in the construction of industrial, agricultural, storage facilities, during the operation of which are increased requirements for resistance to aggressive environments, frost and weather resistance, impermeability. Increased use of sulfur is largely due to the decision of the environmental problem of waste disposal industry, on the one hand, and significantly reduces the cost of the process of obtaining resistant and durable materials.

Thematic Section: Physico-Chemical Research. **Full Paper**
Subsection: Physical Chemistry of Explosives. *Registration Code of Publication:* 15-42-6-11
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Characteristics of thermal decomposition and thermal explosion of certain components of composite energetic materials

© **Vladimir N. Popok**,*+ and **Alexander S. Zharkov**
Joint Stock Company «Federal Research and Production center «ALTAI».
Sotsialisticheskaya St., 1. Biysk, 659322. Altai territory. Russia.
Phone: +7 (3854) 30-19-37. E-mails: vnpopok@mail.ru

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*Supervising author; +Corresponding author

Keywords: mixed energy materials, thermal decomposition, thermal explosion, cocrystals.

Abstract

The article presents the results of experimental studies of the parameters thermal decomposition in transient conditions and characteristics of the thermal explosion of a number of components mixed energy materials. Spend clustering of substances by their functional appointment determined from the compositions of mixed energy materials and the presence of functional groups, recommendations for the selection of materials from the class of oxidizers, fuel-binder components, energy additives for use in the compositions of mixed energy materials.

Thematic Section: Physico-Chemical Research. **Full Paper**
Subsection: Physical Chemistry of High Temperatures. *Registration Code of Publication:* 15-42-6-17
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Ignition of cellulosic materials: measurement of characteristics of ignition

© **Artem V. Kargin**[1+], **Rustem Sh. Enaleev**[2*],
Fidais M. Gimranov[1] and **Vyacheslav S. Gasilov**[1]
[1] *Department of Industrial Safety;* [2] *Department of Chemical Cybernetics. Kazan National Research Technological University. K. Marx St., 68. Kazan, 420015. Tatarstan Republic. Russia.*
Phone: 8-9297239816. E-mail: a_a384@rambler.ru

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*Supervising author; [+]Corresponding author

Keywords: thermal radiation, cellulosic materials, surface temperature, automated experiment.

Abstract

The analysis of domestic and foreign data on the measurement of the ignition characteristics of cellulosic materials has been carried out. A method for contact temperature measurements of wood, textiles, paper is worked out. The design of the automated measuring unit with interchangeable holders for mount samples is substantiated. The results of experiments on the measurement of the ignition characteristics of cellulosic materials are presented.

Thematic Section: Physico-Chemical Research. **Full Paper**
Subsection: Inorganic Chemistry. *Registration Code of Publication:* 15-42-6-25
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Kinetic aspects of recovery of palladium salts(II) in the presence of hydroxyl-containing compounds

© **Aleksander V. Krylov**,* **Ekaterina A. Bakhtieva**,+ and **Vitaly R. Flid**
M.V. Lomonosov Moscow State University of Fine Chemical Technologies.
Vernadskogo prospect, 86. Moscow, 119571. Russia.
*Y.K. Syrkin Department of Physical Chemistry. Phone: +7 (495) 246-05-55*916.*
E-mail: ekaterinabakhtieva@gmail.com

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*Supervising author; +Corresponding author

Keywords: nanoparticles, palladium, alcohol, polymer.

Abstract

In this paper has been investigated the reducing ability of hydroxyl-containing compounds in the $PdCl_2$ - H_2O - R $(OH)_n$ - NaCl with the formation of nanoscale particles of palladium. It has been shown that in aqueous-organic media particle sizes Pd^0 largely determined by the nature and concentration of hydroxyl-containing compounds, which allows to obtain the required size of the palladium particles. It has been established that the reactivity of the compounds increases in the order: aliphatic alcohols - double, trihydric alcohols - hydroxy acids.

Mechanism of the reaction that has been proposed includes the stage of forming aquachloride complexes of palladium with alcohols or hydroxy acids, stage of aggregation and stabilization of palladium nanoparticles using molecules of hydroxyl compounds. It has been shown, that the introduction of water-soluble polymers PVA and PVP significantly increases the stabilizing effect of the nanoparticles Pd^0 and leads to a decrease of their size, and in the case of the PVA was observed polymer flocculates containing particles Pd^0.

The influence of UV - radiation leads to a noticeable increase the rate of reaction of reduction of palladium ion in agreement with the mechanism of the UV-activation of water molecule in aquachloride complexes of palladium.

Thematic Section: Preparative Research. **Full Paper**
Subsection: Organic Chemistry. *Registration Code of Publication:* 15-42-4-33
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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

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*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, ^1H NMR and $^{13}C\ \{^1H\}$.

Full Paper ____ *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 15-42-6-48 *Subsection:* Inorganic Chemistry.
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Local electrophysical properties of conductive ZnO films

© **Natalia A. Lashkova**,[1+] **Alexander I. Maximov**,[1]* **Lev B. Matyushkin**,[1]
Vyacheslav A. Moshnikov, [1,2]* **Andrey A. Ryabko**,[1]
Pavel A. Somov,[3] and **Stanislav S. Tulenin**[4]
[1] *Department of Micro- and Nanoelectronics. St. Petersburg State Electrotechnical University "LETI". Pr. Popova., 5. St. Petersburg, 197376. Russia. Phone: +7 (812) 234-31-64. E-mail: lashkovanat@yandex.ru.*
[2] *St. Petersburg State Polytechnic University, St. Petersburg. Polytechnicheskaya St., 29. Petersburg, 197376. Russia*
[3] *JSC Svetlana-Rost. Engelsa pr., 27. St. Petersburg, 194156. Russia.*
[4] *Ural Federal University named after the first President of Russia B.N. Yeltsin. Mira St., 19. Ekaterinburg, 620002. Russia.*

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*Supervising author; [+]Corresponding author

Keywords*:* zinc oxide, spray-pyrolysis, chemical vapor deposition, scanning electron microscopy, scanning probe microscopy.

Abstract

Zinc oxide nanostructures are promising candidates for the development of novel electronic devices due to their unique electrical and optical properties. Zinc oxide films were obtained by two methods (spray-pyrolysis and low pressure chemical vapor deposition) and were investigated by scanning electron microscopy and atomic-force microscopy. Obtained results show that polycrystalline layers consist of grains 100-550 in length, and the main conductivity occurs at grain boundaries.

Full Paper ____ *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 15-42-6-54 *Subsection:* Inorganic Chemistry.
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Modification of clay excavated from Klyuchishchenskii deposit of the Republic of Tatarstan

© **Liliy N. Nazharova**,[1]* **Tatiana S. Kvashnina**,[1+] and **Gulfia G. Mingazova**[1]
The Department of Inorganic Substances and Materials . Kazan National Research Technological University.
Karl Marx St., 68. Kazan, 420015. Tatarstan Republic. Russia.
Phone: +7 (843) 231-41-31. E-mail: tatka.100@mail.ru

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*Supervising author; +Corresponding author

Keywords: clay, diatomite, chemical and mineral composition, diffraction and thermal analysis, samples, physical and mechanical properties, photomicrogram, microstructure, X-rayogram.

Abstarct

The paper presents the results of comparative analysis for chemical and mineral composition of clay from Klyuchishchenskii deposit of the Republic of Tatarstan and diatomits from Inzenskii and Irbitskii deposits. The results show a good agreement between them and their applicability for the production of construction wall materials. Physical and mechanical properties of clay samples with diatomite additives were defined. The dependence of particle size, mixture ratio and burning temperature on physical and mechanical properties was given. Sample microstructure was studied using laser microscope. The phase composition analysis was conducted. The authors propose the optimal conditions for the production of ceramic materials with high thermal and physical properties.

Thematic Section: Physico-Chemical Research. **Full Paper**
Subsection: Phase Equilibrium. *Registration Code of Publication:* 15-42-6-59
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Experimental research and computer modeling of stable triangle LiF–KI–K_2CrO_4 of quaternary reciprocal system Li,K||F,I,CrO_4

© **Alexander V. Burchakov**,*$^{+}$ **Ekaterina M. Dvoryanova**, and **Igor M. Kondratyuk**
Samara State Technical University. Molodogvardeyskaya St., 244. Samara, 443100.
Russia. E-mail: turnik27@yandex.ru

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*Supervising author; $^{+}$Corresponding author

Keywords: phase equilibria, differential thermal analysis, stable triangle, quasi-ternary system, liquid phase stratification, monovariant monotectic equilibrium, T-x-y-phase diagram, phase complex.

Abstract

In this work we experimentally studied the quasi-ternary system LiF-KI-K_2CrO_4 for the first time. It's a stable triangle of the quaternary reciprocal system Li,K||F,I,CrO_4.The ternary eutectic is formed in this system. LiF-richer terminal solid solution field is formed in this system, so LiF-crystallizing vertex is situated inside the triangle. The liquid phase stratification occupies a large area in the concentrated triangle. Based experimental data we designed 3D solid state model of phase complex for the system in the form of *T-x-y* diagram and constructed isotherms of the liquidus surface, isothermal and polythermal sections, calculated coexistent phase material balance for some composition, using this model.

Full Paper *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 15-42-6-68 *Subsection:* Phase Equilibria.
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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Experimental study and modeling of phase transformations in a stable triangle NaF-KF-CsBr of quaternary reciprocal system Na,K,Cs||F,Br

© **Andrew S. Kirsanov**,*+ and **Alexsander V. Burchakov**
Samara State Technical University. Molodogvardeyskaya St., 244. Samara, 443100.
Russia. E-mail: andryxa07-92@mail.ru

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*Supervising author; +Corresponding author

***Keywords**:* phase equilibria, differential thermal analysis, quasi-ternary system, stable triangle, quaternary reciprocal system, eutectic, T-x-y phase diagram.

Abstract

Quaternary reciprocal system Na,K,Cs||F,Br consists of three stable separated by two tetrahedrons triangles. The paper presents a system partition on the stable elements and described the chemical interaction of components in the form of mass balance for each stable element. We did the analysis of the elements of faceting of Na,K,Cs||F,Br. Quasi-ternary system NaF-KF-CsBr is studied experimentally by differential thermal analysis and we identified characterizations of the nonvariant point. T-x-y phase diagram 3D model build for the system.

Thematic Section: Physico-Chemical Research. **Full Paper**
Subsection: Phase Equilibrium. *Registration Code of Publication:* 15-42-6-75
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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Experiment investigation of partitioning elements NaF-Na_2MoO_4-KI in the quaternary reciprocal system Na,K||F,I,MoO_4

© **Elizaveta V. Terentyeva**,[+] **Ekaterina M. Dvoryanova**,*
Ivan K. Garkushin,* and **Mikhail A. Krasnov***
Chair of General and Inorganic Chemistry. Samara State Technical University.
Main Building. Molodogvardeyskaya St., 244. Samara, 443100. Samara region. Russia.
Phone: +7 (846) 242-36-92. E-mail: Here.and.now-1@yandex.ru

*Supervising author; [+]Corresponding author

Keywords: differential thermal analysis, eutectics, phase equilibrium, graph theory, tree of phases.

Abstract

The quaternary reciprocal system Na,K||F,I,MoO_4 was partitioned into simplexes using geometrical method and graph theory. A tree of phases of the system was constructed, and stable elements were identifies. Phase equilibrium in partitioning triangles NaF-Na_2MoO_4-KI were studied by differential thermal analysis. Defined eutectic composition (EQ. %): NaF-2%, Na_2MoO_4-60%, KI-38% with a melting point of 506 ^{o}C. The melting specific and molar enthalpies were identified for eutectic composition.

Thematic Section: Physico-Chemical Research. **Full Paper**
Subsection: Phase Equilibrium. *Registration Code of Publication:* 15-42-6-75
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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Experiment investigation of partitioning elements KCl-KBr-LiKCrO$_4$ and KCl-KBr-Li$_2$CrO$_4$ in the quaternary reciprocal system Li,K||Cl,Br,CrO$_4$

© **Elena Yu. Voronina**,$^+$ and **Marya A. Dyomina***
Chair of the Common and Inorganic Chemistry. Samara State Technical University.
Molodogvardeiskaya St., 244. Samara, 443100. Samara region. Russia.
Phone: +7 (846) 242-36-92. E-mail: vor31@inbox.ru

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*Supervising author; $^+$Corresponding author

Keywords: differential thermal analysis, phase diagram, continuous series of solid solutions.

Abstract

In this paper, the quaternary reciprocal system Li,K||Cl,Br,CrO$_4$ was partitioned into simplexes using geometrical method and graph theory. A tree of phases of the system was constructed, and stable elements were identifies. Phase equilibrium in partitioning triangles KCl-KBr-LiKCrO$_4$ and KCl-KBr-Li$_2$CrO$_4$ were studied by differential thermal analysis. In these systems, the stability of continuous series of solid solutions based on kalium chloride and bromide is preserved.

Full Paper ____ *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 15-42-6-86 *Subsection:* Phase Equilibrium.
The article is published on materials of the report on “International Scientific Forum
Butlerov Heritage – 2015”. http://foundation.butlerov.com/bh-2015/ *(English Preprint)*
Submitted on March 28, 2015.

Thermodynamic evaluation sulphur-absorption ability slag system CaO – CaF_2

© **Svetlana E. Pratskova**,[+] and **Alexander G. Tyurin***
Analytical and Physical Chemistry Division. Chelyabinsk State University. Br. Kashirinykh St., 129.
Chelyabinsk, 454136. Russia. Phone: +7 (351) 799-70-69. E-mail: se_pratskova@mail.ru.

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*Supervising author; [+]Corresponding author

Keywords: oxide-fluoride melts, state diagram, the generalized theory of "regular" ionic solutions.

Abstract

In the framework of the generalized theory of "regular" ionic solutions designed triple phase diagram of CaO – CaF_2 – CaS, its isothermal (1500-1700 ^{o}C) in a cross-section of two-phase equilibrium melt – CaO (s) and the melt – CaS (s). Estimated sulfide capacity of synthetic slag based on CaO – CaF_2.

Full Paper *Thematic Section:* Preparative Research.
Registration Code of Publication: 15-42-4-96 *Subsection:* Organic Chemistry.
The article is published as a material of correspondence participation in International Scientific Forum "Butlerov Heritage-2015". http://foundation.butlerov.com/bh-2015/ *(English Preprint)*
Submitted on April 15, 2015.

High-temperature transformation of cyclic aromatic sulfides in the presence of Lewis acids

© **Lyubov A. Korneeva**,[1+] **Vladimir I. Nedel'kin**,[2*] and **Boris A. Zachernyuk**[2]
[1] *Chemistry and Electric-Chemical Energetic Division. National Research University "MPEI".*
Krasnokazarmennaya St., 14. Moscow, 111250. Russia.
Phone: +7 (495) 362-70-31. E-mail: korneevala@bk.ru
[2] *Inorganic and Analytical Chemistry named after Y.A. Klyachko Division. K.G. Razumovski Moscow State University of Technologies and Management. Zemlyanoy Val St., 73. Moskow, 109004. Russia.*
Phone: +7 (495) 236-72-95. E-mail: zachern@rambler.ru

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*Supervising author; [+]Corresponding author

***Keywords**:* cyclic aromatic sulfides, aluminum chloride, thianthrene, phenoxathiine, dibenzothiophene, poly(arylene sulfide)s, polysulfudation, polymerization of cycles.

Abstract

High-temperature interaction of cyclic aromatic sulfides (thianthrene, phenoxathiine and dibenxothiophene) with $AlCl_3$ was investigated. It was determined that the reaction is accompanied by breaking the sulfide bonds and the formathion of structures of poly(arylene sulfide)s type. It was shown that unlike dibenxothiophene and phenoxathiine in the case of thianthrene breaking of both C-S bonds in the cycle is probable and it causes the release of benzene and formation of polythianthrene structure of cycle-chain type.

Full Paper ____ *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 15-42-6-100 *Subsection:* Phase Equilibrium.
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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The analysis and prediction of the systems liquidus Li(Na),K||Hal,CrO_4 (Hal – F, Cl, Br, I)

© **Ekaterina M. Dvoryanova**,[+1] **Elena O. Ignatieva**,[2*]
Marina V. Chugunova,[3] and **Ivan K. Garkushin**[1*]
[1] *General and Inorganic Chemistry Department;* [2] *Drilling Oil and Gas Wells Department.*
Samara State Technical University. Molodogvardeiskaya St., 244. Samara, 443100.
Samara region. Russia. Phone: +7 (846) 242-36-92. E-mail: dvoryanova_kat@mail.ru
[3] *Technology of Storage and Processing of Animal Products Department.*
Samara State Academy of Agriculture. Russia.

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*Supervising author; [+]Corresponding author

Keywords: prediction of liquidus, analysis series, differential thermal analysis, T-x diagram, eutectic, phase equilibria.

Abstract

The prediction liquidus, the analysis similar series of ternary reciprocal systems Li(Na),K||Hal,CrO_4 (Hal – F, Cl, Br, I) founded, was conducted. The prediction results in the systems Na,K||Br,CrO_4 и Na,K||I,CrO_4 was confirmed by differential thermal analysis.

Thematic Section: Physico-Chemical Research. **Full Paper**
Subsection: Phase Equilibrium. *Registration Code of Publication:* 15-42-6-105
The article is published as a material of correspondence participation in International Scientific Forum "Butlerov Heritage-2015". http://foundation.butlerov.com/bh-2015/ *(English Preprint)*
Submitted on April 09, 2015.

Calculation and prediction of critical temperatures of binary systems of *n*-alkanes

© **Anna N. Trunova,**[1] **Ivan K. Garkushin,**[1]* **Alyanus G. Nazmutdinov,**[1]
and **Alexey I. Garkushin**[1]
Samara State Technical University. Molodogvardeyskaya St., 244. Samara, 443100. Russia.
Phone: +7 (846) 242-36-92. E-mail: chemsstu@mail.ru

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*Supervising author; +Corresponding author

Keywords: critical temperature, *n*-alkanes, the method of calculation, analytical description.

Abstract

A description of the method of calculating the critical temperature for the compositions of the system C_3H_8–C_9H_{20} based on analytical description and graphical plotting isoconcentrational dependencies $Tc = f(n)$ number of C_3H_8–C_nH_{2n+2} (n = 4…10) is presented.

We construct graphical dependences in different coordinate systems. The obtained dependences allow to determine the missing values T_c in the systems of *n*-alkanes.

Thematic Section: Physico-Chemical Research. **Short Communication**
Subsection: Phase Equilibrium. *Registration Code of Publication:* 15-42-6-109
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Investigation of the phase equilibria in the system diphenyl – *n*-hexadecane

© **Ivan K. Garkushin**,* **Alexander V. Kolyado**, and **Ivan G. Yakovlev**+
Chair of General and Inorganic Chemistry. Samara State Technical University.
Pervomayskaya St., 18. Samara, 443100. Samara region. Russia.
Phone: +7 (846) 278-44-77. E-mail: yakovlev.ivan.g@gmail.com

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*Supervising author; +Corresponding author

Keywords: the differential scanning calorimetry, biphenyl, *n*-hexadecane, the phase equilibrium.

Abstract

The phase equilibria in the system diphenyl – *n*-hexadecane was considered. Melting temperature and composition of the eutectic were determined. Liquidus of the system was constructed according to the experimental data. Furthermore, the phase equilibrium was calculated by the method of Schroeder – Le Chatelier and physical and chemical properties of the eutectic composition's alloy were identified, such as the flash point and density. The dependence of the kinematic viscosity of the alloy of the eutectic composition at temperatures ranging from 25 to 50 °C was constructed.

Short Communication *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 15-42-6-112 *Subsection:* Phase Equilibrium.
The article is published on materials of the report on “International Scientific Forum Butlerov Heritage – 2015”. http://foundation.butlerov.com/bh-2015/ *(English Preprint)*
Submitted on March 15, 2015.

Study of the stable tetrahedron LiBr-LiVO$_3$-NaBr-KBr of the quaternary reciprocal system Li,Na,K||Br,VO$_3$

© **Nurlana A. Mamedova, Inna N. Samsonova** $^{+}$ **,**
Tatyana V. Gubanova * and Ivan K. Garkushin
Department of General and Inorganic Chemistry. Samara State Technical University. Molodogvardeiskaya St., 244.Samara, 443100. Russia. Phone: +7 (927) 759-72-95. E-mail: inna7774@yandex.ru

Keywords: phase equilibria, T-x diagram, differential thermal analysis (DTA), stable tetrahedron eutectics.

Abstract

By differential thermal analysis there have been studied phase equilibria in stable tetrahedron LiBr-LiVO$_3$-NaBr-KBr of quaternary reciprocal system Li,Na,K||Br,VO$_3$. The composition of the components of the eutectic alloy (%mol.): 54.88% LiBr, 2.0% LiVO$_3$, 7.35% NaBr, 35.77% KBr with the melting point 324 ºC has been defined. We described the invariant and univariant equilibria.

Thematic Section: Physico-Chemical Research. **Letter to the Editor**
Subsection: Phase Equilibrium. *Registration Code of Publication:* 15-42-6-115
The article is published on materials of the report on "International Scientific Forum
Butlerov Heritage – 2015". http://foundation.butlerov.com/bh-2015/ *(English Preprint)*
Submitted on April 08, 2015.

Research the two-component system of sebacic acid – adipic acid

© **Ivan K. Garkushin**,[1]* **Alexander V. Kolyado**,[1] **Saule M. Alenova**,[1+]
Filipp K. Sukochev,[1] and **Alexander M. Shterenberg**[2]
[1] *Department of General and Inorganic Chemistry. Samara State Technical University.*
Molodogvardeyskaya St., 244. Samara, 443100. Russia.
Phone: +7 (846) 242-36-92. E-mail: saule-alenova@mail.ru.
[2] *Department of General Physics and Physics of Oil and Gas Production. Samara State Technical University.*
Molodogvardeyskaya St., 244. Samara, 443100. Russia.

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*Supervising author; [+]Corresponding author

Keywords: differential thermal analysis, sebacic acid, adipic acid, eutectics.

Abstract

In a two-phase equilibrium system of sebacic – adipic acid were studied by differential thermal analysis (DTA). Found eutectic composition with a melting point of 120 °C, containing (wt.%) adipic acid – 46.3%, sebacic – 53.7%. Study of the system of dibasic organic acids is of interest for practical use as a heat accumulating material.

Thematic Section: Physico-Chemical Research. **Full Paper**
Subsection: Physical Chemistry. *Registration Code of Publication:* 15-42-6-117
The article is published on materials of the report on "International Scientific Forum
Butlerov Heritage – 2015". http://foundation.butlerov.com/bh-2015/ *(English Preprint)*
Submitted on March 27, 2015.

Acidity of aromatic sulfoacids in gas and water phase

© **Evgeny Nikolaevich Krylov**,[1]*+ **Matvey S. Gruzdev**,[2] and **Lyudmila V. Virzum**[3]
[1] *Chair of Physical and Organic Chemistry. Ivanovo State University. Ermak St., 39. Ivanovo, 153025.*
Russia. Phone: +7 (4932) 37-37-03. E-mail: enk2000S@yandex.ru
[2] *Institute of Solution Chemistry RAS. Academic St., 1. Ivanovo, 153045.*
[3] *Chair of Chemistry. Belyaev Ivanovo State Agricultural Academy. Soviet St., 45.*
Ivanovo, 153012. Russia. E-mail: virzum@ivgsxa.ru

*Supervising author; +Corresponding author

Keywords: aromatic sulfoacids, deprotonation, pKa, local electrophility, electrostatic potential, quantum-chemical descriptors.

Abstract

The acidity of aromatic sulfoacids is described within the framework of quantitative Pearson`s HSAB theory on base of conceptual DFT. It Is discovered that values their pKa are in linear correlation on local electrophilicity of reaction centre (the atom of the oxygen) and its electrostatic potential, both in gas phase, and water ambience. That dependence is consider in accordance with physical sense of electrophilicity as electron capacity of reaction centre.

Full Paper *Thematic Section:* Physicochemical Research.
Registration Code of Publication: 15-42-6-124 *Subsection:* Physical 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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Thematic course: Hydrochemical synthesis of metal chalcogenide films. Part 23.

Chemical bath deposition kinetics of indium(III) sulfide in tertaric-hydroxylamine solution by thioacetamide

© **Stanislav S. Tulenin,**[1+] **Vyacheslav F. Markov,**[1,2*]
Larisa N. Maskaeva,[1,2] and **Andrey V. Tretyakov**[1]
[1] *Department of Physical and Colloidal Chemistry. The Ural Federal University n.a. the first President of Russia B.N. Yeltsin. Mira St., 19. Ekaterinburg, 620002. Sverdlovsk area. Russia.*
Phone: +7 (343) 375-93-18. E-mail: stast1989@mail.ru
[2] *Department of Chemistry and Burning Processes. Ural institute GPS of the Ministry of Emergency Measures of Russia. Mira St., 22. Ekaterinburg, 620022. Russia.*
Phone: +7 (343) 360-81-68. E-mail: v.f.markov@ustu.ru

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*Supervising author; [+]Corresponding author

***Keywords**:* indium(III) sulfide, chemical bath deposition, formal chemical kinetic, rate of chemical reaction.

Abstract

The chemical bath deposition kinetics of indium(III) sulfide by means of thioacetamide in tartaric and hydroxylamine solutions at 333-363 K in spontanious nucliation conditions of solid phase was studied. The formal-kinetic equation of indium(III) sulfide formation rate was determined. The formal-kinetic equation of indium(III) sulfide formation rate with determination of individual orders on all component in system and an activation process energy was made.

Thematic Section: Physico-Chemical Research. **Short Communication**
Subsection: Physical Chemistry. *Registration Code of Publication:* 15-42-6-129
The article is published on materials of the report on "International Scientific Forum Butlerov Heritage – 2015". http://foundation.butlerov.com/bh-2015/ *(English Preprint)*
Submitted on March 24, 2015.

Invariant kinetic portraits of linear two-stage reaction

© **Vladislav Kh. Fedotov,**[1+] and **Nikolay I. Koltsov**[2*]
[1] *Department of Information Sistems. Chuvash State University. Moskovsky pr., 15. Cheboksary, 428015. Chuvash Republic. Russia. Phone: +7 (352) 58-67-95. E-mail: fvh@inbox.ru*
[2] *Department of Physical Chemistry and Macromolecular Compounds. Chuvash State University. Moskovsky pr., 15. Cheboksary, 428015. Chuvash Republic. Russia. Phone: +7 (352) 45-24-68. E-mail: koltsovni@mail.ru*

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*Supervising author; [+]Corresponding author

***Keywords**:* linear two-step reaction, kinetic portraits, nonlinear transformations, invariants, stationary states.

Abstract

It is shown that the non-linear conversion of the kinetic model of a linear two-step the reaction allowed to use it to describe the of complex behavior reactions which are characterized a number of stationary states with different values of rate for different initial values concentrations of reactants.

Full Paper *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 15-42-6-132 *Subsection:* Electrochemistry.
The article is published on materials of the report on "International Scientific Forum Butlerov Heritage – 2015". http://foundation.butlerov.com/bh-2015/ *(English Preprint)*
Submitted on March 25, 2015.

Application of electrode modified with carbon nanofibers and cationic surfactant for simultaneous voltammetric determination of syringaldehyde and vanillin

© **Guzel K. Ziyatdinova**,[+] **Ekaterina V. Kozlova**,
Endzhe R. Ziganshina, and **Herman C. Budnikov**
Analytical Chemistry Department. A.M. Butlerov Institute of Chemistry. Kazan Federal University.
Kremlevskaya St., 18. Kazan, 420008. Tatarstan Republic. Russia.
Phone: +7 (843) 233-77-36. E-mail: Ziyatdinovag@mail.ru

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*Supervising author; [+]Corresponding author

***Keywords**:* differential pulse voltammetry, chemically modified electrodes, carbon nanofibers, surfactants, phenolic antioxidants.

Abstract

Syringaldehyde and vanillin are oxidized at 0.77 and 0.88 V, respectively, on the glassy carbon electrode modified with carbon nanofibers and cationic surfactant cetylpyridinium bromide in Britton-Robinson buffer pH 2.0. Two-fold increase of oxidation currents and cathodic shift of oxidation potentials on 10-20 mV as well as improvement of voltammograms shapes have been observed in comparison to bare electrode. Analytes peaks potential separation of 110 mV allows to perform their simultaneous determination. Variation of one component concentration at fixed concentration of the second one has shown that oxidation of syringaldehyde and vanillin runs independently. Voltammetric method for simultaneous determination of syringaldehyde and vanillin has been developed. The linear dynamic range is 2.5-30 and 5.0-40 μM for syringaldehyde and vanillin, respectively with detection limits of 0.53 and 1.17 μM.

Full Paper ____ *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 15-42-6-138 *Subsection:* Electrochemistry.
The article is published on materials of the report on "International Scientific Forum
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Submitted on April 08, 2015.

On the peculiarities of passivation of copper in sulfuric acid solutions

© **Alexander I. Biryukov**,[+] **Alexander G. Tyurin**,* and **Artem P. Tronov**
Department of Analytical and Physical Chemistry. Chelyabinsk State University.
Br. Kashirinykh St., 129. Chelyabinsk, 454136. Russia. Phone: (351) 799-70-69. E-mail: st4857@yandex.ru

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*Supervising author; [+]Corresponding author

Keywords: copper sulfate-containing aqueous solutions, electrochemical equilibrium diagram E – pH, polarization curves.

Abstract

Building a cross-section diagrams Fe – pH systems SO_4^{2-} – H_2O and Cu – H_2SO_4 – H_2O was presented. Polarization curves of copper in the solution of 1M H_2SO_4 were demonstrated. Thermodynamic and kinetic features of passivation of copper in sulfuric acid medium have been analyzed.

Thematic Section: Physico-Chemical Research. **Full Paper**
Subsection: Electrochemistry. *Registration Code of Publication:* 15-42-6-145
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Electrochemical properties of nickel(II) complexes with 2,2'-bipyridine in the presence of diphenylphosphinic acid

© **Alia F. Khusnuriyalova**,[1,2] **Leonid E. Kalugin**,[1,2]
Alexey B. Dobrynin,[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: aliya15071993@mail.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

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*Supervising author; +Corresponding author

Keywords: 2,2'-bipyridine, diphenylphosphinic acid, nickel(II) complexes, cyclic voltammetry.

Abstract

The electrochemical properties of nickel(II) / 2,2'-bipyridine complexes of type $[Ni(bpy)_n]^{2+}$, where n = 1-3, in the presence of diphenylphosphinic acid $Ph_2P(O)OH$ have been investigated. It was established that diphenylphosphinic acid $Ph_2P(O)OH$ is more strong ligand in comparison with monophenylphosphinic acid PhP(O)(H)OH, and can substitute 2,2'-bipyridine in the coordination sphere of nickel forming new octahedral complex $[Ni(Ph_2P(O)O)_2(Ph_2P(O)OH)_2(DMF)_2]$. The structure of the new complex was elucidated by X-ray crystal structure analysis. It was found that electrochemical reduction of the obtained new nickel complexes proceeds at more negative potentials than the potential of the electrochemical reduction of nickel(II) / 2,2'-bipyridine system.

Full Paper ____ *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 15-42-6-152 *Subsection:* Physical Chemistry of Polymers.
The article is published as a material of correspondence participation in International Scientific Forum "Butlerov Heritage-2015". http://foundation.butlerov.com/bh-2015/ *(English Preprint)*
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The determination of fatty acids in liquids using piezoelectric sensors based on molecular imprinting polymers

© **Irina A. Krivonosova**[1+], **Olga V. Duvanova**[1], **Alexander N. Zyablov**[1]*,
Svetlana A. Sokolova,[2] and **Olga V. Dyakonova**[2]
[1] *Department of Analytical Chemistry. Voronezh State University. Universitetskaya Sq., 1. Voronezh, 394006. Voronezh region. Russia. Phone: (473) 220-89-32. E-mail: duvanovaov@mail.ru*
[2] *Department of Chemistry. Voronezh State Agricultural University n.a. Peter I. Michurina St., 1. Voronezh, 394087. Voronezh region. Russia. Phone: (473) 253-76-78. E-mail: sokolova_chm@mail.ru*

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*Supervising author; [+]Corresponding author

***Keywords**:* vegetable oils, molecular imprinting polymers (MIPs), oleic acid, palmitic acid, polyamide acid (PAA), polyimides RD, DFO, piezoelectric sensor.

Abstract

Molecular imprinting oleic and palmitic acids polymers (MIPs) on the basis of polyimides PAA, RD, DFO were synthesized on the surfaces of piezoelectric sensors. The analysis of model solutions of fatty acids was conducted in the concentration range: oleic acid 0.16-0.86 g/dm^3; palmitic acid 0.14-0.34 g/dm^3. The imprinting factor and the selectivity coefficient of defined acid in relation to the chemicals of the same class were calculated. These piezoelectric sensors tested in the analysis of vegetable oils.

Full Paper ______________________________________ *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 15-42-6-158 *Subsection:* Spectroscopy of the Artifacts.
The article is published as a material of correspondence participation in International Scientific
Forum "Butlerov Heritage-2015". http://foundation.butlerov.com/bh-2015/ *(English Preprint)*
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An inductively coupled plasma optical emission spectrometry for the research of bronze age artifacts in Kemerovo region

© **Roman P. Kolmykov**
Kemerovo State University. Krasnaya St., 6. Kemerovo, 650043. Russia.
Kemerovo scientific center, the Siberian Branch of Russian Academy of Sciences (SB RAS),
Sovietskij pr, 18. Kemerovo, 650000. Russia. E-mail: kolmykoff.roman@yandex.ru

Keywords: ICP-OES, archaeology, bronze.

Abstract

The elemental compound of nine artifacts of an archaeological monument in Kemerovo region was investigated. This method allows determining the concentrations of bronze basic components and impurities. Thus archaeologists can determine the time, the technology, the ore sours of each ware.

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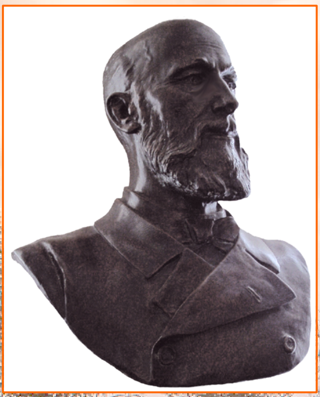

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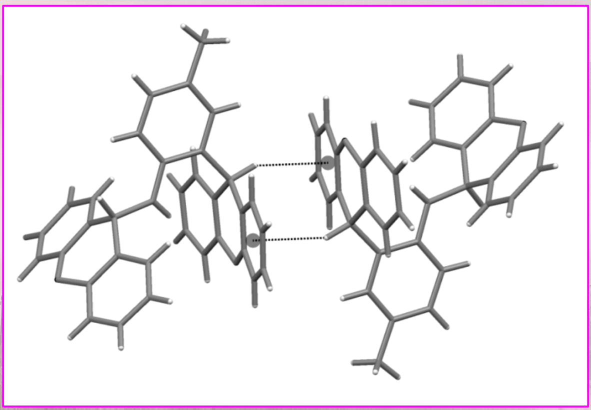

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Thematic Section: Research of Reactivity. **Full Paper**
Subsection: Organic Chemistry. *Registration Code of Publication:* 15-43-7-1
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Thematic course: Theme: Kinetics and mechanism of acyl transfer reactions. Part 10.

Reactivity of dipeptides and esters of carboxylic acids at their interaction in aqueous dioxane solutions

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

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*Supervising author; +Corresponding author

Keywords: acylation, dipeptides, esters, aqueous dioxane, specific solvation, quantum chemical simulation.

Abstract

An influence of a binary system water – 1,4-dioxane and of esters structure on kinetics of glycyl – glycine and *L*-α-alanyl – *L*-α-alanine reactions with 4-nitrophenyl acetate and phenyl benzoates activated by nitro group is studied. It is shown that rate constants enhancement at increase of water part in the solvent is connected with specific solvation of the dipeptides. Kinetic data are compared with results of quantum chemical simulation of the reagents molecules. It is established that Hammet's constants, values of leaving groups pK_a and orbital characteristics of the esters molecules can be used as reactivity descriptors in acylation of the dipeptides.

Full Paper *Thematic Section:* Technological Research.
Registration Code of Publication: 15-43-7-12 *Subsection:* Organic Chemistry.
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5-Amino-3-methylthio-1,2,4-triazole as a key intermediate in the synthesis of antiviral drug Triazavirin®: the synthesis on an industrial scale and quantitative determination by HPLC

© **Andrey A. Tomasov**, **Gregory A. Artemiev**,* **Dmitry S. Kopczuk**,[2+] **Vladimir L. Rusinov**,[2]
Eugeny N. Ulanski,[2] **Oleg N. Chupakhin**[1,2] and **Valery N. Charushin**[2]
[1] *Institute of Organic Synthesis m.a. I.Ya. Postovskogo UB RAS.*
Kovalevskaya St, 22/Akademicheskaya St., 20. Ekaterinburg, 620990. Russia.
Tel./Fax: +7 (343) 369-30-58. E-mail: dkopchuk@mail.ru
[2] *Ural Federal University. World St, 19. Ekaterinburg, 620002. Russia.*
Tel./Fax: (343) 375-45-01.

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*Leader of the thematic course; [+]Corresponding author

Keywords: HPLC, 5-amino-3-methylthio-1,2,4-triazole, column "Kromasil"

Abstract

Designed by hardware scheme of obtaining 5-amino-3-methylthio-1,2,4-triazole (the key intermediate product) during the synthesis of the antiviral drug "Triazavirin" on an industrial scale, as well as the methods of quantitative determination using the method of HPLC.

Full Paper *Thematic Section:* Preparative Research.
Registration Code of Publication: 15-43-7-18 *Subsection:* Bioorganic Chemistry.
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Synthesis and cytotoxic activity of novel transition metal porphyrinates based on chlorophyll *a* derivatives

© **Irina S. Tarabukina**,[1+] **Yana I. Pylina**,[2] **Ilia O. Velegzhaninov**,[2]
Olga M. Startceva,[1] **Dmitry M. Shadrin**,[2] and **Dmitry V. Belykh**[*+1]
[1] *Institute of Chemistry. Komi Scientific Center. Ural Division. Russian Academy of Sciences. Pervomaiskaya St., 48. Syktyvkar, 167982. Russia. E-mail: TarabukinaIS@mail.ru, belykh-dv@mail.ru*
[2] *Institute of Biology. Komi Scientific Center. Ural Division. Russian Academy of Sciences. Kommunisticheskaya St., 28. Syktyvkar, 167982. Russia.*

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*Supervising author; +Corresponding author

Keywords: Methylpheophorbide-a, chlorin e_6, complexes, photo independent cytotoxicity, antitumor cytotoxicants.

Abstract

The number of new transition metal porphyrinates based on chlorophyll *a* derivatives were synthesized and their photo independent cytotoxic activity against HeLa cells were studied. The influence of the central atom nature and the ligand structure on the dark toxicity of the porphyrinates based on chlorophyll *a* derivatives was found. It has been shown that zinc cation introduction results in a sharp increase in the toxicity of the compounds, while the introduction of nickel and copper cations reduces toxicity most cases. A potential antitumor dark cytotoxicant were found among the investigated compounds.

Full Paper ____ *Thematic Section:* Preparative Research.
Registration Code of Publication: 15-43-7-24 *Subsection:* Chemistry of Polymers.
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 bis(2-hydroxyethyl)terephthalate from waste polyethylene terephthalate

© **Nazigul S. Satbaeva,**[1+] **Tatiana M. Bogachyova,**[1]
Alevtina P. Rakhmatullina,[1]* and **Rafinat S. Yarullin**[1,2]
[1] *Department of Synthetic Rubber Technology. Kazan State Technological University.*
K. Marx St., 68. Kazan, 420001. Republic of Tatarstan. Russia.
[2] *JSC "Tatneftekhiminvest-Holding".*
Phone: +7 (843) 23-43-91. E-mail: 1) *nazgul-satbaeva@mail.ru* ; 2) *E-mail: rah-al@yandex.ru*

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*Supervising author; +Corresponding author

Keywords: waste polyethylene terephthalate, glycolysis, ethylene glycol, zinc acetate.

Abstract

The process of depolymerization of waste polyethylene terephthalate (PET) bottles by glycolysis in the presence of a catalyst – zinc acetate was investigated. Degradation of PET was performed in two ways: 1) using conventional heating to 140-180 °C; 2) using microwaves (MW). The process led to a homogeneous mass. The conditions for selection of the desired product – bis(2-hydroxyethyl)terephthalate (BHET) were found. It was studied that the use of MW substantially increases the yield and significantly reducing the time of depolymerization. The concentration of the catalyst (from 0.125 to 1.0 % wt.) has no significant effect on the yield of bis(2-hydroxyethyl)terephthalate when using MW unlike with conventional heating. The resulting product is a white crystalline powder with a melting point 108 °C with hydroxyl number = 436 mg KOH/g, which substantially corresponds to the literature data.

Thematic Section: Preparative Research. **Full Paper**
Subsection: Inorganic Chemistry. *Registration Code of Publication:* 15-43-7-29
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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Synthesis of nanostructured powders of silver from dispersions AgBr

© **Polina V. Lapsina**,[1+] **Evgeny I. Kagakin**,[2*] **Vadim G. Dodonov**,[3] and **Valery M. Pugachev**[3]
[1] *Center shared equipment. Kemerovo Scientific Center SB RAS. Soviet pr., 18. Kemerovo, 650000. Russia.*
Phone: +7 (923) 608-02-71. E-mail: lpv110185@rambler.ru
[2] *Chemical Engineering and Environment Solid Fuel Department. T.F. Gorbachev Kuzbass State Technical University. Vesennyaya St., 28. Kemerovo, 650000. Russia. E-mail: kagakin55@mail.ru*
[3] *Chemistry of SolidsDepartment. Kemerovo State University. Krasnaya St., 6.*
Kemerovo, 650043. Russia. E-mail: 233191@mail.ru

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*Supervising author; [+]Corresponding author

Keywords: nanostructured power, silver, reduction.

Abstract

The synthesis of nanostructured silver reduction crystal salt AgBr by water solutions of reducing agents are proposed. Morphology of the obtained nanostructured powders of silver are considered. The influence of the nature of the reducing agent on the dimensional characteristics of the metal was investigated.

Thematic Section: Preparative Research. **Full Paper**
Subsection: Organoelemental Chemistry. *Registration Code of Publication:* 15-43-7-33
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Synthesis and intramolecular cyclization of ketostabilized phosphorus bisylide under microwave irradiation

© **Rauilya N. Malikova**,[1+] **Ilshat M. Sakhautdinov**,[1]* **Lilya M. Gainetdinova**,[2]
Fanur Z. Galin,[1,2] and **Marat S. Yunusov**[1]
[1] *Ufa Institute of Chemistry. Russian Academy of Sciences. October St., 71. Ufa, 450054. Republic of Bashkortostan. Russia. Tel: +7 (347) 235-58-01. Fax: +7 (347) 235-60-66. E-mail: rolimalika@mail.ru*
[2] *Bashkir State University. Z. Validi St., 33. Ufa, 450074. Republic of Bashkortostan. Russia. Tel.: +7 (347) 273-48-42. E-mail: ioh039@mail.ru*

*Supervising author; [+]Corresponding author

Keywords: ketostabilized phosphorus bisylide, intramolecular cyclization, substituded 2*H*,6*H*-indolizino[2,1-f]pyrido[2,1-*a*]isoindole.

Abstract

The synthesis of phosphorus bisylide based on β-phenyl-β-alanine and pyromellitic dianhydride is implemented and its intramolecular cyclization under microwave irradiation is studied. As a result poly-heterocyclic product with symmetric structure – 4,10-diphenyl-3,4,8,10,11-tetrahydro-2*H*,6*H*-indolizino[2,1-f]pyrido[2,1-*a*]isoindol-2,6,8,12-terion is received regioselectively.

Thematic Section: Preparative Research. **Short Communication**
Subsection: Organic Chemistry. *Registration Code of Publication:* 15-43-7-37
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Butlerov Heritage – 2015”. http://foundation.butlerov.com/bh-2015/ *(English Preprint)*
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Synthesis of uracil derivatives containing in their structure the remains of succinic and maleic acids

© **Inna B. Chernikova**,+ and **Marat S. Yunusov***
Ufa Institute of Chemistry RAS. Prospekt Oktyabrya, 71. Ufa, 450054. Russia.
Phone: +7 (347) 235-58-39. Fax: +7 (347) 235-60-66. E-mail: leben_87@mail.ru

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*Supervising author; +Corresponding author

Keywords: 5-aminouracil, 6-aminouracil, succinic anhydride, maleic anhydride.

Abstract

The 4-[(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-5-yl)amino]-4-oxobutanoic acid and 4-[(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-5-yl)amino]-4-oxabut-2-enoic acid were obtained by a simple method with high yields using the substrate 5-aminouracil and succinic or maleic anhydrides, respectively. It is shown that 6-aminouracil in similar conditions in the reaction does not enter.

Short Communication ______________________ *Thematic Section:* Preparative Research.
Registration Code of Publication: 15-43-7-40 *Subsection:* Organic Chemistry.
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Submitted on April 26, 2015.

Synthesis and antimicrobic activity of 5-aril-4-aroil-3-hydroxy-1-[2-(2-hydroxyetoxy)ethyl]-3-pirrolin-2-ones

© **Sergey N. Rogachyov**,[+] **Alexandra A. Bobyleva**,
Valentina V. Novikova, and **Vladimir L. Geyn***
BGOU VPO "Perm State Academy of Pharmacy". Polevaya St., 2. Perm, 614081. Russia.
Phone: +7 (342) 236-90-50. E-mail: geinvl48@mail.ru; rogachevsergei@mail.ru

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*Supervising author; [+]Corresponding author

***Keywords**:* 5-aryl-4-aroyl-3-hydroxy-1-[2-(2-hydroxyethoxy) ethyl]-3-pyrrolin-2-ones, synthesis, antimicrobial activity.

Abstract

The 5-aril-4-aroil-3-hydroxy-1-[2-(2-hydroxyethoxy)ethyl]-3-pyrrolin-2-ones have been received by the interaction 2-(2-aminoethoxy)ethanol with mixtere of aromatic aldehyde and methyl esther the aroilpyrivic acids. Antimicrobic activity of the synthesized compounds has been studied. Structure of the received 5-aril-4-aroil-3-hydroxy-1-[2-(2-hydroxyethoxy)ethyl]-3-pyrrolin-2-ones was proved on the basis of spectroscopy ^{1}H NMR.

Thematic Section: Preparative Research. **Short Communication**
Subsection: Organic Chemistry. *Registration Code of Publication:* 15-43-7-43
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Development of the method of liquid-phase synthesis vinyl chloride dichloroethane dehydrochlorination

© **Rustem R. Daminev**,[1] **Radik N. Asfandiyarov**,[2] **Lilia R. Asfandiyarova**,[1]*+
and **Guzel V. Yunusova**[1]
[1] *Branch of Ufa State Petroleum Technological University in Sterlitamak.*
October St., 2. Sterlitamak, 453118. Russia.
[2] *JSC “Bashkir Soda Company”. Tekhnicheskaya St., 32. Sterlitamak. Republic of Bashkortostan. Russia.*
Phone: +7 (3473) 24-25-12, +7 (9649) 64-26-06. E-mail: asfand_lilya@mail.ru

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*Supervising author; +Corresponding author

Keywords: ethylene dichloride, vinyl chloride, synthesis, technology, dehydrochlorination, alkyltin, electrochemistry.

Abstract

We have established the possibility of the synthesis of vinyl chloride by the reaction of 1,2-dichloroethane (DCE) with a quaternary ammonium alkoxides; conducted a series of experiments on the synthesis of vinyl chloride by liquid phase dehydrochlorination of DCE quaternary ammonium alkoxides derived electrochemically from alcoholic solutions of quaternary ammonium salts. The main factors affecting the results of the synthesis of vinyl chloride, are temperature, duration of the process and the concentration of alcohol solution, quaternary ammonium alkoxide. It is found that vinyl chloride is released at 0 °C in a yield of 85-90%, with an increase in temperature, an increase yield of vinyl chloride and at a temperature of 20 °C was 98.0-99.7%. Raising the temperature above 250 °C leads to intensive foaming, as a result of the entrainment of the liquid reaction zone and its accumulation in the receiver BX to collect. Isolation of vinyl chloride in a dehydrochlorination reaction occurs fairly quickly, so the determining factor for the output time of dosing is DCE. In the course of the experiments it was found that as dehydrochlorinated agents may use different quaternary ammonium alkoxides, it is therefore of interest to explore the possibility of using alkoxide synthesized from waste products of allyl chloride in the synthesis of VC.

Letter to the Editor ____ *Thematic Section:* Preparative Research.
Registration Code of Publication: 15-43-7-46 *Subsection:* Organic Chemistry.
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Three-component synthesis of *N*-arylmethyl-4-(5*H*-dibenzo[a,d]cyclohepten-5-yl)anilines

© **Tatiana A. Akentieva**
Department of General Chemistry. Perm State Agricultural Academy"
m.a. academician D.N. Pryanishnikov. Petropavlovskaya St., 23. Perm, 614000. Russia.
Phone: +7 (342) 212-95-68. E-mail: akentjeva-perm@rambler.ru

Keywords: 5*H*-dibenzo[a,d]cyclohepten-5-ol (dibenzosuberone), *N*-arylmethyl-4-(5*H*-dibenzo[a,d]-cyclohepten-5-yl)aniline, imine.

Abstract

Carried out one-pot three-component synthesis of *N*-arylmethyl-4-(5*H*-dibenzo[a,d]cyclohepten-5-yl)anilines in the system – imine : dibenzosuberenone : tetrahydroborate sodium.

Full Paper *Thematic Section:* Preparative Research.
Registration Code of Publication: 15-43-7-48 *Subsection:* Physical Chemistry of Explosives.
The article is published on materials of the report on “International Scientific Forum
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Molecular complexes and interaction 1,3-dinitriloxide-2,4,6-trietilbenzol and stabilizers of chemical firmness composition of power materials

© **Vladimir N. Popok,**[*+] **Natalia A. Fedoricheva**
Joint Stock Company «Federal Research and Production Center «ALTAI»
Sotsialisticheskaya St., 1. Biysk, 659322. Altai territory, Russia.
Phone: +7 (3854) 30-19-37. E-mails: vnpopok@mail.ru

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[*] Supervising author; [+] Corresponding author

Keywords: 1,3-dinitriloxide-2,4,6-trietilbenzol, molecular complexes, sewing agents, thermal decomposition, IR-spectroscopy.

Abstract

Results of pilot studies of interaction by 1,3-dinitriloxide-2,4,6-trietilbenzol components the composition of power materials, including stabilizers of chemical firmness are presented in article. The ratio of components corresponding to formation of molecular complexes are defined. Parameters thermal behavior of molecular complexes, their IR spectrums are established. It is offered to apply the received complexes on the basis of 1,3-dinitriloxide-2,4,6-trietilbenzol as the curing agent with possibility regulation of time of curing the composition of power materials.

Full Paper ____ *Thematic Section:* Analytical Research.
Registration Code of Publication: 15-43-7-64 *Subsection:* Organic Chemistry.
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Abiogenic synthesis of biologically important and optically active molecules adsorption on carbon in the early Archean

© Vladimir M. Zhmakin
Public Joint-Stock Company Southwestgeology. Geologists Settlement, 307207. Oktyabrsky District.
Kursk Region. Phone: +7 (47142) 2-13-92. E-mail: v.zhmakin@mail.ru

Keywords: archaean, the atmosphere, carbon, adsorption, synthesis of optically active, amino acids, ribose.

Abstract

Reasons for appearance of optically active organic molecules in nature have not been ascertained up to the present, but clarification of conditions on the Earth during the period of their appearance can contribute to this. H_2 and gases, containing H_2, were oxidized by CO_2 with selection of carbon and H_2O or CH_2O and CHO(OH) in volcanic gas and in the early atmosphere. During adsorption by carbon of CH_2O dissolved in water there might take place synthesis only of R (rectus, in Latin) ribose, and with NH_3 and CHO(OH) synthesis of glycine and only of S (sinister) serine, and on its bases of other S amino acids. Adsorption on the carbon provided in complex of basic properties of organic molecules.

Full Paper ____ *Thematic Section:* Physicochemical Research.
Registration Code of Publication: 15-43-7-70 *Subsection:* Organic Chemistry.
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Effect of the defect structure of the alumina support on the adsorption properties of supported palladium particles in the hydrogenation of 1,3-butadiene

© **Avgustina V. Boretskaya,**[+] **Alexandr A. Lamberov,***
Ildar R. Ilyasov, **Artem I. Laskin**, and **Alexey Yu. Kirgizov**
Physiacal Chemistry Departament. Kazan (Volga Region) Federal University.
Kremlin St., 18. Kazan, 420008. Tatarstan Republic. Russia.
Phone: +7 (843) 233-75-36. E-mail: ger-avg91@mail.ru

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*Supervising author; [+]Corresponding author

Keywords: pseudoboehmite, alumina, palladium catalysts, 1,3-butadiene hydrogenation.

Abstract

Supported palladium catalysts based on γ-Al_2O_3 with varying acidity were investigated. The acidity of the support was varied by introducing to the aluminum hydroxide of acetic acid. It was established that the introduction of acid does not change the phase composition, but is accompanied by a change of textural characteristics and the increase in the number of acid centers. The subsequent deposition of palladium was accompanied by the formation of highly dispersed state of the active component with a strong metal-support interaction. This caused an increase in the conversion of 1,3-butadiene hydrogenation and decrease in selectivity to butenes.

Full Paper ____ *Thematic Section:* Physicochemical Research.
Registration Code of Publication: 15-43-7-76 *Subsection:* Organic Chemistry.
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EPR study of radicals of phenolic antioxidants with terpene substituents

© Rais A. Sadykov,[1]* **Gulnaz D. Safina,**[1] **Konstantin A. Kozhanov,**[2]
Irina Yu. Chukicheva,[1] and **Alexandr V. Kuchin**[1]
[1] *Institute of Chemistry. Komi Scientfic Centre. Russian Academy of Sciences (Ural Branch).*
Pervomayskays St., 48. Syktyvkar, 167982. Russia.
Phone: +7 (8212) 21-90-95. E-mail: sadykov-ra@chemi.komisc.ru
[2] *G.A.Razuvaev Institute of Organometallic Chemistry of Russian Academy of Sciences.*
Tropinina St., 49. Nizhny Novgorod, 603950. Russia. E-mail: kostik@iomc.ras.ru

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*Supervising author; [+]Corresponding author

Keywords: ESR spectra, hindered phenoxyl radicals, hyperfine coupling.

Abstract

First recorded and studied the EPR spectra of phenoxyl radicals of a series of phenols with isobornyl and isocamphyl substituents having high antioxidant activity and promising as drugs. Hyperfine interaction constants of the unpaired electron with the protons was found. Phenoxyl *orto*-isobornyl substituents radicals are less stable than *tert*-butyl substituents radicals was found.

Full Paper ____ *Thematic Section:* Theoretical Research.
Registration Code of Publication: 15-43-7-82 *Subsection:* Thermodinamics.
The article is published on materials of the report on "International Scientific Forum
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Necessary and sufficient conditions for the existence and uniqueness temperature of Boyle and Joule-Thomson, the volume of Boyle and the inflection point of the second virial coefficient

© **Ichtier H. Umirzakov**
Laboratory Simulation. Federal State Budget Institution "Institute of Thermophysics of SB RAS".
Lavrentieva Pr., 1. Novosibirsk, 630090. Russia. Tel: +7 (383) 354-20-17. E-mail: tepliza@academ.org

Keywords: temperature, Boyle, volume boyl, temperature Joule, temperature Joule-Thomson, the second virial coefficient of the interaction potential.

Abstract

The necessary and sufficient conditions were found that are imposed on the spherically symmetric interaction potential that existed the Boyle temperature and Joule-Thomson, the volume of Boyle and the inflection point of the second virial coefficient. The uniqueness of temperatures of Boyle and Joule-Thomson, the volume of Boyle and the inflection point of the second virial coefficient of volume were proved. It is proved that the second virial coefficient has no point touches the temperature axis at finite temperature.

Thematic Section: Theoretical Research. **Full Paper**
Subsection: Thermodinamics. *Registration Code of Publication:* 15-43-7-91
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The second partial derivative of specific volume on pressure at the critical point of phase transition liquid-gas one-component substances

© **Ichtier H. Umirzakov**
Laboratory Simulation. Federal State Budget Institution "Institute of Thermophysics of SB RAS".
Lavrentieva Pr., 1. Novosibirsk, 630090. Russia. Tel: +7 (383) 354-20-17. E-mail: tepliza@academ.org

Keywords: phase transition, equation of state, critical point, fluctuation theory.

Abstract

The second partial derivative of the specific volume on pressure with the equation of state of fluctuation the theory of the critical point and equation of state of Van der Waals forces were analytical investigated. It is shown that this derivative at the critical point of phase transition liquid-gas has no defined value. It is shown that the second partial derivative of the specific volume on pressure is not a continuous function and therefore is not a function of state.

Full Paper ____ *Thematic Section:* Theoretical Research.
Registration Code of Publication: 15-43-7-94 *Subsection:* Metallurgy.
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Calculation of parameters of vibration mixing metal composites of copper-gallium

© **Igor E. Ignatiev**,* **Alexey B. Shubin**, and **Elena V. Ignatieva**+
Laboratory of Physical Chemistry of Metallurgical Melts. Institute of Metallurgy of UB RAS.
Amundsen St., 101. Ekaterinburg, 620016. Russia. Tel.: +7 (343) 232-90-35. E-mail: l.ig_a@mail.ru

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*Supervising author; +Corresponding author

Keywords: gallium, copper, wettability, powder, vibratory mixing.

Abstract

The problem of determining the parameters of the vibratory effect on the mixture of powder copper and gallium liquid at room temperature, to ensure the wetting of the particles forming the copper gallium and gallium copper paste was regarded. The prognostic contact angle dependence of the amplitude, frequency and number of cycles of vibration, which allows to determine the necessary duration of forming a paste was built.

Full Paper ____ *Thematic Section:* Technological Research.
Registration Code of Publication: 15-43-7-100 *Subsection:* Organic Chemistry.
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Improvement of technology dehydrogenation of light paraffins on the catalyst prepared in an electromagnetic field

© **Rustem R. Daminev**,* **Oleg Kh. Karimov**,$^+$ **Lilia Z. Kasyanova**, and **Eduard Kh. Karimov**
Division of General Chemical Technology. Ufa State Petroleum Technological University, Branch of USPTU
in Sterlitamak. Pr. Oktyabrya, 2. Sterlitamak, 453118. Bashkortostan Republic. Russia.
Phone: +7 (3473) 24-25-12. E-mail: karimov.oleg@gmail.com

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*Supervising author; $^+$Corresponding author

Keywords: microwave radiation, the monomers, isoprene, dehydrogenation, chromia-alumina catalyst, isobutylene, methylbutane.

Abstract

The results of the improvement of industrial technology dehydrogenation of light paraffins to alumina-chromium catalysts synthesized in a new way – by impregnation using an electromagnetic microwave radiation were presented. The technology of synthesis of the chromia-alumina catalysts under influence of the microwave field at various stages of its preparation allows to obtain a catalyst with a high catalytic properties, the olefin yield is increased by 4.3%, the selectivity increased by 3.8%. The advanced technological scheme of the process of dehydrogenation of light paraffin hydrocarbons in the prepared catalyst were proposed. The most significant advantages of catalysts, allowing to improve the existing technology for the dehydrogenation of hydrocarbons are: high mechanical strength, low rate of coke formation of the catalyst and high thermal stability. As a result of improvement of technological scheme of the site wet cleaning of dusty hydrocarbon stream from the reactor was replaced with dry cleaning that allows the use of spent catalyst recycled. Low coking of the catalyst will reduce the amount of coke formation of lumps in the reactor, deforming the internal structure of the reactor and in violation of the hydrodynamic regime. The business case for improvement were presented.

Full Paper ____ *Thematic Section:* Research into New Materials.
Registration Code of Publication: 15-43-7-106 *Subsection:* Innovation Technology.
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The synthesis inhibitory composition to prevent corrosion of oilfield equipment

© **Rustem R. Daminev**,*+ **Aygul A. Islamutdinova**,*+
Aleksandr N. Ivanov, and **Ildar R. Hamzin**
Department of General Chemical Technology, Branch of Ufa State Petroleum
Technological University in Sterlitamak. October St.t, 2. Sterlitamak, 453118. Russia.
Phone: +7 (3473) 24-08-58. E-mail: aygul_ru@mail.ru

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*Supervising author; +Corresponding author

Keywords: chemical corrosion, oil, metals, polyamine, dichloroethane, the synthesis of inhibitor of corrosion, protection of metals, the electrochemical method.

Abstract

The corrosion inhibitor on the basis of the condensation products of polyethylene polyamine (PEPA) and 1,2-dichloroethane was received. The reaction was carried out in the apparatus equipped with a stirrer at a temperature of 75 °C for 4 hours. The resulting mixture was subjected to a single distillation to extract from the rest of the components that represent the greatest value in terms of defensive ability. The separation of the mixture was estimated by the change of the refractive index of the distillate. Inhibitory composition subjected to the study on the anticorrosion properties of the electrochemical method using analyzer corrosion rate "Monicor-2M". The obtained data on the value of the corrosion current is processed using specially developed software, which allows to calculate the magnitude of the protective ability of the inhibitor. Also its basic physical and chemical properties: appearance, density, solubility, and flashpoint was studied. Discovered that this inhibitor has high stopping power and can be used as corrosion inhibitor of oil field equipment.

Full Paper ____ *Thematic Section:* Technological Research.
Registration Code of Publication: 15-43-7-112 *Subsection:* Organic Chemistry.
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Peculiarities of salt-free *N,N*-dimethyl-*N,N*-diallilammoniyhlorid polymer and on the basis thereof

© **Rustem R. Daminev,**[1] **Radik N. Asfandiyarov,**[2] **Rail N. Fatkullin,**[2]
Lilia R. Asfandiyarova,[1] and **Guzel V. Yunusova**[1]
[1] *Branch of Ufa State Petroleum Technological University in Sterlitamak. October St., 2.*
Sterlitamak, 453118. Russia.
[2] *JSC "Bashkir Soda Company". Tekhnicheskaya St., 32. Russia. Republic of Bashkortostan.*
Phone: +7 (3473) 24-25-12, +7 (9649) 64-26-06. E-mail: asfand_lilya@mail.ru

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*Supervising author; $^+$Corresponding author

Keywords: polymerization, salt-free polymer, monomer, synthesis, flocculation, chemistry, reaction, technology.

Abstract

One highly effective flocculants currently in use is poly-*N,N*-dimethyl-*N,N*-diallilammoniyhlorid synthesized by radical polymerization of *N,N*-dimethyl-*N,N*-diallilammony chloride in aqueous solution. The aim of the research is to develop methods and technologies of production polyDADMAC not containing in its composition of sodium chloride. For the experiments to determine the feasibility of synthesis of salt-free monomer it was analyzed the chemistry of the process of obtaining DMDAAC. The experiments revealed that this method has the following disadvantages: in the synthesis accumulate in the system, sodium chloride, which is necessary to deduce therefrom; water introduced into it from each new batch of sodium hydroxide. Increasing the amount of water in the system involves losses of product since DMAC part is in the aqueous phase within the solubility. It has been proposed a process flow diagram of the monomer unit for production of salt-free DMDAAC. The advantage of the proposed method and technology is the lack of education is organically polluted wastewater, which distinguishes it from the known technologies for producing salt-free polyDADMAC.

Thematic Section: Technological Research. **Full Paper**
Subsection: Chemical Technology. *Registration Code of Publication:* 15-43-7-117
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Application of flocculants for wastewater treatment of chemical industry

© **Rustem R. Daminev**, **Lilia R. Asfandiyarova**,*[+] **Ramil R. Nasyrov**, and **Guzel V. Yunusova**
Branch of Ufa State Petroleum Technological University in Sterlitamak. October St., 2.
Sterlitamak, 453118. Russia. Phone: +7 (3473) 24-25-12, +7 (9649) 64-26-06. E-mail: asfand_lilya@mail.ru

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*Supervising author; [+]Corresponding author

Keywords: distilled liquid, flocculation, wastewater treatment, coagulant, polyelectrolyte, filtering.

Abstract

The problem of reducing the negative impact on the environment of waste production of soda ash by ammonia method is relevant in all countries, producing soda by this method. One of the effective ways of intensification of the existing wastewater treatment technologies is the use of high-molecular flocculants alone or together with coagulants. To select an effective flocculant used in order distiller thickening suspension was carried out analysis of the applicability of the following types of flocculants – Kaustamin-15, VPK-402, Polyacrylamide, SCF-25, Flopam. Analysis of the results of a series of experiments showed that the consideration of the best indicators of flocculants for the deposition rate, the content of suspended solids in purified suspension, the relative degree of compaction have the following brands: Kaustamin-15, Polyacrylamide and Flopam.

Full Paper ____ *Thematic Section:* Technological Research.
Registration Code of Publication: 15-43-7-122 *Subsection:* Electrochemistry.
The article is published on materials of the report on "International Scientific Forum Butlerov Heritage – 2015". http://foundation.butlerov.com/bh-2015/ *(English Preprint)*
Submitted on April 30, 2015.

Electrochemical processing of distiller fluid of the ammonia-soda manufacture

© **Nikolay A. Bykovsky**,*⁺ **Ludmila N. Puchkova**, and **Nadezhda N. Fanakova**
Branch of Ufa State Petroleum Technological University in Sterlitamak. October St., 2.
Sterlitamak, 453118. Russia. Phone: +7 (3473) 24-25-12. E-mail: nbikovsky@list.ru

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*Supervising author; [+]Corresponding author

***Keywords*: distiller fluid, soda ash, electrolyzer, membranes.

Abstract

It was studied the treatment of wastes of soda ash, that represents a distiller fluid, with obtaining of calcium hydroxide, sodium hydroxide and hydrochloric acid. Distiller fluid was treated by sodium hydroxide to convert calcium into the maximal insoluble form that is calcium hydroxide. After sediment separated the filtrate, consisting mainly from sodium chloride, was treated in a three-chambered membrane electrolyzer. Main regularities of distiller fluid treatment are studied upon the mentioned method. It was shown, that a technological process may be realized without any chemical reagents.

Thematic Section: Technological Research. **Full Paper**
Subsection: Electrochemistry. *Registration Code of Publication:* 15-43-7-127
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Reducing the rate of corrosion of oil and gas equipment by polarization surface

© **Oleg R. Latypov**,[1] **Evgeny V. Boev**,[2] and **Dmitry Ye. Bugay**[1]
[1] *Department of Petroleum Technology Eqipment. Ufa State Petroleum Technological University.*
Cosmonauts St., 1. Ufa, 450062. Bashkortostan. Russia.
*Phone: +7 (347) 242-08-36. E-mail: latypov83@mail.ru**
[2] *Department of Equipment Petrochemical Plants. Ufa State Petroleum Technological University,*
Branch in Sterlitamak. OctoberSt., 2. Sterlitamak, 453118. Bashkortostan. Russia.
Phone: +7 (3473) 24-25-12. E-mail: 9196011116@mail.ru

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*Supervising author; +Corresponding author

Keywords: corrosion rate, polarization, electrode potential, pH, redox potential, field medium.

Abstract

The article describes a new method for reducing the rate of corrosion of a metal surface by its polarization. The primary cause of metal corrosion is the thermodynamic instability of its electrode potential. Shifting the stationary potential to the equilibrium value results in the polarization of the metal surface, and consequently to reduce the corrosion rate. Studies have shown that when the basic electrochemical characteristics of the work medium - pH and redox potential, there is a shift of the electrode potential at the metal surface. The shift of the electrode potential of steel 20 to the reversible potential of significantly reduced the rate of corrosion. Application of this method and apparatus will significantly reduce the amount used in the oilfield corrosion inhibitors or completely eliminate them, which will lead to a reduction in material costs and reduce contamination of finished products inhibiting substances.

Thematic Section: Technological Research. **Full Paper**
Subsection: Chemical Equipment. *Registration Code of Publication:* 15-43-7-135
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Development of the construction and method of calculating the vortex devices for gas cleaning

© **Vitaly G. Afanasenko**,*+ and **Evgenie V. Boev**
Equipment Petrochemical Plants Division. USPTU. Kosmonavtov St., 1. Ufa, 450062.
Bashkortostan Republic. Russia. Phone: +7 (347) 243-11-45. E-mail: awirus@rambler.ru

*Supervising author; +Corresponding author

Keywords: separation, cleaning of gases, vortex motion, centrifugal force.

Abstract

Gas cleaning is one of the most important processes of the petrochemical industry. It is carried out on various stages of production, for preparing a feed gas of organic synthesis and purification products thereof. Also subjected to cleaning gases before atmospheric emission in order to reduce the content of harmful impurities that negatively affect the environment. This article describes the features of the process of separation of inhomogeneous gas mixture in a vortex motion, and shows the structure of a device for carrying out this process.

Full Paper ____ *Thematic Section:* Research into New Materials.
Registration Code of Publication: 15-43-7-140 *Subsection:* Innovation Technology.
The article is published on materials of the report on "International Scientific Forum
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Plasticizer for PVC compositions on the basis of VAT residue rectification 2-ethylhexanol

© **Rustem R. Daminev**,*+ **Raylia F. Nafikova**,* **Aygul A. Islamutdinova**,*+
Ildar R. Hamzin, and **Aleksandr N. Ivanov**
General Chemical Technology Division. Branch of the Ufa State Petroleum Technological
University in Sterlitamak. Pr. Oktyabrya, 2. Sterlitamak, 453118. Bashkortostan Republic. Russia.
Phone: +7 (3473) 24-08-58. E-mail: aygul_ru@mail.ru

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*Supervising author; +Corresponding author

Keywords: plasticizer, polyvinyl chloride, dioctyl phthalate (DOP), PVC adhesive tape.

Abstract

The paper proposed an improved method for the production of plasticizer for PVC compositions when used in the quality of raw materials VAT residue rectification 2-ethylhexanol (COREG). As a catalyst for the esterification reaction suggested the use of zinc stearate, which is a PVC heat stabilizer. Study of the kinetics of the esterification of phthalic anhydride with COREG in the presence of zinc stearate showed that it catalyzes the esterification process. By results of researches it is concluded that the obtained plasticizer possesses good plasticizing properties and meets the requirements.

The article is intended for teachers and students of technical universities, as well as for engineers in the chemical and petrochemical industries.

Full Paper ______________________________ *Thematic Section:* Technological Research.
Registration Code of Publication: 15-43-7-144 *Subsection:* Innovation Technology.
The article is published on materials of the report on "International Scientific Forum
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A study of municipal solid waste generated in the city of Sterlitamak for the possibility of their use in the furnaces of cement production

© **Ramil R. Nasyrov**,* and **Elena Yu. Bryazgin**⁺
Division of General Chemical Technology. Ufa State Petroleum Technological University, Branch of USPTU
in Sterlitamak. Pr. Oktyabrya, 2. Sterlitamak, 453118. Bashkortostan Republic. Russia.
Phone: +7 (3473) 24-25-12. E-mail: 86elen86@mail.ru

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*Supervising author; ⁺Corresponding author

Keywords: alternative fuels, municipal solid waste, calorific value, waste, natural gas, energy source, cement, kiln, clinker.

Abstract

The analysis of existing methods of recycling of solid waste and the volume of his education in the Republic of Bashkortostan was carried out. The results of laboratory tests of samples of municipal solid waste generated in the city of Sterlitamak, to determine its morphology, elemental composition, as well as the calorific value was presented. The possibility of using municipal solid waste in the furnaces of cement production as an alternative source of energy was considered.

Thematic Section: Biochemical Research. **Full Paper**
Subsection: Physical Chemistry. *Registration Code of Publication:* 15-43-7-149
The article is published on materials of the report on "International Scientific Forum
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Identification several of NSAIDs in blood screening by solid-phase extraction and gas chromatography-mass spectrometry

© **Oksana N. Dvorskaya**,[1]*[+] **Sergey S. Kataev**,[2+] and **Ilia P. Krokhin**[2]
[1] *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
[2] *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

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*Supervising author; [+]Corresponding author

Keywords: the non-steroidal anti-inflammatory agents, screening, solid phase extraction, gas chromatography, mass spectrometry.

Abstract

The possibility of determining the several of NSAIDs in blood screening procedure for drugs and medicines using the methods of solid-phase extraction and gas chromatography with mass spectrometric detection was investigated. Ibuprofen, diclofenac, ketorolac, indomethacin, naproxen, and ketoprofen may be identified in the blood directly to the screening procedure.

Full Paper ____ *Thematic Section:* Preparative Research.
Registration Code of Publication: 15-43-7-154 *Subsection:* Organic Chemistry.
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Xanthynilation of arylamines: synthesis and structure of new reaction products

© **Valery Yu. Gorokhov**,*[+] and **Lydia P. Unicov**[+]
Department of General Chemistry. 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, yunnikova@yahoo.com

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*Leader of the thematic course; [+]Corresponding author

Keywords: 9*H*-xanthyn-9-ol, perchlorate cantile, symmetric xanthyne, *ortho*- and *N*-xanthynilation, *ortho*-xanthynilation and *N*-acetylation.

Abstract

Three new destinations for the reaction of arylamines with 9*H*-xanthyn-9-ol or perchlorate cantile, consisting in the possibility to simultaneously was observed: 1) the symmetric xanthylium two *ortho*-positions of arylamine with the preservation of a free amino group; 2) *ortho*- and *N*-xanthynilation or 3) *ortho*-xanthynilation and *N*-acetylation. The receive of new connections carried out by two methods: first – xanthynilation *N*- or *ortho*-anilines containing fragment 9*H*-xanthyne, the second synthesis in the system: arylamine – perchlorate cantile or 9*H*-xanthyn-9-ol – solvent.

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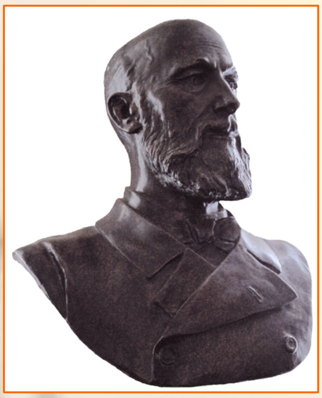

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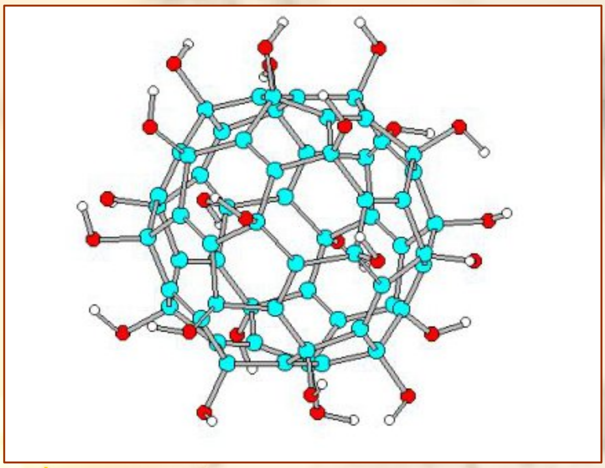

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Subsection: Chemistry History. *Registration Code of Publication:* 15-43-8-1
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About the role of A.M. Butlerov and his school in the formation scientific beekeeping in Russia

© **Eugeny N. Ofitserov**
Department of Chemistry and Technology of Biomedical Drugs. Faculty of Chemical and Pharmaceutical Technology and Biomedical Drugs. Russian Chemical-Technological University n.a. D.I. Mendeleev. Miusskaya sq., 9. Moscow, 125047. Russia.
Phone: +7 (495) 978-32-61. E-mail: ofitser@mail.ru

Abstract

In our ears "Butlerov chemical school," the pride of the scientific community of Kazan. However, there is the history and other Butlerov school – scientific beekeeping. About A.M. Butlerov by his disciple and follower, a famous musician and Director of the Mariinsky theatre G.P. Kondratiev was written: "the leader of Russian beekeeping". The famous scientists-chemists M. Kittary, A. Chugunova, I. Kablukov, the above-mentioned G. Kondratiev and several others can be attributed to Butlerov’s beekeeping school. As written by academician Yu. Zolotov: "For some reason, the chemists have always been drawn to bees". Indeed, in the biographies of many famous and great chemists have sections related to beekeeping. Moreover, these sections in importance is often comparable to chemical activity. Maybe it is because many chemists-beekeepers began his scientific career as a biologist. Examples of this quite a lot: M. Kittary, A. Butlerov, I. Kablukov, and others. To paraphrase Yu. Zolotov, it is can write slightly differently: "For some reason zoologists, entomologists, ichthyologists have always been drawn to chemistry", as most of these chemists began his scientific career as a biologist.

Thematic Section: Historical Heading. ________________________ (It is printed as the appendix) **Historical Review**
Subsection: Chemistry History. *Registration Code of Publication:* 15-43-8-19
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Apicultural Research articles by I.A. Kablukov, Honorary Academician of USSR Academy of sciences, disciple of A.M. Butlerov and V.V. Markovnikov

© **Sergey N. Smarygin**
Inorganical and Analitical Chemistry Department. Russian State Agrarian University – Timiryazev Moscow Agricultural Academy. Timiryazevskaya St., 49. Moscow, 127550. Russia.
Phone: +7 (916) 842-28-12. E-mail: smaryguin@mail.ru

***Keywords**:* Butlerov` school, A.M. Butlerov, V.V. Markovnikov, I.A. Kablukov, beekeeping, chemistry of honey, chemistry of beewax.

Abstract

I.A. Kablukov (1857-1942), honorary academician of URSS Academy of Sciences, was a student of Professor V.V. Markovnikov at Moscow University, and later an interne of A.M. Butlerov at St.-Petersburg University. Therefore he can be indubitably considered as a follower of Butlerov` school of thought in chemistry. From his teacher A.M. Butlerov he took over a passion for apiculture. His scientific and public activities in chemistry and beekeeping were tied up throughout all his life.

This essay offers a survey of three lines of I.A. Kablukov scientific studies: 1) research in chemistry of honey, beeswax and bee-glue as well as methods of revealing counterfeit in these apiculture products; 2) organization of apiculture department attached to Russian Imperial Society of acclimatization animals and plants (the activity of the department was also managed by A.M. Butlerov) and included the organization of travelling apiculture exhibitions; 3) writing articles about apiculture in Europe and America.

Analytical Review ____ *Thematic Section:* Biochemical Research.
Registration Code of Publication: 15-43-8-30 *Subsection:* Physico-Chemistry of Dyes.
The article is published on materials of the report on "International Scientific Forum
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Natural acid-base indicators based on anthocyanins in the treatises of scientists of India

© **Rustem R. Daminev**,* **Aleksandr N. Ivanov**,+ **Ildar R. Hamzin**,
Pahlavon S. Saytmuratov, and **Oleg Kh. Karimov**
Department of General Chemical Technology, Branch of Ufa State Petroleum Technological University
in Sterlitamak. October St., 2. Sterlitamak, 453118. Russia.
Phone: +7 (3473) 24-08-58. E-mail: aspirantdragon@yandex.ru

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*Supervising author; +Corresponding author

Keywords: chemical indicators, acid-base titration, anthocyanins, Ipomoea species biloba, Hibiscus rosa-sinensis, Catharanthus roseus, Nerium oleander, Nerium Odoratum.

Abstract

One of the most common types of chemical indicators are acid-base indicators, which have found wide application in analytical chemistry and are used in qualitative and quantitative methods of analysis. Due to the fact that the preparation of indicators on the basis of natural raw materials is a more simple, cheap and safe way to manufacture than synthetic compounds, conducted numerous studies in the field of new natural indicators. Special attention is paid to the anthocyanins – natural dyes contained in a wide array of plants. One of the leading countries in this matter is India, where different research groups have conducted experiments with various species of plants to extract from the flowers and leaves extracts with further tests on the potential use as indicators. This paper presents an overview of the most significant works of the scientists of India for the last decade aimed at studying changes color depending on the acidity of plant extracts containing anthocyanins, and the ability to replace the last used on date synthetic acid-base indicators.

Full Paper ____ *Thematic Section:* Biochemical Research.
Registration Code of Publication: 15-43-8-36 *Subsection:* Bioorganic 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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The change in the level of lipid peroxidation in cultured cells tissue *Polyscias filicifolia* under the influence of a constant magnetic field

© **Margarita A. Strelkova**, **Nadezhda V. Kirillova**,*[+] and **Nadezhda S. Kuzmina**
Department of Biochemistry. Saint-Petersburg State Chemical-Pharmaceutical Academy.
Prof. Popova St.,14. Saint-Petersburg, 1977376. Russia.
Phone: +7 (812) 234-90-33. Факс: +7 (812) 234-60-44.
E-mail: kirillovanv47@mail.ru , nadezhda.kirillova@pharminnotech.com

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*Supervising author; [+]Corresponding author

Keyword: cell culture, *Polyscias filicifolia*, constant magnetic field, lipid peroxidation.

Abstract

Changes of the superoxidation of lipids in the cultivated plant cells of Polyscias filicifolia at influence of a weak electromagnetic field are studied. The cultivated cells subjected an effect of a magnetic field within 1, 3, 7 and 9 days (an exponential growth phase) and 12, 16, 19, 25 and 28 days (a stationary growth phase). The intensity of lipid peroxidation was assessed by the level of diene conjugates, conjugated ketatrien, Schiffes bases and malonic dialdehyde. In the exponential growth phase the most the damaging effect on the membranes is shown on 7-9 days of exposition At the end of cultivation (28-30 days of grows) the normalization of lipid peroxidation is shown that indicating on the formation in cultured cells of a resistance to the effects of the magnetic field.

Full Payer *Thematic Section:* Biochemical Research.
Registration Code of Publication: 15-43-8-42 *Subsection:* Human's Biochemistry.
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The state of the enzymatic antioxidant defense system in patients with diabetes mellitus type II

© **Nadezhda V. Kirillova,***+[1] **Marina G. Mescheryakova,**[1] **Olga M. Spasenkova,**[1]
Irina A. Orehova,[1] **Valentina I. Laryonova,**[2] and **Анна N. Voytovych**[2]
[1] *Department of Biochemistry. Saint-Petersburg State Chemical-Pharmaceutical Academy.*
Prof. Popova St., 14. Saint-Petersburg, 1977376. Russia.
[2] *Federal State Budgetary Scientific Institution "Institute of Experimental Medicine".*
Akad. Pavlov St., 12. Saint-Petersburg, 1977376. Russia.
Phone: +7 (812) 234-90-33. Факс: +7 (812) 234-60-44.
E-mail: kirillovanv47@mail.ru , nadezhda.kirillova@pharminnotech.com

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*Supervising author; +Corresponding author

Keywords: diabetes mellitus, catalase, glutathione peroxidase, glutathione reductase, paraoxonase.

Abstract

The decrease of activity of key enzymes of the antioxidativ defence in blood of the patients of saccharine diabetes of the type II: superoxide dismutas, katalase, glutationperoksidase, glutationreduktase and paraoksonase was exposed. The intensification of the oxidative stress for the patients saccharine diabetes of the type II was identified.

Thematic Section: Biochemical Research. **Full Paper**
Subsection: Computer Simulation. Registration Code of Publication: 15-43-8-47
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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The study of linear and star-like macromolecules lignin

© **Anatoly P. Karmanov**,*+ and **Andrey G. Dontsov**
Laboratory of Biochemistry and Biotechnology. Institute of Biology of Komi Scientific Center of UB RAS.
Communist St.,, 28. Syktyvkar, 167982. Republic of Komi. Russia.
Tel.: +7 (8212) 43-68-28. E-mail: dontsov@ib.komisc.ru

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*Supervising author; +Corresponding author

Keywords: lignins, scaling, correlation dimension, configuration of macromolecules.

Abstract

Data of experimental study of natural lignins, as well as the results of simulation computer modeling of macromolecules with a star-like and linear topology on a cubic lattice are discussed. Values of correlation dimension and scaling parameters of linear and star-like macromolecules were calculated.

Full Paper _____ *Thematic Section:* Study of Reactivity.
Registration Code of Publication: 15-43-8-52 *Subsection:* Chemistry of Fullerenes.
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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Interaction fullerenol with biologically active substances in water solutions

© **Irina B. Dmitrieva**,* **Albina R. Nazipova**, **Sergey E. Erdni-Garyaev**,
Aleksandr S. Chukhno,+ **Victor I. Gerasimo**, **Mikhail Yu. Mezyutin**,
Ekaterina A. Klimkina, and **Anastasia A. Vysotskaya**
Chair of Physical and Colloid Chemistry. Saint-Petersburg State Chemical-Pharmaceutical Academy.
Professora Popova St., 14. Saint-Petersburg, 197376. Russia.
Phone: +7 (812) 234-11-38. E-mail: alex-chuhno@yandex.ru, amylee2208@mail.ru

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*Supervising author; +Corresponding author

Keywords: fullerenol, dextran, immunoglobulin, gelatin, glycine, aspartic acid, swelling, microelectrophoresis, isoelectric point.

Abstract

The investigations of a number of physical and chemical properties of aqueous solutions of fullerenol (electrical conductivity, surface tension, optical activity, the effect on the swelling of gelatin and electrokinetic properties of dextran) and its interaction with various biologically active substances are investigated.

It is established that fullerenol has no surface activity, does not significantly affect the electrical conductivity and pH of the water and does not interact specifically with dextran. These results demonstrate that the pharmacological action of aqueous solutions of fullerenol is due to its interaction with proteins.

Full Paper *Thematic Section:* Study of Reactivity.
Registration Code of Publication: 15-43-8-60 *Subsection:* Organometallic 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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Comparative analysis of Cu(II) reactivity upon interaction with octa-(4-bromophenyl)-tetraazaporphyrin and Mg-octa-(4-bromophenyl)-tetraazaporphyrin

© **Svetlana V. Zvezdina**,[1] **Natalia V. Chizhova**,[1] **Olga V. Maltseva**,[1]
Nugzar Zh. Mamardashvili,[1] and **Oskar I. Koifman**[1,2]
[1] *G.A. Krestov Institute of Solution Chemistry of the Russian Academy of Sciences. Akademicheskaya St., 1. Ivanovo, 153045. Russia. E-mail: svvr@isc-ras.ru*
[2] *Institute of Chemistry Macroheterocyclic Compounds. Ivanovo State University of Chemistry and Technology. Sheremetev pr., 7. Ivanovo, 153000. Russia. E-mail: koifman@isuct.ru*

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*Supervising author; +Corresponding author

Keywords: octa-(4-bromophenyl)tetraazaporphyrin, Mg(II)-octa-(4-bromophenyl)tetraazaporphyrin, copper(II) chloride, kinetic of complexation, metal exchange reaction, rate constant.

Abstract

The complexation of copper chloride(II) with octo-(4-bromophenyl)tetraazaporphyrin–ligand and metallosalen with Mg(II)-octo-(4-bromophenyl)tetraazaporphyrin in dimethylformamide (DMF) are studied. Kinetic parameters of the reactions and the comparative analysis of their velocity constants. The first order of salt and metallocomplex in the reaction of metallocene Mg(II)-octo-(4-bromophenyl)tetraazaporphyrin copper chloride(II) in DMF are defined. Reaction mechanism of metallocene are proposed.

Full Paper *Thematic Section:* Physicochemical Research.
Registration Code of Publication: 15-43-8-66 *Subsection:* Inorganic Chemistry.
The article is published on materials of the report on “International Scientific Forum
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A study of crystal-chemical transformations in $LaMnO_{3+\delta}$

© **Larisa B. Vedmid’**, **Aleksandr M. Yankin**,*
Vladislav M. Kozin, and **Ol’ga M. Fyodorova**
Laboratory of Statics and Kinetics of Processes. Institute of Metallurgy UB RAS. Amundsena St., 101.
Yekaterinburg, 620016. Russia. Phone: +7 (343) 232-90-72. E-mail: elarisa100@mail.ru

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*Supervising author; $^{+}$Corresponding author

Keywords: Rare-earth manganites, oxygen stoichiometry, phase equilibria, Jahn-Teller effect.

Abstract

The evolution of structural transformations in $LaMnO_{3.018}$ was considered and theirs temperatures were defined by the combination of methods. The temperature dependency of equilibrium oxygen pressure for $LaMnO_{3.018}$ dissociation reaction was measured by a static method. Changes of standard formation enthalpy and entropy of $LaMnO_{3.018}$ were calculated.

Thematic Section: Physicochemical Research. **Full Paper**
Subsection: Biochemistry. *Registration Code of Publication:* 15-43-8-71
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On molecular mechanism of biologic activity of apigenin

© **Ruslan S. Nasibullin**,*+ **Leonid V. Spiriphin**, **Dinara I. Phakhretdinoda**, and **Rosa I. Galieva**
Bashkir State Medical University. Ufa. Lenin St., 3. E-mail: med-fis@yandex.ru

*Supervising author; +Corresponding author

Keywords: biologic activity, flavonoids, apigenin, the NMR spectroscopy, quantum chemistry.

Abstract

The interaction of the molecule apigenin and of the molecule phosphatidylcholine has been investigated by the methods of NMR spectroscopy and quantum chemistry. Changes of the conformational states of lecithin have been defined.

Thematic Section: Thermodynamic Research. **Full Paper**
Subsection: Phase Equilibria. *Registration Code of Publication:* 15-43-8-75
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Modeling of liquid-liquid phase equilibrium in system triacylglycerides – fatty acid – ethanol

© **Irina A. Permyakova**, **Dmitry A. Kazakov**,$^+$ **Vladimir V. Vol'hin**,*
Natalia S. Voronina, and **Ivan Yu. Zorichev**
Chemistry and Biotechnology Department. Perm National Research Polytechnic University.
Komsomolskiy pr., 29. Perm, 614990. Permskiy krai. Russia.
Phone/fax: +7 (342) 239-15-11. E-mail: kazakovbiotech@mail.ru

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*Supervising author; $^+$Corresponding author

Keywords: modeling, phase equilibrium, liquid-liquid system, UNIFAC model, triacylglycerides, ethanol, oleic acid, stearic acid, lauric acid.

Abstract

The aim of the paper is to estimate the possibility of using UNIFAC model for the analysis of phase equilibria in systems TAG – CarbA – EtOH, where TAG – triacylglycerides (sunflower oil), CarbA – fatty carboxylic acids – oleic (OlA), stearic (StA), lauric (LaurA), EtOH – ethanol at temperatures ranging from 30 to 70 °C, which is associated with the disposal of waste oils containing free fatty acids. UNIFAC model with modified group interaction parameters (a_{mn}, a_{nm}) was used. For the studied systems the simulations and experiments were carried out. Obtained data allowed to plot the ternary phase diagrams, determine the composition of reversible transition of the systems from heterogeneous into homogeneous state, calculate residual dispersion and the degree of compliance of calculated and experimental data. It was found that for systems with OlA application of the UNIFAC model with modified group interaction parameters led to results of calculation close to experimental, but it gives substantial deviation for systems with LaurA and especially with StA. Due to the relatively high melting points of these acids the probability of forming of solid phases in the systems increases with growing of overall number of phases up to three.

Full Paper _______________________________________ *Thematic Section:* Research into New Materials.
Registration Code of Publication: 15-43-8-84 *Subsection:* Computational Simulation.
The article is published on materials of the report on "International Scientific Forum
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Simulation and comparison of the mode structure in silver halide hollow- and solid-core PCFs with a single ring of elements for the MIR

© **Dmitry S. Vrublevsky**, **Alexandr S. Korsakov**, and **Lia V. Zhukova***[+]
Ural Federal University Named After the First President of Russia B.N. Yeltsin. Department of Physical Chemistry and Chemistry of Colloids. Mira St., 19. Ekaterinburg, 620002. Russia.
Phone: +7 (343) 375-44-45. E-mail: l.v.zhukova@urfu.ru

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*Supervising author; [+]Corresponding author

Keywords: photonic crystal fibers, computer simulation, fundamental mode, middle infrared, silver halide solid solutions.

Abstract

We simulated the mode structure of photonic crystal fibers with a single ring of elements hexagonally and octagonally arranged around either a solid core or a central defect with either lower or higher optical density, counting upon the refractive indices of $AgCl_{1-x}Br_x$ system, where x = 0.75, 0.82, and 0.84. Mode comparison revealed the advantages of the active-core fiber, i.e. with a higher refractive index of the central rod element. We also predicted such a fiber to be capable of guiding more optical power, comparing with a standard double-layered one with similar dimensions.

Thematic Section: Research of the New Technologies. **Full Paper**
Subsection: New Catalytic Processes. *Registration Code of Publication:* 15-43-8-91
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Mineralization of oxalic acid by ozone in the presence of activated carbon particles

© **Dmitry A. Kazakov**,[+] **Vladimir V. Volkhin**,*
Yulia O. Gulenova, **Marina N. Obirina**, and **Daria A. Rozhina**
Chemistry and Biotechnology Department. Perm National Research Polytechnic University.
Komsomolskiy pr., 29. Perm, 614990. Permskiy krai. Russia.
Phone/fax: +7 (342) 239-15-11. E-mail: kazakovbiotech@mail.ru

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*Supervising author; [+]Corresponding author

Keywords: oxalic acid, mineralization, ozone, activated carbon.

Abstract

The results of the study of the influence of activated carbons (BAU-A and AG-5) with different textural characteristics on the rate of oxalic acid mineralization during ozonation are presented. It was found that in the presence of activated carbons studied mineralization rate of oxalic acid significantly increased. Despite the substantial difference in textural characteristics of the activated carbons studied, the catalytic activity of the sample BAU-A is only slightly lower compared to sample AG-5. Theoretical analysis of the macrokinetic regimes of oxalic acid mineralization during ozonation in the presence of activated carbon particles was carried out. The effect of activated carbon particles size on the degradation rate of oxalic acid was studied. The concentration of the active sites (OH-groups) on the surface of the studied samples of activated carbon using FT-IR spectroscopy was estimated. It was found that the concentration of active sites (OH-groups) on sample BAU-A only slightly lower comparing with the sample AG-5. This was in agreement with the data on the catalytic activity of these samples. It was shown that the rate of oxalic acid mineralization during ozonation significantly increased with decreasing activated carbon particles size. It was concluded that catalytic mineralization of oxalic acid by ozone was realized in external kinetic mode, when macroscopic velocity of rhe process depended on the catalyst particles size and concentration of active sites on its surface and is nearly independent of its textural characteristics.

Full Paper *Thematic Section:* Research of the New Technologies.
Registration Code of Publication: 15-43-8-102 *Subsection:* Electrochemistry.
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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Production of composite powders containing metal carbides

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

[1] *‘Technologii tantala’ Co Ltd. Lenin St., 131. Upper Pyshma, 624096. Sverdlovsk Region. Russia.*
Phone: +7 (922) 211-88-44. E-mail: npp-nauka@yandex.ru

[2] *Laboratory for Physical-Chemistry of Metal Melts. Institute of Metallurgy, Urals’ Division of RAS*
Amundsen St., 101. Ekaterinburg, 620016. Russia. Phone: +7 (343) 267-88-94. E-mail: danaus@mail.ru

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*Supervising author; [+]Corresponding author

Keywords: titanium carbide, tungsten carbide, electrochemical reduction, salt melt, metal matrix.

Abstract

In the work the ways for agglomeration and sintering of nano- and submicron metal-clad composite powders that can be realized in the laboratory environment to produce composite grains of decamicron size were investigated. Two ways of agglomeration were considered: ‘briquetting-grinding-classification-sintering’ and ‘roll briquetting-classification-sintering’. The research was carried out involving titanium carbide powder plated with chromium, iron and titanium, and titanium powder in the metal matrix of mixed nano- and superdispersed chromium, nickel, and titanium. Composite powders with the grain size of +40-125 mkm and +40-160 mkm were produced. The phase composition of the composites, consisted of 3d-metal-clad electrolytic TiC and WC powders in metal matrix, was investigated during thermal treatment and sintering. It is shown the optimum agglomerating performance must be selected each time when the chemical composition of the composite has been changed either in term of quality or quantity.

Thematic Section: Research of the New Technologies. **Full Paper**
Subsection: Electrochemistry. *Registration Code of Publication:* 15-43-8-111
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Method for carbonization of massive refractory metal rods

© **Alexander V. Varaksin**,[1] **Viacheslav L. Lisin**,[2]* **Victor A. Kostilev**,[1]* **Leopold I. Leontiev**,[2]* **Robert G. Zakharov**,[2] **Sophia A. Petrova**,[2+] **Elena V. Ignatieva**,[2] and **Alexey B. Shubin**[2]
[1] *'Technologii tantala' Co Ltd. Lenin St., 131. Upper Pyshma, 624096. Sverdlovsk Region. Russia. Phone: +7 (922) 211-88-44. E-mail: npp-nauka@yandex.ru*
[2] *Laboratory for Physical-Chemistry of Metal Melts. Institute of Metallurgy, Urals' Division of RAS Amundsen St., 101. Ekaterinburg, 620016. Russia. Phone: +7 (343) 267-88-94. E-mail: danaus@mail.ru*

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*Supervising author; +Corresponding author

Keywords: tungsten, titanium, carbonization, chemical transport reaction, electrochemical reduction, salt melt.

Abstract

Carbonization of the volumetric tungsten and titanium rods by chemical transport reactions in salt melts was performed. By X-ray diffraction, X-ray spectrum analysis, and microhardness test it is shown that on the surface of the rods carbide coating of 20-50 mkm thickness was generated. Anodic dissolution was detected as a limiting factor for the carbonization. To prevent the anodic dissolution and to accelerate the carbonization process it is proposed to energize the sample by an alternative current.

Thematic Section: Research of the New Technologies. **Full Paper**
Subsection: Biochemistry. *Registration Code of Publication:* 15-43-8-119
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Тематическое направление: Bioconversion of biomass of *Helianthus tuberosus L* (Jerusalem artichoke) into sugars for biofuel production. Part 1.

Jerusalem artichoke tubers bioconversion

© **Andrey G. Dontsov**
Laboratory of Biochemistry and Biotechnology. Institute of Biology of Komi Scientific Center of UB RAS.
Communist St., 28. Syktyvkar, 167982. Republic of Komi. Russia.
Tel: +7 (8212) 43-68-28. E-mail: dontsov@ib.komisc.ru

Keywords: enzymatic hydrolysis, enzyme compositions, Jerusalem artichoke, biofuels.

Abstract

A comparison of the effectiveness of enzyme preparations with different substrate specificity and their compositions in hydrolysis of biomass artichoke tubers. Set the effect of complementarity of action of cellulolytic, pectinolytic preparations and complex own hydrolases Jerusalem artichoke, leading to a total and indiscriminate destruction of structural polysaccharides, which contributes to the achievement of high speed hydrolytic reactions, increasing the yield of reducing sugars and the degree of conversion of the enzymatic hydrolysis of biomass Jerusalem artichoke tubers.

Thematic Section: Research into New Materials. **Author Review**
Subsection: Photon Infrared Optical Fibers. *Registration Code of Publication:* 15-43-8-127
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Fiber optical system for on-line monitoring of industrial processes

© **Alexandr S. Korsakov**
Department of Physical Chemistry and Chemistry of Colloids. Ural Federal University
n.a. the First President of Russia B.N. Yeltsin. 19 Mira St., 620002. Russia.
Phone: +7 (343) 375-44-45. E-mail: A.S.korsakov@urfu.ru

Keywords: FT-IR spectroscopy; silver and thallium halide solid solutions; structure simulation; photonic crystal fibers.

Abstract

We developed the fiber optical probes for mid-infrared range spectroscopy (2-18 microns). The suitability of using of fiber optical probes for the identification of substances by FTIR spectroscopy is demonstrated by studying the spectra of ink ballpoint pen and ink printer and determining of their application sequence. The principal possibility of using of fiber optical systems for control of industrial processes is presented. The studies of the chemical composition and electrolyte solution concentration in real time, using spectral analysis methods are also shown.

Full Paper *Thematic Section:* Physicochemical Research.
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Rheological feature filled cellulose nitrate lacquer compositions

© **Natalia S. Gainutdinova**,[+] **Tatiana A. Eneykina**,* **Sergey V. Soldatov**,
Anatoly Petrovich Pavlov, **Rose F. Gatina**, and **Yury M. Mikhailov**
Federal State Enterprise "State Scientific-Research Institute of Chemical Products". Svetlaya, 1. Kazan, 420033. Republic of Tatarstan. Russia. Tel: +7 (843) 544-07-21, 544-09-82. E-mail: 173gniihp@gmail.com

*Supervising author; [+]Corresponding author

Keywords: cellulose nitrate lacquer, filler, concentration dependence, the effective viscosity, rheology.

Abstract

The concentration dependence of viscosity is filled with 25% to nitrocell-Loozen lacquer (NC lacquer), which has an extreme character with at least ~50% of the mass. in relation to NTS were presented. The position of the minimum of the corresponding concentration ~50% of the mass does not depend on the concentration of the radio source NC-lacquer. It is shown that the asymptotic dependence of the viscosity is filled with 25% NC-lacquer on the specific surface area of particles of HMX at a constant mass concentration of the filler. The most intensive growth of viscosity, about ~1.6 times, occurs when the values of the specific surface in the range 8000-12500 cm^2/g.

Full Paper *Thematic Section:* Theoretical Research.
Registration Code of Publication: 15-43-8-140 *Subsection:* Physical Organic Chemistry.
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Bond dissociation energy of C-X (X = F, Cl, Br, I) bonds in halogen-containing hydrocarbons: correlation ratios with electronegativity, force constants of bonds and radii of atom X

© **Vladimir E. Tumanov**
Institute of Problems of Chemical Physics RAS. Chernogolovka, 142432.
Russian Federation. Fax: +7 (496) 522-35-07. E-mail: tve@icp.ac.ru

Keywords: bond dissociation energy, enthalpy of radical formation, enthalpy of molecule formation, electronegativity, force constant, atom radius, correlation ratio, regression equation.

Abstract

In this paper dissociation energies of C-X-bonds (X=F, Cl, Br, I) in halogen-containing hydrocarbons are calculated or specified using enthalpies of free radical formation derived from the experimental kinetic data. Comparison of the obtained results with the literary data is made. Correlation connection between the dissociation energy of C-X-bond of the replaced hydrocarbons and their electronegativity, force constant and atom radius of X is established. The regression equations for various groups of halogen-containing hydrocarbons $D_{C-X} = \omega_1\sqrt{D_{X-X}D_{C-C}} + \omega_2 br_{XX} + \omega_3$ are suggested, where $D_{\text{F-F}}$ = 158.670 ± 0.096 kJ/mol, $D_{\text{Cl-Cl}}$ = 242.58 ± 0.004 kJ/mol, $D_{\text{Br-Br}}$ = 193.859 ± 0.120 kJ/mol, $D_{\text{I-I}}$ = 152.25 ± 0.57 kJ/mol, $D_{\text{C-C}}$ are calculated using enthalpies of free radical formation.

Thematic Section: Quantum-Chemical Research. **Full Paper**
Subsection: Chemistry of Fullerenes. *Registration Code of Publication:* 15-43-8-147
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Quantum-chemical study of the structure and energy of formation of isomeric structures $C_{60}N_2^q$ and $C_{60}N_2H^q$, q = 0, -1, -2, based on C_{60}

© **Nikolay Yu. Trifonov**,[+] and **Alexander F. Shestakov***
Laboratory Complex Catalyst Department Kinetics and Catalysis. Institute of Problems of Chemical Physics RAS. Academician Semenov pr., 1. Chernogolovka, 142432. Moscow Region. Russia.
Phone: +7 (4965) 22-17-63. E-mail: viktor-bilyaev@yandex.ru

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*Supervising author; [+]Corresponding author

***Keywords**:* reactivity, catalysis, fullerene C_{60}, nitrogen fixation.

Abstract

In this paper various intermediates of the fixation of molecular nitrogen in the presence of supramolecular complexes of C_{60} with γ-cyclodextrin under electrolysis were considered. Found structures have a relatively small increase of energy during the addition N_2.

Thematic Section: Quantum-Chemical Research. **Full Paper**
Subsection: Physical Organic Chemistry. *Registration Code of Publication:* 15-43-8-153
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Computation of vibrational spectra of furoxane and dimethylfuroxane molecules in coordinates X_δ^0 with an estimation of a force fields in frameworks DFT

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

Keywords: furoxane, dimethylfuroxane, the generalized force constants, coordinates X_δ^0, calculations DFT, vibrational frequencies.

Abstract

Within the framework of approach B3LYP 6-311++G(3df,3pd) the force fields of furoxane and dimethylfuroxane molecules in coordinates X_δ^0 for the first time were received. Frequencies of normal vibrations were calculated. Generalized force constants of molecule was carried out.

Full Paper ______________________________________ *Thematic Section:* Preparative Research.
Registration Code of Publication: 15-43-8-162 *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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The study of oxidative cleavage halogenphenoxycyclopropanes under the influence of nitrous acid

© **Rimma A. Gazzaeva**,*[+] **Larisa B. Koblova**, and **Laura V. Tigieva**
Organic Chemistry Divizion. Chemical-Technological Faculty. North Osetian State University. NOSU.
Vatutina St., 40. Vladikavkaz, 362025. Republic North Osetia-Alania. Russia.
Phone: +7 (928) 067-98-53. E-mail: gazzaevar@mail.ru

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*Supervising author; [+] Corresponding author

Keywords: 2,2-dichlorocyclopropylphenolic ether, 2,2-dibromcyclopropylphenolic ether, oxidative cleavage, 1-phenoxy-1-trifluoromethoxycarbonyl-3,3-dichloro-3-nitrosopropan, 1-phenoxy-1-tribrom-methoxycarbonyl-3,3-dichloro-3-nitrosopropan.

Abstract

We have synthesized 2,2-dichlorocyclopropylphenolic and 2,2-dibromocyclopropylphenolic ethers. Treatment of obtained compounds with nitrous acid formed in situ, led to preferential oxidative cleavage of a small cycle. As the result of the reaction 1-phenoxy-1-trifluoromethoxycarbonyl-3,3-dihalogen-3-nitroso-propanes were obtained and characterized.

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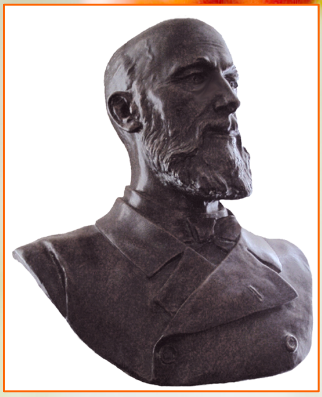

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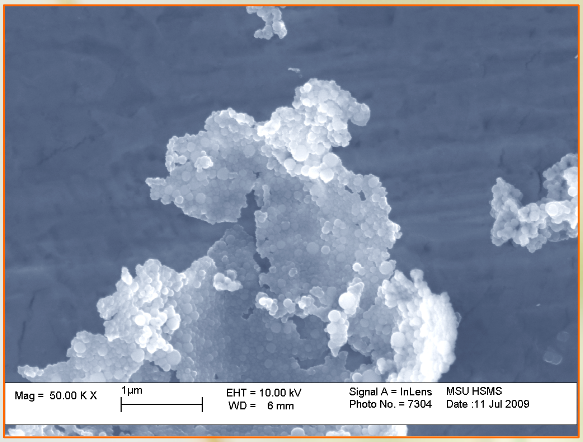

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World market of amorphous silica consumption and Kamchatka hydrotherms as new raw resources for nanosilica production in Russian Federation

© **Vadim V. Potapov**,[1] **Ankhel A. Cerdan**,[2] and **Alexandr N. Kashutin**
[1] *Research Geotechnological Center of Far East Division of Russian Academy of Sciences.*
Severo-Vostochnoe shosse, 30. Petropavlovsk-Kamchatsky-City, Petropavlovsk-Kamchatsky, 683002.
Phone: +7 (84152) 49-54-35. E-mail: vadim_p@inbox.ru
[2] *Lomonosov Moscow State University. Chemistry Department. Lenin Hills, 1, build. 3. Moscow, 119991.*
Russia. Phone: +7 (495) 939-52-57. E-mail: cerdan@mai.ru

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*Supervising author; +Corresponding author

Keywords: sols, silica nanopowders, industrial use of amorphous silica, hydrothermal solution.

Abstract

World demand for different types of amorphous silica is continuously increasing. This trend is evident in the high-tech industries, which are associated with the consumption of ultrafine silica forms, i.e. sols and nanopowders. Hydrothermal solutions are a new source of raw material for SiO_2 sols and nanopowders preparation. There is a need to develop technology for production of nanopowders and sols of SiO2 on the basis of hydrothermal solutions. The technology must take into account the size and concentration of SiO_2 particles, the kinetics of their formation as a result of the polycondensation of orthosilicic acid, the temperature and pH of the aqueous medium.

Thematic Section: Computational Research. **Full Paper**
Subsection: Chemistry of Silicon and its Compounds. *Registration Code of Publication:* 15-43-9-7
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Numerical simulation of orthosilicic acid polycondensation and colloidal particles growth in hydrothermal solutions

© **Vadim V. Potapov**, and **Elena V. Shunina**
Research Geotechnological Center of Far East Division of Russian Academy of Sciences.
Severo-Vostochnoe shosse, 30. Petropavlovsk-Kamchatsky-City. Petropavlovsk-Kamchatsky, 683002.
Phone: +7 (84152) 49-54-35. E-mail: vadim_p@inbox.ru

*Supervising author; +Corresponding author

Keywords: hydrothermal solution, orthosilicic acid polycondensation, silica sol.

Abstract

Hydrothermal solutions – nature water mediums which are potential sources of amorphous silica. There is the problem of research of physical and chemical compounds of colloidal silica in hydrothermal solution for development silica extraction and effective methods of using heat carrier. In the frame of this problem there is the task of studing kinetic of orthosilicic acid polycondensation. Polycondensation is one of basic processes in sol-gel technologies for producing materials oxigens including SiO_2. As the result of silicic acid polycondensation in the water silica sol is forming and the particles of sol are growing. Formation of interface surfaces depends on kinetic of process when solutions turns into sols, thus influence on sols properties and structure of materials through initial conditions.

Thematic Section: Biochemical Research. **Review**
Subsection: Chemistry of Silicon and its Compounds. *Registration Code of Publication:* 15-43-9-17
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Thematic course: Amorphous silica opal-cristobalite rocks as renewable raw materials for the synthesis of organosilicon compounds and silicates. Part 4.

The influence of silicon fertilizers on plants and soil

© **Vladimir V. Matichenkov,**[1]* **Elena A. Bocharnikova,**[2] and **Yana**[3] **M. Amosova**
[1] *Institute of Basic Biological Problems Russian Academy of Sciences. Pushchino, 142290. Russia.*
E-mail: vvmatichenkov@rambler.ru
[2] *Institute of Physicochemical and Biological Problems in Soil Science RAS. Pushchino, 142290. Russia.*
E-mail: vvmatichenkov@rambler.ru
[3] *Faculty of Soil Science of MSU named after M.V. Lomonosov. Moscow, 119899. Lenin hills. Russia.*

*Supervising author; +Corresponding author

Keywords: amorphous silica, silicon fertilizer, rice, sugarcane, wheat, barley, oats, rye, sunflower, maize, sugar beet, clover, tomatoes, cucumbers.

Abstract

This review summarizes data on the influence of silicon fertilizers on plants and soils. A history of these investigations is shortly described. Silicon fertilizers have been shown to benefit the productivity of cultivated plants directly *via* enhancing plant tolerance to biotic and abiotic stresses and indirectly via improving the soil fertility, optimizing the soil phosphate regime, reducing the toxicity of Al and heavy metals as well as improving soil physical properties.

Full Paper *Thematic Section:* Biochemical Research.
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Prospects for the use of nanosized silica in fish farming

© **Anatoly A. Lapin**,*+ **Lada K. Govorkova**, **Yuri V. Chugunov**,
Vadim V. Potapov,[1] **Valery N. Zelenkov**,[2]
and **Anastasia A. Sorokina**
Department of "Water Bioresources and Aquaculture." Kazan State Power Engineering University. Krasnoselskaya St., 51. Kazan, 420066. Tatarstan. Russia.
Phone: +7 (843) 519-43-53. E-mail: lapinanatol@mail.ru
[1] *Scientific-Research Geotechnological Center of the FWB RAS. North East Highway, 30. Petropavlovsk-Kamchatsky, 683002. Russia. Phone: +7 (84152) 49-54-35. E-mail: vadim_p@inbox.ru*
[2] *All Russian Research Institute of Vegetable Breeding of the RAS. Vereya Village. District Ramenskoye. Moscow Region, 140153. Russia. Phone: +7 (910) 451-37-45. E-mail: zelenkov-raen@mail.ru*

*Supervising author; +Corresponding author

Keywords: sols, nanosized silica, feed supplements, toxicity bioassay, lower crustaceans *Daphnia magna Straus*, guppies, antioxidant activity, hydrogen peroxide, ultrasonic dispersion.

Abstract

For the application of nanosized silica from hydrothermal solutions coolants geothermal power stations in fish farming as feed additives carried out tests on samples mortality crustacean *Daphnia Daphnia magna* Straus, who found that nano-dispersed silica has no toxic effect on daphnia doses $4 \cdot 10^{-2}$ g/dm^3 and can be used as a feed supplement in aquaculture.

Full Paper ____ *Thematic Section:* Biochemical Research.
Registration Code of Publication: 15-43-9-40 *Subsection:* Chemistry of Silicon and its Compounds.
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Using of nanodispersed SiO_2 in agriculture

© **Vadim V. Potapov,**[1]*+ **V.A. Sivashenko,**[2] and **Valery N. Zelenkov**
[1] *Research Geotechnological Center of Far East Branch of Russian Academy of Sciences.*
Severo-Vostochnoe Road, 30. Petropavlovsk-Kamchatsky, 683002. Russia.
Phone: +7 (84152) 49-54-35. E-mail: vadim_p@inbox.ru
[2] *Kamchatka Research Institute of Agriculture. Central St., 4. Sosnovka Village. District Yelizovo. Kamchatka Kray, 684000. Russia. Phone: +7 (8924) 780-62-47. E-mail: sivashenko@inbox.ru*
[3] *All Russian Research Institute of Vegetable Breeding of RAS. District Vereya. Ramenskoye Area. Moscow Region. Russia. Phone: +7 (910) 451-37-45. E-mail: zelenkov-raen@mail.ru*

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*Supervising author; +Corresponding author

Keywords: amorphous nanodispersed silica, gel and nanopowder of silica, hydrothermal solution, toxicity, additive in forage, using with agrochemicals, Ca-P exchange.

Abstract

The article discusses the possibility and viability of the use of nanodispersive silica (NDS) obtained from hydrothermal solution. It is shown that the NDS has a non-toxicity and biofility. It is shown rising potato harvest by treatment tubers of NDS and by addition of NDS in soil with N, P, K containing tertilizer. When NDS used as additive in forage for cows it is received the data on influence of NDS dose on morfometric characteristics and rising of Ca, P concentration in blood, optimization of Ca/P.

Thematic Section: Biochemical Research. **Full Paper**
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Silicon-containing preparations on atrnolol basis: practice and prospects of application in plant Russia

© **Vladimir N. Petrichenko**,[1] **Sergey V. Loginov**,[2] and **Oliga**[3] **S. Turkina**
[1] *Research Institute of Vegetable Growing.* [2] *FSUE GNIICHTEOS.* [3] *SEC LLC "Thesis +".*
E-mail: vnpetrich@ yandex.ru, florasilik@yandex.ru, tos060708@yandex.ru

*Supervising author; $^+$Corresponding author

Keywords: plant growth regulators, silicon-containing preparations, productivity, quality of vegetable crops, the correlation between air quality and trace elements.

Abstract

Studied the effect of silicon-containing plant growth regulators. It is shown that the new generation of drugs to stimulate the growth and development of plants, increase the productivity of vegetable crops, improve product quality and affect their chemical composition, reduce the accumulation of heavy metals in agricultural crops. Correlation dependence between the content of microelements in plants and biochemical parameters of products.

Full Paper *Thematic Section:* Biochemical Research.
Registration Code of Publication: 15-43-9-66 *Subsection:* Chemistry of Silicon and its Compounds.
The article is published as a material of correspondence participation in International Scientific Forum “Butlerov Heritage-2015”. http://foundation.butlerov.com/bh-2015/ *(English Preprint)*
Submitted on September 30, 2015.

Subject area: Amorphous opal-cristobalite silica as renewable stuff for organosilicon and silicate synthesis. Pat 4.

Synthesis and structural characteristics of tris(2-hydroxyethyl)ammonium maleate

© **Sergey V. Loginov**,[1] **Dmitry A. Gordeev**,[1] **Igor A. Dain**,[1] and **Evgeny N. Ofitserov**[2]*+
[1] *SRCHTEOC. Enthusiasts Highway, 38. Moscow 111123. Russia. E-mail: florasilik@yandex.ru*
[2] *Russian Chemical-Technological University named after D.I. Mendeleev.*
Miusskaya Sq., 9. Moscow, 125047. Russia. Phone: +7 (495) 978-32-61. E-mail: ofitser@mail.ru

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*Supervising author; +Corresponding author

Keywords: atranes, protatranes, tris-(2-hydroethyl)ammoniummaleate, molecularstructure, hydrogenbond, X-raycrystallography.

Abstract

Crystalline protatranic structure features of triethanolamine and maleic acid salt were studied.

Crystallinestructureof tris(2-hydroxyethyl)ammonium maleate was detected (a = 5.5882(6) Å, b = 10.4152(13) Å, c = 12.2523(17)Å; a = 68.284(10)°, β = 85.301(10)°, γ = 82.432(10)°; Z = 2,group P-1). Crystallinestructuralsubunits – pseudocyclicacidic maleate anion, protatranictris(2-hydroxyethyl)ammonium cation– form the chair structure, stabilized by hydrogen bonds system, electrostatic and π-πinteractions.

There was shown the impact of direct electrostatic interactions and anion structure on protatranic structure stabilization and monosubstituted product formation for maleic acid triethanolammonium salt.

Full Paper ____________________________________ *Thematic Section:* Research the New Technologies.
Registration Code of Publication: 15-43-9-74 *Subsection:* Chemistry of Silicon and its Compounds.
The article is published as a material of correspondence participation in International Scientific
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Submitted on April 28, 2015.

Amorphous nanosilica from hydrothermal solution: technology of production, physical and chemical characteristics, experience and perspectives of innovative application for nonorganic materials

© **Vadim V. Potapov,**[1] **Ankhel A. Cerdan,**[2] and **Alexander N. Kashutin**[1]
[1] *Research Geotechnological Center of Far East Division of Russian Academy of Sciences.*
Severo-Vostochnoe shosse, 30. Petropavlovsk-Kamchatsky-City. Petropavlovsk-Kamchatsky, 683002.
Phone: +7 (84152) 49-54-35. E-mail: vadim_p@inbox.ru
[2] *Lomonosov Moscow State University. Chemistry Department. Lenin Hills, 1, build. 3.*
Moscow, 119991. Russia. Phone: +7 (495) 439-46-38. E-mail: cerdan@mai.ru

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*Supervising author; [+]Corresponding author

Keywords: sols, silica nanopowders, membrane concentration, cryochemical vacuum sublimation, nanoaddives to concrete.

Abstract

Technological scheme of nanosilica production from hydrothermal solution consists of number studies. Basic studies are polycondensation of orthosilicic acid and silica particles rising, membrane concentration of of silica particles by ultrafiltration and production of SiO_2 sols, criochemical vacuum sublimation of sols and production of nanopowders. Nanosilica produced by this technology have physical and chemical characteristics for it application for concrete modification: increasing compressive strength of contrete, cool-resistancs.

Analitical Review ________________________________ *Thematic Section:* Research the New Technologies.
Registration Code of Publication: 15-43-9-78 *Subsection:* Chemistry of Silicon and its Compounds.
The article is published as a material of correspondence participation in International Scientific Forum "Butlerov Heritage-2015". http://foundation.butlerov.com/bh-2015/ *(English Preprint)*
Submitted on April 21, 2015.

Polymer compounds and nanocompounds based on silica

© **Denis V. Sugonyako**,*+ and **Lubov A. Zenitova**
Department of Synthetic Rubber Technology. Kazan National Research Technological University.
K. Marx St., 68. Kazan, 420015. Tatarstan. Russia.
Phone: +7 (843) 231-43-32. E-mail: sugonjako@gmail.com

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*Supervising author; +Corresponding author

Keywords: silica, carbon dioxide, reinforcing filler, the rubber composition, a tire mechanical properties nanocomposites.

Abstract

The practical application of silicon dioxide in the most important polymer systems as a reinforcing filler in rubber compounds in the production of environmentally friendly tires, a modifier of various plastics, adhesives, sealants and so on was considered. The special attention was given to silica as a promising object of modern scientific research. It was found that most studies related to the influence of silica on the properties of polymers include rubber compounds in the manufacture of tires. Thus, the articles on the use of silica as a filler, other polymers (including in comparison with other mineral fillers) much less. It is shown that individual interest and research on the use of silica in nano-region – innovative methods of obtaining it nanopowders and development of polymer nanocomposites.

Full Paper ____________________ *Thematic Section:* Research into New Materials.
Registration Code of Publication: 15-43-9-84 *Subsection:* Silicon in Metallurgy.
The article is published as a material of correspondence participation in International Scientific Forum "Butlerov Heritage-2015". http://foundation.butlerov.com/bh-2015/ *(English Preprint)*
Submitted on September 15, 2015.

Thermodynamic simulation of phase formation in the Mo-Si, alloys doped with scandium or neodymium

© **Aleksey V. Larionov,**[+] **Ludmila Y. Udoeva**, and **Vladimir M. Chumarev***
Laboratory of Pyrometallurgy of Nonferrous Metals. FSBIS Institute of Metallurgy, Ural Branch of RAS.
Amundsen St., 101. Yekaterinburg, 620016. Sverdlovsk Region. Russia.
Phone: +7 (343) 232-90-24. E-mail: a.v.larionov@ya.ru

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*Supervising author; [+]Corresponding author

Keywords: thermodynamic simulation, molybdenum, silicon, scandium, neodymium, phase composition.

Abstract

Thermodynamic simulation of the phase formation in Mo-Si hypoeutectic alloys when doping with scandium or neodymium was carried out. It was determined that scandium or neodymium in the Mo-Si(5.0%)-(Sc, Nd)(0-5.0%) ternary alloys can be found both in the form of silicides and in a metallic state. Their concentrations depend on the temperature and the amount of scandium or neodymium additives in the alloy. To retain the two-phase structure of the Mo-Si hypoeutectic alloys the amount of scandium or neodymium additive should be limited.

Thematic Section: Research into New Materials. **Full Paper**
Subsection: Silicon in Metallurgy. *Registration Code of Publication:* 15-43-9-89
The article is published as a material of correspondence participation in International Scientific Forum “Butlerov Heritage-2015”. http://foundation.butlerov.com/bh-2015/ *(English Preprint)*
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Thermodynamic simulation of phase formation in the Mo-Si alloys doped with yttrium

© **Aleksey V. Larionov**,$^+$ **Ludmila Y. Udoeva**,
Vladimir M. Chumarev,* and **Anastasia N. Mansurova**
Laboratory of Pyrometallurgy of Nonferrous Metals. FSBIS Institute of Metallurgy, Ural Branch of RAS.
Amundsen St., 101. Yekaterinburg, 620016. Sverdlovskregion. Russia.
Phone: +7 (343) 232-90-24. E-mail: a.v.larionov@ya.ru

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*Supervising author; $^+$Corresponding author

Keywords: thermodynamic simulation, molybdenum, silicon, yttrium, phase composition.

Abstract

Thermodynamic simulation of the phase formation in Mo-Si hypoeutectic alloys when doping with yttrium was carried out. It was found that the usage of the values of the thermochemical characteristics of Mo_3Si and Mo_5Si_3 molybdenum silicides laid in HSC Chemistry 6.12 software database in the simulation of binary hypoeutectic Mo-Si alloys led to results, which contradict the Mo-Si phase diagram. It was determined that yttrium in the Mo-Si(5.0%)-Y(0-5.0%) ternary alloys can be found both in the form of yttrium silicides and in a metallic state. Their concentrations depend on the temperature and the amount of yttrium additive in the alloy. To retain the two-phase structure of the Mo-Si hypoeutectic alloys the amount of yttrium additive should be limited.

Thematic Section: Research into New Materials. **Full Paper**
Subsection: Silicon in Metallurgy. *Registration Code of Publication:* 15-43-9-97
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Phase composition and microstructure of the obtained under nonequilibrium crystallization conditions Mo-Si alloys

© **Anastasia N. Mansurova**, **Aleksey V. Larionov**,*+
Stanislav N. Tyushnyakov, and **Larisa A. Marshuk**
Laboratory of Pyrometallurgy of Nonferrous Metals. Institute of Metallurgy of the UB of RAS.
Amundsen St., 101. Yekaterinburg, 620016. Sverdlovsk Region. Russia.
Phone: +7 (343) 232-90-24. E-mail: a.v.larionov@ya.ru

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*Supervising author; +Corresponding author

Keywords: Mo-Si alloy, phase formation, structure, silicides, microhardness, density.

Abstract

Silicide phases close to the stoichiometric compositionwhen vacuum-arc melting of Mo-Si alloys from Mo+(5-12)Si mixtures are formed. The density of alloys regularly decreases as the silicon concentration in them increases. Microhardness of silicide phases in the alloy and of pure molybdenumsilicides have similar values.

Full Paper ____ *Thematic Section:* Research into New Materials.
Registration Code of Publication: 15-43-9-102 *Subsection:* Silicon in Metallurgy.
The article is published as a material of correspondence participation in International Scientific
Forum "Butlerov Heritage-2015". http://foundation.butlerov.com/bh-2015/ *(English Preprint)*
Submitted on October 5, 2015.

Thermodynamic simulation of phase formation during cooling of zinc-containing cooper-smelting slag

© **Stanislav N. Tyushnyakov,**[+] and **Evgeny N. Selivanov***
Laboratory of Pyrometallurgy of Non-Ferrous Metals. Institute of Metallurgy of the UB RAS.
Amundsen St., 101. Yekaterinburg, 620016. Sverdlovsk region. Russia.
Phone: +7 (343) 232-90-24. E-mail: tyushnyakov.sn@gmail.com

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*Supervising author; [+] Corresponding author

***Keywords*:** thermodynamic simulation, iron-silicate slag, zinc, cooper, phase formation.

Abstract

Thermodynamic simulation of phase formation during cooling of the model system from 3500 °C appropriate of the composition of the slag from autogenous smelting of copper-zinc concentrates has been conducted. The thermodynamic simulation results is pointed out on that distillation of zinc from slag simultaneously with a conversion of a portion of iron (up to 24.4%) in the metallic state at high temperatures typical for arc discharge in electric furnace is possible. High polyvalent iron ion content in slag and a low thermal stability of copper and iron oxides provide to the reduction and the pass of zinc (higher 1250 °C) and copper (higher 2200 °C) into a gas.

Full Paper *Thematic Section:* Research into New Materials.
Registration Code of Publication: 15-43-9-108 *Subsection:* Silicon in Metallurgy.
The article is published as a material of correspondence participation in International Scientific
Forum "Butlerov Heritage-2015". http://foundation.butlerov.com/bh-2015/ *(English Preprint)*
Submitted on October 20, 2015.

Thermodynamic simulation of zinc reduction from cooper-smelting slag

© **Stanislav N. Tyushnyakov,**[+] and **Evgeny N. Selivanov***
Laboratory of Pyrometallurgy of Non-Ferrous Metals. FSBIS Institute of Metallurgy of the UB RAS.
Amundsen St., 101. Yekaterinburg, 620016. Sverdlovsk Region. Russia.
Phone: +7 (343) 232-90-24. E-mail: tyushnyakov.sn@gmail.com

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*Supervising author; [+]Corresponding author

Keywords: thermodynamic simulation, reduction, zinc, cooper, iron-silicate slag, blast-furnace dust, gas purification sludge of a steel-making furnace.

Abstract

Thermodynamic simulation of zinc reduction (at 1500 °C) from the model system appropriate of the composition of the slag from autogenous smelting of copper-containing sulfide concentrates has been conducted. The data on simulation of condensed and gas phases compositions during heating of slag together with a carbon monoxide, a blast-furnace dust and gas purification sludge of a steel-making furnace has been given. The thermodynamic simulation results were pointed out on that distillation of zinc from slag together with a conversion of a portion of iron in the metallic state is possible. The subsequent receipt of the oxidized sublimates is due to high zinc concentration in a gas (up to 26-27%). These sublimates can be processing by hydrometallurgical methods.

Full Paper ____ *Thematic Section:* Research into New Materials.
Registration Code of Publication: 15-43-9-116 *Subsection:* Silicon in Metallurgy.
The article is published as a material of correspondence participation in International Scientific
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Submitted on September 10, 2015.

Recieving of Al-Si alloys in KF-AlF$_3$-SiO$_2$ melt

© **Pavel S. Pershin**,*+ **Andrey V. Suzdaltsev**, and **Yurii P. Zaikov**
Laboratory of Electrode Processes. Institute of High Temperature Electrochemistry of the UB RAS.
Akademicheskaya St., 20. Yekaterinburg, 620137. Russia.
Phone: +7 (343) 374-50-89. E-mail: paffka19@yandex.ru Site: www.ihte.uran.ru

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*Supervising author; +Corresponding author

Keywords: aluminum, silicon, silumins, voltammetry, electrolysis, KF-AlF$_3$.

Abstract

Kinetics of silicon and aluminum deposition on the graphite cathode in KF-AlF$_3$ melt with SiO$_2$ addition (0-1.5 mass. %) at the temperature of 720 °C was investigated with cyclic voltammetry method. Peaks of silicon and aluminum deposition at potentials -0.85 and -1.30 V relatively to gas CO/CO$_2$ electrode are noted.

Potentsiostatic (at potentials -0.9 and -1.5 V) and galvanostatic (at cathode current density 0.5 A/cm^2) electrolysis of KF-AlF$_3$-SiO$_2$ is carried out and possibility of receiving silicon and silumins with the content of silicon 37 mass. % is shown.

The article is published as a material of correspondence participation in International Scientific Forum “Butlerov Heritage-2015”. http://foundation.butlerov.com/bh-2015/ *(English Preprint)*
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High-temperature oxidation study of the Nb-18.7Si *in situ* composites doped with yttrium and scandium

© **Vladimir M. Chumarev,**[1]* **Lyudmila Yurevna Udoeva,**[1+]
Leopold I. Leont’ev,[2] and **Alexey V. Larionov**[1]
[1] *Non- ferrous Metal Pyrometallurgy Laboratory. Institute of Metallurgy of the UB RAS. Amundsen St., 101. Yekaterinburg, 620016. Russia. Phone: +7 (343) 232-91-63. E-mail:gulroza@mail.ru*
[2] *Ferrous Metal Pyrometallurgy Laboratory. Institute of Metallurgy. Ural branch of RAS. Amundsen St., 101. Yekaterinburg, 620016. Russia. Phone: +7 (343) 232-91-20. E-mail: leo@imet.mplik.ru*

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*Supervising author; +Corresponding author

Keywords: Nb-Si composites, yttrium, scandium, alloying (doping), oxidation, oxides layers, microstructure, phase composition.

Abstract

In this paper the investigations results of the rare earths (particularly scandium and yttrium) effect on the structure and oxidation resistance of Nb-18.7Si *in situ* composites are presented. Features of the phase composition and microstructure of the eutectic Nb-Si alloys samples with different content of doping components were revealed by optical microscopy and electron probe microanalysis. It’s found that the rare earths doping of the eutectic Nb-Si alloy leads to an increase of microstructure dispersity and stabilization of high-temperature silicide Nb_3Si in the hardening phase. Yttrium and scandium positive effect on the oxidation of composites, reducing the rate of the oxide film formation if doping elements concentration is 1-2 at.% and temperature is lower pesting point (815 ^{o}C). The results of research of the microstructure and composition of the oxide layer indicates the combination of surface and internal oxidations, as evidenced by the formation of internal oxidation zone, keeping the two-phase structure and the initial ratio of elements in composites.

Full Paper *Thematic Section:* Physicochemical Research.
Registration Code of Publication: 15-43-9-130 *Subsection:* Silicon Composites.
The article is published as a material of correspondence participation in International Scientific Forum “Butlerov Heritage-2015”. http://foundation.butlerov.com/bh-2015/ *(English Preprint)*
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Kinetics of Nb-Si *in situ* composites doped with yttrium and scandium

© **Rosa I. Gulyaeva,**[1+] **Anastasia N. Mansuruva,**[1] **Vladimir M. Chumarev,**[1*]
Leopold I. Leont’ev,[2] and **Lyudmila Y. Udoeva**[1]
[1] *Non- ferrous Metal Pyrometallurgy Laboratory. Institute of Metallurgy of the UB RAS. Amundsen St., 101. Yekaterinburg, 620016. Russia. Phone: +7 (343) 232-91-63. E-mail: gulroza@mail.ru*
[2] *Ferrous Metal Pyrometallurgy Laboratory. Institute of Metallurgy. Ural branch of RAS. Amundsen St., 101. Yekaterinburg, 620016. Russia. Phone: +7 (343) 232-91-20. E-mail:leo@imet.mplik.ru*

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*Supervising author; [+]Corresponding author

***Keywords**:* composites, oxidation, kinetics, niobium, silicon, yttrium, scandium.

Abstract

The mechanism and kinetics of Nb-Si in situ eutectic composites, including doped with yttrium and scandium were studied by methods of isothermal heating in an air stream. It is shown that the initial stage of oxidation of the alloy is limited to the chemical interaction oxygen with niobium and the formation of lower valency oxides – NbO, NbO_2, and the second step – the diffusion of oxygen. The oxidation process models are suggested and kinetic parameters of the composites Nb-Si, including doped with yttrium and scandium, are determined.

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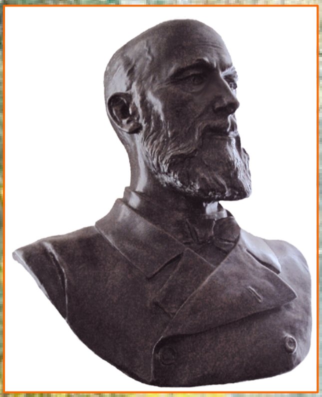

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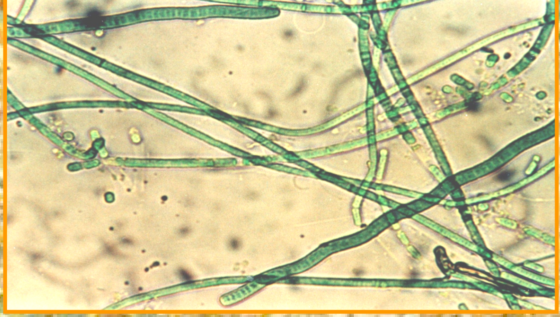

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The theory of ratchet-potential of the oxyhydrate systems

© **Boris A. Markov**, and **Yury***+ **I. Sukharev**
[1] *Department of Computational Mathematics. South Ural State University (National Research University).*
Lenin Ave., 76. Chelyabinsk, 454080. Russia.
[2] *Department of Chemistry of Solids and Some Processing Stages. Chelyabinsk State University.*
Br. Kashirinyh St., 129. Chelyabinsk, 454000. Russia.
Phone: +7 (963) 460-27-75. E-mail: Yuri_Sucharev@mail.ru.

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*Leader of the thematic course; +Corresponding author

Keywords: Lagrangian mappings, electroglobal, fulleroid, multipoles, oxihydrates systems, colloid clusters, spontaneous pulsation flow, diffuse double electric layer, topological continuum, dissociation-disproportion mechanism, Whitney theory, geometry of caustics.

Abstract

The structures formed by the gel particles have been considered. The gel particles formed separate long molecules folding in micellar composition. Due to the peculiarities of the structure of the oxyhydrate gels there is a large number of charged cluster particles. These particles interact with graphite electrodes. While there are currents of free charges, the fluctuations of which are found experimentally. The calculated values of the expected nano-currents give quite good agreement with experiment.

This process of the fluctuated splash motion of particles is determined by a stochastic ratchet-potential, the nature of education which is considered in the work.

Thematic Section: Physicochemical Research. **Full Paper**
Subsection: Physical Chemistry Superconductors. *Registration Code of Publication:* 15-44-10-21
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/ *(English Preprint)*
Contributed: September 25, 2015.

Stability and thermal expansion coefficient of high-temperature superconductors $RBa_2Cu_3O_y$

© **Andrey V. Fetisov**,[1] **Galina A. Kozhina**,[1] **Svetlana Kh. Estemirova**,[1]
Valentin Ya. Mitrofanov,[1] **Sergey A. Uporov**,[1] **Larisa B. Vedmid**,[1] **Stepan V. Pryanichnikov**,[1]
Lyubov A. Cherepanova,[1] **Svetlana G. Titova**,[1]* and **Yulia V. Blinova**+
[1] *Institute of Metallurgy of the UB RAS. Amundsen St., 101. Ekaterinburg, 620016.*
Russia. E-mail: sgtitova@mail.ru
[2] *Institute of Metal Physics of the UB RAS. S. Kovalevskaya St., 18. Ekaterinburg, 620990.*
Russia. E-mail: sudareva@imp.uran.ru

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*Supervising author; +Corresponding author

Keywords: high-temperature superconductors, chemical stability, mechanical activation, crystal structure, cation replacement.

Abstract

Using thermogravimetry, mass-spectrometry and magnetometry chemical stability of high-temperature superconductors $RBa_2Cu_3O_{6+\delta}$ with R = Y, Nd in relation to moisture was studied. To increase the rate of degradation the mechanical activation of powders in a ball mill was used. It is found that the weakening of the diamagnetic signal corresponding to the superconducting phase may be due to both their chemical degradation and suppression of superconductivity by magnetism of unexplored nature. Such magnetism manifests itself in samples containing magnetic R-ion. With the help of X-ray powder diffraction the temperature dependences of unit cell parameters were obtained and linear thermal expansion coefficients were calculated for compounds with R = (Y, Ca), Eu (Nd, Eu). The last composition has a positive and almost constant coefficient of thermal expansion in the temperature range 80–300 K, that makes it perspective for use in superconducting films and composites.

Full Paper ____ *Thematic Section:* Physicochemical Research.
Registration Code of Publication: 15-44-10-26 *Subsection:* Metallurgy.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/ *(English Preprint)*
Contributed: September 23, 2015.

Structural transitions in mechanical activated tulium manganite $TmMnO_3$

© **Olga M. Fedorova**,*+ **Larissa B. Vedmid`**,
Vladislav M. Kozin, and **Alexandr M. Yankin**
Laboratory of Statics and Kinetics of Processes. Institute of Metallurgy of the UB RAS.
Amundsen St., 101. Yekaterinburg, 620016. Russia. Phone: +7 (343) 232-90-72. E-mail: fom55@mail.ru

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*Supervising author; +Corresponding author

Keywords: structural transitions, hexagonal tulium manganite, мechanical activation, X-ray analysis, thermogravimetry.

Abstract

Structural transitions in the hexagonal tulium manganite have been studied by methods of high temperature X-ray diffraction and thermal analysis. The following structural transition are found in macrocrystalline and mechanical activated samples: Jahn-Teller transition in a orthorhombic phase in the range of temperatures 900-970 °C, a transition in a hexagonal phase from structural modification of $P6_3cm$ into $P6_3/mms$ at 1092 °C. Mechanical activation reduces Jahn-Teller transition temperature but does not affect the hexagonal phase transition temperature.

Full Paper *Thematic Section:* Research of the New Processes.
Registration Code of Publication: 15-44-10-30 *Subsection:* Inorganic Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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Thematic direction: Disposal of chromium-containing wastewater. Part 3.

The nature of periodic concentration fluctuations of chromium(VI) when restoring steel shavings

© **Konstantin K. Fazlutdinov**,[1,2]* **Vyacheslav Ph. Markov**,[1,3]
Andrey V. Gorohov,[1,2] and **Larisa N. Maskayeva**[1,3+]
[1] *Department of Physical and Colloid Chemistry. Institute of Chemistry and Technology.*
Ural Federal University named after the First President of Russia B.N. Yeltsin. Mira St., 19.
Yekaterinburg, 620002. Russia. Phone: +7 (343) 375-93-18. E-mail: mln@ural.ru
[2] *Electrochemistry, LTD. Novosvetlovka Plant. Industrial Zone. Building РСЦ, liter ЖЖЖ, POBox 225.*
Ekaterinburg, 620078. Russia.
[3] *Department of Combustion Chemistry and Processes. Ural Institute of State Fire Service*
of the Ministry of Emergency Situations of Russia. Mira St., 22. Yekaterinburg, 620062. Russia.
Phone: +7 (343) 360-81-68.

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*Supervising author; [+]Corresponding author

Keywords: recovery of chromium(VI), chemical kinetics, periodic concentration fluctuations, phase foygerite, layered double hydroxides, waste disposal, electroplating.

Abstract

The experimental data describing the periodic concentration fluctuations in the reaction mixture of six - and trivalent chromium during the process of recovery of Cr(VI) in sulfuric acid solutions of steel shavings. The dependence of the frequency of oscillation and frequency of changes in the concentration of Cr(VI) in the volume of the reaction mixture from temperature, initial content of chromium trioxide, sulfuric acid and hitch steel wool are revealed. Concentration fluctuations of reduced chromium Cr(III) forms are coincided in their early-phase with the oscillations in the concentration of Cr(VI) in solution, but greatly inferior in magnitude. The nature of fluctuations in the concentrations of Cr in the studied process is proposed to explain the cyclic nature of the processes of passivation and depassivation of the surface of the chip based education in the subsurface area and the degradation due to outgassing of chromiferous double hydroxides $Fe^{II}_{y}Fe^{III}_{x}(OH)_{3x+2y-2z}(CrO_4)_z$ with the structure of foygerite.

Full Paper ____________________________________ *Thematic Section:* Research of the New Processes.
Registration Code of Publication: 15-44-10-40 *Subsection:* Inorganic Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/ *(English Preprint)*
Contributed: September 10, 2015.

Thematic division: Hydrochemical synthesis of metal chalcogenides films. Part 27.

Influence of iodine-containing addition on composition, morphology and structure of PbSe thin films

© **Victoria M. Yurk**,[1] **Larisa N. Maskaeva**,[1,2+] **Vyacheslav F. Markov**,[1,2*]
Zulfia M. Ibragimova, **Victoria S. Ustyugova**, and **Elena I. Stepanovsky**
[1] *Physical and Colloidal Chemistry Department. The Ural Federal University of a name of the First President of Russia B.N. Yeltsin. Mira St., 19. Ekaterinburg, 620002. Sverdlovsk Region. Russia.*
Phone: +7 (343) 375-93-18. E-mail: mln@ural.ru
[2] *Chemistry and Burning Processes Department. Ural Institute GPS of the Ministry of Emergency Measures of Russia. Mira St., 22. Ekaterinburg, 620022. Russia. Phone: +7 (343) 360-81-68*

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*Supervising author; +Corresponding author

Keywords: chemical bath deposition, thin films, lead selenide, iodine doping.

Abstract

Influence of iodine addition on elemental composition, structure and surface morphology on lead selenide thin films prepared by chemical bath deposition method was studied by methods of X-ray diffraction analysis and scanning electron microscopy with elemental energy-dispersive analysis. Content of iodine in thin films raised to 4.25 at. % with increasing concentration of ammonium iodide in bath solution. Influence of iodine dopant on lattice constant and crystallite size of lead selenide thin films was found.

Thematic Section: Thermodynamic Research. **Full Paper**
Subsection: Physical Chemistry. *Registration Code of Publication:* 15-44-10-45
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/ *(English Preprint)*
Contributed: September 03, 2015.

The recurrent method to define various sets of clusters and cluster size distribution in the system consisting of finite number of particles

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

Keywords: system with finite number of atoms or molecules, finite system, isolated system, isothermal system, cluster, nanoparticle, cluster size distribution function, thermodynamic equilibrium.

Abstract

The system consisting of finite number of identical particles (atoms and molecules) is considered. The recurrent method to define various sets of clusters consisting of the particles is find. Various sets of clusters are defined for systems consisting of from 1 to 13 particles. Cluster size distribution is defined for these systems. It is shown that the dependence of the cluster appearance probability on the cluster size to the number of particles in the system is weakly depend on the number of particles in the system for the systems with the number of particles greater than ten, and the dependence is rapidly decreased with the increasing of the number of particles in the system.

Full Paper ____ *Thematic Section:* Thermodynamic Research.
Registration Code of Publication: 15-44-10-64 *Subsection:* Physical Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/ *(English Preprint)*
Contributed: September 01, 2015.

About the relation between the critical compressibility factor and maximal size of clusters at the critical point

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

***Keywords**:* cluster, liquid, gas, solid body, crystal, lattice, coordination number, first order phase transition, critical point, critical compressibility factor, cluster model of substance, equation of state, virial coefficient, phase equilibrium, melting.

Abstract

The model of ideal gas of clusters with various number of atoms or molecules of one-component substance is considered. It is shown that the compressibility factor of the gas is inversely proportional to the mean size of clusters. This relation is valid with a good accuracy for many substances. It is shown that the number of clusters in the unite volume does not depend on the number of atoms or molecules in the cluster and it is not equal to zero only up to maximal size of clusters. The formula to define critical compressibility factor via maximal size of clusters is found. It is shown that the formula describes critical factor of compressibility of many of one-component substances with experimental accuracy. The formula to define the value of the triple point temperature via densities and surface tensions of liquid and solid at the triple point temperature is found. The formulae to define the temperature dependencies of compressibility factor at the lines of liquid-gas and solid-gas phase equilibria are found. It is shown that the spinodal lines – boundary lines of thermodynamic stability – of metastable vapor and sublimating ideal gas of clusters do not exist or they coincide with corresponding lines of phase equilibria. The formulae to define the lines of vapor-liquid and gas-solid phase equilibria are found. The temperature dependencies of change of the entropy and the latent heat in liquid-gas and solid-gas phase transitions are found. The change of the entropy and the latent heat in liquid-solid phase transition at the triple point are found.

Full Paper ____ *Thematic Section:* Thermodynamic Research.
Registration Code of Publication: 15-44-10-76 *Subsection:* Physical Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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Contributed: August 27, 2015.

Derivation of the formula of Timmermance-Filippov from the generalized Putilov's equation of state

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

Keywords: critical point, liquid-gas phase transition, critical volume, equation of state, formula of Timmermanse-Filippov, pair interaction potential, cold pressure.

Abstract

The formula of Timmermance-Filippov – the equality of critical factor of compressibility of gas-liquid phase transition to the ratio of densities of substance at the critical point and at the zero temperature and pressure – is derived from the generalized Putilov's equation of state. It is shown that the formula is valid for arbitrary temperature dependences of the parameters of the generalized Putilov's equation of state. The formulas are found to define critical parameters using cold pressure and its first and second volume derivatives.

Full Paper ____ *Thematic Section:* Thermodynamic Research.
Registration Code of Publication: 15-44-10-84 *Subsection:* Physical Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/ *(English Preprint)*
Contributed: September 16, 2015.

The method to define the critical compressibility factor of one-component substance using Boyle temperature and the low temperature parameters of liquid

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

***Keywords**:* critical point, gas-liquid phase transition, critical volume, Boyle temperature, ideal curve, line of unite compressibility, rectilinear diameter law, formula of Timmermans-Filippov, critical pressure, equation of state, Van-der-Waals.

Abstract

The relation between the compressibility factor and temperature at the critical point of the gas-liquid phase transition of one-component substance and the Boyle temperature is obtained on the basis of the Van-der-Waals equation of state. It is shown that the relation is valid with a good accuracy for many substances. It is shown that the Van-der-Waals equation of state is useful to obtain the new relations between thermodynamic parameters.

Full Paper ____ *Thematic Section:* Thermodynamic Research.
Registration Code of Publication: 15-44-10-92 *Subsection:* Physical Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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Contributed: September 13, 2015.

About some consequences from the virial equation of state

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

Keywords: *virial coefficient, critical point, gas-liquid phase transition, critical volume, critical temperature, equation of state.*

Abstract

It is shown that the virial equation of state taking into account only first, second and third virial coefficients gives the relation between values of pressure, temperature and second virial coefficient at the critical point that is valid for many real substances. It is also shown that the additional conditions of equalities to zero of the third and fourth partial derivatives of the pressure with respect to volume at constant temperature at critical point give considerable improvement of the predictions of the virial equation of state for critical point.

Full Paper *Thematic Section:* Thermodynamic Research.
Registration Code of Publication: 15-44-10-98 *Subsection:* Physical Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/ *(English Preprint)*
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About some consequences from the Van-der-Waals equation of state for critical point of liquid-gas phase transition

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

Keywords: critical point, gas-liquid phase transition, critical volume, Boyle temperature, ideal curve, line of unite compressibility, rectilinear diameter law, critical pressure, equation of state, Van-der-Waals.

Abstract

The relations to define critical parameters of gas-liquid phase transition of one-component substance is obtained from the Van-der-Waals equation of state. The relation to define the critical volume using the critical temperature is obtained. The relation to define the critical volume using ratio of the critical pressure and the critical temperature is obtained. The relation to define the critical volume using critical pressure is obtained. The consequences are obtained from the Van-der-Waals equation of state of one-component substance for which the formula of Timmermans relating critical parameters with the density of crystal at low temperatures is valid. It is shown that the Van-der-Waals equation of state gives relations between critical parameters and low temperature properties of liquid and also between critical parameters and Boyle temperature. The relation between critical parameters, Boyle temperature and Boyle volume is established. The relation between critical parameters and the value of the third virial coefficient at the critical temperature is also established. The relation between critical parameters and the substance dependent parameter of the rectilinear diameter law is established.

Full Paper ____ *Thematic Section:* Thermodynamic Research.
Registration Code of Publication: 15-44-10-104 *Subsection:* Physical Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/ *(English Preprint)*
Contributed: August 26, 2015.

Linear dependence of the square of radius of coordination sphere of crystal on the order number of coordination sphere

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

Keywords: crystal, coordination number, simple cubic lattice, bode centered cubic lattice, face centered cubic lattice, hexagonal close packing, packing of diamond, tetrahedral packing, lattice of hexagonal ice, lattice of β-tungsten, quasi-crystalline model.

Abstract

It is shown that the dependence on the order number of coordination sphere of the square of the radius of coordination sphere of simple, bode centered and face centered cubic lattices, crystals with hexagonal close packing, packing of diamond, tetrahedral packing, lattice of hexagonal ice , lattice of β – tungsten can be described with good accuracy by linear function. On the basis of this dependence is established that order number of first vanishing peak of the radial distribution function of crystal is inverse proportional to the temperature.

Thematic Section: Thermodynamic Research. **Full Paper**
Subsection: Physical Chemistry. *Registration Code of Publication:* 15-44-10-109
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/ *(English Preprint)*
Contributed: September 18, 2015.

The Van-der-Waals equation of state with temperature dependent parameters to describe the lines of liquid-gas, solid-gas and liquid-solid phase

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

Keywords: line of phase equilibrium, critical point, first order phase transition, critical volume, Van-der-Waals equation of state, bimodal line.

Abstract

The Van-der-Waals equation of state with temperature dependent parameters is considered. It is shown that the line of phase equilibrium can be described using the Van-der-Waals equation of states with temperature dependent parameters. The parameters are defined via temperature dependencies of the phases which are in thermodynamic state of phase equilibrium.

Full Paper *Thematic Section:* Thermodynamic Research.
Registration Code of Publication: 15-44-10-114 *Subsection:* Physical Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/ *(English Preprint)*
Contributed: September 10, 2015.

The relation between the critical and Boyle temperatures of one-component substance. The relation between the critical and Boyle volumes.

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

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

Abstract

The linear relation between the critical temperature of the gas-liquid phase transition of one-component substance and Boyle temperature is obtained on the basis of the Van-der-Waals equation of states. The linear relation between the critical and Boyle volumes is also obtained. It is shown that the relations are valid with a good accuracy for many substances.

Full Paper ____ *Thematic Section:* Thermodynamic Research.
Registration Code of Publication: 15-44-10-118 *Subsection:* Physical Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/ *(English Preprint)*
Contributed: September 13, 2015.

The method to define critical volume of one-component substance using Boyle temperature and critical pressure

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

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

Abstract

The relation between the values of volume and pressure at the critical point of the gas-liquid phase transition of one-component substance and Boyle temperature is obtained on the basis of the Van-der-Waals equation of states. It is shown that the relation is valid with a good accuracy for many substances.

Full Paper _______________ *Thematic Section:* Preparative Research.
Registration Code of Publication: 15-44-10-122 *Subsection:* Supramolecular Chemistry.
Publication is available for discussion within the functioning of the permanent internet-
Conference "New methods of synthesis, structure and application of organoelemental compounds"
http://butlerov.com/synthesys/ *(English Preprint)*
Contributed: August 28, 2015.

Tris(1-amino)triphosphonates based on tris(2-aminoethyl)amine: modeling complexes with proteinogenic amino acids

© **Konstanin V. Shabalin**, **Olga A. Mostovaya**,
Maya V. Adelshina, and **Ivan I. Stoikov**
Organic Chemistry Department. A.M. Butlerov Chemical Institute.
Kazan (Volga Region) Federal University. Kremlevskaya St., 18. Kazan, 420008. Russia.
Phone: +7 (843) 233-74-62. E-mail: ivan.stoikov@mail.ru

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*Supervising author; +Corresponding author

Keywords: aminophosphonates, "host-guest" complexes, quantum-chemical modeling.

Abstract

The modeling of complexes of tris(1-amino)triphosphonates based on tris(2-aminoethyl)amine was carried out. The regularities of the influence of substituents at the α-carbon on the energy of stabilization and geometry of the complexes formed was determined. The binding sites which responsible for the molecular recognition between tris(1-amino) triphosphonate and α-amino acids were identified.

Full Paper ____ *Thematic Section:* Preparative Research.
Registration Code of Publication: 15-44-10-128 *Subsection:* Organic Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/ *(English Preprint)*
Contributed: September 19, 2015.

1,3-Dioxolan in the synthesis 4,4'-bis(arylmethylidene)difenilmetana and substituted 3,4-dihydroquinazolines

© **Victoria V. Esenbaeva**, **Lydia***+ **P. Yunnikova**,
George N. Nikonov, and **Irina D. Akimova**
[1] *Perm State Agricultural Academy named after Academician D.N. Pryanishnikov. Petropavlovskaya St., 23. Perm, Russia, 614990. Perm Krai. Russia. E-mail: yunnikova@yahoo.com*
[2] *Eigenchem Technologies Inc., Biotecnhology Sid Martin Incubator, University of Florida. 12085, Research Drive, Suite 141, Alachua, Florida, 32615.*

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*Supervising author; +Corresponding author

Keywords: amines, imine, 1,3-dioxolane; 4,4'-bis(arylmethylidene)diphenylmethane, 3,4-dihydroquinazolin.

Abstract

The interaction of 1,3-dioxolane with imines having a substituent in the *ortho*-, *meta*- or *para*-position of the aldehyde fragment leads to the formation of 4,4'-bis(arylmethylidene)diphenylmethans. Imines having the substituents at the *para*-position of the aniline fragment, at interaction with the 1,3-dioxolane forms a substituted 3,4-dihydroquinazolin.

Full Paper *Thematic Section:* Preparative Research.
Registration Code of Publication: 15-44-10-132 *Subsection:* Organic Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/ *(English Preprint)*
Contributed: September 5, 2015.

Synthesis and photophysical properties difluoroborate complexes of 2-(2'-hydroxyphenyl)-3*H*-quinazoline-4-ones

© **Emilia V. Nosova**,[1+] **Tatiana N. Moshkina**,[1]
Galina N. Lipunova,[2] and **Valery N. Charushin**[1,2]*
[1] *Ural Federal University named after the Frst President of Russia B.N. Yeltsin.*
Mira St., 19. Ekaterinburg, 620002. Russia. Phone: +7 (343) 375-45-01. E-mail: emily74@rambler.ru
[2] *Institute of Organic Synthesis named. I.J. Postovskogo of the UB RAS. Ul. S. Kovalevskaya, 22.*
Ekaterinburg, 620137. Russia. Phone: (343) 362-30-65. E-mail: lipunova@ios.uran.ru

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*Supervising author; [+]Corresponding author

Keywords: *N,O*-bidentate ligands, BF_2 complexes of 2-(2'-hydroxyphenyl)-3*H*-hinzelin-4-one, photophysical properties, fluorescence.

Abstract

The synthesis of new derivatives of 2-(2'-hydroxyphenyl)-3*H*-quinazoline-4-ones were carried out and obtained its BF_2 complexes. Coordination compounds characterized by the data of ^{1}H, ^{19}F, ^{11}B NMR spectroscopy and mass spectrometry. The fluorescence of the complexes in acetonitrile solution was investigated and presented data on the effect of substituents in the phenol fragment on photophysical properties.

Short Communication *Thematic Section:* Preparative Research.
Registration Code of Publication: 15-44-10-136 *Subsection:* Organic Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/ *(English Preprint)*
Contributed: September 14, 2015.

Synthesis and the relationship between structure and antihypoxic activity of 5-aril-4-benzoil-3-hydroxy-1-[2-(2-hydroxyetoxy)ethyl]-3-pirrolin-2-ones

© **Sergey N. Rogachyov**,+ **Alexandra A. Bobyleva**, **Natalia A. Alikina**,
Danila Y. Apushkin, **Genrikh A. Gartman**, and **Vladimir L. Geyn***
GBOU VPO "Perm State Academy of Pharmacy". Polevaya St., 2.
Perm, 614090. Russia. Phone: +7 (342) 236-90-50. E-mail: rogachevsergei@mail.ru

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*Supervising author; +Corresponding author

Keywords: 5-aryl-4-benzoyl-3-hydroxy-1-[2-(2-hydroxyethoxy)ethyl]-3-pyrroline-2-ones, synthesis, and hemic normobaric hypoxia.

Abstract

The number of compounds of 5-aryl-4-benzoyl-3-hydroxy-1-[2-(2-hydroxyethoxy) ethyl] -3-pyrroline-2-ones was obtained by using preparative techniques. The structures of the compounds has been demonstrated by using IR and ^{1}H NMR spectroscopy.

The antihypoxic activity of the synthesized compounds has been studied by methods normobaric and hemic hypoxia. The relationship between the structure of compounds and their antihypoxic activity have been detected.

Thematic Section: Biochemical Research. **Full Paper**
Subsection: Chemical Composition of Cyanobacteria. *Registration Code of Publication:* 15-44-10-139
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/ *(English Preprint)*
Contributed: April 28, 2015.

Concentration of chemical elements in the cells of cyanobacteria on hydrothermal areas of Kamchatka

© **Valery N. Zelenkov**,[1]* **Vadim V. Potapov**,[2] and **Michael V. Markov**[3]
[1] *All Russian Research Institute of RAS. Vereya Vilage. District Ramenskoye. Moscow Region. Russia.*
Phone: +7 (8910) 451-37-45. E-mail: zelenkov-raen@mail.ru
[2] *Research Geological-Technological Center, RAS. Petropavlovsk-Kamchatsky. Russia.*
[3] *Moskow State Pedagogical University. Moscow. Russia.*

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*Supervising author; +Corresponding author

Keywords: high concentration, cells of cyanobacteria, chemical elements, hydrothermal waters.

Abstracts

In this work the data obtained based on data of RANS on Kamchatka expeditions during the period 2002-2005. The authors investigated the element composition of thermal waters and specimen cyanobacteria in the thermal springs. The authors divided the chemical elements according to the degree of concentration of cells of cyanobacteria. It is shown that for iron, calcium, aluminum, magnesium, silicon, boron, marganeca, germany, phosphorus is the high concentration of cyanobacteria. The authors experimentally revealed fact giperkoncentrirovaniâ of chemical elements by cells of cyanobacteria in the hydrothermal waters of Kamchatka. The authors experimentally revealed a high degree of concentration of chemical elements in the cells of cyanobacteria in the hydrothermal waters of Kamchatka.

Short Communication ____________________________________ *Thematic Section:* Biochemical Research.
Registration Code of Publication: 15-44-10-146 *Subsection:* Antioxidant Properties of Biological Raw.
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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Contributed: September 26, 2015.

Ascorbic acid and stabilization of phenolic compounds in water-alcohol extraction of amaranth in the manufacture of fish products

© **Anatoly A. Lapin**,*+ **Valery N. Zelenkov**,[1]
Laysan R. Akhmerova, and **Aliya A. Islyamova**
Department of "Water Bioresources and Aquaculture." Kazan State Power Engineering University.
Krasnoselskaya St., 51. Kazan, 420066. Tatarstan. Russia.
Phone: +7 (843) 519-43-53. E-mail: lapinanatol@mail.ru
[1] *All-Russian Research Institute of Vegetable Growing, Vereya Vilage. Moscow Region. Russia*

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*Supervising author; +Corresponding author

Keywords: amaranth, ascorbic acid, antioxidant activity, phenolic compound.

Abstract

Amaranth is characterized by the presence of a large variety of antioxidants, including phenolic compounds. In the work it is shown that the Ascorbic acid for stabilization of phenolic compounds of amaranth in formulating biologically active raw material to produce nutritional supplements in a segment of the world market of food.

Thematic Section: Analytical Research. **Full Paper**
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Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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Development and validation of analytical methods for quality control of active pharmaceutical substance Lamivudine

© **Svetlana A. Petukhova**, **Valeria N. Veselova**, **Yulia E. Budanova**, and **Sergey A. Ivanovsky***+
Department of Organic and Inorganic Chemistry. Yaroslavl State Pedagogical University
named after K.D. Ushinsky. Respublikanskaja St., 108. Yaroslavl, 150000. Russia.
Phone: +7 (8452) 73-15-29. E-mail: s.petukhova@yspu.org

*Supervising author; +Corresponding author

Keywords: lamivudine, validation.

Abstract

Developed analytical methods of quality control of the active pharmaceutical substance Lamivudine on indicators: chromatographic purity and enantiomeric purity. The validation of methods was performed and the suitability of its using for the quality control of APS was confirmed. Appropriate sections of the draft monograph were prepared. On the basis of the validation report appropriate section of the registration dossier was made.

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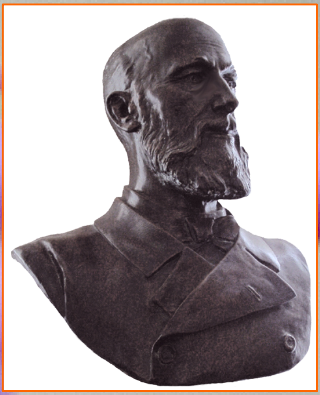

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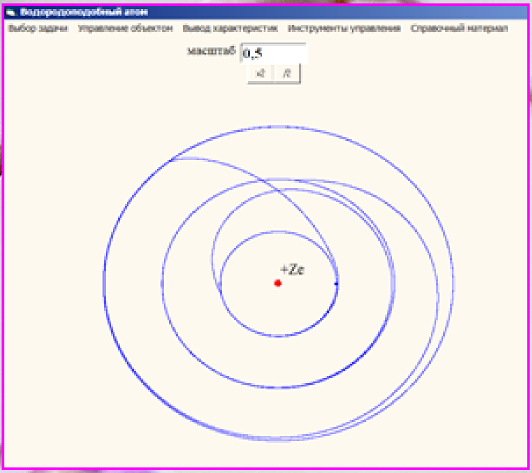

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Thematic Section: Theoretical Research. **Full Paper**
Subsection: Theory of Structure of Matter. *Registration Code of Publication:* 15-44-11-1
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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Planetary model of the hydrogen atom and hydrogen-like structures

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

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*Supervising author; +Corresponding author

Keywords: hydrogen atom, electron, potential and kinetic energy, resistance, electron capture.

Abstract

The article discusses planetary model of Rutherford-Bohr in the application to the hydrogen atom and hydrogen-like structures. The basis of the theory has been based on the laws of conservation of energy and momentum of an amount of movement. The discrete nature of the optical spectrum of the hydrogen atom has been described. The mechanism of electron capture by the nucleus of an atom has been proposed. The program for computer modeling has been developed. The examples of computer research presented for the hydrogen atom and hydrogen-like of cations.

Full Paper *Thematic Section:* Thermodynamic Research.
Registration Code of Publication: 15-44-11-16 *Subsection:* Physical Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/ *(English Preprint)*
Contributed: October 30, 2015.

Van-der-Waals equation of state, second virial coefficient, interaction potential and the minimum condition of free energy

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

***Keywords**:* equation of state, line of unite compressibility (zeno-line), ideal curve, second virial coefficient, interaction potential, polar molecule, free energy.

Abstract

The modified Van-der-Waals equation of state is obtained using the minimum condition of the free energy. It is shown that the Van-der-Waals equation of state can describe the properties of substance near line where the factor of compressibility is equal two number one. It is shown that the parameter of the Van-der-Waals equation of state that is usually considered as parameter of attractive forces can actually include the part of repulsive forces. The integral equations for the interaction potential are obtained using condition of minimum of free energy that is a function of one of two related with each other parameters of the Van-der-Waals equation of state. One- and two-temperature expansions with coefficients that are defined via interaction potential are theoretically obtained for the second virial coefficient.

Thematic Section: Thermodynamic Research. **Full Paper**
Subsection: Physical Chemistry. *Registration Code of Publication:* 15-44-11-29
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/ *(English Preprint)*
Contributed: October 07, 2015.

Thematic direction: About some consequences from the virial equation of state. Part 2.

Definition of the critical parameters from second and third virial coefficients

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

Keywords: virial coefficient, critical point, liquid-gas phase transition, critical volume, critical temperature, critical pressure, equation of state.

Abstract

It is shown that the virial equation of state gives the relations between temperature, pressure, volume and second and third virial coefficients at the critical point of liquid-gas phase transition of one-component substance. It is shown that the critical values of pressure, temperature and volume can be defined with good accuracy using relations. The relation between temperature, pressure and second virial coefficient at the critical point is find that gives the values of critical pressure for 17 various substances with accuracy equal to 5% . The values of critical temperature for 17 various substances with accuracy equal to 4% can be obtained using the relation between second and third virial coefficients at the critical point if the experimental (or simulated) temperature dependences of second and third virial coefficients are known. The relations obtained can be used to determine the critical parameters of substances.

Full Paper ____ *Thematic Section:* Thermodynamic Research.
Registration Code of Publication: 15-44-11-44 *Subsection:* Physical Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference “*Butlerov readings*”.
http://butlerov.com/readings/ *(English Preprint)*
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Derivation of the Van-der-Waals equation of state from classical equilibrium statistical mechanics of two particle system

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

Keywords: potential of London, hard spheres, equilibrium, Van-der-Waals equation of state, isothermal system, partition function, finite system of particles.

Abstract

Two particle system in the spherical volume is considered in the framework of classical equilibrium statistical mechanics. Interaction potential of particle with the wall of the spherical volume is equal to hard sphere potential. It is shown that Van-der-Waals equation of state can be obtained approximately for two particles interacting via potential of London if the center of mass of the particles is fixed at the center of spherical volume.

Thematic Section: Preparative Research. **Full Paper**
Subsection: Nanochemistry. *Registration Code of Publication:* 15-44-11-49
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Sonochemical synthesis of nanocomposites MnO_2/C

© **Nadezhda V. Pechishcheva**,[1] **Svetlana Khusainovna Estemirova**,[2]*+
Galina A. Kozhina,[2,3] **Konstantin Yu. Shunyaev**,[1] and **Maria Yu. Skrylnik**[1]
[1] *Laboratory of Analytical Chemistry;* [2] *Laboratory of Statics and Kinetics of Processes. Federal State Institution of Science Institute of Metallurgy UB RAS. Amundsen St., 101. Ekaterinburg, 620016. Russia.*
[3] *Ural State University of Economics. 8th March St., 62. Ekaterinburg, 620144. Sverdlovsk region. Russia.*
Phone: +7 (8434) 232-90-40. E-mail: k_shun@mail.ru, esveta100@mail.ru

*Supervising author; +Corresponding author

Keywords: sonochemical synthesis, carbon materials, mechanical activation, nanocomposites.

Abstract

Nanocomposites MnO_2/C were obtained by two methods, both of which included an ultrasonic impact and did not involve chemically active substances. The first method was conducted in a single stage; activated charcoal BAU-A served as a matrix material. Sonochemical synthesis of nanocomposites based on spectrally pure graphite (the second method) required its modifications realized by mechanical activation. According to X-ray data all synthesized composites were nanocrystalline and contained two phases – manganese oxide(IV) and carbon. The average crystallite size of MnO_2 adsorbed on the porous structure of the carbon materials was about 5 nm.

Thematic Section: Preparative Research. **Full Paper**
Subsection: Nanochemistry. *Registration Code of Publication:* 15-44-11-55
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Obtaining of nickel and cobalt nanostructured oxides

© **Polina V. Lapsina**,[1+] **Evgeny I. Kagakin**,[2]* **Anna N. Popova**,[1] and **Vadim G. Dodonov**[3]
[1] *Kemerovo Scientific Center SB RAS. Soviet pr., 18. Kemerovo, 650000. Russia.*
Phone: +7 (923) 608-0271. E-mail: lpv110185@rambler.ru
[2] *Chemical Engineering and Environment Solid Fuel Department. T.F. Gorbachev Kuzbass State Technical University. Vesennyaya St., 28. Kemerovo, 650000. Russia. E-mail: kagakin55@mail.ru*
[3] *Chemistry of Solids Department. Kemerovo State University. Krasnaya St., 6.*
Kemerovo, 650043. Russia. E-mail: 233191@mail.ru

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*Supervising author; +Corresponding author

Keywords: nanostructured powders, nickel oxide, cobalt oxide.

Abstract

The synthesis of nickel and cobalt nanostructured oxides from nanostructured metal powders is proposed. The morphology and phase structure of obtained nanostructured oxides is considered by mean of XRD-analysis and scanning electron microscopy (SEM). It is found that the oxides have a size comparable with the size of corresponding metal precursors.

Full Paper ____ *Thematic Section:* Preparative Research.
Registration Code of Publication: 15-44-11-60 *Subsection:* Nanochemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/ *(English Preprint)*
Contributed: October 19, 2015.

Synthesis of silver nanoparticles by borohydride method and determination of they size by photon correlation spectroscopy

© **Vladimir V. Kuznetsov**,*[+] **Veronica V. Smagina**,* **Alexander F. Krivoschepov**,*
Grigory V. Avramenko,* and **Svetlana P. Katuleva**
D. Mendeleev University of Chemical Technology of Russia. Panfilov Heroes St., 20.
Moscow, 125480. Russia. Phone: +7 (962) 964-91-68. E-mail: vladimir19927@yandex.ru

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*Supervising author; [+]Corresponding author

Keywords: silver nanoparticles, sodium borohydride, photon correlation spectroscopy, polyvinylpyrrolidone, poly(4,9-dioxadodecane-1,12-guanidinium) chloride.

Abstract

The article is devoted to obtaining silver nanoparticles by borohydride method using as stabilizer the polyvinylpyrrolidone (PVP), polyvinyl alcohol or poly-(4,9-dioxadodecane-1,12-guanidinium) chloride (PDDG). The size of the silver particles and their change during the time was determined; the influence on this feature of the synthesis conditions and the used stabilizer was evaluated.

It was found that the growth of nanoparticles occur during the time by using PVP, that may be connected with its recovering capability. A promising direction is the use of PDDG chloride that allows obtaining the size of the particles practically unchanged during the time and has the pronounced biocidal properties.

Thematic Section: Preparative Research. **Full Paper**
Subsection: Organic Chemistry. *Registration Code of Publication:* 15-44-11-65
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http://butlerov.com/readings/ *(English Preprint)*
Contributed: November 06, 2015.

Synthesis and biological activity of 2,5-substituted derivatives of 6-hydroxypyrimidine-4(*3H*)-one

© **Anastasia E. Potapova**,+ **Elena V. Kuvaeva**, **Igor P. Yakovlev**,*
Elena V. Fedorova, and **Alexander E. Shchegolev**
Department of Organic Chemistry. St.Petersburg Chemical- Pharmaceutical Academy. Prof. Popov St., 14. Saint-Petersburg, 197376. Russia. Phone: +7 (812) 234-11-72. E-mail: elena.kuvaeva@pharminnotech.com

*Supervising author; +Corresponding author

Keywords: 6-hydroxypyrimidine-4(3*H*)-one, cute toxicity, analgesic activity, anti-inflammatory activity.

Abstract

The series of new 2,5-substituted derivatives of 6-hydroxypyrimidine-4(3*H*)-ones were synthesized. It was established that the reaction rate and the product yield determined by the electronic nature of the substituent in the original amidine hydrochlorides molecules and malonic ester. The derived compounds exhibit a significant analgesic and anti-inflammatory activity.

Thematic Section: Research of the New Technologies. **Full Paper**
Subsection: Organic Chemistry. *Registration Code of Publication:* 15-44-11-69
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http://butlerov.com/readings/ *(English Preprint)*
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Thematic direction: Solid nanoreactor. Part 5.

Polymer nanocontainers for benzocaine

Heinrich N. Altshuler,[1]* **Galina Yu. Shkurenko**,[1+] **Sergey Yu. Lyrschikov**,[2]
Alexey A. Gorlov,[1] and **Olga H. Altshuler**[1]
[1] *Institute of Coal Chemisry and Material Science. Siberian Branch of Russian Academy of Sciences.*
Sovetsky pr., 18. Kemerovo, 650000. Russia.
[2] *Kemerovo Scientific Center. Siberian Branch, Russian Academy of Sciences.*
Sovetsky pr., 18. Kemerovo, 650000. Russia.
Phone: +7 (384-2) 36-80-22. E-mail: altshulerh@gmail.com

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*Supervising author; [+]Corresponding author

Keywords: polymer nanocontainers, immobilized benzocaine, sulfonated polymers.

Abstract

The possibility of immobilization of benzocaine in polymer nanocontainers based on sulfocationites (cationite KU 23 30/100, sulfonated polycalixresorcinarene) has been shown. The Immobilization performedby ion exchange sorption of protonated benzocaine from aqueous solutions. The kineticsofdesorption of neutral molecules and cationsof benzocaine from polymernanocontainers has been investigated.

Thematic Section: Research of the New Technologies. **Full Paper**
Subsection: Colloidal Chemistry. *Registration Code of Publication:* 15-44-11-73
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/ *(English Preprint)*
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Thematic division: Synthesis and research of properties of catalysts of reburning. Part 1.

Influence surfactant on viscous properties of suspension $Pd(NO_3)_2$-Al_2O_3-La_2O_3-HAc-H_2O for afterburning catalysts

© **Alena E. Bezdetnova**,[1] **Vyacheslav F. Markov**[1,2]*
Viktor I. Zelenin,[1] and **Larisa N. Maskaeva**[1,2+]
[1] *Physical and Colloidal Chemistry Department. Ural Federal University named after the first President of Russia B.N. Yeltsin. Mira St., 19. Ekaterinburg, 620002. Sverdlovsk Region. Russia. Phone: +7 (343) 375-93-18. E-mail: mln@ural.ru*
[2] *Chemistry and Burning Processes Department. Ural Institute GPS of the Ministry of Emergency Measures of Russia. Mira St., 22. Ekaterinburg, 620022. Russia. Phone: +7 (343) 360-81-68.*

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*Supervising author; +Corresponding author

Keywords: afterburning catalysts, viscosity, suspensions, ion equilibrium, surface-active substances, palladium(II) nitrate, lanthanum oxide.

Abstract

In system "$Pd(NO_3)_2$ – Al_2O_3 – La_2O_3 – HAc – H_2O" calculation of ion equilibrium with use of thermodynamic constants are determined by boundary conditions of formation of hydroxides of metals Possibility of decrease in dynamic viscosity of the "$Pd(NO_3)_2$ – Al_2O_3 – La_2O_3 – HAc – H_2O", suspension having pH = 3 at addition of 1% of an aqueous solution is experimentally shown cation-active surfactant at 1.74 time: with 850.62 to 488.95 mPa·s. The morphology of particles of suspension before and after the addition in it surfactant cation-active Praestol 655 FC is investigated.

Thematic Section: Research of the New Technologies. **Full Paper**
Subsection: Inorganic Chemistry. *Registration Code of Publication:* 15-44-11-79
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/ *(English Preprint)*
Contributed: October 13, 2015.

Theoretical and experimental studies of the effectiveness of sample preparation methods of non-ferrous metals sulfide raw materials for the determination of the micro- and macro-components by ICP-AES

© **Anna V. Maiorova**,*+ **Nadezhda V. Pechishcheva**, and **Konstantin Yu. Shunyaev**
Institute of Metallurgy UB RAS. Amundsena St., 101. Yekaterinburg, 620016.
Russia. Phone: +7 (343) 267-89-36. E-mail: imeturoran@mail.ru

*Supervising author; +Corresponding author

Keywords: non-ferrous metals sulfide raw materials, polymetallic ore, determination of silver, gold, iron, silicon, sulphur, nickel, cobalt, copper, thermodynamic modeling, inductively coupled plasma atomic emission spectrometry.

Abstract

The efficiency of the sample preparation procedures of non-ferrous metal sulfide raw material for determination of silver, gold, iron, silicon, sulfur, nickel, cobalt, copper by inductively coupled plasma atomic emission spectrometry (ICP-AES) was investigated. Two methods were concidered: acid digestion in a mixture of $HCl:HNO_3$ (3:1) and an fusion with Na_2O_2. Using thermodynamic modeling («HSC» software) shows that at the acidic sample preparation of copper ore with $HCl:HNO_3$ (3: 1) there is loss of one of the target analytes - silicon; fusion with Na_2O_2 prevents loss of analytes. The simulation results of the polymetallic ore sample preparation show similar behavior of the analytes with the exception of sulfur, which in the barium presence forms a $BaSO_4$ precipitate, whereby the sample preparation techniques discussed can not be used for ICP-AES determination of sulfur in barium-containing ores. Experimental studies confirm the obtained theoretical conclusions. Analysis of the certified reference materials showed the effectiveness of proposed methods of sample preparation.

Thematic Section: Research of the New Technologies. **Full Paper**
Subsection: Inorganic Chemistry. *Registration Code of Publication:* 15-44-11-87
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http://butlerov.com/readings/ *(English Preprint)*
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Study on the possibility of measuring the content of nitrosylsulfuric acid in a mixture of acids

© **Nadezhda Yu. Kozlova**,*+ **Alexey I. Harrynov**,* and **Rosa F. Gatina***
[1] *Federal State Enterprise "State Research Institute of Chemical Products". Svetlaya St., 1. Kazan, 420033. Tatarstan. Russia. E-mail: kozlova_nadezhda_2014@mail.ru.*
[2] *Department of Technology of Inorganic Substances. Kazan National Research Technological University. K. Marx St., 68. Kazan, 420015. Tatarstan. Russia.*

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*Supervising author; +Corresponding author

Keywords: nitrate, a mixture of nitric and sulfuric acids, potentiometric titration, nitrogylcerin acid.

Abstract

The investigations of solutions of mixtures of nitric and sulfuric acids in the concentration range of HNO_3 20-23%, H_2SO_4 50-65%, H_2O-10-20% were curried out. It is shown that the interaction of nitric and sulfuric acids, a mixture of nitrosylsulfuric acid is formed. The process of formation of the nitrosylsulfuric acid finished in one day after preparation of the mixtures. By potentiometric titration it is possible to determine nitrosylsulfuric acid in mixtures of nitric and sulfuric acids.

Thematic Section: Research of the New Technologies. **Full Paper**
Subsection: Radiochemistry. *Registration Code of Publication:* 15-44-11-91
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http://butlerov.com/readings/ *(English Preprint)*
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The characteristic of lignocellulosic materials as radionuclides sorbents

© **Ludmila S. Kocheva**,[1] **Anatoly P. Karmanov**,[2]*+
Ida I. Shuktomova,[3] **Natalia G. Rachkova**,[3] and **Olga B. Kotova**[4]
[1] *Chemistry Mineral Raw Material Laboratory. Institute of Geology, Komi Scientific Center, Ural Division, Russian Academy of Sciences. Pervomajskaja St., 54. Syktyvkar, 167982. Komi Republik. Russia. Phone: +7 (8212) 24-54-16. E-mail: lskocheva@geo.komisc.ru*
[2] *Biochemistry and Biotechnology Laboratory. Institute of Biology, Komi Scientific Center, Ural Division, Russian Academy of Sciences. Kommunisticheskaja St., 28. Syktyvkar, 167982. Komi Republik. Russia. Phone:+7 (909) 120-81-63. E-mail: apk0948@ib.komisc.ru*
[3] *Radionuclides migration and radiochemistry Laboratory. Institute of Biology, Komi Scientific Center, Ural Division, Russian Academy of Sciences. Kommunisticheskaja St., 28. Syktyvkar, 167982. Komi Republik. Russia. Phone: +7 (8212) 24-01-63. E-mail: shuktomovaii@ib.komisc.ru*
[4] *Technology Mineral Raw Material Laboratory. Institute of Geology, Komi Scientific Center, Ural Division, Russian Academy of Sciences. Pervomajskaja St., 54. Syktyvkar, 167982. Komi Republik. Russia. Phone: +7 (8212) 24-51-60. E-mail: kotova@geo.komisc.ru*

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*Supervising author; +Corresponding author

Keywords: lignocellulosic materials, sorbtion, radionuclides, uranium, radium, thorium.

Abstract

The results of research of straw oats and rye lignocellulosic materials were presented. The principled opportunity of creation on its basis of universal radionuclide's sorbents was illustrated. It is shown the perspectivity of lignocellulosic sorbents's use for cleaning of water environments contaminated with long-lived radioactive isotopes U^{238}, Ra^{226} and Th^{232}.

Thematic Section: Biochemical Research. **Full Paper**
Subsection: Biochemistry. *Registration Code of Publication:* 15-44-11-97
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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Thematic direction: The possibilities of application of eichornia in the purification of the waters of pulp and paper mill. Part 1.

The specificity of chemical composition of the water in the Volga reach of the Kuibyshev reservoir

© **Marina L. Kalayda**, and **Madina F. Khamitova**
Department of "Water Bioresources and Aquaculture". Kazan State Power Engineering University.
Krasnoselskayast St., 51. Kazan, 420066. Tatarstan. Russia.
Phone: +7 (843) 519-43-53. E-mail: kalayda@mi.ru

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*Supervising author; +Corresponding author

Keywords: environmental pollution, Kuibyshev reservoir, waste water, heavy metals, X-ray fluorescence analysis, concentrations of pollutants.

Abstract

The chemical composition of the water in the area Lopatinskay Volozhka of the Volga reach of the Kuibyshev reservoir. The features of the chemical composition of the water in the areas above the discharge of waste water from the secondary clarifier, below discharge, in place of mixing the waters and in the secondary clarifier of "MTSBK" on the island Lopatinsky of the Kuibyshev Reservoir were studied. Proportion of heavy metals in different conditions shown in a comparative perspective.

Full Paper *Thematic Section:* Biochemical Research.
Registration Code of Publication: 15-44-11-104 *Subsection:* Biochemistry.
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Thematic direction: The possibilities of application of eichornia in the purification of the waters of pulp and paper mill. Part 2.

The specificity of chemical composition of bottom sediments in the Volga reach of the Kuibyshev reservoir

© **Marina L. Kalayda**, and **Madina F. Khamitova**
Department of "Water Bioresources and Aquaculture". Kazan State Power Engineering University.
Krasnoselskayast St., 51. Kazan, 420066. Tatarstan. Russia.
Phone: +7 (843) 519-43-53. E-mail: kalayda@mi.ru

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*Supervising author; $^+$Corresponding author

Keywords: environmental pollution, Kuibyshev reservoir, bottom sediments, heavy metals, X-ray fluorescence analysis, concentrations of pollutants.

Abstract

The chemical composition of the bottom sediments in the area Lopatinskay Volozhka of the Volga reach of the Kuibyshev reservoir. The features of the chemical composition of the bottom sediments in the areas above the discharge of waste water from the secondary clarifier, below discharge, in place of mixing the waters and in the secondary clarifier of Pulp and Paper Mill on the island Lopatinsky of the Kuibyshev Reservoir were studied. Proportion of heavy metals in different conditions shown in a comparative perspective.

Thematic Section: Biochemical Research. **Full Paper**
Subsection: Biochemistry. *Registration Code of Publication:* 15-44-11-113
Publication is available for discussion in the framework of the on-line Internet conference “*Butlerov readings*”.
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Thematic direction: The possibilities of application of eichornia in the purification of the waters of pulp and paper mill. Part 3.

The specificity of chemical composition of *Eichhorniacrassipes*

© **Marina L. Kalayda**, and **Madina F. Khamitova**
Department of "Water Bioresources and Aquaculture". Kazan State Power Engineering University.
Krasnoselskayast St., 51. Kazan, 420066. Tatarstan. Russia.
Phone: +7 (843) 519-43-53. E-mail: kalayda@mi.ru

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*Supervising author; +Corresponding author

Keywords: environmental pollution, Kuibyshev reservoir, waste water, water purification, biohydrobotanical method, aquatic plants, Eyhorniya, heavy metals, X-ray fluorescence analysis.

Abstract

The chemical composition of Eyhorniya contained in the secondary sedimentation tank of pulp and paper mill in the area Lopatinskay Volozhka in the Volga reach of the Kuibyshev reservoir was studied. The peculiarities of accumulation of heavy metals in comparison with other water plants were examined.

Full Paper ____ *Thematic Section:* Biochemical Research.
Registration Code of Publication: 15-44-11-122 *Subsection:* Biochemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/ *(English Preprint)*
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The using of vermiculture in the purification of sewage sludge: heavy metals in sewage sludge of municipal wastewater treatment plants.

© **Marina L. Kalayda**, and **Rail R. Abdullin**
Department of "Water Bioresources and Aquaculture". Kazan State Power Engineering University.
Krasnoselskayast St., 51. Kazan, 420066. Tatarstan. Russia.
Phone: +7 (843) 519-43-53. E-mail: kalayda@mi.ru

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*Supervising author; ⁺Corresponding author

Keywords: sewage sludge, soil, environmental pollution, heavy metals, vermiculture, earthworms, Eisenia foetida, X-ray fluorescence analysis, concentration of the chemical elements.

Abstract

The chemical composition of sewage sludge from municipal wastewater treatment plants in Naberezhnye Chelny and experimental substrates on the basis of sewage sludge and garden soil from Kazan territory, which contained earthworms was studied. The peculiarities of the chemical composition of substrates, in which the cultivation of *Eiseniafoetida* was carried out at varying degrees of humidity were investigated. Highlighted the heavy metals – lead, chromium and zinc, which should be given special attention in biotechnological purification of sewage sludge through vermiculture.

Full Paper *Thematic Section:* Biochemical Research.
Registration Code of Publication: 15-44-11-130 *Subsection:* Biochemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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Biochemical basis of inclusion of worms *Eisenia foetida* into the fish feed as bioadditives

© **Marina L. Kalayda**, and **Rail R. Abdullin**
Department of "Water Bioresources and Aquaculture". Kazan State Power Engineering University.
Krasnoselskayast St., 51. Kazan, 420066. Tatarstan. Russia.
Phone: +7 (843) 519-43-53. E-mail: kalayda@mi.ru

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*Supervising author; $^+$Corresponding author

Keywords: environmental pollution, heavy metals, vermiculture, earthworms, *Eisenia foetida*, X-ray fluorescence analysis, concentration the chemical elements, trace elements in aquaculture, bioadditives for fish food.

Abstract

Peculiarities of the microelement composition of the experimental soil on the basis of wastewater sludge and grown in it earthworms. The possibility of using *Eisenia foetida* in biotechnology of wastewater purification on municipal wastewater treatment plants, and later as bioadditives to fish feed in aquaculture was shown. Peculiarities of the microelement composition of *Eisenia foetida* compared to aquatic organisms were shown.

Full Paper ____ *Thematic Section:* Biochemical Research.
Registration Code of Publication: 15-44-11-136 *Subsection:* Biochemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/ *(English Preprint)*
Contributed: October 06, 2015.

The using of vermiculture in the wastewater sludge purification: the results of cultivation of *Eisenia foetida* in the substrate of wastewater sludge

© **Marina L. Kalayda**, and **Rail R.Abdullin**
Department of "Water Bioresources and Aquaculture". Kazan State Power Engineering University.
Krasnoselskayast St., 51. Kazan, 420066. Tatarstan. Russia.
Phone: +7 (843) 519-43-53. E-mail: kalayda@mi.ru

---

*Supervising author; +Corresponding author

Keywords: soil, sewage sludge, heavy metals, environmental pollution, biotechnology, vermiculture, earthworms, *Eisenia foetida*, X-ray fluorescence analysis, concentration of the chemical elements.

Abstract

The features of the chemical composition of of earthworms *Eisenia foetida*, used in biotechnology of water puruification on municipal wastewater treatment plants were studied. Shown the change in concentration of of heavy metals in the substrate, the worms bodies and its coprolites. Earthworms when cultured in substrates with high concentrations of trace elements and dangerous heavy metals is capable of processing sewage sludge. The highest coefficient of biological absorption is observed for the zinc, the smallest in the lead.

Thematic Section: Biochemical Research. **Full Paper**
Subsection: Biochemistry of Plant. *Registration Code of Publication:* 15-44-11-141
Publication is available for discussion in the framework of the on-line Internet conference "*Chemical basis for the rational use of renewable natural resources*".
(English Preprint) http://butlerov.com/natural_resources/
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The content and composition of carbohydrates from leaves of some species of the genus *Filipendula*

© **Nelly V. Sklyarevskaya**,[*+] **Yulia A. Gladkaya**, and **Sergey V. Tolstikov**
Department of Pharmacognosy. Laboratory of Analytical Methods.
Saint-Peterburg State Chemical Pharmaceutical Academy.
Prof. Popov St., 14. Saint-Peterburg, 197376. Russia.
Phone: +7 (812) 234-43-62. E-mail: nelly.sklyarevskaya@pharminnotech.com

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*Supervising author; [+]Corresponding author

Keywords: monosaccharides, water-soluble polysaccharides, pectins, gas-liquid chromatography, *Filipendula ulmaria*, *Filipendula camtschatica*.

Abstract

Water-soluble polysaccharides and pectins were isolated from leaves of species of the genus *Filipendula – Filipendula ulmaria, Filipendula camtschatica*. Monosaccharide composition of these carbohydrate complexes was investigated by gas-liquid chromatography. Quantity contents of free monosaccharides, water-soluble polysaccharides and pectins in the leaves of *Filipendula ulmaria, Filipendula camtschatica* were determined.

Full Paper ____ *Thematic Section:* Biochemical Research.
Registration Code of Publication: 15-44-11-146 *Subsection:* Molecular biology.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
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Thematic direction: the Polysaccharides of microalgae. Part 1.

General chemical characteristics of extracellular polysaccharides of cyanobacterium *Nostoc muscorum* Ag. ex Born. et Flah.

© **Anatoly A. Shubakov,**[1]*+ **Elena N. Patova**,[2]* **Oksana V. Popeyko,**[1]
Fedor V. Vityazev,[1] and **Elena A. Mikhailova**[1]
[1] *Department of Molecular Immunology and Biotechnology. Federal State Budgetary, Institute of Physiology, Komi Science Centre, The Urals Branch of the Russian Academy of Sciences. Pervomayskaya St., 50. Syktyvkar, 167982. Komi Republic. Russia. Phone: +7 (8212) 241-001.*
E-mail: shubakov@physiol.komisc.ru
[2] *Laboratory of Geobotany and Comparative Floristic. Federal State Budgetary Institution of Science, Institute of Biology, Komi Science Centre, The Urals Branch of the Russian Academy of Sciences. Komunisticheskaya St., 28. Syktyvkar, 167982. Komi Republic. Russia.*

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*Supervising author; +Corresponding author

Keywords**:** polysaccharides, cyanobacteria, *Nostoc muscorum*.

Abstract

For the cyanobacterium *Nostoc muscorum* the general chemical characteristics of polysaccharides isolated from the culture fluid is given. The content glycuronic acids and protein in the extracellular polysaccharides are respectively 22.1 and 7.3%. In the composition of extracellular polysaccharides is dominated by four monosaccharide: mannose (9.0%), galactose (7.9%), glucose (6.9%) and xylose (5.9%).

Thematic Section: Technological Research. **Full Paper**
Subsection: Mathematical modeling. *Registration Code of Publication:* 15-44-11-151
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Mathematical model reator block ethylene glycol production

© **Ramil M. Latyipov**,[1] **Eduard V. Osipov**,[2+] and **Eduard Sh. Telyakov**[2*]
[1] *JSC “TAIF-NK”*
[2] *Department “Mechanical Engineering for Chemical Industry”.*
Kazan National Research Technological University. Karl Marx St., 68. Kazan, 420015.
Tatarstan. Russia. Phone: +7 (843) 231-42-41. E-mail: mahp_kstu@mail.ru

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*Supervising author; +Corresponding author

Keywords: reactor; kinetics of chemical reaction; ethylene glycol; technology of glycol production; hardware design; mathematical modeling; modeling programs.

Abstract

Using modeling program Chemcad created mathematical model of reactor block for glycol production. Model takes into account using equipment (reactors, heat exchangers, pipelines) and was identified by productions dates. Shown the prospects of using model for solution design and optimization problems of high complexity.

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Dynamics of thermo-vacuum-impulsive drying of inert burning construction material

© **Vladimir F. Magakin**,* **Tatiana A. Eneykina**, **Anastasia Yu. Osipova**,
Sergey V. Soldatov,+ **Svetlana Yu. Ignatieva**, and **Rosa F. Gatina**
Federal Sate Enterprise "State Research Institute of Chemical products". Svetlaya St., 1. Kazan, 420033.
Tatarstan. Russia. E-mail:gniihp@bancorp.ru

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*Supervising author; +Corresponding author

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Abstract

The influence of drying regimes of burning hard caps from an inert material (cellulose – polyvinylacetate – aluminum) on the rate of dehumidification was investigated. It is shown that convective drying even at the highest temperature equal to 110 °C is the least effective. It is found that of the four variants of the thermo-vacuum-impulsive drying the highest rate of moisture removal is characteristic for condition of combining thermo-vacuum-impulsive pass of hot fluid (70 °C, the vacuum 5 kPa) through the layer of material for 5 minutes with simultaneous heating of the form heated to the desired temperature. The number of pulses depends on the material moisture. This condition allows to reduce the drying time about in 8 times compared with the staffing process.