



XXII MENDELEEV CONGRESS
ON GENERAL AND APPLIED CHEMISTRY

BOOK OF ABSTRACTS

IN 7 VOLUMES

VOLUME 7

7 — 12.10.2024

Federal Territory "Sirius", Russia



XXII MENDELEEV CONGRESS ON GENERAL AND APPLIED CHEMISTRY

*Dedicated to the 190th anniversary
of D.I. Mendeleev and the 300th anniversary
of the Russian Academy of Sciences*

BOOK OF ABSTRACTS

Volume 7

Book of abstracts in 7 volumes

October 07-12, 2024
Federal Territory "Sirius", Russia

XXII Mendeleev Congress on General and Applied Chemistry, October 7-12, 2024, Federal Territory "Sirius", Russia. Book of abstracts in 7 volumes. Volume 7. — M.: "Buki Vedi" LLC, 2024. — 288 p. — 978-5-00202-679-1 (v. 7)

ISBN 978-5-00202-672-2

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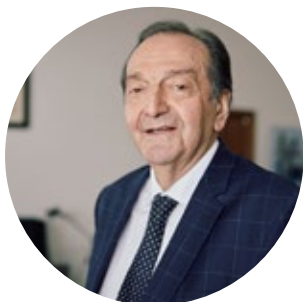
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Section 6

ANALYTICAL CHEMISTRY: NEW METHODS AND TOOLS FOR CHEMICAL RESEARCH AND ANALYSIS

RESEARCH OF THE SOIL PROFILE OF THE VINEYARDS IN THE ANAPA REGION

Abakumov A.G., Gipich E.Y, Abakumov P.G., Temerdashev Z.A.

*Kuban State University,
350040, Krasnodar, Stavropolskaya Street 149,
e-mail: abakumovleks@gmail.com*

The soil has a significant influence on the formation of the chemical composition of plants. The vine selectively absorbs mostly the elements it needs from the soil¹. However, a traceable consistent correlation between the elemental composition from soil to wine has not been revealed. The influence of soil chemical properties on the formation of the elemental composition of different grape varieties is also not entirely clear.

The work studied soil samples taken from the territory of six vineyards of the Anapa region of the Krasnodar Territory. The soil was selected during the ripening period by the envelope method from 8 different depths (0-20 cm, 20-40 cm, 40-60 cm, 60-80 cm, 80-100 cm, 100-120 cm, 120-140 cm, 140-160 cm). The elemental composition of soil samples was determined by inductively coupled plasma atomic emission spectrometry (iCAP 7400, ThermoScientific, USA). The analysis was carried out taking into account the possible forms of metals in the soil: total and mobile. X-ray phase analysis of the studied soils was performed using an X-ray diffractometer (Shimadzu XRD-7000, Japan). Thermal analysis of soils was carried out on the STA-409 PC Luxx derivatograph (Netzsch, Germany).

According to the results of X-ray phase analysis, soil samples were divided into three groups. Thermal analysis has made it possible to evaluate the contents of the main phases (quartz, calcite, hydrosilicates, smectites and zeolites) in the soil samples based on their temperature transformations. Using ICP-spectrometric analysis, it was found that the total contents of elements within the formed groups have great similarity, while there are significant differences between different groups. The contents of the mobile forms of the elements have even greater similarity within the groups. The obtained dependences of the distribution of metals by sampling depth differ for mobile forms and total contents of most elements. With increasing sampling depth within the same form of finding, metals also behave differently.

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This research was founded by the Russian Science Foundation, № 23-13-00056

ESTABLISHING THE RELATIONSHIP BETWEEN THE ELEMENTAL COMPOSITION OF SOIL AND GRAPE

Abakunov A.G., Temerdashev Z.A., Gipich E.Y., Khalafyan A.A.

*Kuban State University,
350040, Krasnodar, Stavropolskaya Street 149,
e-mail: abakumovleks@gmail.com*

Analytical approaches are being developed to control the authenticity of wines on a geographical basis, based, as a rule, on the analysis of the mineral composition of wines, grapes and soils corresponding to the area of vine growth¹. These relationships allow us to establish with high reliability the varietal and geographical origin of wine due to the formation of an elemental “image” characteristic of the grape variety cultivated in a particular territory².

In the work, samples of Cabernet Sauvignon grapes were studied, selected from the territory of six vineyards in the Anapa district of the Krasnodarsky Region. The features of the formation of the elemental image of grapes are considered, taking into account the possible forms of extraction of elements from soils: gross and mobile. The elemental composition was analyzed by inductively coupled plasma atomic emission spectrometry (iCAP 7400, ThermoScientific, USA). To determine the total content of elements in soils and grapes, acid microwave mineralization was performed using a microwave decomposition system (Ethos 1, Milestone, Italy). An extract in an ammonium acetate buffer (pH=4.8) was used to analyze the mobile forms of elements in soils.

To describe the degree of transition of metals from soil to grape, the biological absorption coefficient was used – the ratio of the concentration of metal in the grape to its mobile form in the soil. It has been established that the migration of elements from the soil to the grape is individual for each area of cultivation. The analysis of correlations in the soil-grape system showed that for all regions there is a pattern of decreasing correlation between metal concentrations in grapes and soil as the depth increases both for the mobile form and for the total content of elements. It was found that the greatest correlation between metal concentrations in grapes and soil for all regions is observed at a depth of 0-40 cm, while the correlation is weak and statistically insignificant.

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This research was founded by the Russian Science Foundation, № 23-13-00056

DETERMINATION OF INORGANIC FORMS OF ARSENIC IN DRINKING AND NATURAL WATER

Abakumov P.G., Temerdashev Z.A., Abakumov A.G.

*Kuban State University,
350040, Krasnodar, Stavropolskaya Street 149,
e-mail: pg.abakumov@gmail.com*

In water bodies, arsenic is predominantly in the form of arsenites (As^{III}) and arsenates (As^{V}); extraction methods are often used to separate them^{1,2}. The separation of forms is carried out due to the selective interaction of arsenite ions with diethyldithiocarbamates; the resulting complex is extracted into the organic phase, and As^{V} remains in the aqueous phase³. Previous studies have established efficient separation of As^{III} and As^{V} by dispersive liquid-liquid microextraction (DLLME) using carbon tetrachloride (extractant) and methanol (dispersant).

In this work, we investigated the possibility of ICP-MS determination of inorganic forms of arsenic in various types of waters. ICP-MS determination was carried out on an iCAP RQ ICP-MS inductively coupled plasma mass spectrometer (Thermo Fisher Scientific, USA). It was found that the addition of methanol to the test samples increases the analytical signal of arsenic relative to solutions with 1 % vol. nitric acid by 3.7 times for As^{III} and 3.8 for As^{V} . The presence of methanol in analyte solutions also increased the level of the background signal for arsenic, but its fluctuations (noise) did not increase. Therefore, the observed increase in analyte sensitivity leads to a similar increase in the signal-to-noise ratio.

Under optimized separation conditions, the effect of matrix elements on the degree of As^{III} recovery was assessed. In the presence of matrix elements, complete extraction of As^{III} from water is achieved with two- and three-fold microextraction. In drinking and natural water samples, determination of each form of As^{III} and As^{V} at a content level of 10 ng/dm³ is possible with a degree of As^{III} recovery of ~ 95%.

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The work was carried out within the framework of the State Assignment project of the Ministry of Education and Science of the Russian Federation No. FZEN-2023-0006 using scientific equipment of the Center for Shared Use "Ecological Analytical Center" of Kuban State University

DETERMINATION OF ENANTIOMERS OF DRUGS USING A VOLTAMPEROMETRIC SENSOR MODIFIED WITH MOLECULAR-IMPRINTED POLYPYRROLE

Abdullin Y.R., Nazyrov M.I.

*Ufa University of Science and Technology,
 Zaki Validi 32, Ufa, 450076, Russia
 e-mail: yaroslav_abdullin@list.ru*

Determination of enantiomers of medicinal compounds is an actual problem for medicine and analytical chemistry. The use of voltammetric sensors modified with molecularly imprinted polymers (MIPs) is a cheaper and more effective method. There are works in which polypyrrole (PPy) is used, a superconducting, chemically and physically stable polymer with a high specific capacity. Thanks to this number of properties, it is a good material for creating MIPs. The process of creating MIP consists of the interaction of the template with the monomer, polymerization and removal of the template, after which pores are formed that are specific to the original analyte.

In this work, a sensor based on a glassy carbon electrode modified with molecularly imprinted polypyrrole (miPPy) synthesized electrochemically was developed for the determination of drug enantiomers. Polypyrrole was polymerized on the electrode surface by electrochemical polymerization using cyclic voltammetry in the potential range from 0 to 1 V with a scan rate of 100 mV/s for 3 cycles in a solution containing 100 mM LiClO₄, 1.5 mM pyrrole and 0.5 mM drug enantiomer. The sensor was developed for further analysis of enantiomers of substances such as tryptophan, propranolol, atenolol and clopidogrel.

The resulting miPPy film was studied using cyclic voltammetry, electrochemical impedance spectroscopy and scanning electron microscopy. The analytical performance of the sensor was also studied, including its selectivity towards structurally similar substances, as well as its reproducibility in the analysis of biological fluids such as blood plasma and urine.

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FORMS OF NICKEL IN BOTTOM SEDIMENTS OF SMALL RIVERS

Belousova Y.O., Larina N.S.

*Tyumen State University,
625003, Tyumen, Volodarskogo 6,
e-mail: belousova1485@gmail.com*

Heavy metals pollution of river systems is interest due to their ability to bioaccumulate and high toxicity, and the degree of toxicity depends on the chemical form of the element¹⁻². The object of the study was the bottom sediments of the small Barsuk River, which were fractionated into sizes using a set of sieves. The forms of nickel in the fractions were determined by five-step extraction³.

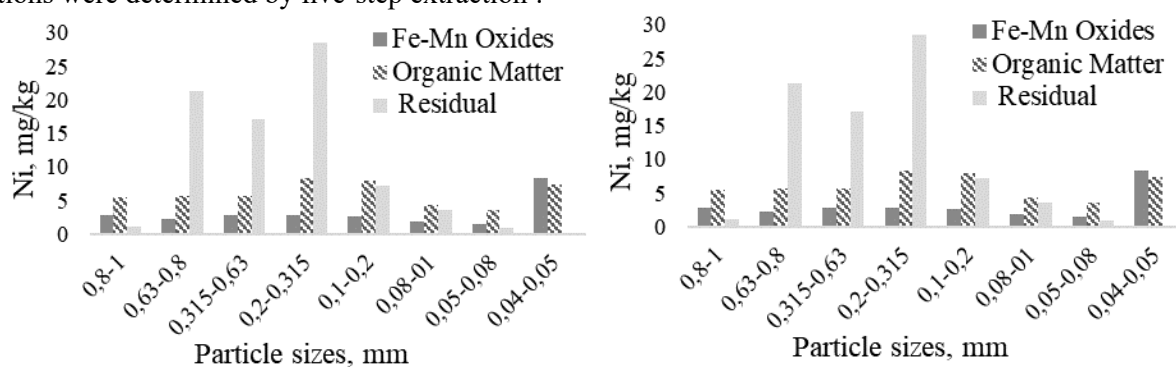


Figure 1. Distribution of nickel's forms (in extractable fractions) in various particle size fractions of bottom sediments of the Barsuk river

Content of Ni in exchangeable and bound to carbonates fractions is insignificantly (fig.1) and equal to 0.3 and 2.4% of the total content respectively. Despite the high mobility of these forms, they cannot have a significant impact on the river ecosystem. The fraction Bound to Fe-Mn oxides amounted to 15.9% of the total content and is mainly represented in the 0.05-0.04 mm fraction. The form of Ni bound to organic matter is presented in all size fractions and averaged 30.9%. The mobility of these forms of metal can increase significantly when environmental conditions change. The share of the residual form of Ni from the total content was 50.6%, while migration of this form into the water is unlikely. The maximum content of residual and exchangeable forms of Ni was observed in the fraction 0.2-0.315 mm, organic - in fractions 0.2-0.315, 0.1-0.2 and 0.04-0.05 mm.

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PHYTOSYNTHESIS METAL AND OXIDE NANOPARTICLES

**Bukharinova M.A., Khamzina E.I., Tarasov A.V.,
Kolotygina V.Yu., Stozhko N.Yu.**

*Ural State University of Economics
620144, Ekaterinburg, 8 Marta/Narodnoy Voli st, 62/45,
e-mail: m.a.bukharinova@usue.ru*

Metal and oxide nanoparticles continue to be one of the most popular nanomaterials in medical, cosmetic, environmental, (bio)sensoric and other areas of economic activity for a long time. Modern synthetic strategies for producing nanoparticles try to follow the principles of “green” chemistry, to which the use of plant extracts is fully consistent. A measure of the reducing ability of plant extracts is antioxidant activity (AOA), which can be used as a prognostic criterion for the kinetics of the phytosynthesis process and the properties of “green” nanoparticles. In our studies using phytosynthesized gold and silver nanoparticles as an example, it was shown that increasing of the plant extract AOA makes it possible to obtain smaller particles with improved optical and electrochemical properties. Nanoparticles obtained using plant extracts have some advantages compared to nanoparticles obtained using chemical reagents. These include bioactivity, biocompatibility and stability, which offer broad prospects in various applications. Gold phytonanoparticles turned out to be more stable to the ultrasound and the electrolyte-destabilizer sodium chloride treatment compared to citrate gold nanoparticles obtained using the Turkevich method. The absorption maximum and surface plasmon resonance wavelength of phytosynthesized nanoparticles did not undergo significant changes in contrast to citrate nanoparticles. Electrodes modified with gold phytonanoparticles demonstrated an increase in sensitivity, a decrease in the detection limit, and an expansion of the linear range in the determination of ascorbic and uric acids. In the catalytic photodegradation of the E133 dye, phytosynthesized zinc oxide nanoparticles were 16 % more effective compared to chemically synthesized zinc oxide nanoparticles

The study was supported by a grant from the Russian Science Foundation № 23-23-00353 (<https://rscf.ru/project/23-23-00353>).

SYNTHESIS AND EXTRACTION OF RARE EARTH ELEMENT CARBOXYLATES BY AQUEOUS AND ORGANIC MEDIA

Chaykin D.Y., Ermakov R.A., Tupikova E.N., Platonov I.A.

*Samara National Research University named after Academician S.P. Korolev,
Moskovskoe shosse 34, Samara, 443086, Russia,
e-mail: dmchaykin@mail.ru*

Carboxylic acid salts are used in REE chemical technology due to their high activity and solubility in both polar and non-polar solvents. Precipitation of REE carboxylates and extraction with aqueous solutions from organic phases are used for their separation and concentration¹.

The aim of the work is to study the extraction processes of neodymium palmitate and lanthanum, yttrium, and gadolinium oxalates by aqueous solutions as well as by oil, including from polymer matrices.

Neodymium palmitate was synthesized from neodymium oxide and palmitic acid in heptane. It was then extracted from the organic solvent with aqueous solutions of hydrochloric acid with pH 1, 2, 4 and 6. The neodymium content in the obtained aqueous solutions was analyzed by spectrophotometric method at a wavelength of 522 nm. Extraction of neodymium palmitate from crude oil was carried out with aqueous solutions with pH=1, 5, 7, 9, 11.

Lanthanum, yttrium, and gadolinium oxalates synthesized from aqueous solutions of REE chlorides by oxalic acid precipitation were placed in polymer matrices. The extraction was carried out with crude oil, a mixture of water and crude oil (1:1) and distilled water at 25°C and 80°C for 6 h. The extracts were analyzed by optical emission spectrometry with inductively coupled plasma.

Studies have shown that Nd is extracted from palmitate solution in heptane according to the molar content of hydrochloric acid in the extractant. Maximum extraction of Nd from crude oil is achieved at pH=1, with increasing pH the degree of extraction practically does not change. The degree of extraction of La, Y and Gd from oxalates in polymer matrix by aqueous solutions is 30 times higher than the degree of extraction by crude oil. REEs can be arranged in a row by increasing degree of extraction: Gd, Y, La. Extraction by both organic and aqueous medium is enhanced by heating.

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EXTRACTION OF VOLATILE ORGANIC COMPOUNDS FROM CHAMOMILE FLOWERS WITH ULTRASONIC RADIATION

Chubukina T.K., Kiseleva N.V.

*Kuban State University,
Stavropolskaya street 149, Krasnodar, 350040, Russia,
e-mail: t.chubukina@yandex.ru*

Ultrasound-assisted extraction is widely used to extract biologically active substances (BAS) of different classes from medicinal plant raw materials. This effect contributes to the destruction of cells containing essential oils and the extraction of BAS, is not difficult to implement, is rapid and allows the use of a large list of extractants¹. Identification and quantification of volatile components is usually carried out by gas chromatography with mass spectrometric detector.

As part of this study, the possibility of extracting volatile organic compounds from the wild chamomile flowers (*Matricaria chamomilla* L.) under the effect of ultrasonic radiation into acetone was studied. Chromatomass spectrometric studies were carried out on a chromatograph Shimadzu GC-2010 with a mass spectrometric detector GCMS-QP2010 Plus (Japan) on a quartz capillary column HP-ULTRA 1 (50 m × 0.20 mm, 0.33 μm) (Agilent Technologies, USA). The identification of volatile components of wild chamomile was carried out by comparing the obtained mass spectra with data from the libraries NIST07 and WILEY8.

During the experimental studies, the influence of the fraction size of the plant raw material, the ratio of its mass and volume of the extractant on the degree of analyte extraction was evaluated. In the extracts obtained, in addition to the essential oil components (en-in-dicycloether, α-bisabolol oxide B, β-farnesene), linoleic, stearic and palmitic fatty acids were identified. In contrast to those obtained by traditional methods (hydrodistillation and subcritical extraction), under the proposed conditions for the extraction of analytes under the action of ultrasonic radiation, the major component of the analyzed extract is en-in-dicycloether.

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This work was supported by Ministry of Science and Higher Education of the Russian Federation [FZEN-2023-0006].

USE OF ULTRASOUND STANDING WAVE FOR CONCENTRATION AND FRACTIONATION OF POLYMER PARTICLES

Dzhenloda R.Kh., Shkinev V.M.

*Vernadsky Institute of Geochemistry and Analytical Chemistry,
Russian Academy of Sciences, 119991, Moscow, 19 Kosygin str.,
e-mail: dzhenloda@geokhi.ru*

The solution of tasks of ecological monitoring on pollution by polymers in the environment is impossible without studies of their micro- and nanosized particles. To obtain reliable information on quantitative and qualitative composition of polymer particles in environmental objects and their dispersibility, sample preparation is necessary before analysis.

Currently, many different methods are used to concentrate and fractionate polymer particles, such as filtration, gravity and centrifugal field fractionation and others, but all of them have various limitations.

In this report, an approach for flow-through fractionation of aqueous suspensions using ultrasonic standing waves of polymer particles is proposed. A schematic diagram of the setup for carrying out the fractionation process is proposed. The ultrasound parameters for separation of a mixture of polymer particles of different densities and sizes in an ultrasonic column into size fractions have been determined.

The zones of retention, separation, and washout of polymer particles at different values of ultrasound intensity (2-20 W/cm²), liquid flow rate (0.5-5 ml/min) and ultrasound frequencies (2.5-2.9 MHz) were determined.

The conducted studies allow qualitative planning of experiments on fractionation and concentration of polymer particles.

The work was carried out within the framework of the state assignment of GEOCHI RAS.

DETERMINATION OF CEFOTAXIME IN MILK BY A MODIFIED AMPEROMETRIC SENSOR

Pham Thi Gam^{a,b} Zyablov A.N.^a Pham Thi Bich Ngoc^{b,c}

^a*Voronezh State University,*

1 Universitetskaya pl., Voronezh, 394018, Russia, I,

e-mail: alex-n-z@yandex.ru

^b*Hanoi University of Business and Technology, Hanoi, Vietnam*

^c*Master of Hanoi University of Pharmacy, Hanoi, Vietnam*

Currently, antibiotics are widely used in animal husbandry. Uncontrolled use of them used as therapeutic and prophylactic agents for farm animals leads to the formation of antibiotic residues in food products, for example, in milk, eggs, meat, which poses a danger to human health. In this regard, it is relevant to develop rapid methods for the determination of antibiotics in non-laboratory conditions. To solve these problems, the use of amperometric sensors is promising. In this regard, the goal of the work is to develop amperometric sensors based on polymers with molecular imprints of the antibiotic cefotaxime for its determination in liquid media.

The synthesis of polymers with molecular imprints (MIPs) on the surface of amperometric sensors was carried out on the basis of a copolymer of 1,2,4,5-benzenetetracarboxylic acid and 4,4'-diaminodiphenyloxide produced by OAO MIPP NPO «Plastik», Moscow.

To determine the concentration of cefotaxime in solutions, the method of graduation graphs was used. It has been established that the detection limit of the antibiotic for cefotaxime is $1,0 \cdot 10^{-6}$ g/l, the range of determined antibiotic concentrations is $1,0 \cdot 10^{-5}$ - $1,0 \cdot 10^{-1}$ g/l, and the relative standard deviation of the determination does not exceed 10%.

In order to determine residual amounts of antibiotics in milk, samples of industrial and farm milk were examined. In all samples, the antibiotic cefotaxime was not detected in the studied concentration range.

Thus, the work developed an amperometric sensor based on a polymer with a molecular imprint of cefotaxime, developed a method for determining the antibiotic in model solutions, and tested the resulting sensors on real objects. It was shown that this method can detect cefotaxime in the analyte in the concentration range of $1,0 \cdot 10^{-5}$ - $1,0 \cdot 10^{-1}$ g/l.

DEVELOPMENT OF A METHOD FOR DETERMINING AMINOGLYCOSIDE ANTIBIOTICS USING FUNCTIONALIZED CARBON QUANTUM DOTS

Farafonova O.V., Puchkova A.Yu., Moskaleva A.A., Ermolaeva T.N.

*Lipetsk State Technical University,
398600, Lipetsk, Moskovskaya str., bld. 30,
e-mail: OV.Farafonova@yandex.ru*

Carbon quantum dots (CQDs) have proven themselves as efficient fluorescent labels with unique optical properties, high hydrophilicity, and developed functional surfaces in immuno- and biosensing, immunoassay chromatography, and enzyme-linked immunosorbent assay (ELISA) methods. Their application in the determination of antibiotics using polarization fluorescent immunoassay (PFIA) is an interesting direction. The work was carried out on the Abbott Diagnostics polarizer, therefore the synthesis of CQDs was limited by the conditions: excitation wavelength (λ_{ex}) – 485 nm, emission (λ_{em}) – 525–550 nm. Ascorbic and citric acids, ammonium citrate were used as carbon sources for CQD creation. Urea and glycine were used as amino-functionalizing agents (CQD-1, CQD-2, CQD-5), thiourea for thiolation (CQD-3), APTES for silanization (Si-CQD), and ethylene glycol for creating hydroxyl groups on the surface (CQD-4). Synthesis was performed using hydrothermal, microwave, and solid-phase methods. It was found that CQD-2, Si-CQD-2, CQD-4, and CQD-5 met the specified emission range, which were further used for the synthesis of tracers with aminoglycoside antibiotics – kanamycin and gentamicin. The functionalization of dots and their conjugation with antibiotic molecules were monitored using Fourier transform infrared spectroscopy (FTIR). Particle sizes were estimated by atomic force microscopy. All nanomaterials had sizes up to 6 nm. When developing a method for determining kanamycin and gentamicin using functionalized carbon quantum dots, optimal dilutions of antibodies and tracers were established. The detection limit of kanamycin and gentamicin with tracers labeled with CQD-2, CQD-4 was (ng/ml) 20, 70, 30, 80; the range of detectable concentrations (ng/ml) 30-1000, 100-3000, 50-1000, 100-3000, respectively.

The developed method for determining aminoglycoside antibiotics was tested on “Prostokvashino” milk brands with 2.5% fat content and “LebedyanMoloko” with 3.2% fat content. No antibiotics or their traces were detected in the samples.

ANALYTICAL MONITORING OF WATER OBJECTS IN THE TECHNOLOGY OF REACTIVE AND HIGH-PURITY PRODUCTS

Averina Yu.M.,^a Guseva N.V.,^a Bessarabov A.M.^b

*^aD.I. Mendeleev University of Chemical Technology of Russia,
Miusskaya square 9, Moscow, 125047, Russia,
e-mail: averina.i.m@muctr.ru*

*^bR&D Centre "Fine Chemicals",
Krasnobogatyrskaya 42, Moscow, 107564, Russia,
e-mail: bessarabov@nc-mtc.ru*

The systematization of management tasks for water resources has been carried out at three levels of hierarchy: country, industry, company^{1,2}. At the lower level of the analysis, the main tasks of the water management of the chemical enterprise are highlighted: recycled water supply, collection and treatment of contaminated water, steam generation, hot water supply.

An integrated water management system² has been created for one of the leading manufacturers of reactive and high-purity products of JSC «EKOS-1», in which there are 9 types of water objects: main water, concentrate, recycled water (direct and return), osmotic and high-purity water, saturated steam, hot water, domestic and industrial wastewaters.

To improve the efficiency of analytical monitoring of water objects, a computer-based quality management system (CQM-system) has been developed. The development was carried out on the basis of CALS technology (Continuous Acquisition and Life cycle Support - continuous information support of the product life cycle)^{2,3}.

At the upper level of the information model of the system, there are water objects used in the manufacture. At the second level of the hierarchy, the main quality indicators are implemented for each water object, which are characterized at the 3rd and 4th hierarchy levels by the appropriate analysis methods and devices. The CQM-system (as well as the LIMS - Laboratory Information Management System) allows to improve analytical quality control of products, increase the efficiency of using laboratory resources (personnel, instruments and reagents), reduce the time of analytical research³.

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THE STUDY OF IR SPECTRA PROCESSING FOR THE ATENOLOL QUANTITATIVE ANALYSIS

Khisyamov M.M., Red'kin N.A., Onuchak L.A.

*Samara National Research University,
443086, Samara, Moskovskoye shosse, 34,
e-mail: hisiamov@yandex.ru*

In recent years, there has been an increasing use of computer technologies in analytical chemistry. Various methods for processing analytical data based on mathematical tools have been developed.

In this paper are compared the IR spectrometry quantitative determination results of atenolol in tablet using the method of absolute calibration and chemometric.

At the first stage, quantitative analytical methods were developed and verified using the absolute calibration method. However, it was found that two absorption bands can be used for analysis, although they are difficult to associate with specific functional groups in atenolol and they do not correspond to the strongest absorption bands in the spectrum.

At the second stage, the projection to latent structures was used to construct calibration dependencies. It has been demonstrated that the spectra of the atenolol compound are not suitable for such analysis, since there are significant differences in the IR spectra of pure atenolol compared to that extracted from tablets during the extraction process. However, using the spectra of atenolol isolated from tablets with known concentrations of the active ingredient, it became possible to develop a model for estimating the content of atenolol in tablets.

Both methods can potentially be used for the analysis of pharmaceuticals. The traditional method is suitable for small batches, while the chemometric approach can be used when comparing samples from different batches.

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NON-TARGETED SEARCH IN DETERMINATION OF PROCESS FLUIDS COMPOSITION

**Kiseleva M.G., Novikov R.I., Sakovich M.V.,
Povarov I.G., Aleksenko S.S., Novikova I.V.**

*FSUE «State Scientific Research Institute of Organic Chemistry and Technology»
State research center of Russian Federation,
111124 Moscow, shosse Entuziastov, 23.
e-mail: centrlab@gosniokht.ru*

Determination of complex mixtures' composition is one of the most challenging and interesting analytical tasks. It is usually necessary to use the entire arsenal of available methods. NMR spectroscopy, gas and liquid chromatography with mass spectrometric detection are the main tools for elucidation of the structure of organic compounds. Atomic spectroscopy and ion chromatography help to quantify metals and inorganic ions. The simplest, routine methods often suggest the direction of the research: pH measurement, visual characteristics of the sample (chromaticity, fluidity, uniformity), solubility in water, polar and non-polar organic solvents. The determination of the dry residue at different temperatures and even the characteristics of the stain on the filter paper after drying can provide valuable information. All available data need to be taken into account. The component composition of process fluids is determined by the scope of their application, thus the literature and, in particular, patent search is important stage of investigation. The joint work of the analysts allows us to make an assumption about the composition of the sample.

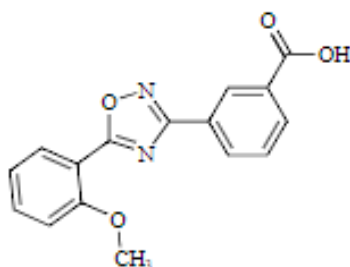
Based on the experience of the conducted research, the laboratory has developed a scheme for sample preparation and analysis of samples of unknown composition using general laboratory (pH-metric, determination of dry residue, miscibility and solubility), chromatographic (liquid and gas chromatography with mass spectrometric detection, ion chromatography) and spectral (atomic spectroscopy, NMR spectroscopy) methods. Special attention is paid to the identification of analytes missing in available databases. The correctness in this case is confirmed by the consistency of the results obtained by different methods. The report presents interesting cases of mutual complementation of information obtained by different methods, only it's joined consideration allowed to make an assumption about the structure of compounds.

ISOLATION AND IDENTIFICATION OF THE ALKALINE HYDROLYSIS PRODUCT OF THE ACTIVE PHARMACEUTICAL SUBSTANCE ATALUREN

Korobkina M.P., Popova Yu. V., Ivanov R.A.

*ANOO VO "Sirius University",
354340, Krasnodar Territory, village g.g.t. Sirius, Olimpiysky pr. 1,
e-mail: korobkina.mp@talantiuspeh.ru*

An urgent task of modern pharmaceutical development is the study of stability of pharmaceutical substances. ICH Q10 and GF RF place high demands on the resolution of methods for the isolation and structure determination of impurities. In a stress experiment under conditions of alkaline hydrolysis of ataluren, a limited set of impurities are formed which can be separated by liquid chromatography. To evaluate the resolution of the chromatographic system, an impurity peak with a relative retention time of 0.84 to the atalurene peak was selected. The resolution with the main peak ($R_s=5.5$), number of theoretical plates (15,523), asymmetry factor (1.109), signal-to-noise ratio and signal reproducibility allowed us to accept this impurity as a marker of the resolving system of the chromatographic method. The impurity was isolated by preparative liquid chromatography. The substance was identified by NMR as 2-Methoxy-atalurene. The molecular weight of the impurity was confirmed by mass spectrometry.



Ataluren Impurity 1

CAS No. 775304-03-5

$C_{18}H_{12}N_2O_4$

M.W. 296.28

Impurity 2-Methoxy-ataluren

The advantage of all performed works is analytical availability for independent preparation of chromatographic system suitability solution and minimization of enterprise resources costs when purchasing a third-party standard for impurity identification.

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2. GF RF XV OFS.1.1.0009 Stability and shelf life of medicinal products;
3. Stability testing of new drugs and preparations (ICH Q1A).

The work was financially supported by RNF, project 23-90-04000.

LUMINESCENCE OF LANTHANIDE(III) COMPLEXES IN SOLS OF NANOANIONITES

Koroleva M.V., Yagov V.V., Dolgonosov A.M., Khamizov R.H.

*V.I. Vernadsky Institute of Geochemistry and Analytical Chemistry of the Russian Academy of Sciences,
119991 GSP-1, Moscow, Kosygin str., 19
e-mail: koroleva.mv@geokhi.ru*

Lanthanide(III) complexes have characteristic intense luminescence caused by intramolecular energy transfer from the triplet level of the ligand to the emissive level of the lanthanide ion ("antenna effect"), which allows them to be used in analytical chemistry for the determination of both REEs themselves and ligands. More efficient luminescence is facilitated by the use of organized media (micelles, modified sorbents), which ensure rigidity of the environment of luminescent complexes, which reduces the likelihood of non-radiative deactivation of the excited state¹.

We were the first to propose using a sol of anionite nanoparticles (NIA)², which is highly stable in aqueous solutions and characterized by a low level of intrinsic luminescence, as an organized medium for enhancing the luminescence of lanthanide(III) complexes. The unique properties of the NIA sol lie in the ability of charged nanoparticles, acting as nanoreactors, to locally concentrate large anions in their volume, creating conditions for the formation of multiligand complexes with the displacement of water from the coordination sphere of the cation.

The effect of NIA on the luminescence of lanthanide(III) complexes (Eu^{3+} , Sm^{3+} , Tb^{3+}) with β -diketones (thenoyl-trifluoroacetone, avobenzene, etc.), tetracyclines and quinolones was studied. It has been established that when NIA is added to such systems, the luminescence intensity can increase by three orders of magnitude, which makes it possible to significantly reduce the detection limit of the analyte (REE ion or ligand).

Thus, it has been shown that the use of nanoionites sols as organized media is a promising direction in luminescent analysis.

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The work was carried out on the topic of the state assignment of the Institute of Geochemistry and Analytical Chemistry of the Russian Academy of Sciences.

ETAAS DETERMINATION OF ELEMENTS IN HIGH SALT SOLUTIONS WITH PRELIMINARY CONCENTRATION WITH SILICA GEL MODIFIED WITH A THIOSEMICARBAZONE GROUP AND SUBSEQUENT DOSING OF SORBENT SUSPENSIONS INTO AN ELECTROTHERMAL ATOMIZER

Burylin M.Yu., Kostuchenko E.S.

*Kuban State University,
350040, Krasnodar, st. Stavropolskaya, 149
e-mail: Kostuchenko_01@mail.ru*

A method has been developed for the electrothermal atomic absorption determination of Hg(II) and Sn(II) in natural (fresh and salty) waters after concentration with modified silica gel and dosing of the sorbent into the graphite furnace of an electrothermal atomizer in the form of suspensions.

The modes of the program for electrothermal atomization of elements have been determined, which make it possible to eliminate the influence of the silica gel matrix. The maximum permissible concentrations of silica gel suspensions should not exceed 10 mg/cm³ when determining both elements. The possibility of using a calibration dependence constructed using standard solutions of the element being determined when determining Sn in a sorbent based on modified silica gel is substantiated. When determining Hg, it is necessary to use a calibration curve based on suspensions of silica gel containing a known amount of the element. Range of linear calibration dependencies (ng/ml): 20–200 for Hg, 5–200 for Sn. Modes of simultaneous sorption of elements have been developed.

The proposed scheme was tested by determining Hg and Sn in fresh natural and sea waters; mineral water of the Essentuki brand using the «spiked samples» method. The found element contents coincided quite well with the introduced amounts. The relative error in all cases did not exceed 15%. The detection limits (3s criterion) were (ng/dm³): 50 (Hg) and 7 (Sn), respectively. The concentration factor was 100.

The work was carried out with the financial support of the Russian Science Foundation, project 23-23-00019.

EXTRACTION OF RARE EARTH ELEMENTS IN AQUEOUS BIPHASIC SYSTEMS BASED ON QUATERNARY AMMONIUM SALTS FOLLOWED BY INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY DETERMINATION

Lebedeva L.M., Emelianov A.E., Smirnova S.V.

*Lomonosov Moscow State University, Leninskie gory 1,
Moscow, 119991, Russia,
e-mail: lebedevaliliiiia@gmail.com*

The growing demand for safe and environmentally friendly “green” chemistry is a key trend in the development of modern analytical methods. In particular, the development of liquid extraction techniques involves the use of new extraction systems that do not contain conventional organic solvents. An alternative to traditional heterogeneous liquid-liquid systems are aqueous biphasic systems (ABSs), both phases of which consist mainly of water, more than 50 mol. %¹. ABSs are formed in the combined presence of water-soluble substances, for example, organic and inorganic salts, at a certain concentration ratio. The choice of the phase-forming components of the ABS determines the availability and properties of the resulting ABS, for example, the ability to ion exchange and extraction without a complexing reagent.

The present work describes the patterns of group extraction of rare earth elements (REEs) in the new ABSs based on quaternary ammonium halides (tetrabutylammonium bromide, TBAB, and benzethonium chloride, BX) and potassium thiocyanate. The boundaries of the phase separation region for ABSs have been determined. The optimal conditions for obtaining new ABSs and quantitative extraction and preconcentration of REEs (10-5000 µg/l) have been established: the total concentration ($c_{\text{TBAB} + \text{KSCN}} = 0,016\text{--}0,4 \text{ M}$ and $c_{\text{BX} + \text{KSCN}} = 0,6\text{--}0,8 \text{ M}$) and the ratio of molar concentrations of components TBAB : KSCN and BX: KSCN (from 3:1 to 1:3), the pH range (5–8), the ratio of phase volumes, and the phase contact time (no more than 10 min). The possibility of REEs determination by inductively coupled plasma mass spectrometry in surface and marine water samples after back-extraction with nitric acid solutions has been demonstrated. The preconcentration of REE in the proposed new ABSs with subsequent back-extraction significantly reduces matrix effects and provides low limits of detection for REE determination in complex samples.

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MICROFLUIDIC PLANAR CONCENTRATORS FOR DEFINITIONS OF VOLATILE ORGANIC COMPOUNDS (VOC)

Margarian A.E., Platonov I.A., Kolesnichenko I.N., Novikova E.A.

*Samara National Research University,
443086, Samara, ул. Moskovskoye shosse, 34,
e-mail: pia@ssau.ru*

Recently, noninvasive medical diagnostics has become one of the most relevant areas and is coming to the fore. An important area of noninvasive medical diagnostics is the analysis of exhaled air¹.

Exhaled air consists of compounds such as nitrogen, oxygen, carbon dioxide, inert gases, water vapor and traces of VOCs. Some of these components have illustrated their value as biomarkers in various diseases.

One of the promising volatile components associated with metabolism is acetone. To date, various studies have been conducted on the clinical significance of exhaled acetone and its reliable relationship with blood glucose levels.² However, the concentration of acetone in the exhaled air is at the level of trace impurities, which makes it necessary to pre-concentrate.

In the framework of this study, a configuration of microfluidic planar concentrators has been proposed for the concentration of acetone in exhaled air, which are plates based on Silagerm 8040 with microchannels filled with Porapak-Q sorbent.

Optimal concentration conditions were established ($t_{\text{sorb}} = 0^{\circ}\text{C}$; $t_{\text{des}} = 70^{\circ}\text{C}$, $V_{\text{sorb}} = 45 \text{ ml}$, $t_{\text{des}} = 1 \text{ sec}$) using microfluidic planar concentrators filled with Porapak-Q sorbent, at which the maximum concentration coefficient was reached, which is 43.

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APPLICATION OF THE AUTOMATED ELECTRODE SYSTEM FOR MEDIUM EXCHANGE IN STRIPPING VOLTAMMETRY

Martynov L.Yu.^a, Sadova M.A.^a, Zaitsev N.K.^b

^aMIREA - Russian Technological University, Lomonosov Institute of Fine Chemical Technologies,
 Vernadsky Avenue 86, Moscow, 119454, Russia
 e-mail: martynov_leonid@mail.ru

^bLLC «Econix-Expert», Akademika Bakuleva st. 6, Moscow, 117513, Russia

Stripping voltammetry (SVA) is a highly sensitive method for determining trace amounts of organic and inorganic substances. The reproducibility and accuracy of the method is often limited due to the influence of the sample matrix on the recorded analyte signal, as well as to the necessity of renewing the surface of the working electrode. One of the most promising ways to solve this problem is to use electrode systems that make it possible to vary the composition of the background solution at individual stages of the inversion cycle without opening the circuit¹.

This work is devoted to the development and application of a combined electrochemical cell, called a «3 in 1» sensor in the literature, Fig. 1.



Figure 1. The «3 in 1» sensor: (A) – general view and (B) – photograph of working surface:
 1 – working electrode (impregnated graphite), 2 – auxiliary electrode, 3 – reference electrode

The developed sensor was used for the voltammetric determination of heavy metals (Pb(II), Cd(II), Zn(II), Cu(II)) in natural water², Se(IV) and As(III) in seawater and seafood, In(III) and Ge(IV) in electronic waste by medium exchange at different stages of the measurement cycle³. The advantages of the “3in1” sensor over using conventional electrode systems are discussed.

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UNIFIED SAMPLE PREPARATION SCHEME IN THE DETERMINATION OF GOLD AND SILVER IN NON-FERROUS METAL CONCENTRATES

**Losev V.N., Maznyak N.V., Didukh-Shadrina S.L., Borodina E.V.,
Metelitsa S.I., Buyko O.V.**

*Siberian Federal University,
prospect Svobodnyy, 79, Krasnoyarsk, 660041, Russia,
e-mail: metelitsa_sl@mail.ru*

Known methods of sample preparation of non-ferrous metal concentrates include assay concentration stages followed by the determination of silver and gold by gravimetric or spectrometric methods or acid decomposition with the addition of an insoluble residue or its discarding (which can lead to partial losses of precious metals). The schemes are characterized by long duration, labor intensity, and require consideration of the characteristics of the matrix composition for the selection of appropriate reagent compositions for decomposition.

The proposed universal sample preparation scheme is used in the determination of gold and silver in copper, lead, and zinc concentrates. The sample weight is pre-subjected to high-temperature oxidative and reagent decomposition in the presence of ammonium salts (NH_4F , NH_4Cl), resulting in the phase composition changes, the sulfide, silicate and carbon-containing parts are removed. The sintered mass is highly porous and easily dissolves in a mixture of mineral acids (HCl , HNO_3) without forming an insoluble precipitate in systems with microwave or resistive heating. Nitric acid after decomposition is neutralized by the introduction of carbamide or 2-fold boiling-down with concentrated hydrochloric acid

A significant difference of the proposed scheme is the conversion of all forms of gold and silver into chloride complexes, which allows their direct determination by available instrumental methods. This scheme is successfully combined with any isolation, separation and concentration schemes, including extraction with individual or mixed dialkyl sulfides or co-precipitation on tellurium (selenium).

The work was performed using the the Joint Scientific Center of the Siberian Federal University “High-tech methods of research and analysis of new materials, nanomaterials and mineral raw materials”.

DETERMINATION OF METHYL METHACRYLATE IN AQUEOUS MEDIA BY CAPILLARY ELECTROPHORESIS

Stakhanova S.V., Ermolenko Yu.V., Kobets U.L., Mikhailova N.V.

*D. Mendeleev University of Chemical Technology of Russia,
Miusskaya Ploshchad 9, Moscow, 125047, Russia,
e-mail: mikhailova.n.v@muctr.ru*

The development of an accessible, rapid methodology for determining residual monomers of biocompatible polymers released into biological fluids is an urgent task for medicine. This work is devoted to the determination of methyl methacrylate – the monomer of polymethylmethacrylate used in dentistry as the main material for prosthetics – in aqueous solutions and physiological media¹. Due to the complexity and incompleteness of biological experiment data, the amount of methyl methacrylate eluted into the liquid is used as an indicator of the polymer's allergenic activity.

During the study, the capabilities of methods such as visible and UV spectrophotometry, high-performance liquid chromatography, and capillary electrophoresis were evaluated. It has been shown that the capillary electrophoresis method has higher accuracy and reliability compared to other methods, as it allows the separation of substances with similar molecular weights and natures that absorb UV radiation at the same wavelength. A methodology for determining methyl methacrylate in aqueous media by micellar electrokinetic chromatography using sodium dodecyl sulfate as the pseudo-stationary phase has been developed, which, unlike capillary zone electrophoresis, allows the separation of neutral molecules². The determination of the monomer by this method is possible with detection and quantitation limits of 0.021 µg/mL and 0.069 µg/mL, respectively.

The methodology has been successfully tested on samples of aqueous extracts of polymethylmethacrylate obtained from actual dental practice.

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PALLADIUM DETERMINATION WITH DIRECT INJECTION OF THE EXTRACT INTO A DROP-SPARK DISCHARGE

Mokhodoeva O.B., Yagov V.V., Bykov D.A., Shkinev V.M.

*Vernadsky Institute of Geochemistry and Analytical Chemistry, Russian Academy of Sciences,
19, Kosygin street, Moscow 119991, Russia,
e-mail: olga.mokhodoeva@mail.ru*

Despite the wide possibilities of modern instrumental methods, sample preparation still plays a key role in obtaining reliable analytical results. This is especially true for elements such as platinum metals, for which the mutual and matrix influence is always critical; therefore, the development of hybrid methods for their determination, providing selective separation and preconcentration, is an important task.

Previously, aqueous biphasic systems (ABS), whose phase-forming components are water-soluble, non-hazardous, biocompatible, and commercially available, were proposed as alternative extraction systems¹. It has been demonstrated that polyethylene glycol (PEG)-based ABSs can be used for extraction of platinum metals from chloride solutions².

In the present work, a hybrid method for the determination of palladium is proposed, including its extraction by PEG-based ABS and analysis of the PEG-rich phase by drop-spark discharge atomic emission spectrometry. Drop-spark discharge is a pulsed microplasma source oriented for application in portable devices³. It was found that the upper phase of the ABS based on PEG and ammonium sulfate is suitable for direct injection into the drop-spark discharge, and the discharge stability and metrological characteristics of the determination are comparable to the values obtained in mineral acids commonly used for this purpose.

Experimental data showed that the relative standard deviation of palladium signal intensity at 363.5 nm wavelength does not exceed 10%. The detection limit is 1 mg/L, and the linearity range of palladium concentration is 5-100 mg/L.

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INFLUENCE OF THE OLIGOHEXAMETHYLENE GUANIDINE DERIVATIVE CONTENT IN THE POLYMER COMPOSITE MATRIX ON THE BIOFOULING OF THE OPTICAL SENSOR OF MOLECULAR OXYGEN

Naumova A.O., Melnikov P.V.

*Institute of Fine Chemical Technologies named after M.V. Lomonosov, MIREA - Russian Technological University,
 119454, Moscow, Vernadskogo Avenue, 86,
 e-mail: alina.naumova.92@bk.ru*

Biocidal agents are used to protect against biofouling of various coatings in environments with high biomass content¹. In this work, we used the biocidal polymer oligohexamethylene guanidine (OHMG), which was additionally modified with para-aminosalicylic acid (PAS) to enhance its properties against microorganisms with lipid membrane. Bactericidal activity was tested against strains *Mycobacterium smegmatis* ATCC 607 and *Pseudomonas chromraphis* 449.

We prepared a series of samples with different contents of OHMG-PAS in the polymer matrix of the composite material of the optical oxygen sensor. It has been established that the ratio of components significantly changes the surface morphology and wetting angle. The optimal content of OHMG-PAS was 3 wt.%, when the water contact angle reaches almost 122°, and the rate of biofouling, according to the MTT-assay and confocal microscopy with staining, decreases almost five times (Fig. 1).

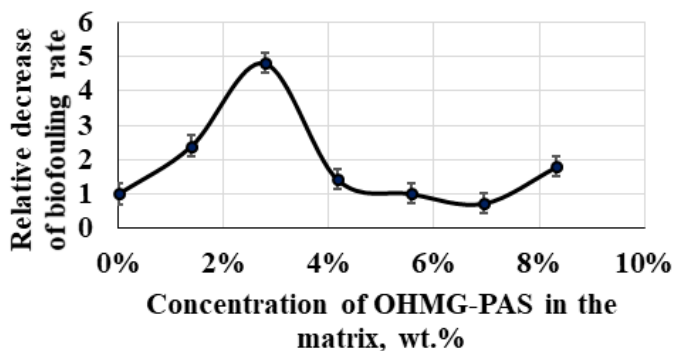


Figure 1. The relative reduction in the rate of biofouling on the content of OHMG-PAS in the sample

The demonstrated approach opens up prospects for creating stable and biofouling-resistant sensor elements, which is relevant for use in environments with a high biomass content, such as aeration tanks or seawater.

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CHROMATOGRAPHIC DETERMINATION OF BIOLOGICALLY ACTIVE SUBSTANCES IN SPEARMINT

Nazarova D.V.^a, Temerdashev Z.A.^a, Vinitskaya E.A.^b

^a *Kuban State University,
Stavropolskaya 149, Krasnodar, 350040, Russia,
e-mail: nazarovadv1999@gmail.com*

^b *Subtropical Research Centre, RAS,
Jan Fabricius 2/28, Sochi, 354002, Russia*

Spearmint (*Mentha spicata* L.) is widely used in herbal medicine and other areas of industry due to the presence in its composition of a complex of biologically active substances (BAS) - essential oil components (EOCs) and phenolic compounds (PCs). To assess the possibility of therapeutic use of plant raw materials, it is necessary to know the component composition, because its formation is influenced by growing conditions, the type and chemotype of the plant, the method of extracting components from the plant matrix, etc.; it is also not species-specific for plants of the mint genus.

Spearmint was collected in Maykop in 2023 during the flowering phase. Before testing, the sample was dried and crushed according to the recommendations of the Pharmacopoeia of the Russian Federation. The extraction of EOCs from spearmint was carried out by subcritical extraction using acetone as an extractant.¹ The extract was analyzed by GC-MS in the programmable column heating mode. Analyte identification was performed using the NIST05 and WILEY8 libraries. The main EOCs of spearmint were monoterpene alcohols - 4-thujanol and eucalyptol. PCs from mint was extracted by microwave extraction with a water-ethanol mixture. The extracts were analyzed by HPLC-DMD, and the identification and determination of PCs was carried out using standard samples. The main component of the aqueous-alcoholic extract of spearmint was rosmarinic acid, the content of which was 35.5 mg/g in terms of air-dried raw materials.

BAS identified in extracts are one of the most valuable classes of substances for aroma and herbal medicine; they exhibit antioxidant, chelating and enzyme inhibitory activity.

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LUMINESCENCE OF THE COMPLEX OF EU(III) WITH AVOBENZONE

Nesterovich D.S., Yagov V.V., Koroleva M. V., Bykov D.A.

*Institute of Geochemistry and analytical chemistry. V. I. Vernadsky
Russian Academy of Sciences, 119991 GSP-1, Moscow, Kosygina, 19
e-mail: nesterovich@geokhi.ru*

Avobenzene is an organic substance that is used in cosmetic products as a sunscreen component. Recently, studies have been carried out on the photostability of avobenzene and its negative impact on marine ecosystems, in particular on corals¹. In this regard, the task of determining trace amounts of avobenzene in waters, sand, corals and other environmental objects is relevant. In this work, in order to develop a new method for the determination of avobenzene, the luminescence of its complexes with Eu(III) in micellar media was studied.

Like other aromatic β -diketones, avobenzene can form luminescent complexes with lanthanide(III) ions. The “antenna effect” was observed for the Eu^{3+} complex with avobenzene², but without connection with chemical analysis. We studied the possibility of determining avobenzene in aqueous solutions in the presence of various surfactants.

It has been established that weakly alkaline solutions containing avobenzene and Eu(III) luminesce intensely in the presence of cationic surfactants and nanoanion exchangers. In terms of the glow intensity of complexes with europium, avobenzene is not inferior to the most effective “antennas”, such as thenoyltrifluoroacetone and dibenzoylmethane. To determine avobenzene, an LED with a maximum emission of 370 nm was used. The peak of the most intense transition $5D_0 \rightarrow 7F_2$ corresponds to a wavelength of 613 nm. The best determination conditions are realized when using a nanoanion exchanger obtained from AB-17-8 resin³. The possibility of luminescent determination of avobenzene in water in the range of 10-10000 nM with a detection limit of 3 nM has been demonstrated.

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The work was carried out with the support of the Ministry of Science and Higher Education as part of the implementation of work on State assignments of the Federal State Budgetary Institution of Geochemistry and Analytical Chemistry of the Russian Academy of Sciences at the expense of budget funding.

GC-MS DETERMINATION OF PAHS AND PCBs IN WATER USING EXTRACTIVE FREEZING-OUT

**Ovsepyan S.K.,^a Chervonnaya T.A.,^a Musorina T.N.,^a
Temerdashev Z.A.,^a Bekhterev V.N.^b**

^a *Kuban State University,
Russian Federation, Krasnodar, 3
50040 Stavropolskaya Street 149
e-mail: arttat718@gmail.com*

^b *Forensic Medical Examination Bureau No. 2 of the Ministry of Health of Krasnodar Region in Sochi,
Ministry of Health of Krasnodar Region,
Russia, Sochi, 354057, Tuapsinskaya Street, 1*

16 priority polycyclic aromatic hydrocarbons (PAHs) and 7 indicator polychlorinated biphenyls (PCBs) are common pollutants in the environment, regulated for determination in environmental objects by the monitoring programs of the US Environmental Protection Agency (US EPA). PAHs and PCBs enter water bodies through air transport from sources, secondary pollution, with wastewater, etc. The search for effective sample preparation methods for water, ensuring high extraction and concentration of analytes from complex matrices, is relevant. The study of the features of extractive freezing-out as a method of analyte concentration under the influence of centrifugal forces is of interest, as extraction, concentration of analytes, and purification of extracts from major matrix components occur in one step.

This paper presents the results of studies of extraction mixtures with varying contents of the extractant (acetonitrile) for simultaneous extraction of PAHs and PCBs from water. The influence of chloroorganic pesticides on the extraction rates of analytes in the concentration range corresponding to the content of interfering components in real objects was evaluated. The absence of influence of *n*-paraffin hydrocarbons on the analysis of water samples contaminated with petroleum products was demonstrated: under optimized conditions, hydrocarbons were not extracted into acetonitrile extracts. The extraction rates of analytes exceeded 90% in the range of 0.1 – 100 µg/l for PCBs and 0.2 – 100 µg/l for PAHs in their GC-MS determination.

The work was supported by Ministry of Science and Higher Education of the Russian Federation [FZEN-2023-0006].

RATIONALE FOR THE CHOICE OF EXTRACTANT FOR THE EXTRACTION OF PAHS IN SOILS OF VARIOUS COMPOSITION

Ovsepyan S.K., Chervonnaya T. A., Musorina T. N., Temerdashev Z.A.

*Kuban State University,
Krasnodar, 350040 Russia,
e-mail: suzannadd7@mail.ru*

Control of the content of polycyclic aromatic hydrocarbons (PAHs) is one of the priority areas of monitoring natural objects. Soils are the main natural matrix for the accumulation of PAHs, and their accumulation is mainly based on sorption processes and is largely determined by the mineralogical composition and organic matter of the soil.

Soils with high humus content are the most problematic when determining PAHs in natural objects, due to the strong interaction of the substances to be determined with the analyzed matrix of the sample. Experimental studies have shown that the extraction of penta- and hexacyclic PAHs from soils with an organic matter content of more than 5% is inefficient under conditions optimized for low humus samples¹. The extraction of these PAHs requires the development of new sample preparation schemes for analysis.

This work presents the results of studies on the application of binary extraction mixtures of different compositions – acetonitrile: dichloromethane, acetonitrile: acetone, hexane: acetone, chloroform: acetone, dichloromethane: acetone, and dichloromethane: ethyl acetate. The extracts were analyzed by gas chromatography-mass spectrometry in the selective ion monitoring mode on the “Shimadzu GCMS-QP 2020” instrument. The greatest extraction of PAHs of various structures (more than 90%) was achieved by the extraction mixture acetone: dichloromethane due to the higher elution power of chlorinated hydrocarbons and ketones in charge transfer mode, due to the destruction of complexes formed in the analyzed soil matrix and the release of analytes.

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A COMPARABILITY OF SARA-ANALYSIS' RESULTS FOR DIFFERENT PETROLEUM SAMPLES OBTAINED BY OPEN-COLUMN LIQUID ADSORPTION CHROMATOGRAPHY

Panyukova D.I.^a, Savonina E.Yu.^a, Ossipov K.^b, Maryutina T.A.^a

*^aVernadsky Institute of Geochemistry and Analytical Chemistry of Russian Academy of Sciences,
Kosygin str. 19, Moscow, 119991, Russia
e-mail: daria.paniukova@gmail.com*

^bLLC Strata Solutions, Institutskiy per. 9, Dolgoprudny, 141700, Russia

The group-type hydrocarbon composition of a petroleum object is determined to obtain information about its quality and chemical behavior.

Chromatographic SARA-analysis is a traditional scheme for establishing the group-type composition, which makes it possible to divide a petroleum sample into four groups: saturates, aromatics, resins and asphaltenes followed by their quantitative determination.¹⁻²

The most available method for SARA-analysis is open-column liquid adsorption chromatography (LAC). Standard and research procedures of LAC have been developed for the analysis of high boiling point petroleum products¹.

Despite the strict adherence to the requirements of both standard and research procedures of LAC, researchers obtain incomparable results of SARA-analysis using different procedures within the same method for a particular object.²⁻³ It is possible that opposite trends will be revealed in a similar analysis of other petroleum samples.

The determination of group-type hydrocarbon composition for a wide range of petroleum samples (oils of different classes, petroleum products) was carried out in this work using two procedures of LAC: standard procedure – ASTM D4124 and research procedure developed at the Joint-Stock Company VNII NP. The goal of the research was to fix the comparability or incomparability of the results. The obtained data of group-type hydrocarbon composition of oil samples allowed to assess the possibility of applying the selected procedures to them. It's shown that the selected procedures of LAC can be recommended for SARA-analysis of heavy and bituminous oils.

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This work was performed within the framework of the government assignment for the GEOKHI RAS.

DEVELOPMENT OF A PNEUMATIC FLOW BLURRING NEBULIZER FOR ANALYTICAL SPECTROMETRY

Burumov I.D.^{a,b}, Putmakov A.N.^{a,b}, Trunova V.A.^a, Komin O.V.^{a,b}, Pelipasov O.V.^{a,b}

^a*LLC «VMK-Optoelectronica»,
Akademika Koptyuga 1, Novosibirsk, 630090, Russia, 1,
e-mail: pelipasov@vmk.ru*

^b*Institute of Automation and Electrometry, SB RAS,
Akademika Koptyuga 1, Novosibirsk, 630090, Russia*

The type of nebulizer used in ICP-OES, ICP-MS, MIP-OES and flame spectrophotometry significantly affects the basic plasma parameters and, consequently, analytical characteristics such as accuracy, sensitivity and reproducibility.

To solve research problems and import substitution problems of foreign nebulizer, a serial production of pneumatic nebulizer with “flow blurring” technology has been developed and established¹. The appearance of the developed nebulizer is shown in Figure 1 (b). The article compares the analytical characteristics of the created pneumatic nebulizer with the Burgener MiraMist, OneNeb2, Glass Expansion and Mainhard A-type and C-Type nebulizer obtained on the Grand-ICP spectrometer².

The highest plasma temperature and electron concentration were obtained using the created nebulizer and OneNeb2. The MiraMist showed the lowest efficiency of aerosol transportation to plasma. Comparable detection limits, reproducibility and accuracy with the OneNeb2 nebulizer have been obtained and are several times higher than Glass Expansion and MiraMist.

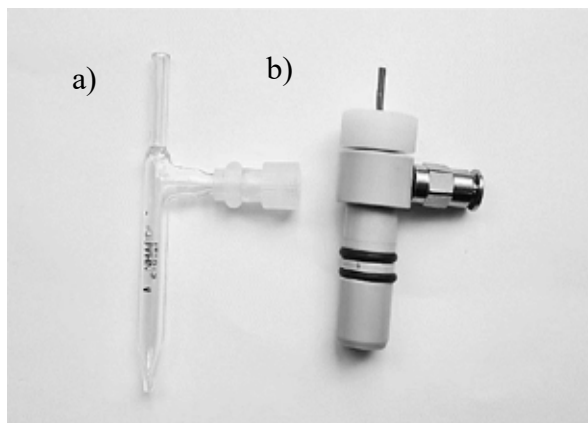


Figure 1. Photos of pneumatic nebulizer: a – Mainhard, b – designed by the authors

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USING PHASE VALUES FOR PEAK CLASSIFICATION IN ORBITRAP MASS SPECTRA OF NATURAL ORGANIC MATTER

Potemkin A.A., Volkov D.S., Proskurnin M.A.

*Chemistry Department of Lomonosov Moscow State University,
Leninskie Gory 1-3, Moscow, Russia, 119991,
e-mail: skypehoper@yandex.ru*

Fourier transform mass spectrometry, including the Orbitrap method, is widely used tool for studying natural organic matter (NOM). The Orbitrap method is used for nontargeted analysis of NOM, which consists in assigning molecular formulas to the peaks in mass spectra.¹ However, uninformative peaks associated with noise must be removed before such a procedure, because formula assignment algorithms find the appropriate elemental composition for these signals as well.² This aspect interferes with the correct estimation of the chemical composition of NOM samples.

In this study, we propose using the phase values obtained during the Fourier transform to classify and remove uninformative peaks. The measured phases of ion oscillations in the Orbitrap method change systematically³, making it possible to distinguish analytical signals from the noise, which has random phase values.

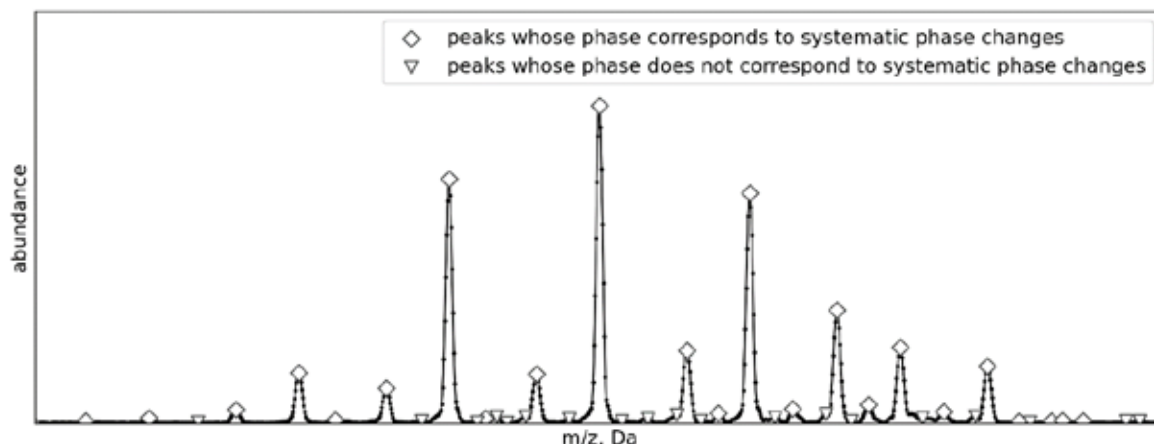


Figure 1. The result of peak classification for a NOM mass spectrum.

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The work was supported by the Russian Science Foundation, project number 21-73-20202.

PECULIARITIES OF RARE EARTH ELEMENTS PRECONCENTRATION USING COPRECIPITATION OF THEIR CHELATES WITH BISAZO SUBSTITUTED CHROMOTROPIC ACID WITH ORGANIC MATRICES IN X-RAY FLUORESCENCE ANALYSIS

Prokopenko Y.R., Kuznetsov V.V.

*D. Mendeleev University of Chemical Technology of Russia,
125047, Moscow, Miusskaya Square, 9, Russia,
e-mail: prokopenko.i.r@muctr.ru*

The efficiency of rare earth elements (REE) preconcentration from solutions by coprecipitation of their chelates with bisazosubstituted chromotropic acid with different functional groups (arsenazo III, nitkhromazo, carboxyarsenazo and chlorophosphonazo III) has been studied. The blocking of hydrophilic analytically active sulfogroups in the reagents was achieved due to their association with sufficiently large cations of arylmethane dyes. The high coprecipitation efficiency is ensured because of sufficiently large similarity of chelate associates with reagents and these with an excess of reagent with dye cations.

A fundamentally important solution is also the introduction into the system of a water-insoluble polymer precipitator that is indifferent to REE¹. This technique ensures almost complete coprecipitation and, after filtering the concentrate through a standard dense paper filter, prepare solid-phase compact concentrate-emitter with an adjustable layer thickness and a flat surface. Maximum coprecipitation is achieved when using polyvinylbutyral as an indifferent film-forming coprecipitant, added in the form of a small amount of alcohol solution. The achieved preconcentration coefficients are $1.5 \cdot 10^4$. This makes it possible to reach LOD (IUPAC) $0.007 \mu\text{g/ml}$ when concentrating samples from 50 ml solutions. Practical examples of REE determination in bottom sediment extracts are considered.

The list of used reagents allows to flexibly select the best option for solving practical problems.

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THE POSSIBILITY OF USING FTIR SPECTROMETRY IN DETERMINING COUNTERFEIT LINOLEUMS

Redkin N.A., Lobacheva I.V., Lobachev A.L., Shumska N.Yu.

*Samara University,
443086, Samara, Moskovskoye shosse, 34,
e-mail: redkin.na@ssau.ru*

Linoleum is one of the most common flooring types that can be used in residential, office and industrial premises. The wide distribution of this coating is facilitated by its high resistance to direct sunlight, some chemicals, and abrasion resistance. At the same time, the growth in demand in the linoleum market has led to a natural increase in the share of counterfeit products.

Counterfeit linoleums, imitations of well-known brands, are sharply inferior in quality to the originals due to the use of cheaper and lower quality raw materials, and therefore can serve as a source of increased danger to human health due to the release of toxic components from these materials. Identification of counterfeit linoleum samples makes it possible to prevent the use of counterfeit goods by consumers and minimize risks to their health.

In this work, a technique was proposed for analyzing polyvinylchloride linoleums using Fourier transform infrared spectrometry.

It was proposed to compare the IR spectra of extracts with chloroform from the linoleum layer on which the pattern was applied. For different brands of linoleum, spectra are obtained in which a number of absorption bands retain their intensity constant, while for a number of bands significant differences are observed both when moving from one brand to another, and within samples of the same brand. The ratios of the intensities in the IR spectra to the intensity of the absorption band of the C=O group, which has the highest intensity, were taken as analytical signals. The obtained characteristics made it possible to identify group characteristics suitable for determining the brand of linoleum and identifying counterfeits.

THE STUDY OF IR SPECTRA PROCESSING FOR THE ATENOLOL QUANTITATIVE ANALYSIS

Khisiyamov M.M., Redkin N.A., Onuchak L.A.

*Samara National Research University,
443086, Samara, Moskovskoye shosse, 34,
e-mail: hisiamov@yandex.ru*

In recent years, there has been an increasing use of computer technologies in analytical chemistry. Various methods for processing analytical data based on mathematical tools have been developed.

In this paper are compared the IR spectrometry quantitative determination results of atenolol in tablet using the method of absolute calibration and chemometric.

At the first stage, quantitative analytical methods were developed and verified using the absolute calibration method. However, it was found that two absorption bands can be used for analysis, although they are difficult to associate with specific functional groups in atenolol and they do not correspond to the strongest absorption bands in the spectrum.

At the second stage, the projection to latent structures was used to construct calibration dependencies. It has been demonstrated that the spectra of the atenolol compound are not suitable for such analysis, since there are significant differences in the IR spectra of pure atenolol compared to that extracted from tablets during the extraction process. However, using the spectra of atenolol isolated from tablets with known concentrations of the active ingredient, it became possible to develop a model for estimating the content of atenolol in tablets.

Both methods can potentially be used for the analysis of pharmaceuticals. The traditional method is suitable for small batches, while the chemometric approach can be used when comparing samples from different batches.

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DETERMINATION OF POLYCYCLIC AROMATIC HYDROCARBONS IN ATMOSPHERIC AIR

Roeva N.N., Kulikova N.E., Chernobrovina A.G., Zaitseva I.A., Yakovlyuk R.O.

*FSBEI “ Russian Biotechnological University”,
Volokolamskoe shosse, d.11, Moscow, 125080, Russia,
e-mail: roeva@mgupp.ru*

Man-made human activity has a negative impact on the ecological state of natural ecosystems. The atmosphere is not an exception, since the contribution of emissions of various pollutants into it, both of inorganic and organic origin.

Polycyclic aromatic hydrocarbons, which have pronounced carcinogenic properties, are of particular concern among pollutants of organic origin.

The authors conducted monitoring of enterprises in the Kaluga and Tula regions and assessed the degree of emission of 3,4-benz(a)pyrene and 1,12-benzoperylene entering the atmosphere as a result of their activities.

The sampling conditions have been optimized to ensure the completeness of extraction of analyzed PAHs from the atmosphere.

Concentration levels of 3,4-benz(a)pyrene and 1,12-benzoperylene in atmospheric aerosols were determined by liquid chromatography and quasi-linear luminescence spectra using additives.

It was found that the minimum detectable amounts of 3,4-benz(a)pyrene and 1,12-benzoperylene in the chromatographed volume (50 μ l) were 0,4 and 0,6 ng, respectively. When using quasi-linear luminescence spectra using additives, the range of detectable concentrations of 3,4-benz(a)pyrene ranged from 10^{-7} to 10^{-2} mg/m³.

METAL-ORGANIC FRAMEWORKS APPLICATION FOR MERCURY CONCENTRATION AND SPECIATION

Romanova T.E.^{a,b} Volynkin S.S.,^c Shuvaeva O.V.^{a,b}

^a*Nikolaev Institute of Inorganic Chemistry, SB RAS,
Ac. Lavrentieva ave. 3, Novosibirsk, 630090, Russia,
e-mail: romanova@niic.nsc.ru*

^b*Novosibirsk State University,*

Pirogova str. 1, Novosibirsk, 630090, Russia

^c*V.S. Sobolev Institute of Geology and Mineralogy, SB RAS,
Ac. Koptuga ave. 3, Novosibirsk, 630090, Russia*

Metal-organic frameworks (MOFs) are a new promising class of materials. These materials have found several applications including storage and separation of gases, sensors, catalysis and functional materials, but in the last decade, they have also attracted interest as stationary phase in separation technologies¹. Their key properties are high porosity, large pore volume, high surface areas, uniform structured cavities and uniform pore size, wide possibilities of direct design of polymers. Due to this properties MOFs can be regarded as promising materials for use in gas chromatography (GC), high performance liquid chromatography (HPLC), and solid phase extraction (SPE) as a stationary phase.

Despite the fact that some MOFs, such as UiO-66, can be synthesized by a method that provides a low cost of the product with a yield of more than 90%, it seems promising to obtain regenerated sorbents, so the possibility of regenerating sorbents will be studied.

From this point of view, Zr-ttdc, a zirconium and thienthiophene dicarboxylic acid based MOF, appears to be a promising compound. Theoretically, this coordination polymer can be used for selective sorption or separation of chemical species of mercury and a number of chalcophile elements. An important difference between this MOF and UIO-66 is the implementation of chemisorption, due to the formation of coordination bonds between active sorption centers and mercury atoms. Moreover, unlike MOFs with sulfhydryl groups, this MOF allows not only to selectively concentrate mercury, but also to ensure regeneration of the sorbent due to weaker interactions with Hg.

This work was supported by the Russian Science Foundation (project No 23-73-01154).

NEW SUPRAMOLECULAR SYSTEMS BASED ON SILVER NANOPARTICLES AND NANOIONITE

Romanovskaya G. I., Koroleva M. V.

*Vernadsky Institute of Geochemistry and analytical chemistry
Russian Academy of Sciences, 119991 GSP-1, Moscow, Kosygina, 19
e-mail: gromanovskaya@yandex.ru*

Methods of synthesis of new supramolecular systems of two types are proposed. To obtain them, we used a method of targeted modification of the surface of silver nanoparticles (NPs) and high-base nanoanionite with various chemical compounds.

Supramolecular systems of the first type contain anisotropic silver NPs¹ of 10 nm size stabilized with citrate ion, the surface of which is covered with spontaneously formed ordered micelle-like aggregates of cetyltrimethylammonium bromide molecules.

Supramolecular systems of the second type contain nanoparticles of a highly basic anionite² with a styrene copolymer matrix and 8% divinylbenzene with a size of 50÷250 nm. On the outer surface and in the pores of this nanoanionite there are spontaneously formed inclusion complexes of the “host-guest” type from chemical compounds of inorganic and organic nature (for example, negatively charged silver NPs and complexes of doxycycline with europium 3⁺).

Studies of the processes of self-assembly of starting molecules into the corresponding supramolecular systems were carried out using the fluorescent probe method. In the first case, pyrene served as the molecular probe, in the second – the doxycycline complex with europium 3⁺. Optimal conditions for obtaining new supramolecular systems have been determined.

Supramolecular systems can be used to create various composite optical and luminescent materials, and can also be used for luminescent control of chemical compounds in various objects. Moreover, the presence of anisotropic silver NPs in these new supramolecular systems makes it possible to obtain the maximum analytical signal.

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The work was carried out with the support of the Ministry of Science and Higher Education as part of the implementation of work on State assignments of the Federal State Budgetary Institution of Geochemistry and Analytical Chemistry of the Russian Academy of Sciences at the expense of budget funding.

MONOAZATRIPHENYLENE DERIVATIVES AS SELECTIVE CHEMOSENSORS FOR PICRIC ACID

Sadieva L.K.,^a Khasanov A.F.,^{a, b} Taniya O.S.,^a Valieva M.I.,^{a, b} Starnovskaya E.S.,^a Kopchuk D.S.,^{a, b} Kovalev I.S.,^a Zyryanov G.V.^{a, b}

^aUral Federal University named after the first President of Russia B.N.Yeltsin,
 620002, Ekaterinburg, Mira St.19,
 e-mail: l.k.sadieva@urfu.ru

^bInstitute of Organic Synthesis named after I.Y. Postovsky, Ural Branch of Russian Academy of Sciences,
 620219, Ekaterinburg, S. Kovalevskaya St.22

The development of effective chemosensors for fluorescent detection of nitro-explosives (NEs) is relevant for modern society. This study examined the applicability of previously obtained monoazatriphenylenes^{1,2} for the fluorimetric “turn-off” detection of such explosive substances as 2,4-dinitrotoluene (DNT), 2,4,6-trinitrotoluene (TNT) and 2,4,6-trinitrophenol (picric acid, PA). Monoazatriphenylenes showed a sensory response to all NEs, with the most pronounced response to PA, which indicates their selectivity to this analyte.

Compound **1** gave the maximum response to PA with a quenching constant up to $5.93 \times 10^6 \text{ M}^{-1}$ (compared to that for TNT – $2.54 \times 10^3 \text{ M}^{-1}$, with no response to DNT) with a quenching efficiency of 99.68% and a detection limit of 33.4 ppm (Figure 1). All this indicates the prospects of searching for chemosensors for NEs in these series.

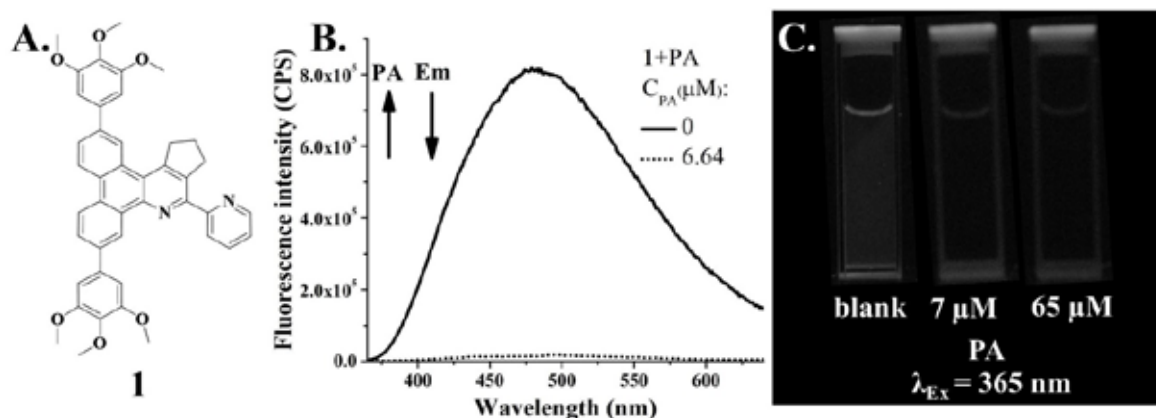


Figure 1. Structure of compound **1** (A), spectrum (B) and photo (C) of fluorescence quenching of **1** in the presence of various concentrations of PA.

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This work is supported financially by RSF #24-73-00297.

POTENTIOMETRY IN THE STUDY OF ANTIRADICAL PROPERTIES OF OBJECTS

Salimgareeva E., Kirillova V., Gerasimova E., Ivanova A.

*Ural Federal University named after the First President of Russia B. N. Yeltsin,
19 Mira st., Ekaterinburg, 620002,
e-mail: e.r.gazizullina@urfu.ru*

Currently, the study of the inhibition processes of free radical oxidation by antioxidants, as well as the development of approaches for studying these processes, is the relevant objective. Known optical methods and the EPR, studying the antiradical properties, have a number of limitations, such as the complexity of the technique and equipment, the narrow range of analyzed concentrations, the complexity of studying colored objects, etc. Since the antioxidant action is based on electron-proton-donor properties, the use of electrochemical methods, characterized by simplicity, accessibility, and rapidity, is possible for the study of antiradical properties.

For the first time, we proposed the use of the potentiometric method to study the antiradical properties of objects.

Approaches using as a model oxidant both stable radicals 2,2-diphenyl-1-picrylhydrazyl [1], the radical cation 2,2'-azinobis-3-ethylbenzothiazoline-6-sulfonate, and generated oxygen peroxy radicals of similar nature with radicals in the body [2], and the model system for the degradation of protein substrates in the Fenton reaction have been proposed.

Antioxidants were conditionally divided into "fast" and "slow" based on the obtained kinetic patterns. The standard approach was used to assess the inhibitory properties of "fast" antioxidants, in which the antiradical capacity was assessed by the induction period. The potentiometric approach, which consists in calculating the area above the kinetic curve of the $\text{Exp}(\Delta E)$ dependence, which is directly related to the amount of inhibited peroxy radicals, was proposed for "slow" antioxidants [3].

Model antioxidants, food, biological, and pharmaceutical objects were studied using the proposed approaches. The data, obtained using the developed approaches, are consistent with accepted methods for studying antiradical properties.

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SERS SUBSTRATES FOR DETECTING LOW CONCENTRATIONS OF ANALYTES IN DIRECT AND INDIRECT FORMATS OF SERS SPECTROSCOPY

Serebrennikova K.V., Zherdev A.V., Dzantiev B.B.

*A.N. Bach Institute of Biochemistry, Research Center of Biotechnology of the Russian Academy of Sciences,
Leninsky prospect 33, 119071 Moscow, Russia,
e-mail: ksenijasereb@mail.ru*

In recent years, interest in sensor systems for the determination of various compounds based on surface-enhanced Raman spectroscopy (SERS) is growing. SERS method allows obtaining spectra of both the detected compounds themselves (direct SERS spectroscopy) and reporter molecules included in specific complexes with analytes (indirect SERS spectroscopy). The analytical parameters achieved using SERS sensors vary over a wide range depending on used SERS substrate and structure of formed specific complexes. Therefore, a reasonable choice of SERS substrates that provide a high signal enhancement and effective binding of analytes is in demand.

This study proposes substrates modified by nanoparticles that make it possible to detect low concentrations of analytes of different classes in direct and indirect formats of SERS spectroscopy. Spherical gold nanoparticles with an average diameter of 31.4 ± 3.6 nm labeled with 4-mercaptobenzoic acid as the reporter molecule were used to detect the SARS-CoV-2 spike protein (RBD) in lysates of infected cells by immunochromatography coupled with indirect SERS spectroscopy. A low detection limit of 0.1 ng/mL and an assay time of 20 min were achieved using a SERS substrate based on gold nanoparticles. A substrate based on cellulose membrane and silver nanostructures of different morphologies and sizes was successfully applied for direct detection of malathion, an organophosphorus insecticide. To form plasmonic nanostructures on the substrate surface, silver nanoparticles were synthesized using the silver mirror reaction and subsequent growth of large raspberry-like silver nanostructures with simultaneous immobilization on a membrane. The proposed flexible SERS-active substrate, which combines easy manufacturing and high SERS signals, ensured the detection of malathion in low concentrations - up to 0.15 $\mu\text{g/mL}$.

The study was carried out with the financial support of the Russian Science Foundation, project 21-74-20155.

DETERMINATION OF TOXIC METALS BY MASS SPECTROMETRIC METHOD IN MEDICINAL RAW MATERIALS AND PHARMACEUTICALS

Sharapova E.K., Bardyugov N.S., Nebera E.A.

*The Russian State Center for Animal Feed and Drug Standardization and Quality,
Moscow, Russia
e-mail: kate-dronova@ya.ru*

Medicinal plant preparations and drugs are widely used in veterinary practice to improve the effectiveness of treatment due to their availability, ease of use and relatively safe pharmacological effects. However, medicinal plants are capable of accumulating toxic elements. The development of unified approaches to measuring the content of toxic elements in medicinal plant preparations and drugs will provide a reliable assessment of the content of toxic elements and minimize the risk of ingestion when using preparations based on medicinal plant raw materials.

In this work we developed a technique for the determination of toxic elements by inductively coupled plasma mass spectrometry. The advantage is the simultaneous determination of several elements, which greatly simplifies the task of large-scale monitoring, and is more cost-effective than the study of toxic elements separately. In the course of the work, herbal medicines and remedies in two forms were selected: solid (tablets, powders) and liquid (alcohol and infusion solutions) with different known contents of toxic elements. For more efficient decomposition of selected samples, the method of acid mineralization at elevated pressure in microwave systems Mars-5 (CEM, USA) and Ethos Up (Milestone, Italy) was chosen. Decomposition of samples was carried out using nitric acid with the addition of internal standard (In, Bi) and gold solution.

Operation parameters of Varian 820-MS and Agilent 7900 inductively coupled argon plasma mass spectrometers were optimized for all determined elements (necessity to use CRI and KED cells), absolute sensitivity, specificity, reproducibility of the technique were evaluated with respect to all determined elements. The range of measurements of the mass fraction of the determined elements (As, Cd, Hg, Pb, Cr, Mn, Co, Ni, Cu) was from 50 to 50000 mg/kg.

BIOPOLYMERS BASED ON CHITOSAN CONTAINING TETRAZOLE CYCLES AS COMPLEXING PALLADIUM SORBENTS

Shaulina L.P., Kizhnyaev V.N.

*Irkutsk State University,
Irkutsk, Lermontova, 26
e-mail: Shaulinalp@mail.ru*

Biopolymers in analysis are a modern direction, closely related to the study of their properties and the possibility of use. Biopolymers based on chitosan are of particular interest, but their use in sorption concentration of elements requires modification of the structure, which allows expanding the range of properties. To concentrate palladium, samples of chitosan obtained by deacetylation of chitin with subsequent transformation of nitrile fragments into tetrazole rings were studied. Deacetylation of chitin for sample ChTS-2 was carried out using a hot solution of sodium hydroxide.

The study of sorption properties and establishment of characteristics was carried out in a static mode for the powder form of the compound. Palladium was determined by the atomic absorption method.

Sorption was studied in the pH range 7-4M for solutions of hydrochloric, sulfuric and nitric acids. Palladium is extracted throughout the entire indicated acidity range with a decrease in sorption at acidity above 2M and at pH greater than 3. Maximum extraction at pH 2. Based on the obtained nature of the dependence on acidity, a conclusion was made about the proposed mechanism of formation of solid-phase complexes. In solutions of molar concentration, ion exchange interaction dominates, in the pH region - coordination interaction. The composition of the putative complexes and the extraction mechanism were confirmed by elemental IR spectroscopy data. The time to establish equilibrium and half-sorption is 20 and 8 minutes, respectively. The sorption capacity calculated from the equilibrium distribution curves is 260 and 640 mg/g, the distribution coefficients of palladium are $2,0 \cdot 10^3$ and $7,5 \cdot 10^5$ for ChTZ-1 and ChTZ-2, respectively. Under conditions of quantitative extraction of palladium, sorption of non-ferrous metals and platinum is observed. Metal acid complexes react with nitrogen-containing ligands, which are chitosan, both due to coordination and ion exchange interaction. Palladium is quantitatively eluted from the sorbent phase with a hydrochloric acid solution of thiourea. The sorbent retains its sorption activity in four sorption-desorption cycles.

STUDY OF THERMODYNAMICS SORPTION OF COPPER IONS (II) BY A SORBENT OF PLANT ORIGIN

Silaeva V.A.

*Astrakhan Tatishchev State University, Tatishcheva 20a, Astrakhan,
414056, Astrakhan Region,
e-mail: belsi2001@mail.ru*

There are many methods for removing heavy toxic metal ions from water. One promising cleaning method is sorption, the efficiency of which is determined by the quality of the sorbent [1].

An experimental study of the thermodynamics of the sorption process of Cu ions (II) from aqueous solutions on the sorbent, obtained by heat treatment of rice husks, has been conducted.

The resulting adsorption isotherms were analyzed at appropriate linearization coordinates of the classical Langmuir, Temkin and Freundlich adsorption equations. The Freundlich model [2] has been found to be the preferred process model. The experiment at three temperatures allowed to calculate the main thermodynamic characteristics of the process (table. 2)

Table 2. Thermodynamic function parameters for copper cation (II) adsorption process at different temperatures

T, K	ΔH , kJ/mol	$-\Delta G$, kJ/mol	ΔS , J/(mol·K)
284	-12,15	6,2	21,7
297		3,9	13,4
313		5,6	17,7

In conclusion, it may be noted that the results of the experiment in the future will be the basis for developing methods of cleaning water bodies of heavy toxic metals.

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RESEARCH INTO METHODS FOR THE QUANTITATIVE DETERMINATION OF BAS SUBSTANCE WITH ANTICOAGULANT ACTIVITY

Berezina E.S., Nepogodina E.A., Sobin F.V., Pulina N.A.

*Perm State Pharmaceutical Academy of the Ministry of Health of the Russian Federation,
 614990, Perm, Polevaya 2,
 e-mail: fff-2005@mail.ru*

The research team of the Perm State Pharmaceutical Academy of the RF Ministry of Health has previously synthesized 2-hydroxy-4-oxo-(4-chlorophenyl)-2-butenate of thiazolinammonium, which exhibits pronounced anticoagulant activity with different administration routes and features low acute toxicity^{1,2}.

Prior to standardizing new BAS every research is focused on the quantitative content of the active substance as the most important quality indicator. The methods must be accurate, objective, selective, reproducible and accessible. The studied BAS contains the following functional groups in its structure: ketone, enol hydroxyl, covalently bound chlorine and sulfur, a tertiary nitrogen atom, a primary amino group, and a carboxyl group.

We have tested the alkalimetric method of quantitative determination, thus displacing the organic base from the salt. The experiment has showed that fixing the equivalence point is difficult so far; in addition, the reaction may possibly proceed non-stoichiometrically.

When developing methods for identifying the new BAS³, it is revealed that the absorption spectrum of a solution in sodium hydroxide of 0.1 M has an absorption maximum at 333 nm, which is stable for solutions of different concentrations, and the optical density has an acceptable value for the spectrophotometric method to be applied. As a result, we have proposed a spectrophotometric method for standardization with calculations based on the specific absorption index.

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The work was carried out with financial support within the framework of the state task of the Perm State Pharmaceutical Academy of the Ministry of Health of the Russian Federation (code 720000F.99.1.BN62AB06000), 2024.

QUANTITATIVE ASSESSMENT OF THE COORDINATION STATE OF ATOMS IN THE NEAR-SURFACE LAYER OF SOLID

Sosnov E.A.

*Saint-Petersburg State Institute of Technology,
26, Moskovskii prospect,
St. Petersburg, 190013, Russia,
e-mail: sosnov@lti-gti.ru*

Various functional (sorption, catalytic, etc.) properties of solids are largely determined by the chemical composition and structure of their surface, which makes it necessary to identify not only the structure of the bulk phase of the substance, but also the structure of its surface layer. An effective method to evaluate the coordination state of atoms on the surface of solid-phase materials (and on this basis to predict the functional properties of solid-phase material) is electron spectroscopy of diffuse reflectance (ESDR) in the ultraviolet and visible spectral region, which allows to identify the composition of the near-surface layer 1.5 - 2 nm thick¹. However, when atoms with different coordination environment are present on the surface, it is rather difficult to quantitatively characterize the composition of the surface layer.

On the example of a number of TiO₂ samples (anatase and rutile) of different genesis and two-phase pyrogenic titanium dioxide AEROXIDE TiO₂ P25 (Evonik Degussa Corp.) the possibilities of program division of ESDR spectra into components corresponding to polyhedra with different coordination environment of titanium atom^{2,3} are demonstrated.

The results of spectra separation are compared with other methods of ESDR spectra representation (determination of the absorption band edge by the tangent method, representation in Gurevich-Kubelka-Munk (F_R) and Tauc $(\alpha h\nu)^m \propto (h\nu - E_g)$ coordinates) and with the data of spectra hardware differentiation. Based on the results of separation of ESDR spectra of two-phase titanium dioxide P25 and XRD data, a relation linking the intensities of spectral transitions corresponding to anatase- and rutile-like coordination of titanium with the quantitative ratio of the corresponding structures on the TiO₂ surface was proposed.

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DIFFERENCES IN THE ION MOBILITY SPECTRA OF SATURATED NITROGEN-CONTAINING HETEROCYCLES

Stepanova D.V., Alexandrova D.A., Melamed T.B., Luzyanina L.A., Baberkina E.P., Yakushin R.V.

*Dmitry Mendeleev University of Chemical Technology of Russia,
 125480, Moscow, Geroyev Panfilovtsev str., 20, building 1,
 e-mail: stepanovad02@mail.ru*

Differences in the ion mobility spectra of piperazine, morpholine, 2-methylpiperazine, N-methylpiperazine, N-aminopiperazine and 1-amino-4-methylpiperazine in the field of positive ionization were established using the Kerber-T ion drift spectrometer from Yuzhpolymetal-Holding Group in Moscow. The proton affinity (PA) values for these substances were calculated using the ab initio quantum chemistry program package ORCA version 5.0.4, using the hybrid B3LYP functional with a def2-SVPD1 basis sets. Figure 1 illustrates the correlation of the reduced ion mobility values (K0) with the molecular weight (Mr) and proton affinity (PA).

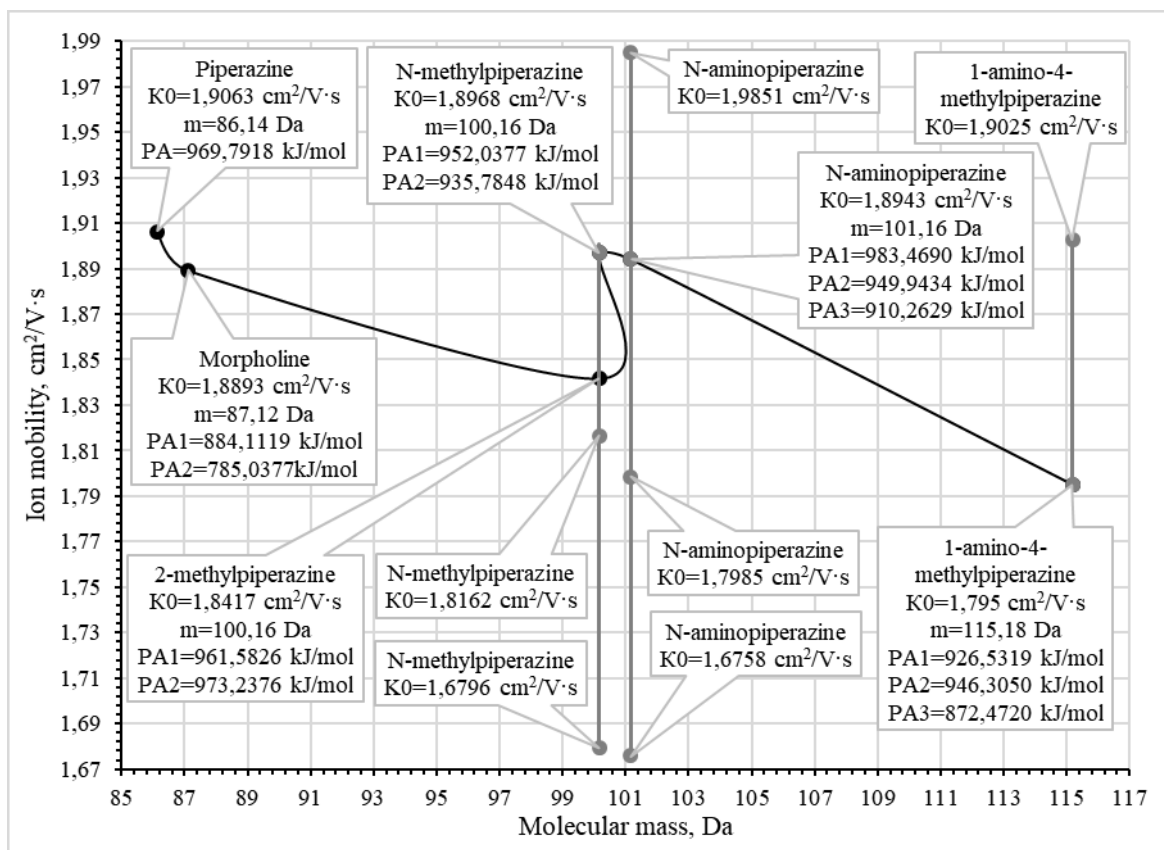


Figure 1. Values of K0, Mr and PA of saturated nitrogen-containing heterocycles.

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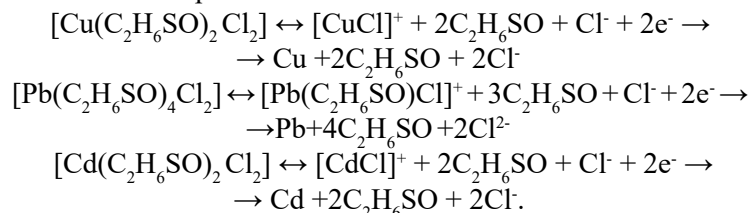
SIMULTANEOUS VOLTAMMETRIC DETERMINATION OF CU(II), PB(II) AND CD(II) USING DMSO-CONTAINING BACKGROUND ELECTROLYTES

Trubachev A.V., Trubacheva L.V.

*Udmurt State University,
Universitetskaya str., 1, Izhevsk, 426034,
e-mail: trub_av@mail.ru*

The use of mineral-organic background electrolytes in voltammetry containing organic solvents with high solvating ability makes it possible to increase the selectivity and accuracy of the determination of metallocations due to the formation of metal complexes in solution, which include in the coordination sphere molecules of organic solvents and electrochemically active particles of various compositions. Among organic solvents with high donor numbers, the greatest effect is achieved when using dimethylformamide (DMFA, DN=26.6) and dimethylsulfoxide (DMSO, DN=29.8).

It was found that in acidic chloride media (pH=2; 0.1 M KCl + 0.1 M LiCl) in the presence of 4-6 M DMSO, Cu(II), Pb(II) and Cd(II) are reduced at the electrode with the formation of clear cathode current peaks, while their potentials are shifted to the region of more negative values with an increase in the difference of $\Delta E_{Cu/Pb}$ to 350 mV and $\Delta E_{Pb/Cd}$ to 250 mV (in the absence of DMSO, their values are 200 and 150 mV, respectively). It was found that the following electrochemical reactions take place under these conditions:



Electroreduction is irreversible in the case of copper(II) and cadmium(II), in the case of lead(II) the process is reversible, while the limiting current in all cases is controlled by diffusion. The linear dependence of the limiting current on the content of depolarizers in solution is observed within the following concentration limits: for copper(II) - $4 \cdot 10^{-5} \div 2 \cdot 10^{-3}$ M, for lead(II) - $1 \cdot 10^{-5} \div 6 \cdot 10^{-4}$ M, for cadmium(II) - $5 \cdot 10^{-5} \div 1 \cdot 10^{-3}$ M. A method for the voltammetric determination of copper, lead and cadmium with their simultaneous presence in complex objects against the background of DMSO-containing chloride electrolytes is proposed.

DETERMINATION OF TRACE ELEMENT COMPOSITION OF BIOPSY MATERIAL OF RED BONE MARROW IN PATIENTS WITH HEMOBLASTOSES BY X-RAY FLUORESCENCE ANALYSIS USING SYNCHROTRON RADIATION

Trunova V.A.¹, Pospelova T.I.², Voytko M.S.², Krupovich E.S.¹, Soldatova G.S.²

¹*Institute of Inorganic Chemistry named after: A.V. Nikolaev SB RAS, 630090, Novosibirsk,
Пр. Академика Лаврентьева, 3
valna-t@mail.ru*

²*Department of Therapy, Hematology and Transfusiology (FPK and PPV), Novosibirsk State Medical University,
630091, Novosibirsk, Красный проспект, 52*

Significant advances in the treatment of hematological malignancies associated with the introduction of standardized protocols for chemoradiotherapy, targeted drugs and transplantation technologies have naturally led to an increase in the overall survival of patients. The search for available markers for early diagnosis and determination of the prognosis of tumor diseases of hematopoietic tissue is an urgent task. The search for available markers for early diagnosis and determination of the prognosis of tumor diseases of hematopoietic tissue is an urgent task. Advantages of a synchrotron radiation beam:

- high brightness allows you to reduce sample measurement time and reduce requirements for the size and weight of samples,

- natural SR polarization significantly reduces detection limits,

- the non-destructive nature of the method allows you to create a data bank of samples and use it in subsequent studies.

To study the distribution of trace elements in the bone marrow using X-ray fluorescence using synchrotron radiation (XRF-SR) in patients with hemoblastosis.

The analysis of trace elements in the bone marrow was carried out by X-ray fluorescence analysis using synchrotron radiation (XRF-SR) at the Siberian Center for Synchrotron and Terahertz Radiation at the Institute of Nuclear Physics (BINP SB RAS) on the VEPP-3 storage ring. The following chemical elements were determined: K, Ca, Cr, Mn, Co, Ni, Fe, Cu, Zn, As, Se, Br, Rb, Sr, Mo, La, Th. Carrying out analysis with variations in the energy of exciting quanta makes it possible to reduce the required detection limits. Sample preparation of the material under study eliminates thermal heating and interactions with acids, and this eliminates the possibility of both loss of microelements from the sample and the possibility of introduced contaminants.

The data obtained will allow us to identify early predictors of the refractory-recurrent course of hemoblastosis. The results of the study were tested in clinical practice and approved by the Local Ethics Committee of the hospital.

ELEMENTAL ANALYSIS OF PALLADIUM ALLOYS - MATERIALS FOR HYDROGEN ENERGY

**Volchenkova V.A.^{a,b}, Penkina T.N.^a, Kazenas E.K.^a, Fomina A.A.^a, Roshan N.R.^a,
Gorbunov S.V.^a, Kasyanov V.S.^a, Solntsev K.A.^a, Tarnopolskaya M.V.^b**

*^aA.A. Baikov Institute of Metallurgy and Materials Science, Russian Academy of Sciences,
49 Leninsky Prospekt, Moscow, 119334,
e-mail: volch.v.a@mail.ru*

*^bInstitute of Geology of Ore Deposits, Petrography, Mineralogy and Geochemistry, Russian Academy of Sciences,
35 Staromonetny per., Moscow, 119017*

When conducting research on the creation of new materials for hydrogen energy - palladium alloys of a given chemical composition of systems: Pd - Cu, Pd - Ag, it is necessary to determine the content of both impurity elements and macrocomponents (Cu, Ag).

The use of atomic emission spectrometry with inductively coupled plasma (AES - ICP) and atomic absorption spectroscopy (AAS) - methods of analysis with complementary analytical capabilities, provided high-precision determination of the contents of macrocomponents (Cu, Ag) and functional elements (Ru, In, Y, Sc, Pb, Co) in a wide range of concentrations ($n \cdot 10^{-3}$ - $n \cdot 10\%$) from a limited amount of material (from 5 mg) without the use of certified solid composition standard samples.

Depending on the genesis of the studied compounds, the optimal schemes of sample preparation were found and the composition of acids was selected to obtain stable solutions of easily hydrolyzable matrix and impurity elements. Dissolution of samples was carried out in open or closed systems (Mars 5 microwave oven - CEM Corporation, USA). In the case of difficult-to-open samples (with a ruthenium content of more than 2%), the method of fusion with sodium peroxide was used.

The optimal analytical parameters for AES - ICP and AAS determination of elements were established.

Analytical control techniques provided research on the development of new alloys with enhanced physical and mechanical properties, as well as high specific hydrogen permeability, for hydrogen power generation.

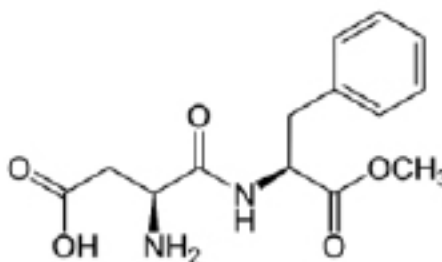
The work was carried out according to the state assignment No. 075-00320-24-00

SENSORY SYSTEMS AS AN AVAILABLE METHOD FOR DETERMINING SWEETENERS IN LIQUIDS

Vybornyi A.Yu., Zyablov A. N.

Voronezh State University, 1 Universitetskaya pl., Voronezh, 394018, Russia
e-mail: antonvyb.job@gmail.com

Sweeteners are one of the most common food additives because they make it possible to produce food that is safe for people with diabetes or metabolic syndrome. However, there are a number of studies that indicate a direct relationship between the consumption of sweeteners and an increased risk of developing various diseases, including cancer. This is especially true for sweeteners such as aspartame¹, which over the past few years has become widely used by soft drink manufacturers in Russia.



In addition, recently sweeteners are also being considered as a new source of environmental pollution, in particular wastewater².

In this work, quartz resonator-based sensors were developed, which are low cost and widely available. These sensors were modified with a molecularly imprinted polymer³ using aspartame molecules as a template molecule. The use of this technology made it possible to achieve selective determination of the target sweetener in a multicomponent liquid medium, which was shown in the analysis of model solutions simulating soft drinks using the “introduced-found” method, and the standard deviation did not exceed 9%.

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ANALYTICAL CONTROL OF THE CONTENT OF CHEMICAL FORMS OF MERCURY IN SURFACE WATER

Roeva N.N., Zaytseva I.A., Buzdakov D.R.

*FSBEI “ Russian Biotechnological University”,
Volokolamskoe shosse, d.11, Moscow, 125080, Russia,
e-mail: roeva@mgupp.ru*

Mercury is the most toxic pollutant of surface waters. The migration of this element and the efficiency of its accumulation in surface waters are determined by chemical forms with different degrees of toxicity. Of these forms of mercury, organomercury compounds are the most toxic to humans and biomes, so it is important to quantify these forms.

Labile forms of mercury in the surface waters of the Kaluga and Moscow regions have been studied.

A scheme for the separation of these forms (suspended, inorganic, organic, dialkylmercury, alkylmercury hydrocarbons) is proposed for the purpose of their differentiated analysis.

The dynamics of the isolated content of these forms depending on the hydrological regime and the distribution from the source of contamination are studied.

The contribution of suspended inorganic and organic forms to the migration of mercury in the surface waters of the Kaluga and Moscow regions is estimated.

It has been established that the dominant migration form is organomercury.

A combined method for the determination of organic and inorganic forms of mercury with a lower detection limit of 0.04 micrograms/l has been developed.

The background of the entire page is a dark, almost black, space filled with intricate, glowing patterns of particles. These particles are arranged in dense, swirling clusters and trails, primarily in shades of bright blue and vibrant orange. The overall effect is reminiscent of a microscopic view of a chemical reaction or a complex molecular structure, with the particles appearing to be in motion, creating a sense of dynamic energy and scientific exploration.

Section 7

CATALYSIS IN SCIENCE AND INDUSTRY

ISOPROPYLATION OF TOLUENE ON BIMETALLIC CATALYSTS BASED ON ZSM-5 ZEOLITE

Abdullaeva N.M.^a, Voskresensky L.G.^b, Gahramanov T.G.^a, Mamedov E.S.^c

^a*Baku State University, AZ 1148, Baku, 23 Zahid Khalilov str.
e-mail: nigaremirova@yandex.com*

^b*Peoples' Friendship University of Russia, 117198, Moscow, Miklukho-Maklaya str.6*

^c*Baku Branch of Lomonosov Moscow State University, AZ1143, Baku, Huseyn Javid Avenue, 133*

The purpose of this work was to study the joint modification of ZSM-5 type zeolite with La and Ni on the para-selectivity of a bimetallic catalyst in the alkylation reaction of toluene with isopropanol.

Bimetallic catalysts with the composition 0.5-1.5% Ni 3%La-HZSM-5 were prepared by impregnation using an aqueous solution (0.03-0.10 g/10 ml) of lanthanum nitrate and nickel acetate. The catalysts were characterized by XRF, BET, BJH and ammonia TPD methods.

Catalytic experiments were carried out in a flow-through installation in a quartz reactor with a load of 2.0 g of catalyst in the temperature range 300-350°C with a volumetric feed rate of 1.0 h⁻¹, molar ratio C₇H₈:i-C₃H₇OH: H₂ = 2:1:0.5.

It was shown that unmodified HZSM-5 zeolite exhibits lower selectivity (54.6-58.2%) for isopropyltoluenes than modified catalysts. The content of the valuable isomer 4-IPT does not exceed 44.2%. Modification of HZSM-5 with lanthanum in an amount of 3.0 wt.% leads to an increase in selectivity for IPT to 69.8%, and selectivity for 4-IPT to 65.8%. The introduction of nickel into the composition of 3%-La-HZSM-5 in an amount of 1.0 wt.% prevents the formation of 2-IPT and promotes an increase in the yield of 4-IPT.

Modification, calcination of the catalyst leads to a dispersed distribution of nanoparticles of La₂O₃ oxide and metallic nickel in the outer surface and in the pores of the zeolite, which causes a decrease in the specific surface area, total pore volume and an increase in the proportion of mesopore volume.

All this has a decisive influence on the selectivity of 4-IPT formation and the stability of the bimetallic catalyst. The maximum selectivity for 4-IPT on the bimetallic catalyst 3% La 1.0% Ni/HZSM-5 is achieved at 330°C and is 73.2% with a toluene conversion of 24.2%.

ETHYLENE OLIGOMERIZATION USING IONIC LIQUID TYPE CATALYTIC SYSTEMS, MODIFIERS AND REACTION AREAS

Khamiyev M.J., Aliyeva R.V., Ibrahimova M.J., Mahammadzade R.Z.

*Institute of Petrochemical Processes named after academician Y.H.Mammadaliyev,
Khojaly pr. 30, Baku, AZ1025, Azerbaijan.
e-mail: alreyhan@yahoo.com*

Interest in ionic liquids (IL) has been growing rapidly in recent years. IL, which are included in the principle of "Green chemistry", also occupy an important position in petrochemical processes.

The presented work studies the results of research on new methods for the accessible synthesis of zirconium aminophenolate complexes with ionic liquid ligands (ZIL) for ethylene oligomerization. Chloroaluminate ionic liquids (CIL) have also been studied as modifiers and reaction media extensively in these processes.

It is known that in the metal complex catalysis of olefins, in comparison with other transition metals, complexes containing zirconium are obtained more easily, and isomerization of α -olefins almost does not occur in their presence. As a result of oligomerization of ethylene in the presence of zirconium-containing ZIL and obtained various organic aluminum compounds, low molecular weight α -olefins (80-90%), which consist of C_4 - C_{10} fractions. In the presence of ethylaluminium dichloride as aluminum organic compound the higher branched structured oligomers (oil fraction) is obtained with >75 % yield. It has been shown that by using electron donor and acceptor type modifiers, it is possible to regulate their molecular and other properties by making purposeful changes in the structures of these catalysts and type of ligands. Electronodonor modifiers were used in the oligomerization process of ethylene in the presence of various zirconium complexes consisting of alkyl aluminum chlorides as activators.

Thus, it should be noted that our research shows once again the special importance of ionic liquids in the metal complex catalysis of ethylene, and in the future these processes can be widely used in recirculating two-phase industrial catalysis.

INVESTIGATION OF THE PROPERTIES OF CeO_2 AND Nd_2O_3 CATALYTIC COMPOSITE WITH ZSM-5 ZEOLITE IN THE CONVERSION OF METHANOL TO $\text{C}_2\text{-C}_4$ ALKENES AND AROMATIC HYDROCARBONS

Babayeva T.A.^a, Mamedov S.E.^a, Mamedova A.Z.^b, Mirzaliyeva S.E.^a

^a*Baku State University, AZ 1148, Baku, 23 Zahid Khalilov str.
e-mail: azeri09@mail.ru*

^b*Azerbaijan State Oil Industry University, AZ1010, Baku, Azadliq Avenue, 20*

The target of this work was to study the properties of catalytic compositions obtained by solid-phase mixing of cerium and neodymium oxide nanopowders with zeolite of ZSM-5 type ($\text{SiO}_2/\text{Al}_2\text{O}_3=40$) in the conversion of methanol into $\text{C}_2\text{-C}_4$ alkenes and aromatic hydrocarbons.

Increasing the concentration of CeO_2 and Nd_2O_3 in the catalytic composition up to 6.0 wt.% promotes an increase in the yield of $\text{C}_2\text{-C}_4$ alkenes up to 32.9-34.3%. The yield of aromatic hydrocarbons passes through a maximum and the highest content of aromatic hydrocarbons (39.5 wt.%) and xylene fraction (24.1 wt.%) is achieved at a modifier content of 4.0 wt.%.

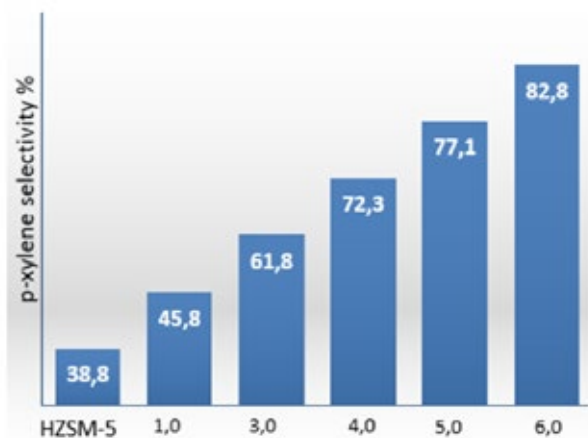


Figure 1. Effect of the concentration of CeO_2 in the catalytic composition on the selectivity for p-xylene ($T=400^\circ\text{C}$, $v=2\text{h}^{-1}$)

Increasing the content of cerium oxide in the catalytic composition is accompanied by an increase in the content of p-xylene in the xylene mixture, i.e. an increase in the selectivity for p-xylene (figure 1). High selectivity for p-xylene (76.8-82.8%) is achieved on catalysts containing 5.0-6.0 wt.% cerium oxide.

SELECTIVE HYDROGENATION OF CARBON DIOXIDE IN THE PRESENCE OF THE FE-CARBON CATALYST

Chemakina I.S.^a, Ivantsov M.I.^b, Elyshev A.V.^a, Kulikova M.V.^b

^a*University of Tyumen, Volodarskogo 6, 625003, Russia, e-mail: i.s.chemakina@utmn.ru*

^b*A.V. Topchiev Institute of Petrochemical Synthesis, RAS, Leninsky prospekt 29, Moscow, 119991, Russia*

The widespread use of fossil fuels is accompanied by excessive release of carbon dioxide (CO₂) into the atmosphere, which negatively affects the environment. Hydrogenation of CO₂ into synthetic methane (CH₄) can not only reduce the greenhouse effect, but also solve the problem of global energy scarcity. The purpose of this work is to evaluate the catalytic activity of a Fe-carbon catalyst on a microcrystalline cellulose (MCC) substrate during the selective hydrogenation of CO₂.

The catalytic system of 20% Fe/MCC was synthesized by hydrothermal synthesis at 230 °C in an inert atmosphere, characterized by XRF, TGA, SEM, and ISP-OES methods. It is shown that spherical structures are formed on the surface of the sample during synthesis (Figure 1).

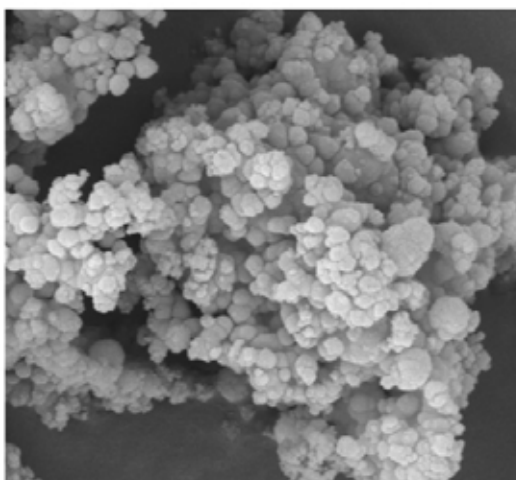


Figure 1. Micrography of the sample.

The test of the sample in the reaction of selective hydrogenation of CO₂ showed that in the presence of the synthesized Fe-carbon catalyst the conversion of CO₂ reaches 74%, and the selectivity for CH₄ reaches 65%, which proves the satisfactory catalytic activity of 20% Fe/MCC.

The study was carried out with the financial support of the Government of the Tyumen Region under the project of the West Siberian Interregional Scientific and Educational Center No. 89–DON (3) and within the framework of the State Task of the A.V. Topchiev Institute of Petrochemical Synthesis of the Russian Academy of Sciences.

RESEARCH OF THE INFLUENCE OF RAW:HYDROGEN RATIO ON THE PROCESS OF NORMAL HYDROCARBONS ISOMERIZATION WITH ALUMINOSILICATE $K_2Al_2Si_6O_{16}$

Chudovskiy A.S., Isaeva D.T., Popova T.S., Lagunov M.A., Ryabchenko T.Y.

*Far Eastern Federal University, Ajax Village 10, Vladivostok, 690922, Russia,
e-mail: chudovskiy.as@dvfu.ru*

The process of isomerization of light gasoline fractions, which leads to the formation of branched isomers from normal paraffins, has become increasingly important in the production of gasoline, due to the ever-stricter requirements imposed on these fuels within the territory of the Russian Federation.

The object of study is the process of n-hexane isomerization on the catalytic flow laboratory setup LabCAT (Neosib, Russia). A zeolite catalyst with the composition $K_2Al_2Si_6O_{16}$, provided by the Institute of Chemistry FEB RAS, was utilized¹. The research focused on investigating the influence of the raw:hydrogen molar ratio on the conversion of n-hexane, as well as the yield of three most significant isomers (2,3-dimethylbutane, 2-methylpentane, 3 methylpentane).

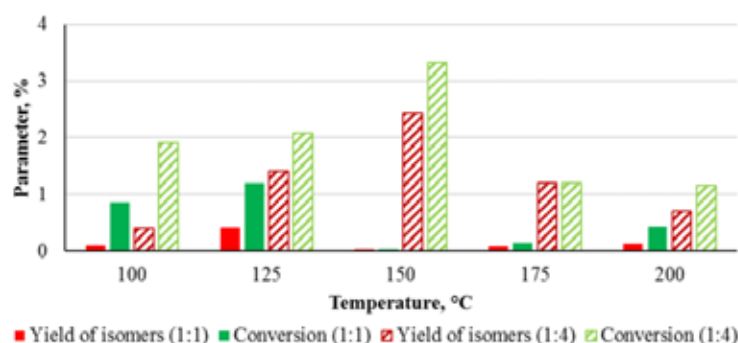


Figure 1. N-hexane conversion and yield of isomers dependence on temperature and raw:hydrogen molar ratio at pressure 15 MPa and volumetric hourly space velocity 2 h^{-1}

The maximum conversion of n-hexane (3.33 %) was achieved during the experiment at 150 °C. A decrease in the conversion was observed as the temperature varied and the raw:hydrogen ratio was reduced. The maximum yield of isomers (2.44 %) was obtained at 150 °C with a raw:hydrogen ratio of 1:4. Among all the isomers, 2-methylpentane demonstrated the highest yield.

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ACTIVATED KAOLINITE IN CRACKING FUEL AND ITS MIXTURE WITH VACUUM GASOIL

**Volkova L.D.^a, Kim O.K.^a, Akurpekova A.K.^a,
Gabdrakipov A.V.^b, Kharlamova T.V.^c**

^aJSC «Institute of Fuel, Catalysis and Electrochemistry named after D.V. Sokolsky», 050010, Almaty, Kunaeva, 142
 e-mail: volkova_ld@rambler.ru

^b Scientific Analytical Center LLP, 050060, Almaty, Tazhibaeva, 124

^c JSC «Institute of Chemical Sciences named after A.B. Bekturov», 050010, Almaty, Ualikhanov, 106

Interest in the study of clays as matrices and catalysts for oil refining. Determined by their abundance in nature and an effect was obtained with a change in surface, structural and acidic characteristics.

The goal of the work was to prepare a catalyst that does not separate zeolite, based on acid-treated kaolinite, modified with a radiation hydrocomplex (2.5 mmol Al₃⁺/g) and hydroxide gel synthesized by the ammonia method in the cracking of fuel oil and its mixtures with vacuum gas oil (VG).

Kaolinite from the Pavlodar region of Kazakhstan (PK-1) was used in this work. Each stage of catalyst preparation was completed by high-temperature treatment. We designated the catalyst as Al(2.5)HPK-1 + Al₂O₃. Chemical analysis of the samples before and after activation was carried out using X-ray fluorescence spectroscopy. The SiO₂/Al₂O₃ value was controlled. Cracking was carried out at 500 and 550°C in a reactor with a stationary bed of catalyst and chromatographic analysis of raw materials and cracking products. The specific surface area of the sample is -125.1 m²/g, the content of mesopores is 70.1%, the total acidity for ammonia adsorption is 80.0 μmol NH₃/g. SiO₂/Al₂O₃ ratio -1.53.

At 500°C for fuel oil and its mixture with VG on the developed catalyst, the yields of the main cracking products (%) are: gasoline 23.8 and 29.6, light gas oil 19.3 and 25.7 with feed conversion 84.3 and 88.7, respectively. Cracking gasolines are distinguished by a significant content of iso-paraffinic hydrocarbons: (25.6 and 27.3%), aromatic (30.7 and 38.3%), naphthenic (8.3 and 5.6%) and unsaturated hydrocarbons (23.0 and 16.3%).

Modified kaolinites can be catalysts for cracking heavy and residual petroleum feedstocks.

COMPOSITE NANOPARTICLES AS A BASE FOR THE CREATION OF SOLID HETEROGENEOUS CATALYSTS WITH A HIGHLY DEVELOPED SURFACE

Isaeva I.Yu.¹, Ostaeva G.Yu.¹, Morenko I.V.¹, Grushina V.V.²

¹*Moscow Automobile and Road Construction State Technical University (MADI), Moscow, Leningradsky prospect 64*

²*ООО "Chemistry XXI century", Moscow, pr-d Entuziastov 19, str. 13*

E-mail: (irina-razumova-xim@yandex.ru)

The possibility of obtaining a catalyst based on modified zeolite (base) with copper and nickel nanoparticles embedded in its pores for the synthesis of quinolines was investigated in this study. Copper and nickel nanoparticles were obtained by chemical synthesis from aqueous solutions. Tert-butylamine-borane was used as a reducing agent. PVP (MM 360000) was used to stabilize the size and growth of copper and nickel nanoparticles. The resulting sol was applied to a pre-prepared zeolite. The polymer matrix was removed by thermal degradation to avoid negative effects. Heating in the muffle furnaces at a speed of 5° C /min to 450° C was carried out within 4 hours. The XRD showed that during cyclic sol deposition and annealing, the increase in particles on the carrier is 10.6 times higher in compare with the one without annealing. This indirectly indicated the removal of a significant amount of PVP. The result was achieved after two stages of annealing. Two stages are enough for saturation.

The study of samples by the TEM method showed a small number of aggregated particles and their uniform distribution over the surface of the catalyst. At the same time, the sizes of the synthesized particles are in the range from 20 to 80 nm.

The samples were tested in the reaction of propanal with nitrobenzene at a temperature of 200° C, for 5 hours to evaluate the effectiveness of the obtained catalysts. As a result, the conversion of nitrobenzene was 11%, and the selectivity of quinoline and tetrahydroquinolinamine was 10 and 77%, respectively. At the same time tetrahydroquinolinamine is a precursor to quinoline. The obtained data indicate the effectiveness and possibility of using the obtained catalyst based on modified zeolite with deposited metal nanoparticles.

SELECTIVE HYDROGENATION OF OXIMES ON HIGH PERFORMANCE 1%Pt/CeO₂-ZrO₂ CATALYST

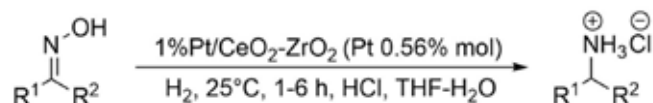
Ivanova I.I.,^{a,b} Redina E.A.^a

^a*N.D. Zelinsky Institute of Organic Chemistry of the Russian Academy of Sciences,
 Leninsky prospekt 47, Moscow, 119991, Russia,
 e-mail: inigiv022@gmail.com*

^b*Higher Chemical College of the Russian Academy of Sciences,
 Mendeleev University of Chemical Technology of Russia, 9 Miusskaya sq., Moscow, 125047, Russia*

Hydrogenation of oximes is a common way to introduce an amino group in the structure a molecule. This step appears to be the most applied in the synthesis of pharmaceuticals due to facile procedure and satisfactory product yields.

Heterogeneous catalysis is widely known as a convenient tool for atom-economic reduction of organic compounds, but it is still not the case with oximes hydrogenation. The majority of oxime hydrogenation catalysts require rather harsh conditions for the reaction to proceed, leading to side reaction products formation.¹



Catalytic system 1%Pt/CeO₂-ZrO₂ has previously shown promising results in carbonyl and nitro compounds reduction under ambient conditions.²⁻⁴ Similar reaction conditions were applied in oximes hydrogenation to examine the effectiveness of 1%Pt/CeO₂-ZrO₂.

The performed catalytic experiments proved an exceptional activity and selectivity of 1%Pt/CeO₂-ZrO₂ catalyst in oxime hydrogenation at room temperature and atmospheric pressure. Corresponding primary amine was the only product observed in ¹H and ¹³C NMR spectra of the reaction mixture.

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The work was carried out with a financial support from the Russian Science Foundation (grant no. 22-73-00183).

THERMOSTABLE HETEROGENEOUS CATALYST FOR LIQUID-PHASE OXIDATION OF SULFUR SULFIDE

**Lai H.D.^a, Akhmadullin R.M.^b, Bao Q. Tranc, Akhmadullina F.Y.^a,
Zakirov R.K.^a, Hoang H.Y.^{d,e}**

^a*Kazan National Research Technological University, Kazan, Russia;
email: laihongdung1997@gmail.com*

^b*R&D Center "AkhmadullinS" LLC, Kazan, Russia;*

^c*Ho Chi Minh City University of Natural Resource and Environment, Viet Nam*

^d*Center for Advanced Chemistry, Institute of Research & Development, Duy Tan University, Danang, Vietnam;*

^e*Faculty of Natural Sciences, Duy Tan University, Da Nang, Vietnam*

Wastewater from industries is one of the main causes of water pollution. In particular, wastewater containing sulfur sulfide is highly toxic and harmful to human health and animals as well as plants in the ecosystem. There are many methods to remove sulfur sulfide, and the method that receives the most attention because of its high efficiency and safety is the catalytic oxidation method. In typical wastewater treatment processes, homogeneous catalysts exhibit a high activity and user-friendly characteristics but have some disadvantages such as difficulty in synthesis and the potential generation of secondary pollutants. Conversely, heterogeneous catalysts are considered a more optimal choice due to their long operating time and high efficiency¹. However, conventional heterogeneous catalysts were recognized for their operation only at low temperatures (below 90°C) and did not yield high oxidation rates for high-sulfur wastewater in this condition.

In this study, we propose a high-temperature-capable a heterogeneous catalyst composed of metal oxides (MnO₂, CuO, TiO, Fe₂O₃, NiO, CdO, Mn₂O₃, Cr₂O₃, PbO, MnO, Cu₂O) embedded in thermally stable polymer - polyphenylene sulfide (PPS). The study on their catalytic activity was carried out in an autoclave under harsh conditions with varying oxygen consumption rate (v), sulfur sulfide removal efficiency (E), and oxidation time (t). The obtained results reveal that in the process of liquid phase oxidation of sulfur sulfide at $[S^{2-}] = 3\%$, $T = 200^{\circ}\text{C}$, $p = 3.6 \text{ MPa}$ and $\omega = 1000 \text{ rpm}$, the catalyst containing MnO₂ immobilized on PPS matrix has the highest activity. Under these conditions, the oxygen consumption rate reached $2.5 \text{ mol}\cdot\text{min}^{-1}$ with a sulfur sulfide removal efficiency of 86% within 11 min; many times higher than the oxidation process without catalyst ($v = 0.39 \text{ mol}\cdot\text{min}^{-1}$, $E = 70 \%$ and $t = 50 \text{ min}$). Overall, the proposed catalyst can be applied in wastewater treatment with high sulfide content.

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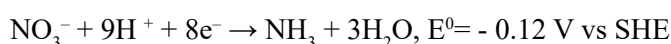
IRON NANOPARTICLES DEPOSITED ON GRAPHITE IN AN ELECTROCATALYTIC NITRATE REDUCTION REACTIONS

Kuznetsova I.I.,^a Lebedeva O.K.,^a Kultin D.Yu.,^a Kustov L.M.^{a,b}, Dunaev S.F.^a

^a*Department of Chemistry, Lomonosov Moscow State University,
119991 Moscow, Russia, e-mail: kuznetsowair@yandex.ru*

^b*N.D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences,
Leninsky Prospect 47, 119991 Moscow, Russia*

The processes related to the field of hydrogen energy in modern scientific literature include not only the reactions of hydrogen synthesis (the so-called "brown", "blue" and "green" hydrogen, depending on the method of production) and the synthesis of hydrogen carriers, but also reactions with the direct participation of hydrogen (molecular or atomic, adsorbed on the surface of the catalyst) to produce valuable organic¹ or inorganic products. The electrocatalytic reaction of nitrate reduction to ammonia (NH₃RR) proposed to replace the energy-intensive and environmentally unsafe Haber-Bosch ammonia production process refers to processes related to hydrogen energy:



Environmentally friendly and energy-efficient materials² can be used for these processes as catalyst electrodes^{3,4}. Electrochemically deposited catalysts containing iron nanoparticles modified with cobalt nanoparticles on a graphite substrate were obtained and tested in an electrocatalytic reaction of reducing nitrates to ammonia. The results show moderate Faraday efficiency values from 25% to 33%, while a sharp increase of (to 50%) is observed with the addition of an insignificant mass of cobalt nanoparticles even at the lowest masses of iron nanoparticles.

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SYNTHESIS OF $\text{La}_x\text{Mg}_{1-x}\text{Al}_2\text{O}_4$ NANOPOWDERS FROM SPINEL STRUCTURE AND RESEARCH OF THE PROPERTIES OF THEM IN COMPOSITION WITH ZSM-5 ZEOLITE IN TRANSFORMATION OF METHANOL IN OLEPHINES $\text{C}_2 - \text{C}_4$ AND P-XYLOL

Mahmudova N.I., Mammadov S.E., Akhmedova N.F., Akhmedov E.I.

Baku State University, Az 1148, Baku, Z.Khalilov Street, 23, Baku.

A promising way to produce $\text{C}_2\text{-C}_4$ olefins and aromatic hydrocarbons from alternative oil feedstock is the transformation of methanol in the presence of catalysts based on zeolite ZSM-5 ^{1,2}.

The aim of the present work was the synthesis of $\text{La}_x\text{Mg}_{1-x}\text{Al}_2\text{O}_4$ nanopowders of spinel structure by combustion of appropriate reagents, preparation of effective catalytic compositions with zeolite NZSM-5 for the process of obtaining $\text{C}_2\text{-C}_4$ olefins and p-xylene from methanol.

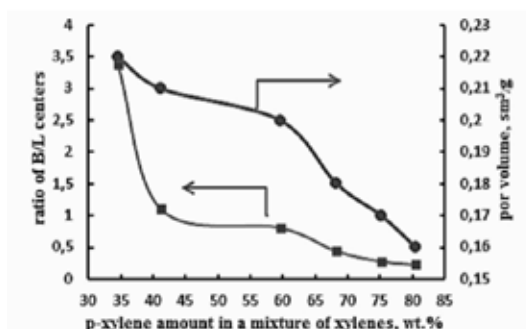


Figure 1. Effect of B/L ratio of acid centres and catalyst pore volume on p-xylene selectivity.

It was found that as a result of interaction of modifier nanoparticles with the zeolite crystal lattice, additional Lewis acid centres are formed, the density of strong acid centres of Brønsted decreases, which leads to a decrease in the B/L ratio of acid centres and a decrease in the zeolite pore volume. These factors play an important role in the selective conversion of methanol to $\text{C}_2\text{-C}_4$ olefins and p-xylene (Fig.1). On catalytic compositions containing 5.0 wt.% of $\text{La}_{0.1}\text{Mg}_{0.9}\text{Al}_2\text{O}_4$ nanopowder at optimal combination of B/L acid centres (0.22), pore volume ($0.16 \text{ cm}^3/\text{g}$) high yield of $\text{C}_2\text{-C}_4$ olefins (31.8%) and p-xylene selectivity (81.2%) were achieved.

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PREPARATION OF FE-FER CATALYSTS FOR N₂O DECOMPOSITION REACTION

Makova A.S.,^{a,b} Kustov L.M.,^{a,b} Ter-Akopyan M.N.^b

^a*N.D. Zelinsky Institute of Organic Chemistry RAS, Leninsky prospekt 47, Moscow, 119991, Russia,
e-mail: makovaas@ioc.ac.ru*

^b*National University of Science and Technology 'MISIS', Leninsky prospekt 4, Moscow, 119049, Russia*

Zeolite with the ferrierite structure (FER) is of great interest as a catalyst due to its activity in acidic reactions and unique molecular sieve properties. The most promising applications of FER are related to skeletal isomerization of linear olefins, N₂O decomposition, dimethyl ether synthesis, etc.

In this work, zeolite with FER structure (SiO₂/Al₂O₃=20) was obtained by hydrothermal method (T=190 °C) with the variation of synthesis time (3-7 days) and use of different organic structure-directing agents (templates) – ethylenediamine, pyridine, cyclohexylamine and tetrahydrofuran.

It was found that the use of different templates and changing synthesis times affect the physico-chemical characteristics of the resulting materials, namely crystallinity, textural and acidic properties, and crystallite sizes. The best physico-chemical characteristics were exhibited by the FER sample synthesized using pyridine as template and synthesis time of 4 days.

The Fe-FER iron-containing catalysts were prepared by incipient wetness method using different iron precursors.

The N₂O decomposition reaction was carried out in a flow-type unit at a temperature of 300-600 °C and a GHSV (gas hourly space velocity) of 3000 h⁻¹. It was shown that 100% conversion at the lowest temperature was achieved on Fe-FER catalysts obtained using iron (III) acetylacetonate and ammonium tris(oxalato)ferrate (III) trihydrate as precursors.

The effect of iron content in Fe-FER catalysts on N₂O decomposition was also studied. The maximum N₂O conversion for the sample containing 7.5 wt.% Fe was obtained at a temperature of 460 °C. For 2.5, 5.0 and 10.0 wt.% Fe catalysts, the maximum N₂O conversion was achieved at higher process temperature.

This research was funded by Russian Science Foundation, grant 23-73-30007.

THE ROLE OF CONJUGATED FORMATION, ISOMERIZATION AND HYDROCRACKING OF BIMOLECULAR INTERMEDIATES IN THE JOINT CONVERSION OF GAS GASOLINE AND PROPANE-BUTANE FRACTION

Mamedova M.T., Abasov S.I., Isaeva E.S., Iskenderova A.A., Imanova A.A. Nasibova A.R.

*Institute of Petrochemical Processes named after Academician
Y.H. Mammadaliyev, the Ministry of Science and Education of the
Republic of Azerbaijan, AZ1024, avn. Khojali 30
Email: memmedova-melahet@mail.ru*

To solve the problem of increasing the raw material sources of C_5 - C_6 isoalkanes, it is possible to explore the possibility of using associated petroleum gases in the process of obtaining fuel (gasoline). For this purpose, a catalytic system composed of sulfated zirconium dioxide and cobalt-modified HZSM-5 zeolite was synthesized and its activity in the isomerization of the mixture of gas gasoline (GG) with the propane-butane fraction (PBF) was studied.

The obtained results (table 1) show that even at a temperature of 160°C, an intensive change in the composition of the GG : PBF (propane-butane fraction) (1:1) mixture occurs. PBF undergoes intensive consumption with complete consumption of C_4 - components. At this time, up to 50% consumption of high-molecular components of QB is observed. In the conversion products of the mixture, the amount of i - C_5 - i - C_6 isomer components increases up to 27%, and the amount of n - C_5 increases 2 times.

T, °C	C_2	C_3	iC_4	C_4	iC_5	C_5	iC_6	C_6	iC_7	C_{7+}
Composition of the initial mixture (QB : PBF = 1 : 1), wt. %										
5		17.8	9.9	16.7	15.1	12.3	8.1	3.7	2.4	9
Composition of the catalysate, wt. %										
160	-	-	-	8.8	24.3	25.8	25.6	3	8	4.5
180	-	-	-	5.4	26.2	27.2	27.6	2.0	9.2	2.4
200	-	-	-	3.5	24	21.2	23.5	1.8	12.5	13.5

Table 1. Effect of temperature on the conversion of mixture of GG and PBF (1:1).
Catalyst: 0.4%Co/HZSM-5/10% ZrO_2 - SO_4^{2-} (2%); WHSV=2h⁻¹, GHSV_{PBF} = 500h⁻¹

Taking into account the lack of appropriate activity in individual components of the catalyst, the products obtained as a result of the process, the hydrocracking activity of Co/H-zeolite, it can be concluded that the conversion of the GG and PBF mixture with the presence of C_{7+} and C_4 components occurs through conjugated formation, isomerization and hydrocracking of bimolecular [C_4 - C_{7+}] intermediates. The result of this transformation is the accumulation of C_5 - C_6 hydrocarbons, that is, the molecular weight averaging of the hydrocarbons in the process.

COMPARATIVE ONIOM MODELING OF 1,3-BUTADIENE POLYMERIZATION USING Nd(III) AND Gd(III) ZIEGLER-NATTA CATALYST SYSTEMS

Masliy A.N.,^a Akhmetov I.G.,^b Kuznetsov A.M.,^a Davletbaeva I.M.^c

^a *Department of Inorganic Chemistry, Kazan National Research Technological University, 420015, Kazan, K. Marx Street 68, Russia;*

e-mail: masliy@kstu.ru

^b *Nizhnekamsk Chemical and Technological Institute (branch), Kazan National Research Technological University, 420015, Kazan, K. Marx Street 68, Russia;*

^c *Technology of Synthetic Rubber Department, Kazan National Research Technological University, 420015, Kazan, K. Marx Street 68, Russia;*

On the base of structural and thermodynamic data using modern methods of quantum chemistry, a comparative theoretical study of the elementary acts of initiation and growth of a polymer chain during the polymerization of 1,3-butadiene was carried out. Ziegler-Natta catalysts based on Nd(III) and Gd(III) were used as polymerization initiators.

As a result of the work carried out, it was shown that the slower initiation of polymerization of 1,3-butadiene by the gadolinium catalytic system in comparison with neodymium is due to a higher activation barrier. The calculated Gibbs free energy of activation of the initiation process for AS(Gd) is 117.7 kJ/mol, and for AS(Nd) is 60.9 kJ/mol.

For the stage of growth of the macrochain of cis-1,4-polybutadiene, the same pattern persists, but to a lesser extent. The Gibbs free energy of activation of the polymer chain growth process for AS(Gd) is 73.6 kJ/mol, and for AS(Nd) – 61.7 kJ/mol.

At the same time, the transition from the stage of initiation of 1,3-butadiene polymerization to the stage of chain growth is accompanied by changes in the nature of the interaction of the central atom AS with the terminal link of the polymer chain. Thus, for a neodymium catalytic system, three of carbon atoms of last polymer chain link are located at approximately equal distances from the Nd(III) ion, amounting to ~ 2.65 Å, which is typical for π -bonding. For the gadolinium catalytic system, the distance between the first carbon atom of last polymer chain link and the Gd(III) ion is ~ 2.5 Å, and the distance between the second carbon atom and the Gd(III) ion is ~ 3.1 Å, which is more typical for σ -bonding. This explains the increased stability of the terminal π -allylic Gd(III)–carbon bond in the anti-configuration and the higher stereospecificity of the gadolinium catalytic system with its lower activity. The higher stereospecificity of AS(Gd) is also indicated by the fact that $i\text{-C}_4\text{H}_9\text{-CC-AS(Gd)}$ is more stable compared to $i\text{-C}_4\text{H}_9\text{-CC-AS(Nd)}$.

CATALYSTS FOR OXIDATION OF ORGANIC POLLUTANTS BASED ON FERRITES NANOPOWDERS

Meshcheryakova A.A.,^a Titov S.A.,^a Solovyova A.A.,^a Tomina E.V.^{a,b}

^a Voronezh State University, 394018, Voronezh, Universitetskaya p., 1,
e-mail: anna-meshcheryakova@internet.ru

^b Voronezh State Forest Engineering University named after G.F. Morozov,
394087, Voronezh, Timiryazeva str., 8

Nanoscale nickel (NiFe_2O_4) and zinc (ZnFe_2O_4) ferrites synthesized and characterized by XRD, TEM, SEM, EDS methods were tested as catalysts for oxidative degradation of organic pollutants in aqueous solutions by hydrogen peroxide under optimized conditions, with control of parameters, including contact time, pH of the tested solution and catalyst dose ^{1,2}.

Index	Ferrite	Prevailing particle fraction, nm	Pollutant		
			Ultraviolet radiation		
			2,4-dinitrophenol	Methyl orange	Methylene blue
Rate constant, $k \text{ min}^{-1}$	ZnFe_2O_4	10-40	$0,0044 \text{ min}^{-1}$	$0,0159 \text{ min}^{-1}$	$0,0168 \text{ min}^{-1}$
	NiFe_2O_4	20-60	$0,0046 \text{ min}^{-1}$	$0,0191 \text{ min}^{-1}$	$0,0137 \text{ min}^{-1}$
	No	-	$0,0021 \text{ min}^{-1}$	$0,0121 \text{ min}^{-1}$	$0,0097 \text{ min}^{-1}$
Degree of destruction, W %	ZnFe_2O_4	10-40	48%	92%	95%
	NiFe_2O_4	20-60	52%	99%	92%
	No	-	37%	82%	76%

Table 1. Summary table of research results

The values of rate constants of phenon-like oxidation reactions and degrees of degradation of toxicants allow us to consider the studied ferrite-spinels and composites with them as promising materials for wastewater treatment and water treatment processes.

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The study was funded by a grant from the Russian Science Foundation № 23-23-00122, <https://rscf.ru/project/23-23-00122/>

NEW NICKEL CATALYSTS FOR THE HYDROGENATION OF BENZENE AND ITS HOMOLOGUES

Mokhov V.M., Nebykov D.N., Lagutin M.A.

*Volgograd State Technical University, Volgograd, Lenin Avenue, 28,
e-mail: tons@vstu.ru*

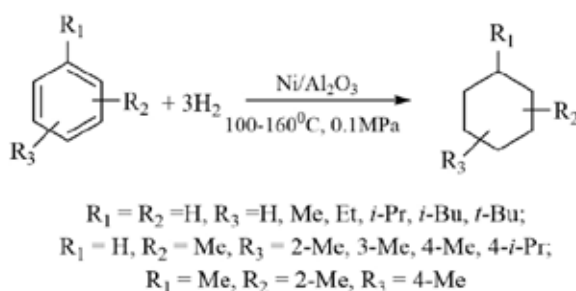
Products of the hydrogenation of aromatic hydrocarbons have found industrial use as organic solvents, additives for oils and fuels, extractants and fragrances, while 7.5 million tons of global benzene production is spent on hydrogenation into cyclohexane, which in turn is the raw material for the production of caprolactam and adipic acid.

Existing catalysts for the hydrogenation of aromatic hydrocarbons based on noble metals allow the process to be carried out at moderate hydrogen pressures and low temperatures, while the use of available nickel catalysts requires the use of harsh conditions, including high pressure.

We have studied the process of hydrogenation of benzene and a number of alkylbenzenes in a continuous mode on nanostructured nickel catalysts at atmospheric pressure and investigated the influence of the nature of the support and nickel loading on their activity and stability.

It was found that the best carrier is $\gamma\text{-Al}_2\text{O}_3$, the method of impregnation of the carrier is the precipitation of nickel(II) chloride with urea in the presence of boric acid, the reduction of the active metal phase is an aqueous solution of sodium tetrahydride borate mixed with hydrazine hydrate.

Using this catalyst, the hydrogenation of benzene and a number of alkylbenzenes was carried out at atmospheric pressure and 100-160 °C with a substrate:hydrogen molar ratio of 1:6.



The dependence of the specific productivity of the catalyst on the number of substituents on the benzene ring, temperature, and nickel content in the catalyst was determined.

The catalyst exhibits high stability, and at 100% conversion of the substrate within 30 h, no loss of activity was observed.

NEW NICKEL CATALYSTS FOR CONTINUOUS HYDROGENATION OF PHENOL AT ATMOSPHERIC PRESSURE

Mokhov V.M., Shemet V.V.

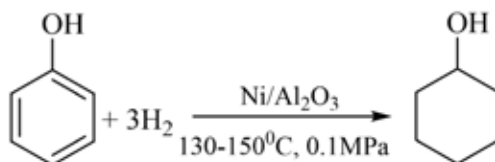
Volgograd State Technical University, Volgograd, Lenin Ave., 28, e-mail: tons@vstu.ru

Hydrogenation of aromatic compounds is one of the main processes in industrial organic synthesis and petroleum chemistry. Thus, by hydrogenation of phenol, cyclohexanol and cyclohexanone are obtained, which are intermediates for the synthesis of caprolactam and adipic acid.

Industrial production of cyclohexanol is carried out on nickel catalysts (nickel supported on aluminum oxide, chromium oxide, etc.) in the vapor phase. Hydrogenation is carried out in flow mode under a pressure of 1.5–2.0 MPa and a temperature of 140–150 °C. In order for phenol to be in a vapor state under conditions of high pressure, a large excess of hydrogen is used - about 80–100 mol of gas per 1 mol of phenol. The yield of the target substance exceeds 96%.

The goal of our work was to study the process of phenol hydrogenation in a flow mode on nanostructured nickel catalysts at atmospheric pressure. During the work, the influence of the composition of catalyst precursors on their activity and stability was studied.

It has been established that for the hydrogenation of phenol the best of the obtained catalysts is Ni/Al₂O₃, modified with urea and boric acid, the method of impregnation of the carrier (γ-Al₂O₃) is the precipitation of nickel(II) chloride with urea in the presence of boric acid, the reduction of the active metal phase is with an aqueous solution of tetrahydride borate sodium mixed with hydrazine hydrate.



Using this catalyst, phenol was hydrogenated at atmospheric pressure and 130-150 °C at a substrate:hydrogen molar ratio of 1:6. The catalyst exhibits high stability and selectivity with 100% substrate conversion; no loss of activity was observed within 24 hours.

BIMETALLIC HYDROGENATION CATALYSTS BASED ON PLATINUM CLUSTERS WITH THE INCLUSION OF 3d METALS (V, Cr): QUANTUM CHEMICAL DFT/NUDGED ELASTIC BAND STUDY

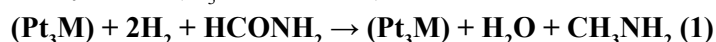
Panina N.S.,^a Klyukin I.N.,^b Fisher A.I.,^a Buslaeva T.M.,^c Zhizhin K.Yu.^b

^aSt. Petersburg State Technological Institute (Technical University), 190013, St. Petersburg, Moscow Avenue, 26,
 e-mail: nataliepanina2707@gmail.com

^bN.S. Kurnakov Institute of General and Inorganic Chemistry, RAS, 119991, Moscow, Lenin Avenue, 31

^cRTU MIREA, 119454, Moscow, Vernadsky Avenue, 78

In order to describe the reaction mechanism and the catalytic properties of bimetallic clusters based on platinum with the inclusion of 3d metals (V, Cr), the quantum chemical DFT/PBE0/def2tzvp method with the NEB functional using the ORCA software package was applied. Minimum energy paths (MEP) were constructed for a two-stage test hydrogenation of formamide to methylamine (Pt_3M , M = V, Cr):



The ability of the atoms of these 3d metals for molecular adsorption of H_2 molecules, in contrast to their dissociative adsorption on platinum centers, was described. It was established how the migration of H atoms between the metal centers and to the hydrogenated substrate occurs. It was found that, at the molecular level of interaction, the highest activation barriers (Table 1) found on the MEP curve upon formamide hydrogenation without a catalyst (reaction (1)) – the E_a values of stages I and II are taken as 100% – in the case of introducing a monometallic Pt₄ cluster (reaction (2)) can decrease by 21 and 55%, respectively, relative to (1). On the Pt₃V cluster (reaction (3)), they decrease by 49% (stage I) and 55% (stage II). The relative decrease in these activation barriers with the participation of the Pt₃Cr cluster in the reaction is even greater: 53% (stage I) and 63% (stage II).

Reaction	E_a , stage I	E_a , stage II
(1) $\{2\text{H}_2 + \text{OC}(\text{H})\text{NH}_2\}$	289 (TS1)	292 (TS2)
(2) $\{2\text{H}_2 + \text{Pt}_3\text{PtOC}(\text{H})\text{NH}_2\}$	191 (TS5), 228 (TS6)	102 (TS4), 163 (TS5), 136 (TS9)
(3) $\{2\text{H}_2 + \text{VPt}_2\text{PtOC}(\text{H})\text{NH}_2\}$	126 (TS3), 121 (TS4), 148 (TS5)	131 (TS5), 102* (TS6), 129 (TS8)
(4) $\{2\text{H}_2 + \text{CrPt}_2\text{PtOC}(\text{H})\text{NH}_2\}$	136 (TS4), 130 (TS5), 124 (TS7)	97 (TS5), 64 (TS6), 71 (TS7), 109 (TS9)

Table 1. Activation energies E_a (kJ/mol) in various catalytic systems
 (the highest E_a values are highlighted in red).

PALLADIUM CARBOXYLATES $[Pd(RCO_2)_2]_n$ AS CATALYSTS FOR THE OXIDATION OF ALCOHOLS: EFFECT OF A SUBSTITUTE IN THE CARBOXYLATE GROUP

Polyakova V.A.^a, Akhmadullina N.S.,^b Flid V.R.,^a Shishilov O.N.^a

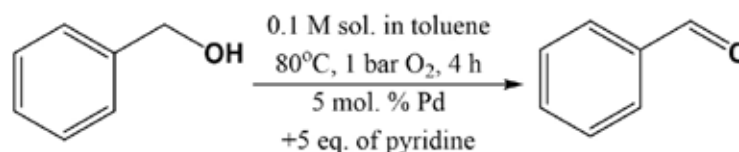
^a*MIREA – Russian Technological University, M.V. Lomonosov Institute of Fine Chemical Technologies,
117571, Moscow, Vernadsky Avenue, 86*

E-mail: valeriya_polyakova_97@mail.ru

^b*A.A. Baikov Institute of Metallurgy and Material Science of Russian Academy of Science,
119991, Moscow, Russia, Leninsky avenue 49*

Palladium carboxylates $[Pd(RCO_2)_2]_n$ are well known as effective catalysts (or their precursors) for a wide range of transformations of organic substrates, including oxidative ones. One of these transformations is the oxidation of alcohols, which is an effective route to carbonyl compounds as important synthons of fine organic synthesis. Palladium acetate is most widely used as a basis for the design of catalytic systems for the oxidation of alcohols. In combination with coordinating bases such as pyridine, it provides efficient and selective oxidation of primary and secondary alcohols under relatively mild conditions (temperatures up to 120°C, oxygen pressure up to 10 atm.). Palladium trifluoroacetate under similar conditions demonstrates low activity, although it retains high selectivity.

Thus, we have shown that in the oxidation reaction of benzyl alcohol under the conditions shown in the diagram below, palladium trifluoro- and trichloroacetate provide a yield of 8-11% compared to 88% for palladium acetate:



However, the yield increases to 92% when using 15 mol. % palladium with the addition of 1.5 eq. pyridine. At the same pyridine content in the presence of 5 mol. % palladium yield is 75-83%. From this we can conclude that the influence of the substituent in the carboxylate ligand is not limited to the stability of the resulting active forms of palladium in general. Apparently, a test under identical conditions cannot always serve to assess the relative activity of palladium carboxylate complexes of similar composition and structure, but differing in substituents on the carboxylate groups.

The work was carried out with the support of the Russian Science Foundation – project No. 23-73-00123.

NANOCOMPOSITE MAGNETIC CATALYSTS FOR HYDROGENATION REACTIONS

Pomogailo S.I.^{a,b}, Jussupkaliyeva .I.R.^c, Chepaikin E.G.^a, Bubelo O.N.^b

^a*A.G. Merzhanov Institute of Structural Macrokinetics and Materials Science, Russian Academy of Sciences, Chernogolovka, 142432 Russia*

^b*All-Russian Institute for Scientific and Technical Information RAS, 125190, st. Usievicha 20, Moscow, Russia
e-mail: pomogsvetlana@mail.ru*

^c*Zhangir Khan West Kazakhstan Agrarian Technical University, 090009, Uralsk, Kazakhstan*

Much research interest in creating efficient catalysts with magnetic properties stems from their unique ability to be easily extracted using an external magnetic field, thereby avoiding cumbersome filtering and centrifugation operations. More often, magnetite nanoparticles are used as catalyst carriers^{1,2}, but in some cases it is magnetite nanoparticles that are the active centers for catalysis. In order to increase the stability of magnetite nanoparticles, they are embedded in various matrices. Production methods have a great influence on the formation of the structure of nanocomposites. The introduction of magnetite nanoparticles is usually carried out in two ways: *ex situ* (when pre-synthesized magnetite is used), or *in situ* (with the formation of magnetite nanoparticles at the time of obtaining the nanocomposite). Magnetic nanocatalysts are used in various reactions of hydrogenation of organic dyes and nitro compounds with sodium borohydride. The hydrogenation reaction of nitro compounds produces the corresponding amines, which are intermediate compounds for use in synthesis and industry in the production of dyes, pigments, pharmaceuticals, synthetic polymers and agrochemicals, pesticides, etc. In reduction reactions, most magnetic catalysts are characterized by high activity and stability in several cycles without a significant decrease in activity.

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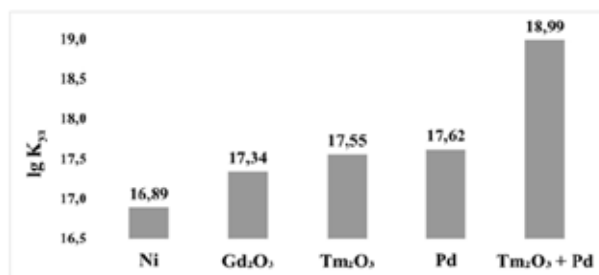
CATALISATORS BASE ON RARE EARTH ELEMENTS COMPOSITES AND BASALT FIBRES FOR LOW-TEMPERATURE ORTHO-PARA CONVERSION OF HYDROGEN

Vinokurov E.G., Pshenitsyn M.B., Boeva O.A.

*D.I. Mendeleev Russian University of Chemistry and Technology, 125047 Moscow, 9 Miusskaya Sq.
e-mail: pshenmichail@gmail.com*

One of the key stages of transition to hydrogen energy is the development of a highly active and stably working catalyst for conversion of *ortho*-H₂ to *para*-H₂ during production and storage of liquid H₂.

The results of investigation of catalytic properties of composites based on Ni-P alloy without/with dispersed phase of Gd₂O₃, Tm₂O₃ oxides, as well as a composite encrusted with Pd nanoparticles are presented. Basalt fibre was chosen as the carrier of the catalytic system because the material is characterised by its lightness, environmental friendliness, and durability. The model reaction is the isomeric conversion of H₂ at a pressure of 0.5 torr and 77 K. The results of this work are presented in the form of dependence of specific catalytic activity K_{sp} (molecules·c⁻¹·g⁻¹) on the composite composition.



The application of Pd nanoparticles on the composite with the addition of Tm₂O₃, which has a high atomic magnetic moment $\mu_{Tm} = 7.62 \mu_V$, resulted in a synergistic effect in the catalytic properties; the Cd of Ni-P-Tm₂O₃ increased by more than 2 orders of magnitude compared to the original nickel coating. Probably, a significant change in the activity of the catalyst is caused by the change of the chemical mechanism of conversion with bond breaking, to the magnetic mechanism - without bond breaking in the H₂ molecule, which is carried out on the magnetic centres of REM atoms.

It is shown that Pd/Ni-P-Tm₂O₃ composite coating and basalt fibres are promising materials for catalysing the reaction of low-temperature conversion of H₂ modifications.

The work was financially supported under the D.I. Mendeleev Russian Chemical Technology University Development Programme "Priority-2030".

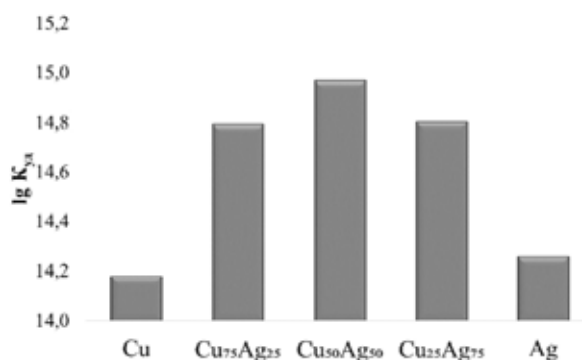
SYNERGIC EFFECTS IN THE CATALYTIC PROPERTIES OF COPPER-SILVER BIMETALLIC NANOPARTICLES

Pshenitsyn M.B., Boeva O.A., Zhavoronkova K.N.

*D.I. Mendeleev Russian University of Chemistry and Technology, 125047 Moscow, 9 Miusskaya Sq.
 e-mail: pshenmichail@gmail.com*

Nanostructures are of interest to many scientific groups. This is due to their unique properties, which open up new applications for substances about which, as it seems to us, we know almost everything. One type of such structures is metal nanoparticles, which exhibit properties uncharacteristic for their element in the macroworld. The catalytic properties of mono- and bimetallic nanoparticles based on copper and silver will be discussed in this work.

The objects of research are nanoparticles deposited on $\gamma\text{-Al}_2\text{O}_3$ with different ratios of copper and silver in the composition. The model reaction is ortho-para conversion of protium. The experiments were carried out at 77 K and a pressure of 0.5 Torr. The research results are shown in the figure below.



The catalysts showed high activity in relation to the isomeric conversion reaction of protium; the activity of bimetallic nanoparticles is 3-6 times higher compared to mononparticles, which cannot be explained by the addition of the properties of metals; therefore, the interaction of copper and silver in a nanoparticle leads to a synergy of catalytic properties.

The work was carried out with financial support within the framework of the development program of the Russian Chemical Technical University named after. D.I. Mendeleev "Priority-2030".

SURFACE MORPHOLOGY OF CATALYSTS BASED ON SYNTHETIC ZEOLITE ZSM-5

Serebryanskaya A.P., Kadirbekov K.A.

*JSC «A.B. Bekturov Institute of Chemical Sciences»
500010, Republic of Kazakhstan, 050010, Almaty, st. Sh. Ualikhanov, 106,
e-mail: srbr-anna@mail.ru*

The catalyst is an important component of any chemical process, on which the yield and quality of the target products depend.

The most promising catalysts for the processes of cracking, alkylation and esterification of alcohols are catalytic systems based on natural and synthetic zeolites. Zeolite catalysts have high catalytic properties, are stable and are capable of regeneration. The bulk of the literature data is devoted to the activity and selectivity of the catalysts used; however, there are very few works devoted to the study of surface morphology in the literature.

As part of our work, studies were carried out to study the surface morphology of catalysts based on synthetic zeolite ZSM-5 modified with silicotungsten (SiW₁₂-HPA) and phosphomolybdenum heteropoly acids (PMo₁₂-HPA).

Determination of morphology was carried out by scanning electron microscopy (SEM) on a Hitachi TM4000 desktop electron microscope.

A comparison of micrographs showed a uniform distribution of spherical ZSM-5 particles on the surface of the studied catalytic systems.

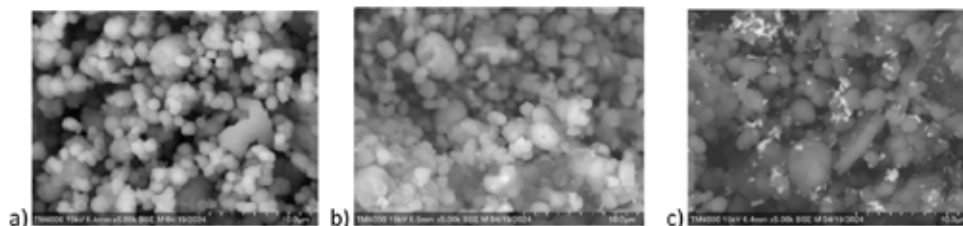


Figure 1. SEM micrographs of catalysts: a) initial ZSM-5 b) ZSM-5 + 5% SiW₁₂-HPA;
c) ZSM-5 + 1 5% PMo₁₂- HPA

The work was carried out within the framework of the targeted funding program of the Committee of Science of the Ministry of Education and Science of the Republic of Kazakhstan No. BR10965255 “Innovative materials for multifunctional purposes based on natural raw materials and man-made waste”

THERMODYNAMIC PROPERTIES OF IMIDAZOLIUM DICATIONIC IONIC LIQUID $[C_4(mim)_2][NTf_2]_2$

Sologubov S.S., Sarmini Yu.A., Markin A.V., Smirnova N.N.

*National Research Lobachevsky State University of Nizhny Novgorod,
 603022 Nizhny Novgorod, 23 Gagarin Avenue, Russia
 E-mail: s.slg90@gmail.com*

Ionic liquids are defined as low-temperature melting salts composed of large asymmetric organic cations and inorganic anions that are liquid at or below 100 °C. Ionic liquids possess unique physico-chemical properties, such as high ionic conductivity, low volatility, and high thermal stability. The most promising areas of the practical application of ionic liquids are organic synthesis, catalysis, energy, pharmaceuticals, and biotechnology.

The potential employment of ionic liquids in the life-science fields requires reliable values of their thermodynamic properties including the heat capacity, the fusion temperature, enthalpy and entropy of the phase transitions, as well as the Gibbs function. In this work, the heat capacity and thermodynamic properties of imidazolium dicationic ionic liquid $[C_4(mim)_2][NTf_2]_2$ (Figure 1) were studied by the low-temperature adiabatic vacuum calorimetry. A set of key fundamental thermodynamic functions of ionic liquid was determined. On the basis of the experimental results and the available literature data, it was established that dicationic ionic liquids are more suitable for possible applications at high temperature conditions than the corresponding monocationic analogues.

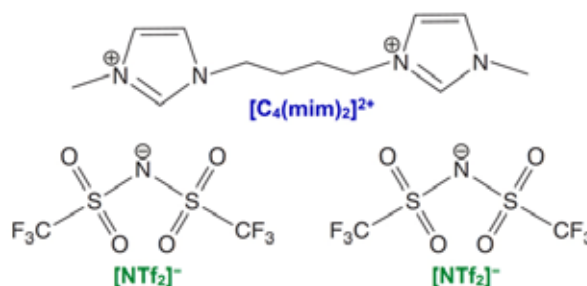


Figure 1. Molecular structure of ionic liquid $[C_4(mim)_2][NTf_2]_2$: $[C_4(mim)_2]^{2+}$ – 1,4-bis(1-*n*-butyl-3-methylimidazolium) dication; $[NTf_2]^-$ – bis(trifluoromethylsulfonyl)imide anion

This work was performed with the financial support of the Ministry of Science and Higher Education of the Russian Federation (FSWR-2023-0025) and the Scholarship of the President of the Russian Federation for young scientists and postgraduate students (SP-1369.2022.4).

APPLICATION OF HKUST-1 AS AN EFFECTIVE HETEROGENEOUS CATALYST FOR THE SYNTHESIS OF β -AMINOPHOSPHONATES VIA HYDROAMINATION OF VINYL PHOSPHONATES

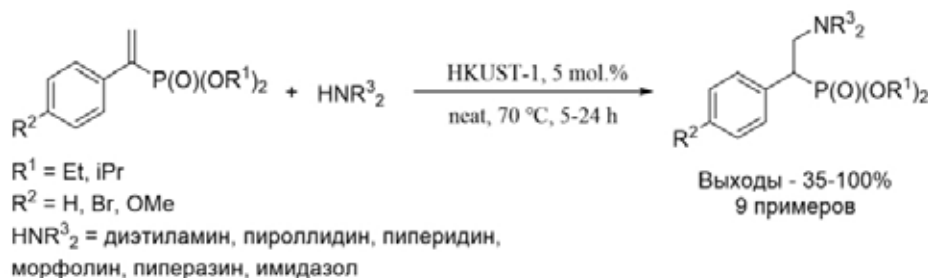
Svishchev V.N., Bondarenko G.N., Ganina O.G.

*Department of Chemistry, Lomonosov Moscow State University, Leninskie Gory 1, GSP-2, 119992, Moscow, Russia.
e-mail: viktor.svishchev@chemistry.msu.ru*

Phosphorus analogues of amino acids, in particular β -amino acids and their esters are important molecules extensively used in agrochemical and pharmaceutical industries¹.

A convenient pathway to β -aminophosphonates is hydroamination of vinylphosphonates. This reaction occurs under mild conditions with unsubstituted vinylphosphonates²; α -substituted vinylphosphonates are significantly less reactive and require harsher conditions with the resulting yield being comparatively low.

Herein we propose a catalytic system utilizing a widely accessible catalyst – HKUST-1, a metal-organic framework (MOF) based on copper and trimesic acid. The use of this catalysts in optimized conditions results in 35-100% yield of target β -aminophosphonates and HKUST-1 can be reused effectively for 5 cycles.



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STUDYING THE POSSIBILITY OF IMMOBILIZATION ENZYMES ON SILICA GEL

**Tagirova M.A.,^a Bakhronova Z.I.,^a Tolmasova M.F.,^a
Mukhamadiyev N.K.,^a Klyachko N.L.^b**

^a *Biochemical Institute of Samarkand State University named after Sharof Rashidov,
140104, Samarkand, University Boulevard, 15.
e-mail: mashxurat@mail.ru*

^b *Faculty of Chemistry, Lomonosov Moscow State University, 119991, Moscow, Leninskiye Gory 1, 11b.*

Immobilized enzymes are attracting significant attention due to their advantages, such as increased mechanical and thermal stability, ease of processing, and reusability in organic environments. Various types of solid supports are used to immobilize the enzyme, such as organic polymers, chitosan, hydrogels, silica gels, zeolite and mesoporous materials. Among them, silica gels have proven to be promising carriers for enzyme immobilization due to their high surface area, special porous structure, thermal stability and biocompatibility.

Catalase belongs to the class of oxidoreductase enzymes, is a chromoprotein having oxidized heme as a prosthetic (non-protein) group, and consists of four identical subunits with a molecular weight of about 60 kDa. However, immobilized catalase on mesoporous materials has received relatively less attention in contrast to intensive research on other enzymes due to the much larger molecular diameter of catalase (10.4 nm). The purpose of this work was to study the possibility of immobilizing catalase on amorphous silica gel and studying the stability of immobilized catalase.

As a result, it was established that immobilization of catalase on amorphous silica gels is possible by varying physicochemical factors and synthesis conditions.

SYNTHESIS OF PYRIDINECARBOXYLIC ACIDS ON A VANADIA CATALYST MODIFIED WITH ZIRCONIA AND NIOBIA

Yugay O.K., Kadirbekov K.A.

*«A.B. Bekturov Institute of Chemical Sciences» JSC,
050010, Republic of Kazakhstan, Almaty, st. Sh. Ualikhanov, 106
e-mail: yu.ok@mail.ru*

Pyridinecarboxylic acids (PCA) have physiologically active properties and are widely used in the production of not only general-purpose medical preparations, but also plant growth regulators and feed additives. Vapor-phase catalytic oxidation of isomeric methylpyridines with atmospheric oxygen is the simplest method for the synthesis of PCA, which meets the conditions of “green” chemistry.

The synthesis of PCA by vapor-phase oxidation of isomeric methylpyridines on a vanadia catalyst modified with zirconia and niobia was studied. The catalyst showed fairly high activity and selectivity in the synthesis of 3- and 4-pyridinecarboxylic acids with a formation selectivity of 83–94% and 69%, respectively. During the oxidation of 2-methylpyridine, the acid decarboxylated to form pyridine.

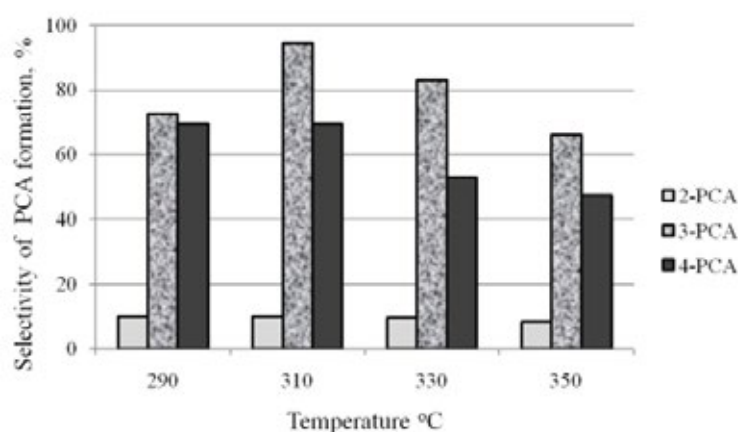


Figure 1. Dependence of the selectivity of formation of isomeric pyridinecarboxylic acids on the oxidation temperature under comparable conditions

The work was carried out within the framework of the targeted funding program for scientific research BR18574042 of the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan.

SYNTHESIS OF OXYGENATE COMPOSITIONS ON MODIFIED ZEOLITE CATALYSTS

Yugay O.K., Kadirbekov K.A.

*«A.B. Bekturov Institute of Chemical Sciences» JSC,
050010, Republic of Kazakhstan, Almaty, st. Sh. Ualikhanov, 106
e-mail: yu.ok@mail.ru*

Issues of ecology and increasing the efficiency of engines are relevant. To reduce harmful emissions into the atmosphere, it is necessary to change the composition of the fuel. To improve the characteristics of gasoline, oxygenate additives are used.

We have conducted studies of the catalytic synthesis of compositions by alkylation of butylene with ethyl alcohol. Catalysts based on synthetic zeolite ZSM-5 modified with polyacrylic acid and silicon-tungsten heteropolyacid have been developed. It has been shown that heat treatment of catalysts at 300°C leads to an increase in the content of ethyl tert-butyl ether in the reaction products by 1.5 times. This probably occurs due to the creation of a developed matrix on the surface of the catalyst on which the heteropolyacid is adsorbed.

The influence of the resulting compositions on the characteristics of commercial gasoline A-92 was studied.

Characteristics of gasoline	A-92	Concentration of the composition in a mixture with gasoline, % vol.			
		2	4	6	8
RON	89.0	95.6	100.6	102.0	104.8
MON	81.5	85.6	90.4	91.6	94.3
AKI	85.2	90.6	95.5	96.8	99.6

Table 1. Dependence of gasoline selectivity indicators for the formation of isomeric pyridinecarboxylic acids on the concentration of the composition

Thus, synthesized compositions consisting of ethyl alcohol and ETBE can be used as oxygenates. Additions of the resulting compositions to A-92 gasoline increase octane numbers calculated using both research and motor methods. The value of the anti-knock coefficient AKI also increases.

The work was carried out within the framework of the targeted funding program for scientific research BR18574042 of the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan.

TRIAZINE DERIVATIVES IN THE REACTION OF ELECTROCHEMICAL NITRATE REDUCTION

Zakharov V.N., Kuznetsova I.I., Kultin D.Yu., Lebedeva O.K., Kalmykov K.B., Chernyshev V.V., Kustov L.M., Aslanov L.A.

*Lomonosov Moscow State University, Department of Chemistry, 119991, Moscow
e-mail: zakharov-valery@mail.ru*

In order to develop effective electrocatalysts for the synthesis of ammonia, we proposed to use graphite as an electrode, with a substrate of 2,4,6-diphenyl-triazine (**I**) coated with cobalt nanoparticles deposited on it. The electrocatalytic reaction of the reduction of nitrates to ammonia was studied. Substrate **I** was synthesized from solutions of cyanuric chloride, biphenyl in n-octane in the presence of aluminum chloride.

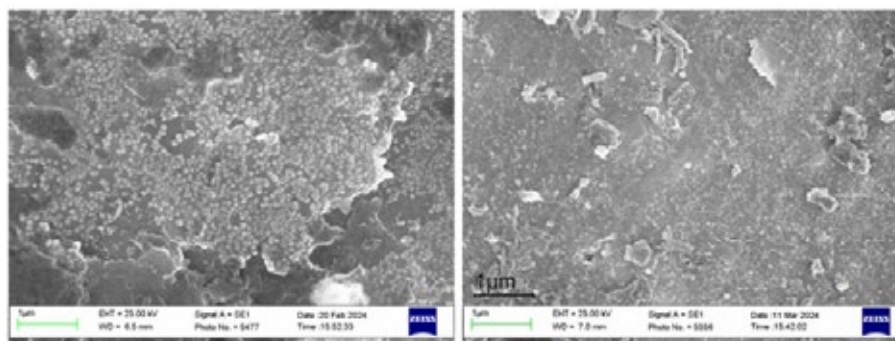


Figure 1. A fragment of the catalyst surface in a scanning electron microscope in the initial state (left) and after 5 operating cycles (right).

It was found that substrate **I** (Fig. 1) significantly increases the durability of the catalyst, and the selectivity of the process (current efficiency) decreases from 40% to 30% after the first two cycles and then remains virtually unchanged.

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*Synthesis of **I** was performed on a NOVA 2S microwave device (China).*

HYDROGENATION OF PHENYLACETYLENE TO STYRENE ON A COPPER MODIFIED COVALENT TRIAZINE FRAMEWORK

**Zakharov V.N.,^a Strekalova A.A.,^b Shuvalova E.V.,^b Kustov L.M.,^{a,b}
Dunaev S.F.,^a Aslanov L.A.^a**

^a *Lomonosov Moscow State University, Department of Chemistry
119991, Moscow, e-mail: zakharov-valery@mail.ru*

^b *Zelinsky Institute of Organic Chemistry RAS,
119991, Moscow*

The processes of hydrogenation of phenylacetylene on a new catalyst - a hybrid material consisting of a covalent triazine framework CTF-1 (I), obtained by ampoule synthesis from 1,4-dicyanobenzene and zinc chloride at a ratio of 1:1 (wt.%) at 400° C for 40 hours, were studied followed by treatment I with copper nitrate (5% wt.) and thermal activation of the catalyst in an inert gas or hydrogen (200° C).

Activation method	Time, min	Conversion, %	Styrene yield, %	Ethylbenzene yield, %
5%Cu(I), 300°C, air calcination	15	5,1	4,93	0,16
	30	8,8	7,9	0,54
	1 h	12	11,21	0,79
	5,5 h	82,4	72,67	7,54
5%Cu(I), 200°C, calcination in Ar	30	0	0	0
	5 h	37,4	32,95	4,4
5%Cu(I), 200°C, reduced in H ₂	15	8,2	5,37	0,12
	30	10,1	6,77	0,26
	1 h	10,8	7,56	0,36
	5 h	45,4	36,1	4,2

Table 1. Catalyst activity in the hydrogenation of phenylacetylene (50 mg of catalyst, 250 mg of phenylacetylene in ethanol (15 ml) at a hydrogen pressure of 13 atm and a temperature of 110°C)

It has been shown that during the hydrogenation of phenylacetylene under mild conditions, the conversion reaches 82%, and the selectivity for styrene exceeds 80%.

SUPPORTED MIXED OXIDES WITH THE PEROVSKITE STRUCTURE LaCoO_3 AS THE EFFECTIVE CATALYSTS FOR N_2O DECOMPOSITION

Zemlianskii P.V.,^a Morozov D.A.,^b Kustov A.L.,^{a,b} Kustov L.M.^{a,b}

^a Zelinsky Institute of organic chemistry RAS, Pr. Leninsky 47, Moscow, 119991, Russia,
e-mail: petrzemlianskii@gmail.com

^b National University of Science and Technology MISIS, Pr. Leninsky 4, Moscow, 119049, Russia

Nitrous oxide (N_2O) is a green-house gas with the global warming potential 310 times higher than that of CO_2 . Perovskite-like materials are the perspective catalysts for the N_2O decomposition due to the thermal stability in the presence of water vapor and low price. A LaCoO_3 bulk mixed oxide with the perovskite structure is known as an effective catalyst for the nitrous oxide decomposition.¹ However, supported systems containing the LaCoO_3 phase has not been investigated in this reaction yet.

Several catalysts of the LaCoO_3 /support type (support: ZrO_2 , $\text{ZrO}_2\text{-La}_2\text{O}_3$, $\text{ZrO}_2\text{-WO}_3$, Al_2O_3 и SiO_2) are synthesized in this work. The zirconia-based materials appeared to be the most active (figure 1 – A). The optimal concentration of the LaCoO_3 phase was 20 wt.% (figure 1 – B). The main contribution to the activity was made by the $\text{Co}^{2+}/\text{Co}^{3+}$ ratio.

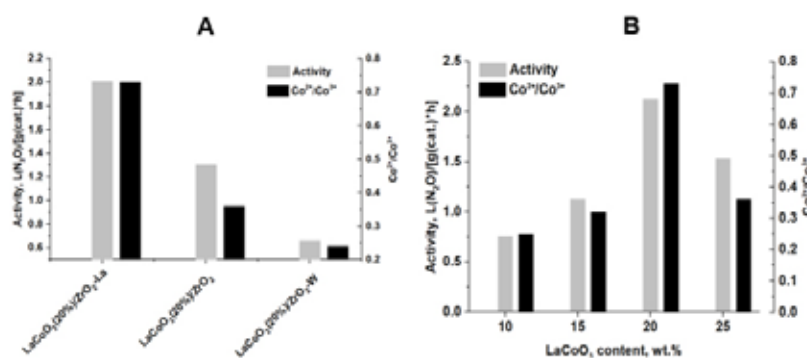


Figure 1. The data on the activity in the N_2O decomposition and $\text{Co}^{2+}/\text{Co}^{3+}$ ratio for the zirconia-based LaCoO_3 catalysts for 20 wt.% LaCoO_3 content – A and for different LaCoO_3 concentrations – B

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This research was supported by the Russian Science Foundation (project no. 23-73-30007).

VOLTAMMETRIC DETERMINATION OF GALLIC ACID AND PROPYL GALLATE AT ELECTRODES MODIFIED WITH TIN AND CERIUM DIOXIDE NANOPARTICLES


Ziyatdinova G.K., Grigoreva I.O., Salakhova L.A.

*Kazan Federal University,
Kremleyevskaya 18, Kazan, 420008, Russia,
e-mail: Ziyatdinovag@mail.ru*

Gallic acid and its esters (ethyl and propyl gallates) are actively used in food industry as antioxidants additives preventing peroxidation of lipids in foodstuff containing fats and vegetable oils. Since high concentrations of gallic acid and its esters can have a negative effect on human health, the content of these additives in foodstuff should be controlled. Therefore, development of simple and reliable methods of their determination is required. Voltammetry with chemically modified electrodes can be applied to solve this problem. Metal oxide nanoparticles, in particular tin and cerium dioxides, are of interest among the modifiers.

Novel voltammetric methods for gallic acid and propyl gallate determination have been developed using glassy carbon electrodes modified with tin and cerium dioxide nanoparticles, respectively. Cationic cetylpyridinium bromide has been applied for the preparation of nanoparticle dispersions. Moreover, surfactant acts as electrode surface co-modifier providing propyl gallate preconcentration. The electrodes fabricated have been characterized by scanning electron microscopy, electrochemical impedance spectroscopy, and voltammetry. The electrooxidation parameters of gallic acid and propyl gallate at the modified electrodes have been calculated, and electrode reaction schemes have been suggested.

Under conditions of differential pulse voltammetry in Britton-Robinson buffer pH 2.0, the linear dynamic ranges of 0.10-2.5 and 2.5-75 μM of gallic acid at the SnO_2 nanoparticle-based electrode and 0.10-2.5 and 2.5-50 μM of propyl gallate at the CeO_2 nanoparticle-based electrode have been obtained. The detection limits of 44 and 67 nM have been achieved. The quantification of propyl gallate in the sunflower and sesame oil extracts has been carried out.



Section 8

**POLYMERS AND POLYMERIC
MATERIALS (INCLUDING 2ND
INTERNATIONAL SYMPOSIUM
“MODERN TRENDS IN DENDRIMER
CHEMISTRY AND APPLICATIONS”)**

QUANTUM CHEMICAL PREDICTION OF CHITIN AND CHITOSAN DISSOLUTION IN IONIC LIQUIDS

Abramova E.S.^a, Muravyev A.A.^b, Novoselov N.P.^a, Skorik Y.A.^b

^aSt. Petersburg State University of Technology and Design, St. Petersburg

^bInstitute of Macromolecular Compounds of the Russian Academy of Sciences, St. Petersburg

Chitin is the second most abundant polysaccharide in nature. A derivative of chitin, chitosan, is produced on an industrial scale. Due to their unique properties, chitin and chitosan are widely used in various industries, but their processing is associated with the use of aggressive media and low level of technological process, which has a significant negative impact on the environment. Ionic liquids (ILs) are promising solvents for chitin and chitosan that meet modern requirements for environmental friendliness and processability of their processing.

Quantum chemical calculations of chitin and chitosan tetramers, chitosan, a series of imidazolium- and pyridine-based ILs, and the known chitin-solubilizing system of 5%LiCl in dimethiacetamide were performed to select the optimal IL dissolving chitin and chitosan, as well as to determine the criteria of chitin and chitosan solubility in ILs of different structures. The structures were optimized by density functional theory using the hybrid density functional B3LYP and the 6-311++G(d,p) basis set. The calculations were performed using Firefly software based on Qcpackage and GAMESS (US).

According to the calculation results, the following parameters were analyzed: bond lengths and angles, charge distribution, energy and dipole moment of the system. The obtained values of bond lengths and angles showed high convergence with literature data, which allows us to judge about the correctness of the chosen method of quantum chemical calculation and the possibility of further calculation of solubility criteria in polymer-IL systems.

STUDY OF PHYSICAL AND MECHANICAL PROPERTIES OF RUBBERS BASED ON MODIFIED BUTADIENE-STYRENE RUBBER REINFORCED WITH SILICA FILLER

Akmyradov A., Ibragimov M.A., Rakhmatullina A.P.

*Kazan National Research Technological University, 420015, Kazan, Karl
Marks Str., 68,
e-mail: akmyradov_2015@mail.ru*

It is well known that the physical and mechanical properties of rubber (hardness, elasticity, tensile strength, abrasion resistance, hysteresis loss, etc.)¹ are improved by reinforcing it with fillers such as black carbon or silicon dioxide. This study investigated the effect of Zeosil 1165MP on the properties of butadiene-styrene based rubber which is modified with polymer microgels (PM)², synthesized by us.

PM modification of butadiene-styrene rubber SKS-30 ARCM-15 was carried out by liquid-phase combination of corresponding latexes. The PM amount ranged from 2.5 to 10 wt. h. (in increments of 2.5) per 100 wt. h. of rubber per "dry" rubber. Rubbers were obtained on the basis of modified rubber and their physical and mechanical properties were investigated. To determine the parameters of the vulcanization mesh, the equilibrium swelling method in toluene was used.

In experimental vulcanizates based on microgel-modified rubber in an amount of 7.5 and 10.0 wt. hours per 100 wt. including polymer (increase in conditional tensile strength by an average of 34%, rebound elasticity by 12% and tear resistance by 72.0% compared to the control vulcanizate) was found a noticeable improvement in properties.

As a result, the polymer microgel introduction leads to an increase in the values of cross-linking density of vulcanizates based on SKS-30 ARKM-15 by 1.3 times. The increase in elastic-strength properties in the experimental samples is due to a higher density of chemically bonded mesh chains.

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PROPERTIES OF PARTIALLY HYDROLYZED MIXTURES ABS COPOLYMER AND POLYAMIDE

Alekseev A.A., Saif Hani Walid Naji Ahmed,

*Al-Otab Hussein Fatehi Mohammed Hassan
 Novomoskovsk Institute (branch) of the Federal State Budgetary Educational Institution
 of Higher Education «Mendeleev University
 of Chemical Technology of Russia», 301665, Russia, Tula region, Novomoskovsky district,
 Novomoskovsk, Druzhby street, 8
 e-mail: alekseev.a.a@muctr.ru*

Polymer blends involving acrylonitrile butadiene styrene plastics (ABS plastics) and polyamide 6 (PA) are a prime example where one quality indicator (notched Izod impact strength) is significantly higher than that of the original components. However, this is achieved by using expensive compatibilizers.

Another way to increase the compatibility of the starting components is seen in the chemical modification of ABS copolymers, in particular, in the partial alkaline hydrolysis of their nitrile groups.

The emulsion ABS copolymer was hydrolyzed with an aqueous solution of NaOH of various concentrations (10, 20 and 30%) and ABS-G1, ABS-G2 and ABS-G3 were obtained, respectively. After washing and drying, ABS-G was mixed with PA 6 in a ratio of 8:2 by weight, granulated, and samples were obtained for injection molding tests.

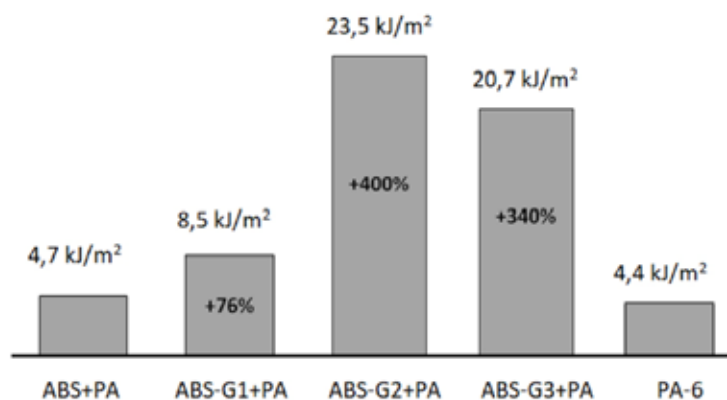


Figure. Izod impact strength of ABS-G+PA mixtures

When moving from ABS to ABS-3G, the yield strength and tensile elongation increase by 34 and 88%, respectively, the melt flow rate decreases by 34%, and the Vicat heat resistance and tensile strength increase slightly.

The work was carried out with the financial support of the Government of the Tula Region, contract DS/100 dated September 27, 2023.

MOLECULAR IMPRINTED POLYMERS FROM COAL WASTE

Arnt O.V., Vassilets Y.P., Zhakina A.Kh.

*LLP "Institute of Organic Synthesis and Coal Chemistry of the Republic of Kazakhstan",
Karaganda, 100008, Kazakhstan,
e-mail: oxana230590@mail.ru*

Solid waste from coal mining and processing makes up a significant part of the total volume of industrial waste generated in the world. In our coal-rich region (Kazakhstan, Karaganda), the authors have carried out a lot of work on the use of oxidized (unsuitable) coals for the energy complex [1-3]. This paper examines the prospects for converting coal waste into adsorption materials to protect the environment. The adsorption materials were obtained by molecular imprinting, where the template is the Zn^{2+} ion. This method of sorption material synthesis makes it possible to copolymerize a functional monomer with a given molecule by crosslinking, and then remove the matrix molecule to form polymers with a molecular imprint (MIPs).

The scheme for obtaining zinc-imprinted polymers is shown in Figure 1.

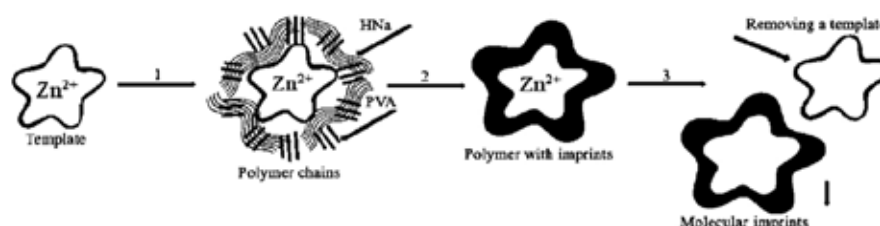


Figure 1. Схема получения молекулярно-импринтированного полимера.

The scheme includes three stages: 1 – formation of a complex between the matrix molecule and polymer chains in solution; 2 – formation of a polymer; 3 – removal of the matrix molecule with the formation of cavities (imprints) in the polymer by compounds. Recognition can be carried out by shape, size, or specific interactions between the functional groups of the matrix molecule and the polymer.

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This research was funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. BR10965230 "Development of "green" technologies for obtaining multifunctional materials based on deep processing of organomineral raw materials of Kazakhstan").

MODIFYING COATINGS BASED ON CHITOSAN AND ALGINATE FOR THE MANUFACTURE OF MEDICAL MASKS

Avdeeva E.V., Rogachev A.A., Agabekov V.E.

*State Scientific Institution "Institute of Chemistry of New Materials of the National Academy of Sciences of Belarus",
 Belarus, 220141, Minsk, st. F.Skorina, 36, Republic of Belarus
 e-mail: avdeeva.katerina86@mail.ru*

Modifying protective coatings from chitosan and sodium alginate (XT-AL) on cotton materials (surface density 174 g/cm², "Blakit", Belarus) were produced using the freeze-drying method. The assessment of the efficiency of air filtration (EAF) was carried out on an experimental laboratory stand, the assessment of the effectiveness of bacterial filtration (EBF) - in the Republican Unitary Enterprise "Scientific and Practical Center of Hygiene" using the test strain *St. aureus* ATCC 6538. The surface properties of the original and modified samples were determined by the contact angle (CA) with water at a drop volume of 5,0 μ L. The morphology of the coatings was studied using a scanning electron microscope JEM-6000, Jeol, Japan.

For samples coated with CT-AL 1:2,3 (molar ratios), the formation of pores of 80-240 μ m, CA less than 5° is shown; HT-AL 1:1,2 - 20-110 μ m, 28±5°. For the system (cotton / cotton / cotton) EAF decreases significantly over time from 78% to 58%, (cotton / HT-AL 1:2,3 cotton / cotton) - with 86,2% to 79,5%, (cotton / HT-AL 1:1,2 cotton / cotton) - from 99,8% to 99,6% (Fig. 1).

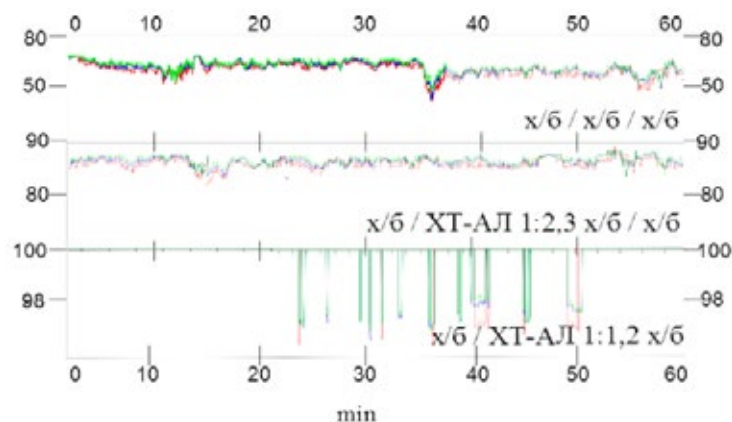


Figure 1. Filtration kinetics of three-layer systems made of modified cotton

It were shown that coating modifying HT-AL 1:1,2 helps to increase the barrier properties and overcome the threshold value of EAF and EBF required for medical masks.

The work was carried out with the financial support of the State Public Research Institute "Chemical processes, reagents and technologies, bioregulators and bioorgchemistry" for 2021-2025, Complex task 2.4.2, Research work 1.

POLYAMIDE 6/6 AEROGELS AND IONOGELS

**Kottsov S.Y.,^a Malkova A.N.,^b Badulina A.O.,^a Lermontov S.A.,^b
Baranchikov A.E.^a**

*^aKurnakov Institute of General and Inorganic Chemistry of the Russian
Academy of Sciences, 31 Leninsky Prospekt, Moscow, 119991,
e-mail: a.baranchikov@yandex.ru*

*^bInstitute of Physiologically Active Compounds FRC Problems of Chemical Physics and Medical Chemistry of the
Russian Academy of Sciences, 142432, Chernogolovka, Severny pr.1.*

A method for the preparation of polyamide 6/6 (nylon 6/6) aerogels was proposed based on the low-temperature supercritical drying of lyogels produced by controlled cooling of polymer solutions in N,N-dimethylacetamide. These highly porous (> 90%, 1.05 mL/g) polymeric materials have a rather high specific surface area (up to 100 m²/g) and high crystallinity (up to 0.86). Their structure and composition were analysed using IR spectroscopy, scanning electron microscopy, thermal analysis, and small angle X-ray scattering.

It was shown that similar highly porous materials can be produced by replacing the organic solvent in the lyogel with water and then freeze-drying.

The polymeric aerogel showed a high sorption capacity for 1-alkyl-3-methylimidazolium ionic liquids, up to 33 mmol/g, as well as for Starks' catalyst (Aliquat 336), up to 18 mmol/g. The stability of the ionogels formed by impregnating polymeric aerogels with ionic liquids upon contact with an aqueous phase was analysed.

The possibility of using these ionogels, based on polymer materials, for extracting transition metals (for example, iron(III)), from aqueous solutions, was evaluated.

The work was supported by Russian Science Foundation, grant 23-73-00028.

SYNTHESIS OF THE BIMETALLIC NANOSCALE BISMUTH-SILVER PARTICLES STABILIZED BY POLYVINYLPYRROLIDONE

Borovikova L.N., Valueva S.V., Volkov A.Ya., Morozova P.Yu.

*Scientific Research Center «Kurchatov Center" Institute of High Molecular Compounds,
 199004, St. Petersburg, Russia, Bolshoy Prospekt, V.O., 31
 E-mail: diadora3@mail.ru*

Recently, bimetallic nanoparticles (BMNP) have been the subject of close attention of the researchers because of their possible use as catalysts for various chemical processes, as well as carriers for targeted drug delivery. The individual physic-chemical properties of metals expand the range of their use, that is explained by the mutually reinforcing effects resulting from the interaction of the metals with each other. It is known that Ag NP and Bi NP are widely used in medicine. The synthesis of BMNPs based on Ag and Bi is of undoubted interest, both for practical application and from the point of view of studying the "internal" structure of BMNPs and developing methods for their stabilization in aqueous solutions.

BMNPs were synthesized by simultaneous introduction of the precursors of the silver nitrate (AgNO_3) and Bismuth nitrate pentahydrate ($\text{Bi}(\text{NO}_3)_3 \cdot 5\text{H}_2\text{O}$) into the reaction system during reduction reactions with sodium borohydride (NaBH_4) in aqueous medium at atmospheric pressure in the presence of PVP (MM10000). The carried out X-ray diffraction analysis of the reduction products showed (Fig. 1) that reflexes at $2\theta^\circ = 27.2^\circ, 38^\circ, 39.6^\circ, 48.7^\circ$ are specific for NP Bi1, whereas reflexes at $2\theta^\circ = 29.8^\circ, 38.1^\circ, 44.09^\circ$ correspond to the pattern observed for Ag^2 NP.

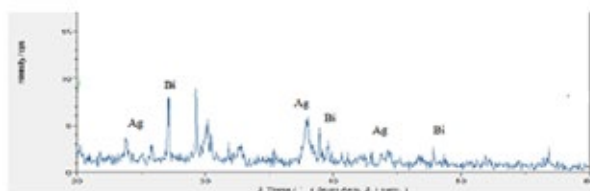


Fig. 1. Diffraction pattern BMNP Bi – Ag.

Thus, it can be argued that as a result of the carried out synthesis, a PVP-stabilized bimetallic NP Bi - Ag was formed.

Literature

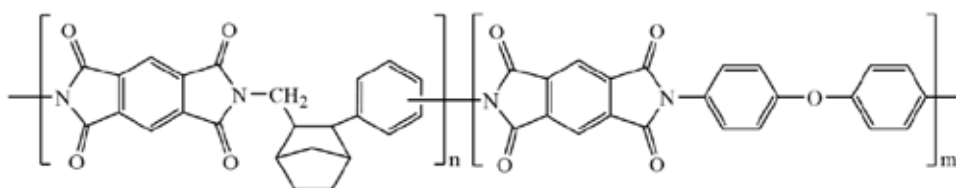
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STUDYING THE FEATURES OF THERMAL DESTRUCTION OF COPOLYIMIDES BASED ON [2-(AMINOMETHYL) BICYCLO[2.2.1]HEPT-3-YL]ANILINES

Novakov I.A., Orlinson B.S., Brunilin R.V.

*Volgograd State Technical University,
Russia, 400005, Volgograd, Lenin Ave. 28, e-mail: brunilin@vstu.ru*

One of the requirements for the development of new polyimide materials is their high heat resistance. In this regard, we studied the features of the thermal destruction of copolyimides based on pyromellitic dianhydride, [2-(aminomethyl) bicyclo[2.2.1]hept-3-yl]anilines and 4,4'-diaminodiphenyl ether.



where $n = 20\%$ (mol.), $m = 80\%$ (mol.).

The kinetics of thermal destruction of copolyimides was studied using the A.W. Coats and J.P. Redfern method. We determined the reaction orders and the values of effective activation energies for thermal destruction processes.

The resulting graphical dependences have several linear sections at $n = 1$. The low-temperature section, in our opinion, is determined by the reactions of hydrolytic cleavage of amide bonds of non-cyclized polyamide acid units (activation energy $E_a = 20 - 40$ kJ/mol). The high-temperature region is probably due to the processes of homolytic decomposition of the polymer chain ($E_a = 130 - 250$ kJ/mol, depending on the structure of the polymer).

Analysis of the data obtained shows that the activation energies of the low-temperature region for bicyclic copolyimides are higher than for completely aromatic ones, which correlates well with their higher hydrolytic stability. In turn, the processes of homolytic decomposition of the polymer chain for a fully aromatic polyimide have the highest activation energy, which corresponds to its greater thermal stability.

The research was carried out with the financial support of the Ministry of Science and Higher Education of the Russian Federation (project No. FZUS-2023-0003 on the basis of agreement No. 075-03-2023-055 dated January 13, 2023) and using the equipment of the Center for Shared Use of the FHMI of the Volgograd State Technical University.

PHYSICAL AND MECHANICAL PROPERTIES OF RUBBERS BASED ON SYNTHETIC POLYISOPRENE, MODIFIED WITH PHOSPHOLIPIDE CONCENTRATE AT THE STAGE OF DEGASSING OF ITS POLYMERISATE

Dauylbek A.A., Rakhmatullina A.P.

*"Kazan National Research Technological University", Kazan, st.
 K. Marksa, 68, Russia, 420015
 e-mail: aidadauylbek@gmail.com*

Synthetic isoprene rubbers, known as SRIs, are the main types of rubbers used in the tire industry. They are the only synthetic polymers that are close in structure and properties to natural rubber. It was previously established [1-3] that modification of SKI-3 with phospholipid concentrate (PLC) makes it possible to bring some properties of its composites closer to the properties of rubbers based on natural rubber (NR).

This work is devoted to finding optimal ways to practically implement the modification of SKI-3. The object of study was rubber polymerizate (a solution of rubber in isopentane), provided by PJSC Nizhnekamskneftekhim with a mass fraction of dry matter of 13.90%. Under laboratory conditions, FLC was introduced into the polymerizate SKI-3 at the stage of its degassing in an amount of 3 to 7 wt. particles per 100 wt. particles in terms of "dry" rubber.

The original polymer SKI-3 was used as a control sample. After degassing, the rubbers were dried to a constant weight and sulfur vulcanizates filled with carbon black were obtained from them.

The influence of FLC concentration on the volcanometric properties of rubber mixtures and the physical and mechanical properties of rubbers was studied. An improvement in elastic-strength characteristics in modified vulcanizates was established with an optimal FLC content in the composite.

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OLIGOMERIC COMPOSITION BASED ON EPOXY RESIN AND PHOSPHORUS-CONTAINING OLIGOETHER METHACRYLATE FOR PRODUCTION OF POLYMER COMPOSITIONS OF REDUCED FLAMMABILITY

**Drozdov E.V., Solomakhin S.M., Donetskova L.Y., Buravov B.A.,
Shevchenko K.E., Tuzhikov O.O.**

"Volgograd State Technical University"
drozdov.ev898@gmail.com

A number of flame retardants based on inorganic (metal hydroxides, inorganic acids), organic and organoelement compounds (phosphorus-containing, halogen-containing, nitrogen-containing) are used to solve the problem of flammability of epoxy compositions. However, many flame retardants have a negative effect on the final properties of compositions and polymers based on them. For example: organic chlorine compounds are capable of releasing toxic corrosive products when heated, inorganic flame retardants negatively affect the strength properties, and phosphorus-containing compounds increase the brittleness of polymers. To solve the above problems, polymerisation-capable phosphorus-containing oligoether methacrylates capable of forming spatially cross-linked structures are used as flame retardants [1].

In the presented work the process of joint curing of ED-20 resin by hot-curing anhydrides and phosphorus-containing oligoethermethacrylate PHOEM-1 cured by dicumyl peroxide was studied. For simultaneous curing of the system components and formation of interpenetrating polymer meshes, polymerisation initiators close in temperature regime of curing were selected: maleic anhydride and dicumyl peroxide.

Samples of investigated compositions with different content of acrylate (from 10 to 90 % wt.) were subjected to thermogravimetric study. The results of the analysis showed that as the content of phosphorus-containing oligomer in the mixture increases, the temperature of the onset of thermal degradation of the material increases from 170 to 260 °C. At the same time, the content of coke residue increases from 1 to 30 wt%.

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ANTI-BACTERIAL ACTIVITY OF ZnS/ EXPANDED PERLITE PHOS-PHORYLATED BUTADIENE RUBBER NANOCOMPOSITE

Edres N.M.,^{1,2} Buniyat-zadeh I.A.,² Suleymanova T.H.,³ Alosmanov R.M.²

¹*Department of Chemistry, Faculty of Education, Khartum University, 406, Khartoum, Sudan*

²*Department of High-molecular Compounds Chemistry, Faculty of Chemistry, Baku State University, Z. Xalilov str., 23, Baku, 1148, Azerbaijan*

³*Department of Medical Microbiology and Immunology, Azerbaijan Medical University, Bakixanov str., 23, Baku, 1022, Azerbaijan
E-mail: nadaedres2010@gmail.com*

Recently polymer-nanocomposites fabricated based on different types of nanofillers (metals, carbon nanotubes, and clays) were reported as the most de-veloped antibacterial materials in various industry applications such as (food packaging, tissue engineering, textile industry, and wearable electronics) due to their attractive structure and optoelectronic properties that efficiency serve their interaction with bacteria disturbing cell wall and inhibit bacterial growth through various interaction mechanisms. Regarding this, numerous reports have been published on the antibacterial activity of ZnS/Polymer composites. In this work, the antimicrobial activity of cubic ZnS of 3 nm immobilized on the expanded perlite/phosphorylated butadiene rubber (ZnS/EP-PhBR) in three cycles of SILAR method was investigated under indoor light toward G – ve and G + ve bacteria. The result of inhibition zones listed in the below table related to different cellular content and thickness of bacteria.

Bacteria	E-coli	P.aeruginoza	C.albicans	K.pneumoniae	B.anthracoidea
Inhibi-tion zone (mm)	5	8	7	5	5

Light activation of ZnS/EP/PhBR induced the hole (h^+) and electron (e) that generate hydroxyl radical ($\cdot OH$) which is responsible for bacterial cell mem-brane degradation.

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POLYMER SURFACTANTS FOR THE DEVELOPMENT OF CATALYTIC ORGANIC CHEMISTRY IN WATER

**Fetin P.A., Kadnikov M.V., Senchukova A.S., Fetina V.I., Solunina A.A.,
Lezov A.A., Zorin I.M.**

*St Petersburg University, 7-9 Universitetskaya Embankment, St Petersburg, Russia, 199034
E-mail: p.fetin@spbu.ru*

Water is the most environmentally friendly solvent for chemical reactions. New polymeric surfactants were formed that can overcome the hydrophobic limits of modern organic reactions and carry them out using only H₂O.

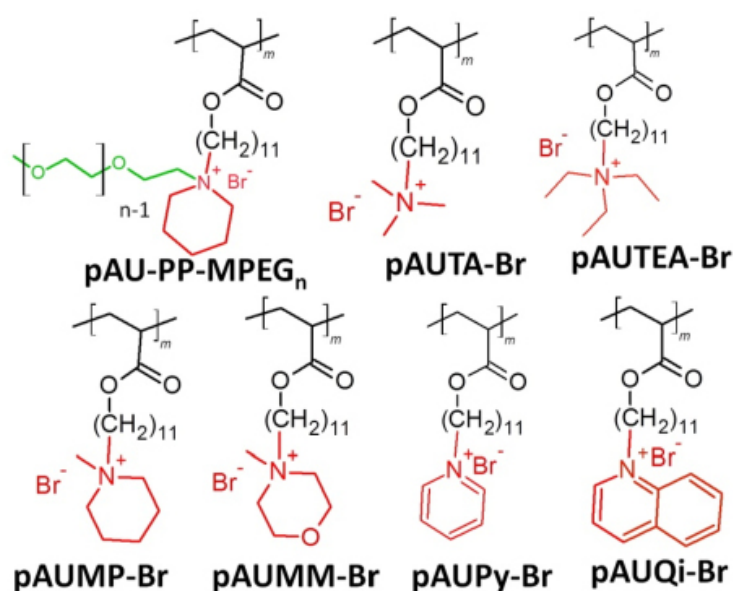


Figure 1. Chemical structures of cationic comb-like polyelectrolytes and their abbreviations used in this work as catalysts for organic reactions.

The comb-like polyelectrolytes obtained in our research group (Fig. 1) turned out to be effective in micellar-catalytic reactions aimed at the destruction of molecules. Acceleration of such reactions is achieved mainly due to local concentration of the substrate and reagent through the mechanism of solubilization and ionic attraction. These polymers also accelerate constructive organic reactions, where the ability to stabilize transition states and steric effects in the micellar pseudophase become important. The key focus of the report will be on studying the peculiarities of the Suzuki and Heck coupling reaction catalyzed by palladium chloride in water, where the comb-like polyelectrolyte acts as a co-catalyst.

This work was supported by a grant of the Ministry of Science and Higher Education of the Russian Federation for large scientific project in priority areas of scientific and technological development (grant number 075-15-2024-553).

INFLUENCE OF STAGED SYNTHESIS ON PROPERTIES WATER DISPERSIONS OF IONOMERIC POLYURETHANES

Golovanova K.V., Zenitova L.A., Tabachkov A.A.

*Kazan National Research Technological University
Russian Federation, Republic of Tatarstan, Kazan, 420015
68, Karl Marx street
e-mail: k.v.golovanova@gmail.com*

Stable water dispersions of ionomer polyurethanes (WDIPU) were synthe-sized based on oligodiethylenadipinate diol (ODAD) and aromatic (TDI) and aliphatic (HMDI) diisocyanates in a molar ratio of 1:3, without the use of high-ly volatile organic solvents (VOR). A study of the effect of the staged synthesis on d of VDIPU particles is presented in Figures 1 and 2.

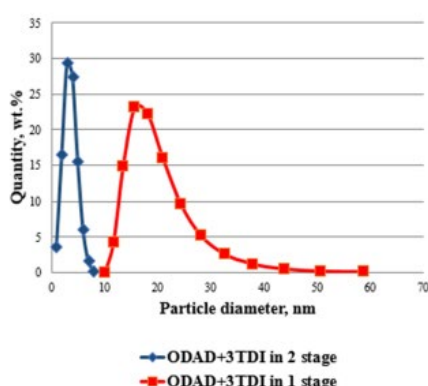


Figure 1. Dependence of particle diameter on the stages of WDIPU synthesis based on ODAD and TDI

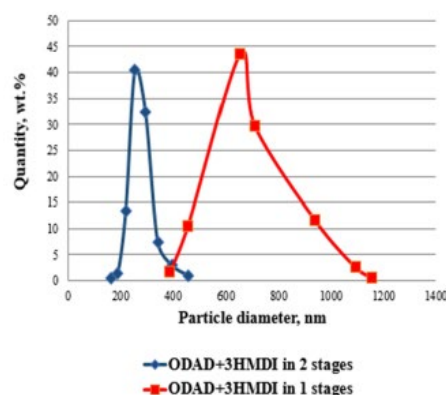


Figure 2. Dependence of particle diameter on the stages of VDIPU synthesis based on ODAD and GMDI

The one-stage method led to a greater scatter of particles in d and the inten-sity of scattering in the width of the transition zone than in the synthesis of WDIPU by a two-stage method, where a narrower distribution of particles is observed due to the ability to control the sequence of addition of reagents and form compositions with a more ordered structure.

Gratitude: The authors thank the Government of the Russian Federation (Grant in the form of subsidies from the Priority 2030 strategic academic leadership pro-gram, approved by Resolution No. 729 of May 13, 2021) for financial sup-port.

POSSIBILITIES OF OBTAINING HEMOSTATIC MATERIALS FROM COLLAGEN-CONTAINING WASTE OF THE FISH PROCESSING INDUSTRY

Grekhneva E.V., Vanina A.S.

*Kursk State University, 305000, Kursk, st. Radishcheva 33,
e-mail: grekhnyovaev@yandex.ru*

Fish collagen has recently been actively competing with collagen of animal origin due to the peculiarities of its structure and properties. The sources of this collagen are fish tissues, which most often represent waste from fish production. This work is a study aimed at obtaining hemostatic sponges from alternative raw materials isolated from waste from the fish processing industry. We considered two types of collagen-containing raw materials: leather and fish scales. Methods for extracting collagen from these materials are now well developed.^{1,2}

Today, among the means of local hemostasis, collagen-based hemostatic sponges are in greatest demand. As a result of the work, two series of sponges were obtained: the first - from collagen of scales and the second - from collagen of the dermal integument of fish. In both cases, the optimal amount of plasticizer (glycerol or PEG-400) and cross-linking agent (glutaraldehyde or glyoxal) was selected. In the resulting materials, parameters such as water absorption, swelling, degradation rate in aqueous solution, elasticity, and average pore size were studied. It should be noted that there are undoubtedly higher sorption and performance properties of sponges made from collagen of the dermal integument with the same ratio and quantity of modifiers. However, fish scale collagen is a much more accessible raw material. Therefore, by introducing additional components into the composition of the sponge, its basic properties can be significantly improved. Such components can be water-soluble cellulose ethers, which significantly increase the sorption properties of the sponge, as well as its flexibility, softness and elasticity.

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A CATALYST FOR THE SYNTHESIS OF SINGLE-COMPONENT HYBRID URETHANE SEALANTS

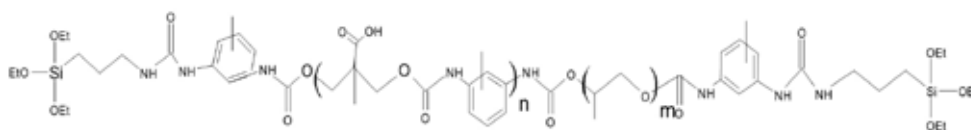
Khairullina I., Tabachkov A., Zenitova L.

*Kazan National Research Technological University,
 420015, Kazan, K.Marksa str., 68,
 e-mail: ntc.gadelshina@mail.ru*

To regulate the curing rate of silylated polyurethane (SPU) binders, it is proposed to use dimethylolpropionic acid (DMPA) as a pre-embedded catalyst in the prepolymer chain in the synthesis of silylated polyurethanes. It was found that the physico-mechanical parameters increase with an increase in the concentration of DMPA and its salt with various methods of introduction into the structure of the SPU.

The prepolymer for SPU was obtained in two ways: single-stage and two-stage. In the first case, polyester, acid and diisocyanate are mixed simultaneously to obtain a prepolymer. In the second case, the reaction was carried out through the stage of formation of a prepolymer followed by the introduction of acid to obtain a prepolymer. To study the effect of the salt of the embedded catalyst, a calculated amount of triethylamine was introduced into the SPU polymer with respect to DMPA.

The resulting SPU with an integrated acid catalyst is a polymer with the general formula:



where: $n = 0,1-0,5$; $m = 1$.

The amount and conditions of DMPA administration at the stage of prepolymer synthesis have an effect on the curing rate of the obtained SPAS. The effect of the salt obtained on the basis of embedded DMPA by neutralizing it with an equimolecular amount of triethylamine after blocking the prepolymer with silane on the formation of a surface film and curing of the SPU in mass is identical to the effect of embedded DMPA.

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THE EFFECT OF FUNCTIONALIZATION ON THE ELECTROPHYSICAL PROPERTIES OF LIGNIN

Khviyuzov S.S.,¹ Bogolitsyn K.G.,^{1,2} Gusakova M.A.¹

¹*N. Laverov Federal Center for Integrated Arctic Research of the Ural Branch of Russian Academy of Sciences, Russia, Arkhangelsk, 163020, Nikolsky Avenue 20.*

e-mail: khviyuzov.s@yandex.ru

²*Northern (Arctic) Federal University named after M.V. Lomonosov, Russia, Arkhangelsk, 163002, Northern Dvina Embankment 17.*

Lignin is the second of the most prevalent natural polymers after cellulose, its content is 18-32%. It has pronounced electrically conductive properties due to their multifunctional aromatic nature, conjugation system, and high reactivity in redox interactions. The production of materials for electric broadband capacitors may be one of the ways of their use. Lignins can change their functional composition when isolated. This is a significant obstacle to the use of the polymer.

Modified samples with different contents of methoxyl, carbonyl, carboxyl and introduced nitro-groups were obtained on the basis of slightly modified preparations of dioxan lignin of coniferous and deciduous species to study the influence of functional nature. The electrophysical properties (specific electrical conductivity σ , real ϵ' and imaginary ϵ'' parts of the complex permittivity) were determined by dielectric spectroscopy in the frequency range from 10^{-2} to 10^7 Hz. A methodical approach to the differentiated isolation of relaxators (charges or charge systems in the structure of a substance) and the determination of their characteristics (frequency, activation energy) was used^{1,2}.

The presence of dielectric relaxation processes at $\nu > 10^5$ caused by the π - electrons of aromatic rings, 10^2 - 10^4 – OH-, 0.1-1 – CO- and OCH₃-, $\nu < 0.1$ Hz - NO₂-groups respectively was established according to the frequency dependences of ϵ' and ϵ'' . The contribution of individual relaxators to the change in σ values was determined. The relationship «functional nature – electrophysical properties» was established for lignin. This will make it possible to predict changes in electrophysical properties during functional transformation, which can simplify the use of the polymer.

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This research was funded from the project agreement No. 122011700252-1. This work was performed using the equipment of Center for Collective Use of Scientific Equipment "Critical technologies of the Russian Federation" in the field of environmental safety of the Arctic (FCIAR).

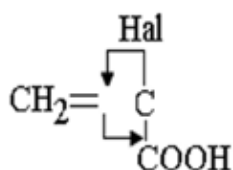
SPONTANEOUS POLYMERIZATION REACTIONS FORMING QUATERNARY AMMONIUM GROUPS

Kokoeva A.A.^a, Malkanduev Yu.A.^a, Dzhalilov A.T.^b

^a*Kabardino-Balkarian State University named after Kh.M. Berbekov, Nalchik,
Kabardino-Balkarian Republic, 360004, Russia,
e-mail: al-aneta@mail.ru*

^b*Tashkent Research Institute of Chemical Technology, Tashkent region, Republic of Uzbekistan*

It is well known that the electronegative carbonyl group in the structure of α -halogenacrylic acids (α -HAC) causes the halide to become sufficiently active and weakens the C–H bond. For this reason, it appears pertinent to take into account reactions in which they are involved.



The study found that when α -halogenacrylic acids (α -HAC) interact with tertiary amines at low temperature, spontaneous polymerization occurs. This allows for the study of the dependence of the process and the properties of the resulting polymers on the structure of the monomer and the groups contained in them, as well as the synthesis of soluble and insoluble polyelectrolytes with a regular structure, high exchange capacity, and When α -HAC interacts with tertiary amines, it forms polymers with quaternary ammonium groups. This contributes to the commencement of the process and the development of polymers with certain structures and molecular weights. These processes were studied, and the key features (medium, temperature, yield, and duration) were determined, as well as the lowered viscosity, nitrogen content, halogen content, and volumetric capacity. It has been proven that the structure of tertiary amines is important: in the absence of vinyl groups, soluble polymer products are generated, whereas when vinyl-containing compounds are utilized as tertiary amines, cross-linked products are formed.

IMPACT-RESISTANT POLYSTYRENE WITH PEARL LUSTER

Korobko E.A., Alekseev A.A. jr., Yarantseva N.V., Pleshkevich D.V.

*Novomoskovsk Institute (branch) of the Federal State Budgetary Educational Institution of Higher Education
«Mendeleev University of Chemical Technology of Russia», 301665, Russia, Tula region,
Novomoskovsky district, Novomoskovsk, Druzhby street, 8
e-mail: korobko.e.a@muctr.ru*

The currently known range of masterbatches will probably satisfy the needs of any manufacturer of products made from polymer materials. There are no problems with purchasing pigments that create special color effects, such as pearlescent ones. However, introduced pigments of this type, at best, do not change the properties of the polymer, and their cost is considerable¹.

In this regard, it may be of interest to obtain impact-resistant polystyrene (HIPS) with a pearlescent luster, based on the combination of polystyrene with a block copolymer of a linear structure of the A–B/A–A type, where A is a polystyrene (PS) block, B/A is a block random copolymer of butadiene and styrene brand StiroTEP-70, containing 70% bound styrene². The capabilities of the method are demonstrated by the data presented in the table.

Index	Content of StiroTEP-70, wt. %					
	0	3	5	10	20	100
Mother of pearl effect	No	No	Yes	Yes	Yes	No
Melt flow index, g/10 min	4,1	4,2	4,4	4,8	5,7	15,2
Impact strength, kJ/m ²	10,8	12,1	14,6	18,1	28,5	HP
Tensile yield strength, MPa	45,2	42,0	38,5	37,0	34,2	13,4
Tensile strength, MPa	43,7	41,3	37,9	34,8	27,6	10,7
Elongation at break, %	2	3	5	7	12	>500

Table. Properties of mixtures PSM-115 + StiroTEP-70

A white pearlescent effect is also achieved when using secondary PS. The complex of properties formed in this case corresponds to the level of HIPS.

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The work was carried out with the financial support of the Government of the Tula Region, contract DS/100 dated September 27, 2023.

METHODS OF INCREASING INTERLAYER ADHESION IN ARTIFICIAL LEATHERS BASED ON POLYVINYLCHLORIDE

Kovalenko G.M., Lototsky N.R.

*The Kosygin State University of Russia, Malaya Kaluzhskaya 1, Moscow, 119071, Russia,
e-mail: gregoryi84@mail.ru*

Artificial leathers are multilayer polymer composite materials that consist of a fibrous type base, as well as one or more polymer layers that differ in composition and/or structure, and have different operational properties depending on their functional purpose.

It is known from the literature data that epoxidian and perchlorovinyl resins, diisocyanates, oligoesteracrylates and various silanes are used to increase the adhesion of polyvinylchloride (PVC) coatings to polyester fabric. In the current economic situation, an urgent task is the selection of new adhesive additives and the study of their mechanism of action in comparison with those already used in production.¹

The purpose of the work is to develop PVC compositions containing adhesive additives of various nature to create polymer composite materials with high adhesive strength between layers.

The paper presents formulations of PVC plastisols for layers of artificial leathers containing various adhesion promoters: epoxy-diane resin of the ED-20 brand, hardener polyethylene polyamine (PEPA), perchlorvinyl (PCV), crosslinking agent diisocyanate «JL-506». The effect of adhesive additives on the rheological properties of plastisols has been established: all systems have a slight viscosity anomaly. The effect of adhesive additives on the bond strength between layers of artificial leather is shown. It was revealed that a composition containing 20 m.h. ED-20 and PEPA in a ratio of 10:1 has a high adhesion index (more than 65 H/5 cm) between the PVC coating and the polyester fabric.

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HYPERBRANCHED POLYMER NANOSYSTEMS CONTAINING IONS AND NANOPARTICLES OF 3D-METALS

**Kutyreva M.P.¹, Khannanov A.A.¹, Gataulina A.R.¹, Rossova A.A.¹,
Burmatova A.E.¹, Kutyrev G.A.², Ulakhovich N.A.¹**

¹ *Kazan Federal University,
420008 18 Kremlyovskaya street, Kazan, Russia*

² *Kazan National Research Technological University, 68 K. Marx street, 420015 Kazan, Russia
E-mail: mkutyreva@mail.ru*

The design of new materials based on complex polymers with 3D architecture - dendrimers and dendrite-like hyperbranched polymers (HBPs) modified by ions and nanoparticles of essential metals is an effective approach to creating promising materials for biomedicine and pharmacy.

The second to fourth generations hyperbranched polyesters G_n -R ($n=2-4$) with terminal OH groups (G_n -OH) and their functional derivatives, where

R - fragments of monoesters of dicarboxylic acids, aliphatic and aromatic amines, aminoalkyltrialkoxysilanes, are used to create metals (iron, cobalt and copper). The following synthetic strategies of metal-polymer materials have been implemented: the first is the doping of G_n -R polymers with metal ions to obtain hyperbranched metal-polymer G_n -OH@ M^{Z+} or hyperbranched coordination

G_n -RM nanosystems. The second strategy is the creation of complex nanocomposites G_n -R@M or G_n -R@ M_xA_y ($A = O, B$) using methods of chemical reduction of G_n -OH@ M^{Z+} , G_n -R@ M^{Z+} , G_n -RM precursors, thermolysis of

G_n -RM, sonochemical and polyol process in G_n -OH@ M^{Z+} systems. The third strategy was the creation of bimetallic organic-inorganic nanohybrids

M_1 @ G_n -R@ M_2 . The structure, physicochemical characteristics, morphology and functional properties (aggregation, thermal and photophysical properties, magnetic activity) of hyperbranched G_n -R polyesters and complex metal-containing nanosystems G_n -RM, G_n -R@M, M_1 @ G_n -R@ M_2 were established. The pool and important parameters of G_n -RM and G_n -R@M, nanosystems with the properties of synthetic modulators of enzymatic activity, antibacterial properties and hemocompatibility have been determined.

This scientific work has been supported by the Kazan Federal University Strategic Academic Leadership Program ('PRIORITY-2030').

MORPHOLOGY OF FATTY AROMATIC POLYAMIDE FIBRIDES

Laguseva E.I.,^a Shiryalin I.M.,^a Ivanova A.I.^b

*^aTver State Technical University, emb. Afanasia Nikitina 22, 170026, Tver, Russia,
e-mail: laguseva@yandex.ru*

*^bCenter for collective use of Tver State
University, str. Zhelyabova 33, 170100, Tver, Russia*

Polyamide fibrilles are produced by reaction molding at gas-liquid polycondensation plants. Reaction molding is a combined process of synthesis of polyamides and molding of fiber-film polymer binders (FPB) directly in the reaction chamber¹.

The properties and behavior of FRB under conditions of processing and operation are significantly influenced by their morphology, which determines the ability of fibrilles to self-bind in mass, i.e. to form relatively stable spatial structures due to capillary forces and mechanical bonding of individual dispersed particles. Polyamide 6I is formed as white loose clumps during synthesis and does not form fibrilles.

During the synthesis of PA-6T, long-fibrous FPB are obtained. The structure of the obtained polyamides largely depends on the structure of acylating monomers and the presence of inter- and intramolecular hydrogen bonds².

Polyamide studies were performed using a Beckman Coulter SA 3100 porosity analyzer. The porous composition of PA-6T and PA-6I polyamide is similar to each other, but the specific area is very different. This is due to the denser pore arrangement caused by the presence of more micropores in PA-6I, which reduces the external surface area.

Micrographs of PA-6T obtained on a JEOL 6610 LV scanning electron microscope revealed that individual layers of the polymer are formed from structures that are bundles of fibrils. The analysis of micrographs of PA-6I polyamide showed the peculiarity of their macrostructure - the PA-6I macromolecule is flexible, capable of twisting into curls.

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GAS-LIQUID POLYCONDENSATION AS A METHOD FOR OBTAINING FATTY AROMATIC FIBRIDES

Laguseva E.I.,^a Shiryalin I.M.,^{a,b} Tulyaev I.P.,^a Kalyuzhny A.P.,^a Hezzieva A.^a

^a*Tver State Technical University, emb. Afanasia Nikitina 22, 170026, Tver, Russia, e-mail: lagusseva@yandex.ru*

^b*Ltd «LPM», Pasha Savelyeva str. 45, 170039, Tver, Russia*

Gas-liquid polycondensation is one way of carrying out non-equilibrium polycondensation processes. It is a two-phase heterogeneous process of synthesis of heterochain polymers by heteropolycondensation, in which the reaction zone is localized at the liquid-gas interface. A distinctive features of the method: the reaction phase (the phase from the side of which the growth of the polymer film) serve only one liquid phase¹.

The foam mode is of greatest practical and scientific-engineering interest. In the conditions of a highly turbularized three-phase mobile layer of the foam mode, combined processes occur: synthesis of polyamides and polyesters with simultaneous reaction formation of fibrides (fiber-film polymer binders, FPB). Fibrides are used for the manufacture of heat-resistant synthetic papers for structural and electrical purposes, filter elements for fine purification of diesel fuel and technological solutions. Three-phase foam mode, accompanied by phase formation - insoluble polymer is formed. In contrast to the classical foam model, it is characterized by an increased linear velocity of the gas phase (based on the cross-section of the reaction zone, $W_g = 30-50 \text{ m/s}$)². Synthesis is carried out in fibridator reactors of special design.

Over 25 polymers of the polyamide and polyester classes were obtained at the gas-liquid polycondensation plant. Homo- and copolyamides with aromatic nuclei in the chain are of most interest. All polyterephthalamides and polyamides obtained on the basis of a monomeric mixture of the gas phase with an isophthalyl chloride content in the range of 10-25% have the properties of fibrides.

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STUDYING THE INTERACTION OF PHOSPHORUS (V) AND ANTIMONY (V) OXIDES WITH POLYPHENYLSILSESQUIOXANE BY MECHANOCHEMICAL ACTIVATION

Libanov V.V., Kapustina A.A., Avilov A.I., Shapkin N.P.

*Institute of High Technologies and Advanced Materials, Far Eastern Federal University,
690922, Vladivostok, Russky Island, Ajax, 10
e-mail: libanov.vv@dvfu.ru*

In this work, the interaction of polyphenylsilsesquioxane (PPSSO) with phosphorus (V) and antimony (V) oxides under conditions of mechanochemical activation was studied. Syntheses were carried out in a "Pulverisette 6" planetary mill at 600 rpm for 3 and 5 minutes at a mechanical activation dose of 2.81 and 4.68 kJ/g, respectively. The initial Si/M ratio in all syntheses was 1:1.

It has been shown that, regardless of the activation time, the interaction of PPSCO and phosphorus (V) oxide leads to the production of two soluble fractions with Si/P ratios different from the specified ones and equal to 8:1 (fraction 1) and 14:1 (fraction 2). According to elemental analysis and IR spectroscopy, both fractions did not contain water molecules and associated silanol groups, and their molecular weights were more than 7000.

When activating PPSSO and antimony (V) oxide, increasing the synthesis time led to a greater inclusion of the antimony atom in the polymer chain, but the expected Si/Sb ratio was also not obtained (19.6:1 for 3 minutes of activation and 13.2:1 for 5 minutes). X-ray phase analysis established that the composition of the insoluble fraction includes the original oxide of antimony (V) (50.7%), antimony oxide (III) in the form of valentinite (20.2%), antimony tetroxide Sb_2O_4 (15.3%), as well as antimony trioxide Sb_2O_3 in the form of senarmontite (13.8%). It has been suggested that the formation of antimony oxides in varying degrees of oxidation in the insoluble fraction could occur due to redox processes involving phenyl radicals and hydroxyl groups. The formation of phenyl radicals is also indicated by the presence of silicon oxide in the insoluble fraction, formed during the destruction of PPSSO. The formation of radicals during the mechanochemical activation of organosilsesquioxanes was established earlier in the works of Streletsky A.N. and Dubinskaya A.M.¹

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PROPERTIES OF POLYPROPYLENE MIXTURES

Lobanov A.V.^a, Alekseev A.A.^a, Osipchik V.S.^b

*^aNovomoskovsk Institute (branch) of the Federal State Budgetary Educational Institution of Higher Education «Mendeleev University of Chemical Technology of Russia», 301665, Russia, Tula region, Novomoskovsky district, Novomoskovsk, Druzhby street, 8
e-mail: lobanov.a.vl@muctr.ru*

^bFederal State Budgetary Educational Institution of Higher Education «D. I. Mendeleev Russian University of Chemical Technology», 125047, Russia, Moscow, Miusskaya square, 9

In actual practice, direct processing of mixtures of primary and secondary polypropylenes (PP) with different fluidity is widely used. However, it is difficult to predict the nature of the formation of their properties under conditions of repeated processing.

The objects of research in this work are products of multiple injection molding of mixtures of primary PPG 1350-21 and PP H030, taken in mass ratios of 75:25, 50: and 25:75, respectively (mixtures SM-1, SM-2 and SM-3) at temperature 190, 205 and 230°C.

The impact strength of the mixtures (at minus 20°C) and their tensile mechanical properties are very stable under repeated casting conditions and correspond to the level of the original PP. The nature of the formation of melt flow index (MFI) values for mixtures SM-1 and SM-3 is similar for PPG 1350-21 and PP H030, processed at temperatures of 180 and 230°C. A noticeable influence of processing conditions on the MFI values was established for the SM-3 mixture (figure), which indicates the heterogeneity of its melt at 200°C.

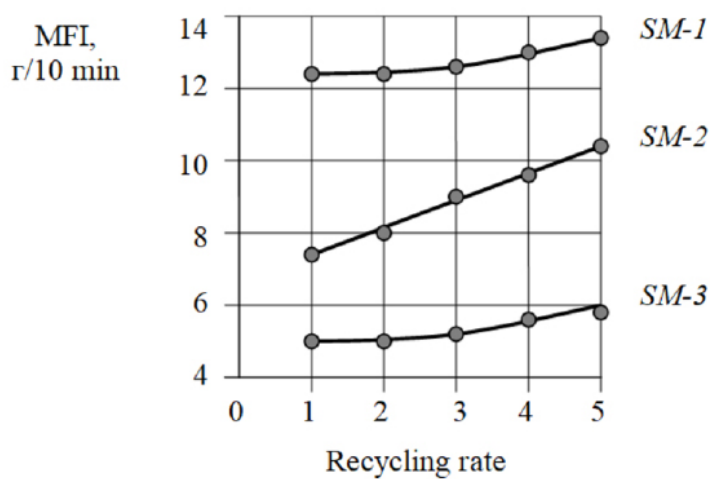


Figure. Dependence of MFI (200 °C/21.18 N) of PP mixtures on the frequency of processing.

Mixtures of these PP can be processed 5 times by injection molding at relatively low temperatures.

The work was carried out with the financial support of the Government of the Tula Region, contract DS/100 dated September 27, 2023.

SPECTRAL CHARACTERISTICS OF NEW TRINARY NANOSYSTEM BASED ON PHOTODITAZINE AND DETERMINATION OF THEIR BIOLOGICAL ACTIVITY

Morozova P.Yu., Valueva S.V., Borovikova L.N., Krasnopeeveva E.L.

*NRC "Kurchatov Institute" Institute of Macromolecular Compounds,
 Saint Petersburg, Bolshoy pr. 31, 199004, Russia.
 e-mail: aravenko_polina@yahoo.com*

One of the most successful Russian photosensitizers (PS) of the chlorine series is Photoditazine (PD), a drug based on the di-N-methylglucamine salt of chlorine e6, used in photodynamic therapy (PDT) in the treatment of cancer.

In order to create new highly effective PS for PDT, we synthesized hybrid ternary nanosystems (HTN) Se⁰/Cell-graft-PMAA/PD based on PD, selenium (Se⁰) nanoparticles (NPs), and a polymer stabilizer (PS) - an amphiphilic molecular brush with cellulose as the main chain and hydrophilic side chains of polymethacrylic acid (PMAA) (Cell-graft-PMAA) with different order of introduction of components¹.

Spectral studies of HTN (Cell-graft-PMAA/Se⁰)/PD (1st synthesis method) and (Cell-graft-PMAA/PD)/Se⁰ (2nd synthesis method) were carried out. First of all, differences for the two synthesis methods in the spectral picture are observed in the region of the Soret band (403 nm) and in the PDT region (Q - bands): for the first method of synthesis, a splitting of the Q - band into two bands is observed, and for the second, one is observed band at $\lambda_{\text{PDT}} = 672$ nm.

The biological activity of HTN was assessed using the African green monkey kidney epithelial cell line (Vero). Survival was assessed both visually, using light microscopy, noting morphological changes in cells, and by the colorimetric method using the MTT test. Both HTNs demonstrated high growth inhibition efficiency in the Vero cell line.

Thus, the synthesized HTNs are promising for the creation of light-sensitive hybrid compounds for PDT on their basis.

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The work was carried out within the state assignment of NRC "Kurchatov Institute".

PREDICTION OF CELLULOSE DISSOLUTION IN PYRIDINIUM IONIC LIQUIDS USING QUANTUM CHEMICAL CALCULATIONS

Muravyev A.A.^a, Petrova E.O.^b, Abramova E.S.^b, Novoselov N.P.^b, Skorik Y.A.^a

^aInstitute of Macromolecular Compounds of the Russian Academy of Sciences, St. Petersburg

^bSt. Petersburg State University of Technology and Design, St. Petersburg

Cellulose is the most widespread natural polymer, and the search for environmentally friendly and technologically suitable solvents for its deep chemical processing remains relevant. Ionic liquids (ILs) are promising cellulose solvents that meet most of the modern requirements in terms of ecology and processability. Pyridine-based ILs are of increasing interest due to the availability of raw materials.

In this work, the optimization of structures within the framework of density functional theory using the hybrid density functional B3LYP and the 6-311++G(d,p) basis set was used to intensify the search for a suitable pyridine-based IL as a cellulose solvent. Calculations were performed using Firefly software based on Qcpackage and GAMESS (US).

Two factors were chosen as solubility criteria: the change in the calculated total energy of the system and the change in the calculated total dipole moment of the system compared to the sum of the parameters for the original components. The dissolution of cellulose occurs if the values of the criteria for both energy and dipole moment are less than zero. The calculations showed a good correlation between the calculated values and the experimental results on the dissolution of cellulose in ILs.

NEW ORGANOSILICONE POLYMER MATERIALS FOR APPLICATION IN MICROELECTRONICS

Neelova O.V.^a, Kubalova L.M.^a, Bekmurzova A.S.^b

^a*North Ossetian State University named after Kosta Levanovich Khetagurov,
 Vatutin St., 44-46, Vladikavkaz, 362025, Russia
 e-mail: o.neelova2011@yandex.ru*

^b*SPC JSC «TsKB RM», «NIEM», Nikolaev St., 4, Vladikavkaz, 362021, Russia*

An urgent task of modern electronic instrument making in the field of micro- and nanoelectronics is the development of new protective polymer materials with special properties that work under conditions of prolonged exposure to high and low temperatures, electrical voltages, humidity, radiation and other harsh factors.

Organosilicon block copolymers of a linear ladder structure, consisting of rigid phenylsilsesquioxane $[C_6H_5SiO_{3/2}]_m$ and elastic dimethylsiloxane $[(CH_3)_2SiO]_n$ blocks, are of greatest interest for the development of new compositions, the coatings of which have high physicochemical properties in the temperature range from -60 to $+300^\circ C$.¹

The authors have shown that polyorganosiloxane block copolymers of the general formula $HO\{[C_6H_5SiO_{1.5}]_m[(CH_3)_2SiO]_n\}H$, synthesized by heterofunctional polycondensation, make it possible to obtain heat-resistant elastomeric coatings characterized by a combination of high strength and hardness, excellent electrical insulation, and moisture protection and adhesive properties, low content of ionic impurities and lack of corrosive action towards aluminum and copper.² The coatings can withstand temperatures of $+300^\circ C$ for 5 hours and $+400^\circ C$ for 0.5 hours.³ High adhesion of coatings to various materials is ensured by a curing system based on polydimethylborozirconsiloxane.⁴

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The work was carried out with the financial support of the Innovation Promotion Fund, project No. 45293, application CI-51344.

PROPERTIES OF POLYPROPYLENE AND IMPACT-RESISTANT POLYSTYRENE MIXTURES

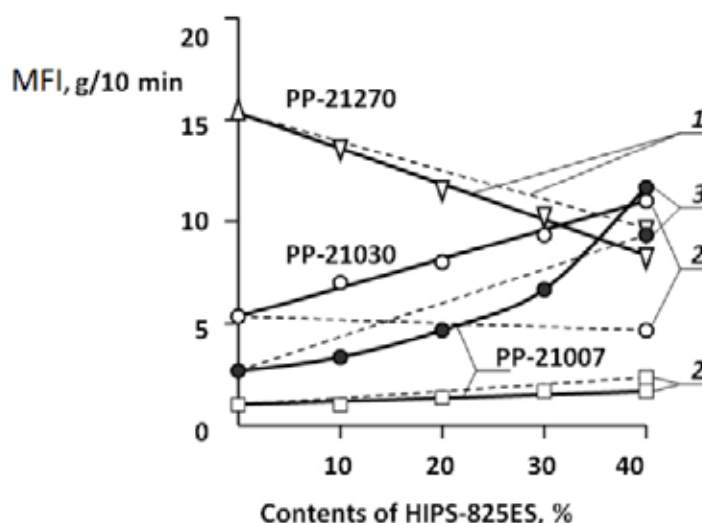
Nikolaev E.S., Lobanov A.V., Alekseev A.A. jr., Yurova I.V.

*Novomoskovsk Institute (branch) of the «Mendeleev University of Chemical Technology of Russia», 301665, Russia, Tula region, Novomoskovsky district, Novomoskovsk, Druzhby street, 8
e-mail: baharamja@mail.ru*

Mixtures involving polypropylene (PP) and HIPS (high-impact polystyrene) can be formed at the stage of crushing both waste from their processing and used disposable tableware. Mixtures can be classified according to the “floating-settling” method, but this requires additional space and considerable energy consumption.

It was interesting to evaluate the possibilities of processing such mixtures directly on model systems involving primary polymers, for example, PP-1250, PP-21030, PP-21007 and HIPS-825ES.

It has been established that the nature of the formation of melt flow index (MFI) values for PP-21030+ HIPS-825ES mixtures is radically different in comparison with other mixtures (Drawing).



Drawing. Dependence of the MFI of PP on the content of HIPS-825ES.
The dotted lines indicate the theoretical additive nature of the formation of MFI mixtures. MFI: 200 °C, 21.2 N (1); 200 °C, 49 N (2); 230 °C, 49 N (3).

The introduction of HIPS-825ES into the composition of PP slightly increases its tensile yield strength and noticeably its tensile strength, while elongation at break and impact resistance are catastrophically reduced.

The work was carried out with financial support from the Ministry of Science and Education of the Russian Federation within the framework of the scientific project «Laboratory of Smart Materials and Technologies», project No FSSM-2024-0005.

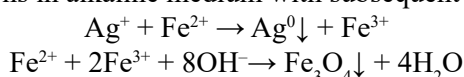
SYNTHESIS OF NANO-SIZED COMPOSITE Ag@Fe₃O₄ BY PARTIAL OXIDATION OF Fe(II) WITH Ag(I) CATIONS IN THE PRESENCE OF LIGNOSULFONATES

Plakhin V.A., Khabarov Y.G., Veshnyakov V.A., Chukhchin D.G., Malkov A.V.

*Northern (Arctic) Federal University named after M.V. Lomonosov,
 Naberezhnaya Severnoy Dviny, 17, Arkhangelsk, 163002, Russian Federation
 e-mail: v.plahin@narfu.ru*

One of the most important issues in the application of nanoparticles is the difficulty of regenerating them from the medium in which they are used. To solve this problem, nanoparticles are deposited on magnetically active materials that can be separated by magnetic separation^{1,2}.

We have developed a one-step synthesis of magnetically active composite of Ag@Fe₃O₄ composition based on the partial oxidation of iron(II) by Ag(I) cations in alkaline medium with subsequent formation of magnetite:



Technical lignosulfonates (LST) were used as stabilizers of the formed particles. The synthesis results in the formation of spherical particles composed of silver plates with a thickness of 30 to 100 nm (Figure 1).

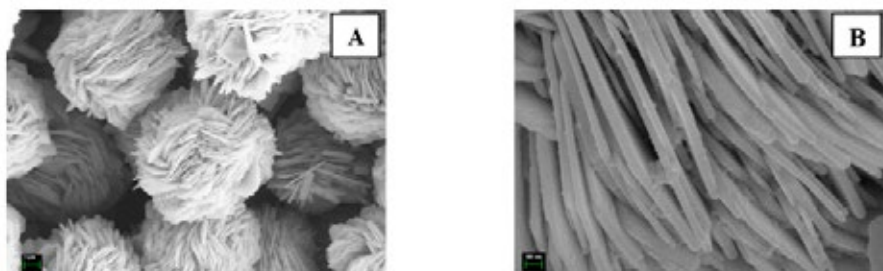


Figure 1. Micrographs of the synthesized composite with the reagent consumption: 0,7 g LST /g Fe(II); 1,3 g Ag(I)/g Fe(II). Scale bar – 1 μm (A) and 100 nm (B).

It was found that, depending on the LST consumption, spherical structures with different packing density of nanosized silver plates are formed, and at LST consumption more than 2 g/g Fe(II) they are not formed.

The resulting composites have high catalytic activity in the reduction of nitrophenols with NaBH₄ and are easily separated by magnetic separation.

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This work was financially supported by the Ministry of Science and Higher Education of the Russian Federation, Project No. FSRU-2024-0010.

MODIFICATION OF ABS PLASTICS WITH EPOXY OLIGOMERS

Pleshkevich D.V., Korobko E.A., Grigorov I.V.

*Novomoskovsk Institute (branch) of the Federal State Budgetary Educational Institution
of Higher Education «Mendeleev University
of Chemical Technology of Russia», 301665, Russia, Tula region,
Novomoskovsky district, Novomoskovsk, Druzhby street, 8
e-mail: pleshkevich.2015@mail.ru*

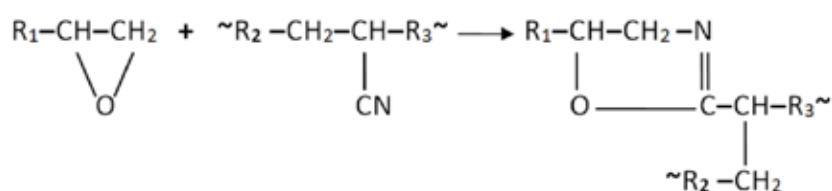
A well-known way to expand the range of extrusion grades of acrylonitrile butadiene styrene plastics (ABS plastics) is to vary the content of the rubber phase in the styrene-acrylonitrile copolymer matrix. In practice, this is realized in a “reactor” version (synthesis) or by carefully mixing injection-molded ABS plastic with expensive graft rubber.

This work demonstrates the possibility of transforming emulsion injection molded ABS plastics into materials for extrusion purposes by partially cross-linking the matrix copolymer with epoxy compounds: epoxy oligomer SM-828 (table) and diglycidyl ether of diethylene glycol brand DEG-1.

Index	SM-828 content, wt. %			
	0	+0,5	+1,5	+3,0
Melt flow index (220 °C, 10 min, 98 H), g/10 min	10,3	11,6	8,4	4,6
Notched Izod impact strength, kJ/m ²	17,3	17,9	16,6	17,1
Tensile yield strength, MPa	36,9	40,1	39,5	43,2
Tensile strength, MPa	27,7	28,0	29,8	32,1
Elongation at break, %	16	16	22	16
Shoulder blade shrinkage No. N 2 (GOST 11262)	0,8	0,8	0,7	0,6

Table. Properties of ABS + SM-828 mixtures

The crosslinking of SAN macromolecules proceeds according to the scheme (fragment):



The use of DEG-1 is less effective.

Further chemical modification of ABS is also possible.

The work was carried out with financial support from the Ministry of Science and Education of the Russian Federation within the framework of the scientific project “Laboratory of Smart Materials and Technologies”, project No. FSSM-2024-0005.

COPOLYMERS OF N,N-DIMETHYLAMINOETHYLMETHACRYLATE AND METHYL METHACRYLATE AS RAFT-AGENTS

**Ponomareva D.A.^a, Morozov N.A.^a, Silantieva E.V.^a, Lobanova N.A.^a,
Serkhacheva N.S.^a, Chernikova E.V.^b, Prokopov N.I.^a**

^a*MIREA - Russian Technological University, Lomonosov Institute of Fine Chemical Technologies,
Vernadsky prospekt 86, Moscow, 119571, Russia,
e-mail: d89169750510@mail.ru*

^b*Lomonosov Moscow State University, Faculty of Chemistry, Moscow, 119991, Russia, Leninskie Gory, 1c3*

Recently, there has been a growing interest in the production of colloidal particles of amphiphilic block copolymers using heterophase controlled radical reversible addition-fragmentation chain transfer polymerization (RAFT). In particular, PISA - polymerization induced self-assembly technology has gained wide popularity^{1,2}. In these reactions, a polymer precursor is used, capable of performing the function of an RAFT-agent by building up the chain to form a block copolymer.

In this work, polymerization of methyl methacrylate (MMA) under the action of copolymers N,N-dimethylaminoethyl methacrylate (DMAEMA) and MMA (5% mol. MMA) with a tritiocarbonate group at the end of the chain of different molecular weights (MM): C1 ($M_n = 6200$ g/mol, $M_w/M_n = 1.27$) and C2 ($M_n = 26200$ g/mol, $M_w/M_n = 1.33$). The reaction was carried out in ethanol (volume phase ratio MMA/medium = 1/10) in the presence of azoisobutyric acid dinitrile (1% by weight) and C1 or C2 copolymer (1% by weight) at 65 °C for 8 hours.

The key point in the mechanism of particle formation in PISA reactions is the ratio of block lengths, namely, solvophilic (RAFT-agent) and solvophobic (PMMA block) fragments. It is shown that with increasing MM of the DMAEM and MMA copolymer, the polymerization rate of MMA also increases. Apparently, in the presence of C2, the nucleation period of the particles is shorter, which is confirmed by the data on the dispersed composition obtained by the method of dynamic light scattering. An hour after the start of the reaction, the particle size during polymerization in the presence of C1 was about 35 nm, and in the presence of C2 – 60 nm. In the future, it is planned to analyze the reaction with copolymers with other MM.

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RHEOLOGICAL PROPERTIES OF STARCH PRODUCTS WITH SUCCINCINE ANHYDRIDE

Shtepenko D.E., Protopopov A.V.

*Altai State Technical University I.I. Polzunova, 656038, Barnaul, Lenin Ave., 46,
e-mail: protopopovav@altgtu.ru*

Although there are many commercially available starches produced by this process, there is relatively little information about them. Therefore, based on existing research, the work examines the possibility of carrying out a reaction between starch and succinic anhydride in a weakly alkaline medium.

Component ratio	Synthesis temperature	
	25°	45°
1:0,5	0,019	0,027
1:1	0,032	0,043

Table 1 - Degree of substitution in reaction products

The degree of substitution in the resulting starch products naturally increases with increasing synthesis temperature, and no side processes of starch polysaccharide destruction are observed. The resulting modified starch products have a low degree of substitution with respect to acid, which favors their use in the food industry if their rheological properties are improved. The study on rheological properties was carried out by determining the viscosity of a 2.5% solution after keeping the solutions at a given temperature, thus a change in gelation was observed in the resulting solutions (Figure 1).

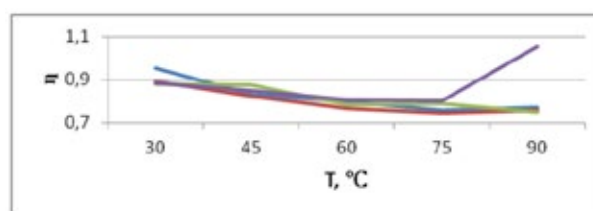


Figure 1 - Graph of viscosity versus temperature

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STUDY OF THE INTERACTION OF STARCH WITH CITRIC ACID AND RHEOLOGICAL PROPERTIES

Gavrilenko G.A., Kurochkina E.V., Protopopov A.V.

*Polzunov Altai State Technical University, 656038, Barnaul, Lenin Ave., 46,
e-mail: protopopovav@altgtu.ru*

We modified starch in two solvents: water and carbon tetrachloride, at different ratios of starch to solvent and at different synthesis temperatures.

Conditions for obtaining the product	Synthesis temperature	
	25°C	45°C
CCl ₄ (3 часа)	0,126	0,15
CCl ₄ (4 часа)	0,393	0,323
H ₂ O ((1:0,25) 4 часа)	0,37	0,37
H ₂ O ((1:0,5) 4 часа)	0,54	0,6

Table 1 - Degree of substitution in the resulting modified starch. Conditions for obtaining the product Synthesis temperature

During the study of the resulting starch modifications, studies of their solubility were also carried out (Table 2).

Component ratio	30°C	45°C	65°C	90°C
КЛБ 1:0,25 4/25	1.08	1.10	1.03	1.03
КЛБ 1:0,25 4/45	1.05	1.12	1.02	1.05
КЛБ 1:0,5 4/25	1.00	1.01	0.99	1.32
КЛБ 1:0,5 4/45	1.04	1.04	0.95	1.08
КЛ CaCl ₂ 3/30	1.05	1.02	0.95	0.9

Table 2 - Viscosity of the resulting starch citrates.

The data obtained show that starch modified with citric acid, under the specified synthesis conditions, does not affect the viscosity of solutions. However, the resulting starch products exhibit a significant decrease in solubility temperature. Also, due to the presence of free groups of bound citric acid in starch, the resulting product is of interest as a regulator of acidity and viscosity.

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FIRE-RETARDANT POLYPROPYLENE-BASED POLYMER COMPOSITES WITH AMMONIUM POLYPHOSPHATE CONTENT

Psyanchin A.A., Zakharova E.M.

*Ufa University of Science and Technology, Zaki Validi 32, Ufa, 450076, Russia,
e-mail: artps96@yandex.ru*

Currently, ammonium polyphosphate (APP) is the most effective halogen-free flame retardant compound, exhibiting activity both in the gas phase and in the condensed phase¹. Piperazine can act as a synergist in the flame inhibition process. Therefore, the aim of this study is to determine the influence of piperazine on the fire-resistant properties of primary polypropylene (PP) homopolymer containing ammonium polyphosphate.

During the investigation, it was found that the minimum content of ammonium polyphosphate and piperazine required to achieve the V-0 flammability class of polypropylene is 20% by mass and 4% by mass, respectively.

Sample	Composition	w, % mass.	Minimum torque of the plastograph, Nm	UL- 94
1	PP	70	5,8	V-0
	APP	25		
	Piperazine	5		
2	PP	73,6	4,4	V-0
	APP	22		
	Piperazine	4,4		
3	PP	6	3,5	V-0
	APP	20		
	Piperazine	4		
4	PP	82	3,4	-
	APP	15		
	Piperazine	3		

Table 1. Indicators of torque and flammability class of composites.

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This research was funded by the Ministry of Science and Higher Education of the Russian Federation (scientific code FZWU-2023-0002).

SYNTHESIS OF NEW ELECTRICALLY CONDUCTIVE POLYMER MATERIALS

Sanakoeva M.O.^a, Musaev Yu.I.^b, Musaeva E.B.^b, Kozhemova K.R.^b

^a South-Osetian State University, 100001, Tskhinval, Putin st., 8
 e-mail: maradonnaa.kbr@mail.ru.

^b Kabardino-Balkarian State University, 360004, Nalchik, Chernyshevsky st., 173

The most polymer materials are dielectrics, but to varying degrees polymers exhibit conductivity characterized by electronic, ionic, and bipolar mechanisms ¹. The main advantage of electrically conductive polymers is that, along with high electrical conductivity, they can combine mechanical properties such as flexibility, strength, elasticity, etc. Using various synthesis methods, it is possible to regulate their properties in the required directions. By reacting the diketoxime 4,4'-diacetylphenyl oxide with p-diethynylbenzene, copolyphenylene ether pyrroles was synthesized ², which has a polyconjugated bond system:

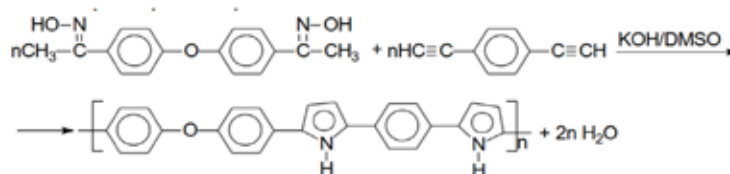


Figure 1. Polymer synthesis scheme

The obtained samples of some copolyphenylene ether pyrroles film (disks $d = 25 \pm 1$ mm, $15\text{--}50$ μm) were studied by impedance spectroscopy. With its help, it is possible to identify the influence of the sample microstructure on its total conductivity ³. The specific electrical conductivity was $2.12 \cdot 10^{-2}$ $\text{Ohm} \cdot \text{m}^{-1}$, which corresponds to literature data ⁴. Also, a method for electrochemical doping of PFEP was developed, as a result of which the conductivity of doped films of polyphenylenedipyrroles can reach ~ 102 $\text{Ohm}^{-1} \cdot \text{cm}^{-1}$.

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INVESTIGATION OF THE EFFECT OF THE VISCOSITY OF THE WORKING FLUID ON THE PARAMETER OF THE MAXIMUM FILLER CONTENT

Savitskaya Y.A., Kharlamova K.I.

*MIREA – Russian Technological University, Lomonosov Institute of Fine Chemical Technology,
Malaya Pirogovskaya street 1b5, Moscow, 119435, Russia,
e-mail: juli.ska@mail.ru*

Dispersed-filled polymer composite materials (DFPCMs) are created by incorporating a dispersed phase into a polymer matrix. The amount and characteristics of the added filler allow to adjust the properties of the final product.

One of the most important parameters for constructing DFPCMs is the maximum filler content parameter φ_m . Its value can be determined by the absorption of liquid oil or oligomer, by compaction curve, by bulk density, and by porosity of the DFPCMs material.¹⁻²

The aim of the study is to investigate the impact of the viscosity of the working fluid on the maximum filler content parameter in the method of oil and oligomer absorption.

During the course of the study, mixtures of ED-20 and DEG-1 oligomers in various proportions were prepared. Full-bodied glass microspheres MSP-55 ($d = 55 \mu\text{m}$, INOTEK AQUA LLC, Russia) were used as the objects of investigation. For each of the experimentally obtained working fluids, the φ_m parameter was determined by oligomer absorption.

When the values of dynamic and kinematic viscosities reach $8.00 \text{ Pa}\cdot\text{s}$ and $6.87 \text{ m}^2/\text{s}$, respectively, the value of the φ_m parameter begins to increase to 0.64 vol/vol ($\eta = 1.00 \text{ Pa}\cdot\text{s}$, $\nu = 0.86 \text{ m}^2/\text{s}$). At this point, the relative systematic error is 3%.

It has been demonstrated that the optimal working fluid viscosity lies within the range of 16 and $8 \text{ Pa}\cdot\text{s}$, as at the lower viscosities the value of φ_m parameter begins to rise. It should be noted that beyond $8 \text{ Pa}\cdot\text{s}$, the complexity of the mixing process for the filler and working fluid increases. Therefore, it is recommended to use a fluid with a viscosity between 16 and $10 \text{ Pa}\cdot\text{s}$.

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OBTAINING OF DRUG'S MATRIX FORMS BASED ON POLYSACCHARIDES

Shevchuk N.O., Kryuk T.V., Tyurina T.G., Grigoriev E.S.

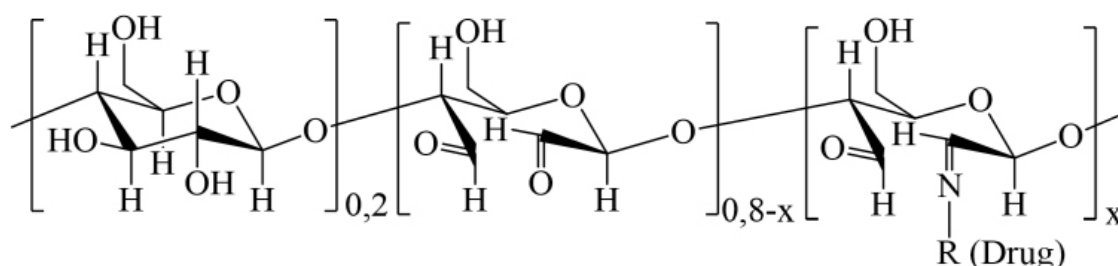
*L.M. Litvinenko Institute of Physical Organic and Coal Chemistry,
 st. R. Luxemburg 70, Donetsk, Russia, 283048,
 e-mail: minarina@mail.ru*

One of the ways to solve the problem of increasing the drugs bioavailability is the formation of their intermolecular complexes or conjugates with polymers through mechanical action. Polysaccharides are being actively studied as potential drug carriers¹⁻³.

The aim of the study was to obtain matrix forms of drugs by interacting with a polymer matrix using mechanochemical methods: impact-shear, microwave (MW) and ultrasonic (US) treatment.

Slightly soluble drugs were used: benzocaine (BC), sulphadimidine (SD), acyclovir (ACV); matrices for conjugation or production of solid dispersions – nature starch (S) or oxidized starch form (OS) and carboxymethylcellulose (CMC). The treatment was carried out in a ball mill (solvent free, 3 h, 20 N); in an ultrasonic generator (1 or 4 % water suspension, 3 min, 23 kHz); MW irradiation – 3 min, 600 W.

It was found that drugs react with OS units to form conjugates:



wherein, the products also contain unbound drugs.

The best results were obtained as a result of ultrasonic treatment of OS with BC and SD. It was found that the OS units reacted completely with the amino groups of the drugs, and the products contained the initial BC and SD in the ratio of 77:23 and 72:28 (bound:free). At the combined mechanical treatment of ACV, S and CMC (extrusion, shear-impact, ultrasound), the drug interacts with polysaccharides via an H-bond type, resulting in an increase of the pharmaceutical substance solubility.

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This work was supported by the Ministry of Science and Higher Education of the Russian Federation (project FRES-2023-0002).

X-RAY STRUCTURAL ANALYSIS OF CARBOXYMETHYL CHITIN IN SALT AND ACID FORM

Shirokova L.N., Alexandrova V.A.

*A.V. Topchiev Institute of Petrochemical Synthesis, RAS, Leninsky prospect 29, Moscow, 119991, Russia,
e-mail: shirokova@ips.ac.ru*

The structure of the initial chitin and the 6-O-carboxymethyl chitin (CMC) obtained on its basis in the salt form (CMC-Na) and acidic form (CMC-H) was studied by X-ray diffraction. The salt form CMC-Na (pH 8.5) were obtained from the acidic form of CMC-H (3.0) by adding 0.1 M NaOH in an amount necessary to convert 100% of –COOH groups to –COONa ones, in accordance with the titration curve of the acidic form.

From analysis of the data and comparison with the parameters described in, it follows that the original polysaccharide is α chitin with the orthorhombic unit cell ($a = 4.74 \text{ \AA}$, $b = 18.86 \text{ \AA}$, $c = 10.32 \text{ \AA}$) and a high degree of crystallinity of 89%, which was determined using the special software. In contrast to the highly ordered structure of the original α chitin, the CMC obtained on its basis has an amorphous structure. At the same time, for CMC-Na and CMC-H, the diffraction pattern shows two regions of amorphous halo. For CMC-Na, the region of the first amorphous halo ($2\theta = 9^\circ$) is more pronounced. This region can be characterized by a certain short-range order of macromolecules with an average distance of about 1 nm. For the CMC-H structure, the region of the second amorphous halo ($2\theta = 21.5^\circ$) is more defined, which indicates the short-range order in the system with an average distance of 0.4 nm. Apparently, the films obtained from CMC-H contain the associates of macromolecules arising via formation of hydrogen bonds between polymer chains. The region of the first amorphous halo is close in position to the reflection at a distance of $2\theta = 9^\circ$ due to the crystal lattice of chitin. The region of the second amorphous halo approaches in position the reflections of the crystal lattice of α chitin which are in the range of $2\theta = 15^\circ\text{--}25^\circ$. This may indicate only a slight displacement of scattering sites in the crystalline α chitin during the reaction of polymer-analogous transformations to obtain CMC, a water-soluble derivative of chitin.

LIQUID PHASE MODIFICATION OF RUBBER BNKS-28 AMN WITH FACTS BASED ON VEGETABLE OILS

Sibgatullina A.M., Tsyganova M.E., Rakhmatullina A.P.

*Kazan National Research Technological University. 420015, Russia, Republic of Tatarstan,
 Kazan, st. Karl Marx, 68,
 E-mail: sam21121984@mail.ru*

Modification of rubbers¹, including in the liquid phase²⁻⁴, makes it possible to obtain composite materials based on them that have an improved set of physical and mechanical properties.

In this work, we used factis⁵ synthesized by us based on vegetable oils and sulfur to modify BNKS-28 AMN rubber by liquid-phase combining its latex with toluene solutions of factis. The mass fraction of rubber in latex is 14.1% wt. The amount of factis varied in the range from 0 to 15 parts by weight per 100 parts by weight in terms of “dry” rubber. Liquid-phase combination was carried out at a temperature of 50-600C, stirring speed 350-400 rpm for 10 minutes. Isolation of modified rubbers from latexes and their drying were carried out using known technology⁴. On their basis, rubber mixtures filled with carbon black and their sulfur vulcanizates were obtained.

The vulcanization characteristics of rubber compounds and the physical and mechanical properties of their vulcanizates have been studied.

In the course of the work carried out, positive results were obtained regarding the influence of the modification on these indicators.

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PREPARATION OF N-VINYLPYRIDINE AND METHYL METHACRYLATE DIBLOCK COPOLYMER PARTICLES BY DISPERSION RAFT-POLYMERIZATION

**Silantieva E.V.,^a Ponomareva D.A.,^a Lobanova N.A.,^a Serkhacheva N.S.,^a
Plutalova A.V.,^b Chernikova E.V.,^b Prokopov N.I.^a**

^a*MIREA - Russian Technological University, Lomonosov Institute of Fine Chemical Technologies,
Vernadsky prospekt 86, Moscow, 119571, Russia,
e-mail: sil.liza02@mail.ru*

^b*Lomonosov Moscow State University, Faculty of Chemistry, Moscow, 119991, Russia, Leninskie Gory, 1c3*

Today, heterophase reversible addition-fragmentation chain transfer polymerization (RAFT) is often used to produce particles of amphiphilic block copolymers, which is called "polymerization induced self-assembly" PISA in english literature. The morphology of particles in such reactions primarily depends on the ratio of block lengths in the copolymer^{1,2}.

Dispersion polymerization of methyl methacrylate (MMA) was performed in the presence of a 4-vinylpyridine copolymer and MMA (P(4VP-co-MMA)) with a tritiocarbonate group at the end of the chain ($M_n = 23200$ g/mol, $M_w/M_n = 1.33$. 5 % mol. MMA) as an RAFT-agent. The reaction was initiated with azoisobutyric acid dinitrile (1% by weight). at 65 °C for 8 hours. The volume ratio of the MMA/medium phases was 1/10. At this stage, special attention was paid to the choice of a dispersion medium, which was used as ethyl and isopropyl alcohol.

When comparing the reaction rates, it was found that polymerization in ethyl alcohol proceeds at a higher rate than in isopropyl alcohol. Probably, in a less polar alcohol, the resulting diblock copolymer, due to the presence of a sufficiently large number of more hydrophilic units, loses solubility faster, self-assembling into particles, the access of the monomer to which is difficult. In addition, the conformation of the P(4VP-co-MMA) block in the dispersion also changes, in ethyl alcohol, with an increase in monomer conversion, particle growth from 6 to 50 nm was recorded, and in isopropyl aggregates with a size of 550-730 nm. Apparently, the stabilizing role of P(4VP-co-MMA) weakens and the particles of P(4VP-co-MMA)-block-PMMA lose their stability.

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CHANGES IN THE FINE STRUCTURE OF AROMATIC POLYAMIDE FIBERS UNDER THE INFLUENCE OF WATER

Smotrina T.V.^a, Popova T.V.^b, Scheglova N.V.^a

^a*Mari state university, Lenin Square 1., Yoshkar-Ola, 424001, Russia,
e-mail: tatyana-smotrina@yandex.ru*

^b*State university of humanities and technologies, Zelenaya Street 22, Orekhovo-Zuevo, 142611, Russia*

Aromatic polyamide fibers are widely used in the production of wear-resistant and heat-resistant materials including composite ones for the aerospace, military and civil industries¹. Increased performance characteristics are provided by the compact molecular structure, rigidity and high degree orientation of the polymer chain, and the ability to form strong hydrogen bonds². Under the influence of water the restructuring of fine structure elements which affect deformation and strength characteristics of aramid fibers can occur despite their low moisture capacity³.

In this work, we studied the effect of long-term treatment with water at 20°C and 100°C on the hydrophilic properties and structure of aromatic polyamide fibers Rusal, Kevlar 49, Technora T 200.

A change in the sorption properties of aramids was discovered when they were treated with water. When describing water vapor sorption isotherms using equations of quasi-chemical and probabilistic sorption models using the Van Krevelen group contribution method, the conditional degrees of crystallinity of aramid fibers were estimated. For untreated fibers, good agreement between the results obtained and the data of X-ray diffraction analysis was found.

It was shown that treatment with water, both under soft and hard conditions, led to a decrease in the degree of ordering of aromatic polyamides, indicating the presence of a mesomorphic phase with short-range three-dimensional order that can be destroyed under the influence of water.

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INVESTIGATION OF THE INFLUENCE OF MODIFIED FILLERS ON FLAME RETARDANT PROPERTIES OF POLYVINYLCHLORIDE PLASTISOL

**Kablov V.F.¹, Keibal N.A.¹, Kharlamov V.O.²,
Krekaleva T.V.¹, Stepanova A.G.¹**

¹*Volzhsky Polytechnical Institute (branch) "Volgograd State Technical University", Volzhsky,*

²*"Volgograd State Technical University", Volgograd,*

404121, Russian Federation, Volgograd region, Volzhsky, Engelsa str. 42a,

e-mail: stepanastya@mail.ru.

Nowadays, the production of plastisols for various purposes has increased due to the technical and economic advantages of this technology.

The presence of modified aluminium hydroxide and modified magnesium hydroxide reduces the temperature on the unheated side by 10.3 °C (modified aluminium hydroxide with amidophosphate) and by 31.8 °C (modified magnesium hydroxide with amidophosphate). The formed coke has a low value of thermal conductivity coefficient and high thermal resistance, which leads to a decrease in the exit of combustible products into the gas phase, reducing the flow of combustible gases to the flame. Thus the blowing coefficient increases 11 times with the addition of modified aluminium hydroxide and 10 times with the addition of modified magnesium hydroxide.

The results of tests on determination of coke residue at temperature 750 °C and exposure time 30 minutes correlate with the above data, so coke residue increases by more than 20% (modified aluminium hydroxide amidophosphate) and by more than 30% (modified magnesium hydroxide amidophosphate).

The presence of modified aluminium hydroxide improves the adhesion strength by 1.6 times and the addition of modified magnesium hydroxide improves the adhesion strength by 1.5 times.

At carrying out research of the received polyvinylchloride plastisols by method of electron microscopy it has been established that at modification of aluminium and magnesium hydroxide reduction of agglomeration of filler particles is observed that promotes its better distribution in a matrix of polymer. Also by the increase of phosphorus peak it is possible to draw a conclusion about the detection of phosphorus on the surface of filler particles - aluminium and magnesium hydroxide, that testifies to the carried out surface modification of fillers that increases their antipyrretic abilities.

MORPHOLOGY AND SIZES OF MONO- AND BIMETAL NANOPARTICLES OF PLATINUM AND SILVER STABILIZED BY CATIONIC POLYELECTROLYTE

Valueva S.V., Vylegzhanina M.E.

*NRC "Kurchatov Institute" Institute of Macromolecular Compounds RAS,
199004, St. Petersburg, Russia, Bolshoy pr. V.O., 31
E-mail: svalu67@mail.ru*

Metal nanoparticles (MNPs) are an excellent material for creating electronic, optical, and sensor devices of a new generation due to a combination of the valuable qualities such as a highly developed surface, high capacity of the double electric layer, and the ability to be self-organized into monolayers, etc. In addition, they are very promising in bioanalytical electrochemistry and biomedicine. Platinum- and silver-containing nanosystems (NS) occupy an important place among nanomaterials for biomedicine, the properties of which are largely determined by the morphology and size of the NP/nanostructures consisting the NS. In particular, the possibility of regulating the shape and size of the NP/nanostructures is important for creation of the dosage forms, since these factors largely determine the degree of toxicity of the NS being formed. In this work, the studies of the morphological and dimensional characteristics of the NS based on the mono-bimetallic silver and platinum nanoparticles stabilized by a biocompatible cationic polyelectrolyte (CP) – poly-N,N,N,N-trimethylmetha cryloyloxyethylammonium methylsulfate ($M_w = 170 \times 10^3$), with a fixed mass ratio of the components $v = 0.1$ have been carried out. A comparative analysis of the absorption spectra for NS CP-Ag⁰, CP-Pt⁰ and CP-(Pt⁰/Ag⁰) revealed significant changes during transition from NS containing monoparticles to NS with bi-particles. Static/dynamic light scattering methods provide information related to the changes in MM and dimensions (RMS radius of inertia and hydrodynamic radius) of the nanostructures. The molecular conformational parameters of the nanostructures based on the bimetallic nanostructures (Pt⁰/Ag⁰) exceeded in magnitude the similar parameters for the nanostructures based on the platinum nanostructures, however, they were less than the corresponding parameters determined for the NS CP-Ag⁰. When analyzing AFM images of the surface of the thin films cast from CP-Ag⁰, CP-Pt⁰ and CP-(Pt⁰/Ag⁰) nanodispersions, discrete spherical nanostructures with a diameter not exceeding 100nm are visualized. A detailed analysis of the AFM images for the studied dispersions has shown that mononuclear morphology is characteristic for NS CP-Ag⁰, and for NS CP-Pt⁰ and CP-(Pt⁰/Ag⁰) – polynuclear one.

NATURAL RUBBER AND RUBBER TREE SEED OIL – BIODEGRADABLE ADDITIVE FOR POLYOLEFINS

Yanov V.V., Gataullina L.I., Zenitova L.A.

*Kazan National Research Technological University,
420015, Kazan, 68 Karl Marx St.,
e-mail: Liubov_zenitova@mail.ru*

The paper presents studies on the effect of additives of natural rubber and rubber tree seed oil both independently and jointly in order to give polyolefins: polyethylene and polypropylene the ability to biodegrade during deposition.

The optimal ratio of additives in the amount of up to 15% by weight has been selected. It has been shown that rubber tree seed oil manifests itself not only as a biodegradable additive, but also as a softener. Thus, the seed oil of the rubber tree increases PTR like natural rubber and reduces viscosity, but more significantly than natural rubber.

Regardless of whether additives are used individually or in a mixture, the strength characteristics of materials decrease slightly with an increase in the number of additives, but remain at a fairly high level.

The tendency of materials to swell in water, 10% H₂SO₄ and NaOH solutions, as well as a change in the wetting edge angle, were evaluated. To assess the biodegradability of polymer compositions, a technique based on their exposure in soil prepared in accordance with GOST 9.060-75 was used.

AMILOIDOGENIC PROPERTIES OF SILK FIBROIN

Zakharov V.V.,^{a,b} Susanin A.I.^c

^a*Institute of Macromolecular Compounds of RAS, 199004, St-Petersburg, V.O. Bolshoy Pr. 31, Russia,
e-mail: vlad.v.zakharov@mail.ru*

^b*Peter the Great St.Petersburg Polytechnic University, 195251, St.Petersburg, Polytechnicheskaya St. 29, Russia*

^c*St.Petersburg State University of Industrial Technologies and Design, 191186, St.Petersburg,
Bolshaya Morskaya St. 18, Russia*

Silk is considered as an example of functional amyloid. According to a hypothesis, production of silk fiber proceeds through the amyloid-like "cross-beta" structure, which further transforms into a silk's "collinear beta" structure when the fiber is stretched. Formation of amyloid fibrils is typically preceded by soluble oligomeric intermediates. We found that an aqueous regenerated fibroin solution contains protein aggregates that interact with conformation-specific antibodies to amyloid oligomers. In transmission electron microscope, the aggregates look like spherical particles of up to 0.5 μm in diameter. These aggregates were previously described as fibroin "micelles". The micelles act as a storage form of unstructured fibroin in the silkworm silk gland to protect it from untimely conformational transition to a beta-sheet-rich structure. Thus, for the first time we have revealed that fibroin micelles are amyloid oligomers on the way to amyloid structure formation. The second protein of silk fiber, sericin, which is usually removed by degumming procedure during silk fibroin regeneration, stabilizes the micellar form of fibroin. We found that the addition of sodium dodecyl sulfate (SDS) to fibroin solution results in rapid fibroin transition into the form of amyloid fibrils. The N-terminal domain of the fibroin heavy chain, which is known to mediate fibroin conformational transition from random coil to the beta-sheets, contains a short polycationic sequence, a probable target of SDS action. The corresponding synthetic peptide undergoes SDS-dependent transition into the form of amyloid fibrils. Consequently, this peptide is a probable amyloidogenic determinant that initiates fibroin transition into the form of amyloid fibrils under the control of anionic cofactors (in nature, the role of SDS can be played by phosphate ions or acid phospholipids). The results obtained suggest that the formation of insoluble silk fiber is a process similar to the transition of amyloid oligomers into amyloid fibrils. This provides a basis for the creation of a biomimetic technology for the production of silk fibroin-based materials with unique properties.

STUDYING THE POSSIBILITY OF PLASTIFICATION OF SILOXANE RUBBERS

Zimina A.S.^a, Mironova Yu.E.^a, Khakimullin Yu.N.^a, Voiloshnikov V.M.^b

*^aKazan National Research Technological University, 68 Karl Marx street
Kazan 420015 Republic of Tatarstan Russian Federation*

^bVESTO LLC, Kazan, st. Rakhimova 8 building 20

Thanks to the unique set of properties of rubbers based on silicone rubber, they are widely used in a wide variety of fields. Considering the high cost and scarcity of silicone rubber, rubber based on it, as a rule, are highly filled. Due to the nature of silicone rubber (its polarity), it is difficult to select a plasticizer (standard ones are ineffective), since plasticizers are effective only, as a rule, under conditions of compatibility with rubber. It has been established that it is possible to achieve a good plasticizing effect when using siloxane rubber destructors, which are well compatible with silicone rubber¹. The introduction of small amounts of plasticizer makes it possible to effectively regulate the viscosity of filled rubber compounds without deteriorating properties.

Taking into account possible compatibility, the possibility of using an organosilicon plasticizer modified with amino compounds was studied. The content of amino compounds in the plasticizer is 3, 5 and 7%.

The possibility of using a plasticizer in siloxane rubbers in standard and highly filled formulations was investigated. The introduction of a plasticizer containing 2 and 5% amino compounds makes it possible to reduce the viscosity and increase the plasticity of rubber compounds. It has been established that the use of a plasticizer in an amount of 2% is effective; this allows one to maintain a complex of physical and mechanical properties, as well as increase the fire resistance of siloxane rubbers (both with and without flame retardants) and reduce weight loss after combustion.

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Section 9

CHEMICAL EDUCATION

PROJECT INTERACTION BETWEEN UNIVERSITY AND SCHOOL

Bigaeva I.M., Agaeva F.A., Simeonidi D.D., Pechenaya V.A.

*North Ossetian State University named after Kosta Levanovich Khetagurov,
362025, North Ossetia-Alania, Vladikavkaz, st. Vatutina 46,
e-mail: bigaeva@mail.ru*

Project interaction between schools and the Faculty of Chemistry, Biology and Biotechnology of North Ossetian State University is being implemented in two ways. The first is project work carried out by schoolchildren who are students of the “School of Young Chemist”¹. The second is project work carried out within the framework of community agreements concluded by North Ossetian State University (NOSU) with a number of schools in the city of Vladikavkaz and regions of the republic. A characteristic feature of this project interaction is the active involvement of students from the Faculty of Chemistry, Biology and Biotechnology in the implementation of projects (as managers). This approach – uniting students and schoolchildren into project groups – is useful and efficient². It is easier for schoolchildren to work when they are supervised by someone closer to their age (there is no age barrier). They acquire skills in both project and research activities. And students, supervising the work of schoolchildren, consolidate the knowledge acquired during training, expand it and acquire mentoring skills³. In addition, universities are better equipped with modern equipment, so the project work carried out at the university is broader in scope and deeper in scale. Upon completion, all schoolchildren’s work completed in collaboration with students participates in the project work competition “PRO CREATIVE 0+”. This competition originated at the Faculty of Chemistry, Biology and Biotechnology two years ago is now held annually in April, as part of the “Science Days” held by North Ossetian State University based on the results of scientific activities. The purpose of the competition is to involve students in research and project activities in the field of natural sciences. The best works are as per usual sent to various All-Russian and International competitions.

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PROBLEMS OF MODERN PROFESSIONAL PEDAGOGICAL EDUCATION

Korotkova A.V., Potemkina N.M., Pluzhnik O.M.

*State Educational Institution of Higher Education of the Moscow region
 "State University of Humanities and Technology",
 142611, Orekhovo-Zuyevo, Zelenaya str., 22,
 e-mail: allakorotkova2018@yandex.ru*

At the present stage, the problems of professional training of chemistry teachers have sharply worsened, which invariably led to a decrease in the quality of the educational process in schools, both basic and advanced training of students.

1. Applicants to pedagogical universities take only one of the core subjects as an entrance exam, despite the fact that the training of future teachers (bachelors) is more often conducted in two profiles. And this exam, as a rule, is biology. The initial level of knowledge in chemistry of such applicants leaves much to be desired.

2. Focusing on the results of the entrance control, teachers are forced to compensate for the subject knowledge, skills and abilities necessary for the educational process of higher education. This requires considerable time, and sometimes correction of the content of academic disciplines.

3. The solution to this problem is seen in changing the rules of admission to universities at the federal level. If a graduate of a school claims to master vocational training programs in two profiles, then he must present the results in two disciplines corresponding to these profiles.

4. Natural sciences, and chemical sciences in particular, always require not only sufficient general pedagogical and methodological training, but also a powerful scientific base. Only then will the subject-based learning outcomes at school fully correspond to the required level of modern education.

5. At the same time, the content of professional pedagogical chemical education requires a certain correction in order to make it more applied, functionally literate and fully contributing to the formation and realization of opportunities for self-development and the formation of a creative personality of the future teacher.

USE OF DOMESTIC EDUCATIONAL RESOURCES IN EXTRACURRICULAR CHEMISTRY CLASSES

Kulikov A.N.^a, Shiryayev S.D.^b, Lobanov A.V.^a

^a*Moscow Pedagogical State University,
Malaya Pirogovskaya Street 1/1, Moscow, 119991, Russia,
e-mail: alexkulikov2003@mail.ru*

^b*The Russian Presidential Academy of National Economy and Public Administration,
prospekt Vernadskogo 82, building 1, Moscow, 119571, Russia*

Chemistry teaching is the most important component of science education^{1,2}. At the time of Covid-19, chemistry education was gradually moving into the information field. Platforms (Zoom, Teams) that were more suitable for the learning process started to replace the resources already available on the market at that time.

The Yandex ecosystem has all the necessary resources for the productive work of both teacher and student – Yandex. teleconference – to conduct a lesson, Yandex.blackboards – for collaborative work on the online whiteboard, Disk – for downloading homework and independent work (with the function of making tests with timers). It is also worth mentioning more specialized information resources, for example, YaClass.ru. Here you can find assignments on any topic from 8th to 11th grade, lesson notes that can be used for additional lessons on the subject. Using the tools of YaClass.ru, a teacher should only monitor the progress of mastering the material and be ready to answer questions that arise from students.

At the same time, the Chemistry application for mobile devices deserves special attention. It has an easy-to-use table of chemical elements, in which you can see the electronic configurations of atoms, and when entering the formula of a substance, the program calculates the molar mass. In the “schemes” tab, the student can find all the necessary methodological materials, among which the solubility table, presented in full, as well as calculations of the solubility constant in digital format, deserve a special comment. In the “reactions” tab, the student can check whether he/she is correctly equating certain reactions and see the interaction conditions of the chemicals of interest.

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DESIGN OF A NEW MASTER'S EDUCATIONAL PROGRAM "NANOBIOTECHNOLOGY"

Kustova T.P.^a, Kiselev M.G.^b

*^aIvanovo State University,
Ermak street 39, Ivanovo, 153025, Russia,
e-mail: kustovatp@ivanovo.ac.ru*

*^bG.A. Krestov Institute of Solution Chemistry of the Russian Academy of Sciences,
Akademicheskaya street 1, Ivanovo, 153045, Russia*

At the present stage of development of society, science has become a sphere where talented youth can find themselves and develop successfully. As part of the national project "Science and Universities," a course has been taken to educate and support a new generation of scientists capable of making breakthrough discoveries. In achieving this goal, consolidation of resources of scientific and educational organizations plays an important role.

In partnership with G.A. Krestov Institute of Solution Chemistry of the Russian Academy of Sciences Ivanovo State University began designing a new educational program "Nanobiotechnologies" in the field of preparation 04.04.01 Chemistry, which will be launched in the 2024/2025 academic year. IvSU has extensive experience in implementing master's educational programs (EP), the profile of which has changed since 2010 depending on the requests of employers and the areas of scientific research of university teachers. When developing a new educational program, it was decided to maintain two types of professional activities for which graduates will be prepared – research and teaching. In this regard, the "pedagogical block" of academic disciplines and practices was retained and transferred from the previous EP "Innovation in Chemistry and Chemical Education", and the "scientific block" was significantly revised and expanded. A new discipline "Physical methods for studying bio- and nanosystems" appeared in it and new modules were added to the discipline "Priority directions for the development of chemistry in the 21st century." Researchers at G.A. Krestov Institute of Solution Chemistry of the Russian Academy of Sciences are developing lectures on supercritical fluid technologies, chemistry of luminescent compounds, plasma chemistry, molecular design of medicinal compounds and preparing practical classes on NMR, IR, Raman spectroscopy, X-ray diffraction analysis, CMS, which will be held in the scientific laboratories of the institute.

We believe that cooperation between the university and the Institute of the Russian Academy of Sciences in the preparation of master's students will make it possible to attract the best undergraduate graduates to the new EP and, in the future, motivate them to engage in serious scientific work and continue their studies in graduate school.

PROBLEMATIC SITUATIONS IN CHEMISTRY LESSONS

Materii Y.M., Lobanov A.V.

*Moscow Pedagogical State University,
Malaya Pirogovskaya Street 1/1, Moscow, 119991, Russia,
e-mail: alexsheremental@yandex.ru*

In teaching chemistry, participants in the educational process at the levels of basic general and secondary general education face problems of a substantive, methodological, adaptive, logistical and personnel nature. The existing questions lead to a number of problematic situations in chemistry lessons. Let's note the most acute of them.

The abstractness of the symbols used – the complexity of chemical formulas and equations can cause difficulties for students in understanding and applying theoretical knowledge. The subject is not interesting to students – lack of motivation of students or their low interest in the subject (lack of understanding of the practical significance of chemistry and its interdisciplinary connections) it can lead to a lack of activity in chemistry class.

Teacher competence – the complexity of the material and thus the deranged explanation of an inexperienced or ignorant teacher can cause confusion and misunderstanding by students. Lack of feedback – insufficient interaction between the teacher and the students, as well as between the students themselves, can hinder effective learning and knowledge sharing.

The time limit for mastering topics or the number of lessons per week – insufficient time in the lesson to complete all tasks and experiments can lead to ineffective assimilation of the material. Illiterate time allocation – insufficient time to prepare for a lesson and organize practical classes can lead to inefficient use of educational material.

Compliance with safety regulations – insufficient attention of students or their non-compliance with safety rules can create dangerous situations in the chemical laboratory. Material support of the chemistry room – insufficient quantity and quality of equipment and tools for conducting demonstration experiments can reduce the interest of students in studying chemistry. The lack of visibility and modern advanced digital tools – the inability to conduct interactive classes and use modern educational technologies can reduce the effectiveness of the chemistry lesson and the interest of students.

TRAINING OF ENGINEERING PERSONNEL FOR THE CHEMICAL INDUSTRY

Movsumzade E.M.^a, Kolchina G.Yu.^b, Loginova M.E.^c

^aFSBEI of HE “Ufa State Petroleum Technical University”,
450064, Ufa, Cosmonauts Str. 1,
e-mail: eldarmm@yahoo.com

^bFSBEI of HE “Ufa University of Science and Technology”,
450076, Ufa, Zaki Validi str. 32,
e-mail: kolchina.GYu@mail.ru

^cRPC Geophysics JSC,
450097, Ufa, Komsomolskaya str. 2/1,
e-mail: ufamel@yandex.ru

Currently, the main tasks of industrial complexes are the creation of new highly efficient processes and the improvement of existing ones, which is only possible through the development and use of computer-aided design systems and optimization of technological processes, the development of which is due to the widespread and deep implementation of computer technology and applied mathematical software. The basis of such systems is applied mathematics, methods of mathematical modeling and mathematical optimization, which consist in representing the properties of objects using mathematical models and mathematical methods.^{1–3}

The creation of powerful software, along with the development of computers itself, has made numerical prediction practically accessible to a wide range of researchers in various fields, chemical reactions and technological processes. The development of an integrated computer-aided design system is due to the widespread introduction and use of computer technology and applied mathematical software.

An important task of chemical technology is to create new highly efficient processes and improve existing ones. Its solution is possible only through the development and use of computer-aided design systems and optimization of chemical technological processes.

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RESEARCH, FORMATION AND DEVELOPMENT OF SCIENTIFIC POTENTIAL IN THE FIELD OF NEW MATERIALS IN ST. PETERSBURG

Pimenova T.F.

*St. Petersburg Scientific Center of the Russian Academy of Sciences,
199034, St. Petersburg, Universitetskaya embankment 5,
e-mail: tpim@spbrc.nw.ru*

The future of information technology, energy, transport, space technology, medicine and chemical technology depends on success in creating new materials. By making full use of the scientific potential in this priority area of research and development, it is possible to make a qualitative breakthrough and take advantage of emerging export opportunities.

The paper presents the results of studies of the state and problems of the formation and development of scientific potential in the field of creating new materials, as one of the most promising areas of development of science and technology in St. Petersburg, which has a competitive advantage in the form of a highly developed intellectual and cognitive component and as the main factor in the innovative development of the region.

In the process of carrying out research, the following were considered: features of the scientific potential of St. Petersburg, institutional and cognitive aspects in this area, leading scientific centers and scientific schools were characterized, it was shown that St. Petersburg is one of the country's leading centers for the study, development and application of promising materials, the innovative component of the ongoing research, priority areas corresponding to global scientific and technological trends have been identified and justified; Specific themes and projects for their implementation have been formed, a section of the regional program for the development of fundamental research in the light of global trends has been justified and developed as an element of a strategic system for managing the formation and development of scientific potential in the region. The results and successes of research in the field of new materials in the scientific laboratories of the megagrant program in St. Petersburg are summarized. The results of a study of the scientific potential of one of the main areas of materials science – nanocomposites in St. Petersburg – are briefly presented.

All this as a whole creates unique prerequisites for the further development of the St. Petersburg scientific cluster in the field of creating new materials and its core – scientific potential through the wider use of competitive advantages, the development of international cooperation, and more intensive investments in human capital.

STEAM APPROACH IN THE PROPAEDEUTICS OF CHEMISTRY TEACHING

Shakirova V.V., Sadomtseva O.S.

*V.N. Tatishchev Astrakhan State University,
 414000, Astrakhan, Tatishchev 20a,
 e-mail: svv_2004@mail.ru*

Many authors, studying the problems of chemical education, note the importance of the propaedeutic stage in the study of chemistry¹. However, it should be noted that the main attention is paid to the development of the content of propaedeutic courses, but not to the methods of their teaching. At the same time, there is an urgent need for methods that would take into account the age characteristics of children, as well as the specifics of the propaedeutic stage.

The solution to this problem is seen through the introduction of STEAM technologies in teaching. STEAM approach is aimed at eliminating the gap between practice and theory, creating logical links between disciplines, gives the opportunity to look at the world globally and notice regularities in different spheres of activity.

We are working on the problem of early learning of chemistry, we have developed both separate lessons and multilevel courses, as well as projects, master classes, using STEAM technologies for children of different age groups. The implementation in the learning process was carried out in extracurricular time in the framework of supplementary education^{2,3}. The implementation of the activities contributed to the development of students' thinking, increased their interest in the subject, which contributed to a more in-depth perception of the material at the next level of education. It should be noted that the key place in all the developed activities was occupied by chemical experiment, which in combination with the use of interactive modules contributes to a more effective mastering of knowledge, skills and abilities.

Thus, the peculiarity of applying the STEM approach is that schoolchildren should not only be included in interesting practical activities, but also fully realize that the world around is a whole, all processes are interrelated and should be studied exclusively in this relationship.

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SCHOOL-UNIVERSITY COOPERATION WITHIN THE FRAMEWORK OF IMPLEMENTING NETWORK INTERACTION

Shershneva A., Dzhigola L.

*Astrakhan Tatishchev State University
414006, Astrakhan, Russia State University, Pushkin street 14,
e-mail: kovalenko09.01@mail.ru*

In the federal project “Modern School” of the national project “Education” it is envisaged that by the end of 2024 more than 70% of schools will implement educational programs in a networking form¹. This is necessary to ensure the opportunity to receive high-quality education in conditions that meet modern requirements, regardless of the place of residence of the child.

Astrakhan Tatishchev State University together with the secondary school p. Trusovo of the Astrakhan region have been implementing “School-University” network interaction since the 2022–2023 academic year. Within the framework of this cooperation specialized chemical and biological 8th and 9th grades are training at the material and technical base university.

Cooperation is carried out in several forms: synchronized development of curricula with the programs of partner schools; conducting master classes in chemistry within the framework of career guidance events of the All-Russian socio-state Movement of Children and Youth “Dvizhenie pervykh” (Movement of the First) and the project “V gostyah u uchennogo” (Visiting a Scientist); students attend laboratory classes once a week for 4 academic hours, which provides a more in-depth study of the subject and succession between general and higher education.

Basing on the results of the implementation of this network program, it can be noted that the type of interaction “School-University” affects both the formation of special knowledge and skills, competencies², and the development of personal qualities of students.

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ON THE ISSUE OF IMPROVING CHEMICAL PEDAGOGICAL EDUCATION IN THE CONTEXT OF FORMING SCIENTIFIC AND TECHNOLOGICAL SOVEREIGNTY OF THE RUSSIAN FEDERATION

Shiryaev S.D.^a, Lobanov A.V.^b

*^aThe Russian Presidential Academy of National Economy and Public Administration,
119571, Russia, Moscow, prospekt Vernadskogo, 82, building 1,
e-mail: shiryaev_ser@mail.ru*

*^bMoscow Pedagogical State University,
119991, Russia, Moscow, Malaya Pirogovskaya St., 1/1*

Previously, we showed and substantiated the relationship between the quality of subject (scientific) training of chemistry teachers and the ability of school graduates to receive higher chemical education, which directly affects the formation of the personnel potential of the Russian state, ensures its strategic stability and the formation of the scientific and technological sovereignty of the country¹.

It should be noted that a great achievement in improving and unifying the subject (scientific) module was the development of Methodological Recommendations for the training of teaching staff for undergraduate programs based on uniform approaches to their structure and content within the framework of the approved “Core of Higher Pedagogical Education”². Nevertheless, a number of problems remain, the solution of which will significantly affect the positive dynamics of the development of chemical pedagogical education: 1) the document is purely advisory in nature; 2) the structure of the subject-methodological module for the “Chemistry” profile does not contain recommendations for the introduction of mathematical and physical disciplines into educational programs; moreover, there is no information about the recommended classroom load.

We believe that increasing the effectiveness of the proposed measures will be ensured by moving away from the discretionary nature of issued legal acts with the establishment of generally binding implementation of the provisions prescribed in them, as well as their scientific refinement.

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EXTRACURRICULAR ACTIVITIES AS A WAY TO INCREASE STUDENTS' INTEREST IN CHEMISTRY AND RESOURCES FOR TEACHERS' PROFESSIONAL DEVELOPMENT

Sobolev A.E.,^{a,b} Isaev D.S.^c

^a*Tver State Technical University, 170026, Tver, A. Nikitin's Emb., 22,*

^b*Tver State Medical University of the Ministry of Health of the Russian Federation,
170000, Tver, Sovetskaya Str., 4,
e-mail: sobolevae@tvgmu.ru*

^c*Secondary school No.43, 170043, Tver, Sklizkova Str., 95.*

The updated federal state educational standards for general education have introduced a new structure for the curriculum at comprehensive schools, which includes extracurricular activities for schoolchildren (EAS) as a separate component that is an integral part of the educational process.^{1,2}

The analysis of scientific and methodological literature has revealed a contradiction between the vast possibilities of EAS in terms of fostering students' cognitive interest in chemistry and the professional development of teachers, on the one hand, and the lack of systematic consideration of these issues in the theory and practice of subject-based education, on the other.^{2,3}

Based on the proposed concept "from cognition to cognitive interest," the authors have developed the conceptual foundations for modernizing the system of extracurricular activities in chemistry in a modern school.² A regional system of EAS in chemistry was created, which includes approximately ten different educational projects in innovative forms. Methods of EAS and means of their implementation were developed and introduced into educational practice. These include an approximate program, plan, algorithms for teacher activities, a theoretical model of the school's methodological service, guides for teachers and students at pedagogical universities, textbooks for students, didactic games, olympiad tasks, educational presentations, and creative works in chemistry. In addition, there are practical tasks of a research nature, and others. The authors also proposed and tested the central idea "from professional growth of teachers to cognitive interest of students," which reflects the essence of the concept of teachers' professional development.

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A NETWORK FORM OF ORGANIZING INDIVIDUAL PROJECTS FOR SCHOOLCHILDREN

Volkova T.G.^a, Shanogina A.M.^a, Talanova I.O.^b

*^aIvanovo State University,
39 Ermaka str., Ivanovo, 153025, Russia,
e-mail: schanoginanastya@yandex.ru*

*^bFSBEI HE "Ivanovo SMU" of MOH of Russia Ivanovo,
Sheremetevsky prospect 8, 153012, Russia*

The development strategy of the Russian Federation necessarily includes the training of personnel who will be able to solve technological challenges. The formation of interest in science, research activities, and the foundations of a research culture should begin from school.

There are a number of problematic issues when implementing projects and research by schoolchildren. This includes difficult communication with experts and technical support for projects, especially for small schools and additional education organizations.

Network research projects can solve these problems and some others, since they have a clear and understandable methodological basis, which allows children to implement a project or research under the guidance of a teacher or parent, as well as receive the necessary expert support. Another positive point is the simplicity of technical and technological support, which allows the project to be implemented by a large number of people interested. Interaction between participants is carried out remotely, and therefore makes it possible to include schoolchildren from small towns and rural schools in the project.

This allows you to scale the network projects, making it systemic for involving schoolchildren in the world of science.

Many network projects are designed in such a way that their implementation addresses not only scientific, but also environmental or social issues. For example, in the project "Young Researchers" <https://vk.com/club224906205> attention is drawn to environmental issues, to the issue of compliance of water consumed by the population with existing sanitary standards.

Schoolchildren not only carry out research, but get acquainted with interesting facts, video recordings of experiments, and results obtained by other project participants.

DEVELOPMENT OF THE EDUCATIONAL AND METHODOLOGICAL COMPLEX OF THE INORGANIC CHEMISTRY COURSE IN ENGLISH FOR FOREIGN STUDENTS

Tyumenova S.I., Rogaleva E.V., Kartasheva M.N.

*National University of Oil & Gas "Gubkin State University",
Faculty of the Chemical Technology and Ecology,
Department of General and Applied Chemistry,
119991 Moscow, Leninsky Prospekt, 65,
e-mail: sv.tyumenova@gmail.com*

The creation and implementation of the educational and methodological complex in inorganic chemistry in English for foreign students for the department of general and applied chemistry in modern conditions is now an urgent task in teaching chemical disciplines.

The educational and methodological complex in English is based on the basic course of the discipline "Inorganic Chemistry" for non-chemical specialties. The educational and methodological complex for the discipline "Inorganic Chemistry" in English includes the work program of the discipline, fund of assessment tools, lecture notes and presentations, glossary, laboratory journal, lecture video materials and laboratory works.

The lectures include short notes in English in accordance with the topics of the course, presentations in English and video lectures with interlinear translations in English. To reinforce the basic concepts of the lecture course we developed a glossary in English with automatic links, comments and practical examples.

To assist laboratory works we now have a bullet journal in English with report forms for five laboratory works and guidelines on how to conduct experiments, sections for recording observations and make conclusions. Reference materials and interlinear translations for video experiments in English are also included.

Control of knowledge of this discipline includes two tests on the chemistry of elements and their compounds and a final test as a form of final certification.

The educational and methodological complex in inorganic chemistry in English can be used as part of the main course in inorganic chemistry, and as an elective course for all university students so as to gain skills and experience in working with technical literature in English and improve the general level of qualifications.

IMPLEMENTATION OF CHEMICAL-TECHNOLOGICAL PRODUCTION TASKS IN THE CONDITIONS OF DIGITAL TRANSFORMATION OF THE EDUCATIONAL PROCESS

Zolotareva N.V.,^a Golda S.U.,^b Goryunov A.V.,^a Akhmedova A.I.^c

^a*Astrakhan Tatishchev State University, 414000, Astrakhan, Shaumyan, 1 sq.,
e-mail: zoloto.chem@mail.ru*

^b*MSEI of Astrakhan, «SGES №12», 414004, Astrakhan, V. Barsova, 8 st.,*

^c*MSEI of Astrakhan, «SGES №52», 414019, Astrakhan, Panfilova, 36 st.*

Scientific and technological progress has brought a lot of new things into modern human life and the economy of our country. It's no secret that breakthrough ideas arise precisely at the intersection of interdisciplinary knowledge and professional skills^{1,2}. However, today, chemistry classes in schools are poorly equipped. Reconstruction of industrial complexes and elements of installations is in demand, but is inaccessible or completely inaccessible for use for specific educational purposes. The intermediate results of joint work within the framework of the “University – School” interaction in the implementation of educational projects below are demonstrated. Undergraduates, 11th grade students and young teachers were involved in the work.

Blender³ program was used for visualize the models, Repetier⁴ program was used to prepare for printing, and printing was carried out on a two-extruder 3D printer «ZONESTAR-P802».



Figure 1. Cutting layers for printing (left). 3D-printed models of objects (right)

As a result, we received a high percentage of schoolchildren who were motivated to achieve results. With the further implementation of the project, it is possible to additionally equip municipal educational institutions with mock-ups of chemical-technological installations created by students under the guidance of specialists and students.

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Repetier <https://www.repetier.com/download-now/>.

FORMATION OF ECOLOGICAL KNOWLEDGE THROUGH PROJECT ACTIVITIES IN CHEMISTRY IN EXTRACURRICULAR TIME

Zubova S.V., Lobanov A.V.

*Moscow Pedagogical State University,
Malaya Pirogovskaya Street 1/1, Moscow, 119991, Russia,
e-mail: sofia.zubova2002@gmail.com*

During the last years at school the project activity of pupils is carried out both at lessons of natural science subjects and in extracurricular time. Pupils choose a topic of research in various areas of the science cycle, and the topics of work can be intertwined in different areas of science (chemistry, ecology, biology and physics).

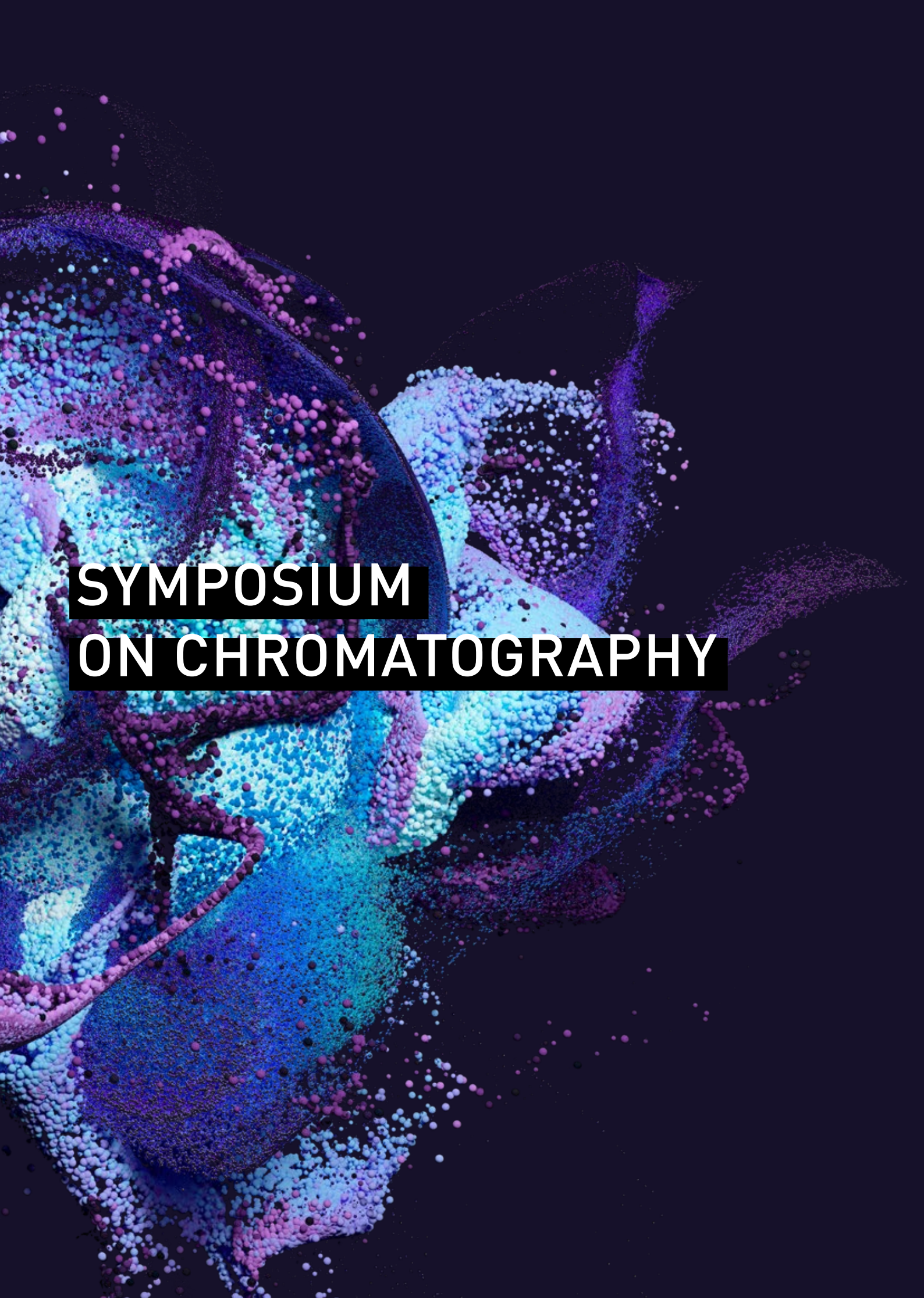
Project activities help students to develop independent work skills, analytical thinking skills and creative approaches to problem solving. It allows them to apply their knowledge in practice and see its relevance in real life. Students also learn to work in a team, communicate with others, acquire communication skills, share ideas and solutions¹.

Project activities in out-of-school time should develop gradually from simple investigations that can be carried out in one activity to more complex ones carried out over a longer period of time, for example, in a school-university link. Project work helps students to better understand the importance of chemical processes in nature, their impact on the environment and how to protect humans and nature. Environmental work, for example, on purifying water from pollution, making environmentally friendly fertilisers or developing new packaging materials can be not only an interesting and educational experience for students, but also a way of engaging them in caring for the environment.

Thus, project activities in chemistry lessons are important not only for in-depth study of the subject, but also for the formation of environmental culture of students and their readiness to solve urgent problems of the modern world.

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SYMPOSIUM ON CHROMATOGRAPHY

FEATURES OF DETERMINATION OF OIL PRODUCTS IN BIOLOGICAL SAMPLES

Brodsky Ye.S.

*IPEE RAS,
Moscow, Leninsky Prospekt, 33, Moscow,
e-mail: efbr@mail.ru*

Petroleum products (PP) and related compounds (n-alkanes, PAHs) are important objects of determination and environmental monitoring. From an analytical point of view, PP is a nonpolar solvent extract from which co-extractable polar compounds have been removed. However, in addition to PP proper - an anthropogenic pollutant, such extract contains other organic compounds, such as natural oil and gas seeps, components of dispersed organic matter, products of vegetation and microorganisms - hydrocarbons, lipids, terpenoids, flavonoids, pheromones and others. When determining PP in living organisms - plants or animals - it is necessary to take into account the presence of metabolites, lipids, steroids, etc. in them. In addition, other anthropogenic pollutants such as phthalates, phosphates, pesticides, etc. may also be present.

Since anthropogenic PP and biogenic compounds are structurally similar, the identification of PP in biological samples is a complex non-trivial task requiring knowledge of the characteristic features of both.

Currently, the main methods of identification of PP and biogenic compounds are: (1) based on the extraction method - extraction with non-polar solvent with removal of co-extracted polar compounds; (2) distribution of n-alkanes and corresponding index values; (3) presence of UCM - «hump» of unresolved compounds on the chromatogram; (4) ratio of different PAHs; (5) presence of certain gopanes and steranes; (6) «fingerprints». These attributes are not always unambiguous and distinguishable.

Modern instruments and methods (GC, HPLC, GC/MS) make it possible to analyse the extract in detail and determine characteristic biomarkers - pristane, steranes, rearranged steranes and methylhopanes, aromatic compounds - perylene, cadalene, etc., and UCM characteristics - presence and distribution of characteristic groups of compounds and molecular weights, considering NP as a system of compounds of a certain structure.

A large set of individual and group characteristics makes it possible to establish the «petroleum» character of compounds in the analysed mixture not only by characteristic individual compounds, but also by «group-type» characteristics and to estimate their kind and content.

ADSORPTION OF ORGANIC COMPOUNDS ON THE SURFACE OF MESOPOROUS SILICA MODIFIED WITH LANTHANUM, CERIUM, EUROPIUM, YTTERBIUM B-DIKETONATES

Faustova Zh.V., Kamotskiy V.V., Slizhov Yu.G.

*National Research Tomsk State University, 634050, Tomsk, Lenin str., 36,
e-mail: zhv.xf@mail.ru*

To obtain highly effective sorbents for gas chromatography, β -dicarbonyl complexes of rare earth elements are promising modifiers. The ability of such compounds to accept additional donor molecules into the outer coordination sphere of the lanthanide provides selective complexation during the separation and concentration of organic compounds.

In this work, sorbents based on mesoporous silicon dioxide modified with lanthanum, cerium, europium and ytterbium benzoylacetonates were studied.

Gas chromatographic studies were performed on a MAESTRO 7820 gas chromatograph (Agilent Technologies) with a flame ionization detector. Metal filled columns with a length of 1 m and an internal diameter of 3 mm were used in the work.

The selected metal cations La^{III} , Ce^{III} , Eu^{III} , Yb^{III} are located at the beginning, middle and end of the series of rare earth elements. With a decrease in the ionic radius of the cation, the strength of the metal–ligand bond in a complex compound increases due to an increase in the polarizing effect of the rare earth element cation on the ligands and an increase in the covalent contribution to the metal–oxygen chemical bond.

It has been experimentally established that with an increase in the serial number of a rare earth element, the chromatographic polarity, selectivity and adsorption capacity with respect to homologs and structural isomers of aromatic hydrocarbons, alcohols, ketones and nitro compounds increases. Maximum adsorption properties in the process of gas chromatographic separation are exhibited by sorbents modified with ytterbium (III) benzoyl acetate due to the preservation of the chelate structure of the complexes during immobilization on the surface of the carrier.

PECULIARITIES OF SORPTION ABSORPTION OF STEROIDAL SAPONINS BY NATURAL POLYMER – CHITOSAN UNDER EQUILIBRIUM CONDITIONS

Ishchenko U.S., Mironenko N.V., Selemenov V.F.

*Voronezh State University, 394006, Russia, Voronezh, Universitetskaya Pl., 1
e-mail: ulia28ischenko@gmail.com*

Steroidal saponins have a wide spectrum of pharmacological action and therefore find very wide application in pharmacological practice. In this work we studied the sorption uptake of saponins by chitosan under equilibrium conditions. The sorption isotherms are shown in Fig. 1 (1, 2).

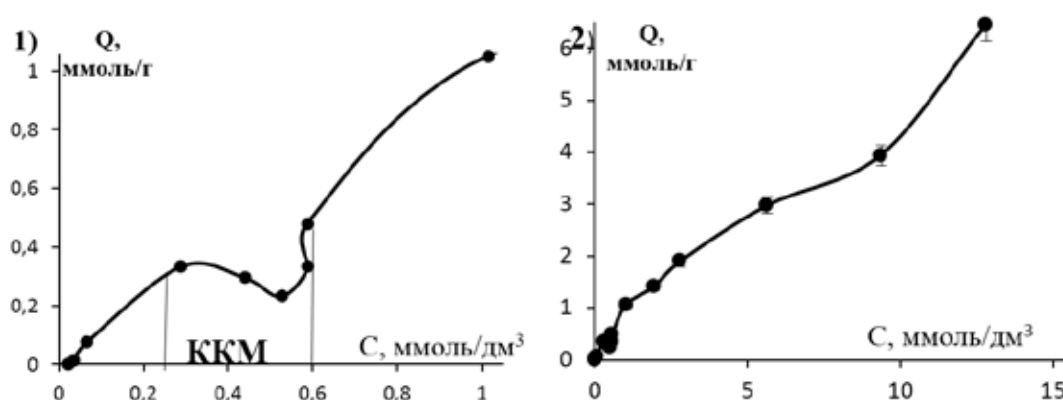


Fig.1. 1) saponin sorption isotherm ($C=0.02 \div 1 \text{ mmol/dm}^3$);
2) saponin sorption isotherm ($C=0.02 \div 13 \text{ mmol/dm}^3$)

At low concentrations of equilibrium solution ($C = 0.02 - 0.29 \text{ mmol/dm}^3$) the isotherm is linear. In the region corresponding to micelle formation processes in solution, a local minimum is observed on the curve, then the sorption parameter increases. It can be assumed that the sharp decrease in the absorption value is due to the emergence of a competing association process in solution and in the sorbent phase. It was found that the increase in absorption in this concentration range is possible as a result of both adsorption of micelles existing in the surfactant solution and association of molecules in the sorbent phase.

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The work was supported by the Ministry of Science and Higher Education of the Russian Federation within the framework of the state assignment to universities in the field of scientific activity for 2023-2025, project FZGU-2023-0009.

HPLC AND GC-MS ANALYSIS OF CAFFEIC AND CHLOROGENIC ACIDS

Ksenofontova T.D.^{a,b} Baranovskaya V.B.^{a,b}

^a*National University of Science and Technology «MISIS», Leninsky prospect 4, str. 1, Moscow, 119049, Russia
e-mail: Ksenofontovat@bk.ru*

^b*IGIC RAS, Leninskiy pr. 31, Moscow, 119991, Russia*

Organic acids play a fundamental role in a number of industries, including chemical, pharmaceutical, medical and food. Caffeic and chlorogenic acids are powerful antioxidants that prevent the oxidation of lipids and proteins making them promising food additives for both food preservation and general health promotion. In addition to its high biological activity caffeic acid is often used as an intermediate in the synthesis of various organic compounds and pharmaceutical substances.

The variety of acid production methods can lead to significant differences in their quality which makes quality control a relevant issue. The reliable analysis of organic acids depends on the accuracy of a set of analytical methods and on the availability and quality of the reference samples used. Despite the absence of specific quantification methods outlined in regulatory documents such as pharmacopoeias, the majority of current scientific literature recommends the use of high-performance liquid chromatography (HPLC) for analysis.¹ HPLC represents a key approach for the separation and analysis of chemical compounds in diverse fields, including agriculture, cosmetics, pharmaceuticals, environmental and food industries. Gas chromatography-mass spectrometry (GC-MS) can serve as an additional method for analysis the purity of acids. Although a derivatization step is required to ensure the stability and volatility of compounds, this method offers significant advantages, including the separation of cis/trans isomers, high sensitivity, and the ability to identify target substances and impurities without the need to use reference samples.²

In this work, the optimal conditions for HPLC and GC-MS analysis of commercially available samples of caffeic and chlorogenic acids were determined.

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This research was performed using the equipment of the JRC PMR IGIC RAS

MICROCOLUMN GAS CHROMATOGRAPHY WITH METAL-ORGANIC FRAMEWORK MIL-101(Cr)

Martina Yu.V., Kopytin K.A., Onuchak L.A., Pariychuk M.Y.

*Department of Physical Chemistry and Chromatography, Faculty of Chemistry,
Samara National Research University, Moscow Shosse St. 34, Samara 443086, Russian Federation,
e-mail: yulya.martina@yandex.ru*

At present, there is a high interest in metal-organic framework (MOFs), a new class of micro- and mesoporous materials with a high diversity of structures, regulated channel geometry and pores, which makes them promising for research in the field of adsorption and chromatographic technologies¹. The aim of the work was to study the adsorption and separation properties of the mesoporous MIL-101(Cr) under microcolumn gas chromatography.

The column (1 mm × 0.5 m) was made using particles with an average diameter of 60 μm. The chromatographic experiment was carried out using the chromatograph Crystal 5000 (Chromatography Ltd.) with a flame ionization detector. According to the study, the retention and thermodynamic characteristics of sorption in homological series of *n*-alkanes and arenas sorption on metal-organic frame MIL-101(Cr) are increased. Branched isomers are found to encounter more steric difficulties during the passage of cavity windows than linear octane molecules due to the presence of a sieve effect in octane sorption. The adsorbent MIL-101(Cr) possessed specific characteristics for octane, decalin (fig. 1), and xylene isomers.

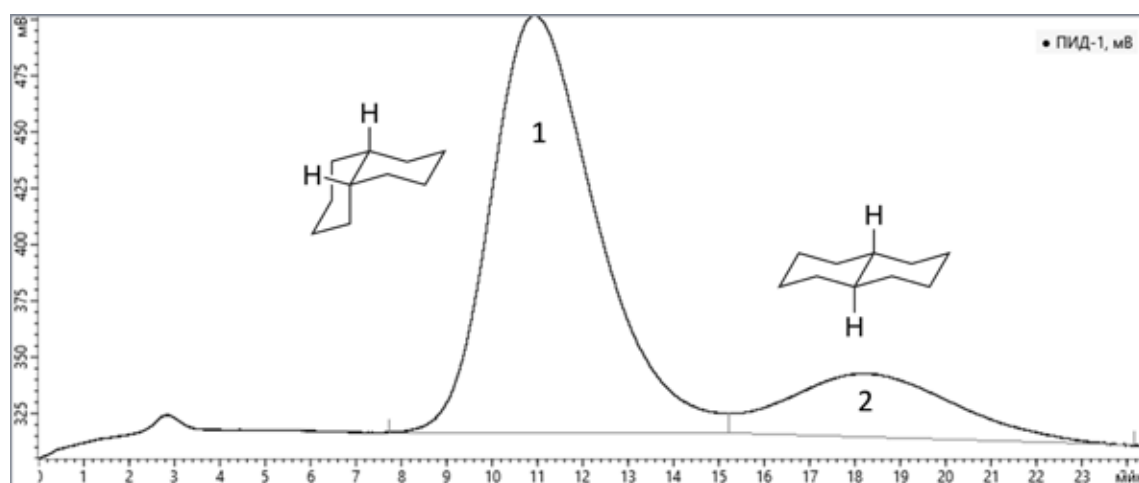


Figure 1. Decalin isomer separation chromatogram:
1 - cis-decalin, 2 - trans-decalin.

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GC-MS ANALYSIS OF THE CHEMICAL COMPOSITION OF *ACHILLEA MILLEFOLIUM* L. ESSENTIAL OIL

Istamkulova M., Mukhamadiev N., Keldiyarov X., Mukhamadiev A.

*Samarkand State University named after. Sh. Rashidova
Uzbekistan, 140104, Samarkand, University Boulevard, 15
e-mail: m_nurali@mail.ru*

Achillea millefolium L. is a medicinal plant that has been used for centuries to treat various diseases. One of its best known components is its essential oil, which has been shown to have a wide range of biological activities, including anti-inflammatory, antimicrobial and antioxidant properties.

The essential oil was extracted from the aerial parts of *Achillea millefolium* L. by hydrodistillation and analyzed using GC-MS method. The chromatogram is shown in the figure.

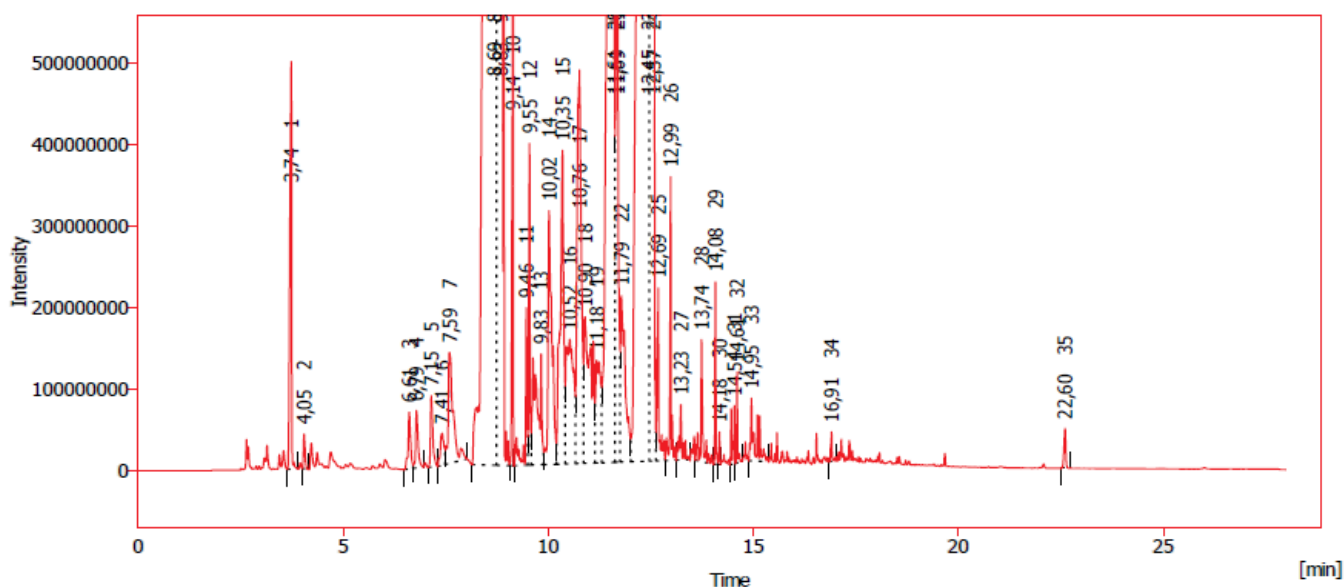


Fig 1. Chromatogram of essential oil of *Achillea millefolium* L.

Analysis of the chemical composition of the essential oil showed the presence of 34 compounds, the main components of which are 2-carene (20.60%), benzene, 1-methyl-3-(1-methylethyl)- (8.78%) and ascaridole (10.06 %). The identified compounds were grouped into several classes, including monoterpenes, sesquiterpenes, oxygenated monoterpenes and sesquiterpenes.

The findings provide valuable information for the potential use of *Achillea millefolium* L. essential oil for various purposes, including the development of new drugs and natural products.

GC-MS ANALYSIS OF CHEMICAL COMPOSITION MELISSA OFFICINALIS ESSENTIAL OIL

Naimova B.K., Mukhamadiev A.N., Mukhamadiev N.K.

*Samarkand State University named after. Sh. Rashidova
Uzbekistan, 140104, Samarkand, University Boulevard, 15
e-mail: nayimovabahora@gmail.com*

The purpose of the study was GC-MS analysis of the chemical composition of the hydrodistillate of the aerial part of *Melissa Officinalis*.

Steam distillation was used to extract the essential oil from the aerial parts of *Melissa officinalis*. The essential oil was analyzed using GC-MS.

The analysis identified more than 20 different compounds, each representing a distinct component with varying degrees of contribution to the overall chemical profile of the oil. The main components included: 1,4-Dioxaspiro[4.5]decane-7-butanoic acid, 6-methyl-, 2-(methylsulfonyloxy)ethyl ester (12.59%); 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-[2,3-bis[(trimethylsilyl)oxy]-2-propenyl]-1,3-dimethyl-5-(1-methylbutyl) (9.77%); 12-Methyl-E,E-2,13-octadecadien-1-ol (8.26% and 4.98%).

Based on the data from the presented table on GC-MS analysis of *Melissa officinalis* essential oil, it can be noted that some chemical compounds indicate optical isomerism. Optical isomers include: Glycine, N-[(3 α ,5 β)-24-oxo-3-[(trimethylsilyl)oxy]cholan-24-yl]-, methyl ester; Pregn-5-ene-3,11-dione, 17,20:20,21-bis[methylenebis(oxy)]-, cyclic 3-(1,2-ethanediyl acetal); Spirost-8-en-11-one, 3-hydroxy-, (3 β ,5 α , 14 β ,20 β ,22 β ,25R), 1.4H,5aH,9H-Furo[2,3-b]furo[3',2':2,3]cyclopenta[1,2-c]furan-2,4; 7(3H,8H)-trione, 9-(1,1-dimethyl-ethyl)dihydro-8,9-bis[(trimethylsilyl)oxy]-, (3aS,5aR,8R,8aS,9R,10aS).

Overall, the chemical composition of *Melissa officinalis* indicates its potential in various applications, including medicine, pharmaceuticals and perfumery.

ISOLATION AND IDENTIFICATION OF POLYPRENOLS FROM CONIFEROUS RAW MATERIAL PROCESSING RESIDUES

Noskova A.G., Matveeva T.N., Khasanov V.V., Slizhov Yu.G.

*National Research Tomsk State University, 634050, Tomsk, Lenin Avenue 36,
e-mail: arina-noskova-01@mail.ru*

The impressive timber reserves in the Russian Federation and substantial volumes of processing make the country one of the leaders in this sphere. However, there is a problem of low efficiency of utilization of all biomass of processed trees¹. Non-volatile residues (cube residues) of hydrodistillation of oil-ether concentrates are poorly studied and have limited usefulness for further processing, despite the fact that they contain valuable biologically active components such as polyprenols, sesqui- and diterpenoids, and carotenoids. Polyprenols are natural long-chain isoprenoid alcohols of the general formula $H-(C_5H_8)_n-OH$ and have a wide range of activity, including antiviral, anti-ulcer, and immunomodulatory actions. In addition, they are important synthons for the production of pharmaceuticals².

During the study, the extraction of polyprenols from the non-volatile residue of hydrodistillation of oil-ether concentrate obtained by carbon dioxide liquid extraction of Siberian fir woody greens was conducted. Preliminary samples were subjected to alkaline hydrolysis followed by liquid extraction of unsaponifiable substances and their separation by column chromatography on silica gel using a gradient of eluents. Identification of the obtained polyprenols and impurities was carried out using high-performance liquid chromatography and chromatography-mass spectrometry methods.

Studies were carried out to evaluate the quantitative content of polyprenols. It was found that most of the polyprenols in the non-volatile residue of hydrodistillation of the oil-ether concentrate are in the form of esters. A significant part of polyprenol esters (up to 60-70%) are precipitated with wax.

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A COMPLEX OF CHROMATOGRAPHIC METHODS AND THERMAL ANALYSIS IN FATS AND OILS IDENTIFICATION

Saranov I.A.,^a Rudakov Ya.O.,^{b,c} Abboud M.,^b Rudakov O.B.^c

^a*Voronezh State University of Engineering Technologies,*

Revolution Avenue 19, Voronezh, 394000, Russia, e-mail: robi57@mail.ru

^b*Voronezh State University, Universitetskaya sq. 1, Voronezh, 394000, Russia*

^c*Voronezh State Technical University, 20 letiya Oktyabrya st., 84, Voronezh, 394006, Russia*

An integrated (complex) approach based on the use of gas chromatographic techniques for analyzing the fatty acid composition (GLC), HPLC techniques for determining the triglyceride composition and differential calorimetry (DSC) were developed to study the chemical composition of natural fats and oils and its effect on the thermophysical properties of fat and oil raw materials, as well as to identify adulteration of fat and oil products valuable varieties.¹⁻⁴

Strong natural correlations between some individual fatty acids, triglycerides and thermophysical parameters of DSC, characteristic of specific lipids, were identified in the work during a statistical analysis of data on the influence of genetic and phenotypic factors on fats and oils chemical composition, on thermophysical parameters (temperatures and thermal effects of melting, polymorphic transformations). Violation of the identified correlations indicates the introduction of substitute fats into the product, fractionation, transesterification or other physical and chemical effects on the sample of fat and oil raw materials.

The application of this complex of GLC, HPLC and DSC techniques allows not only to reliably identify natural raw materials, but also often their origin, i.e. breed of livestock, plant variety, season and climatic conditions in which agricultural products were produced.

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*The study was supported by a grant from the Russian Science Foundation № 23-73-01166,
<https://rscf.ru/project/23-73-01166/>*

MODELING OF QUINOLINE DERIVATIVES SORPTION ON CARBON SORBENTS

Ryzhkin S.A., Kurbatova S.V.

*Samara National Research University
Moskovskoye shosse 34, Samara, 443086, Russia
e-mail: curbatsv@gmail.com*

Molecular modeling of sorption, due to the wide distribution of sorption processes in both natural and technological systems, makes it possible to optimize these processes and predict the sorption characteristics of compounds without resorting to experiment¹. We have carried out modeling of sorption complexes of quinoline derivatives on a carbon surface, while optimization of the geometry of molecules, graphite layer and sorption complexes was carried out in the Gaussian 09 program within the framework of density functional theory at the B3LYP/6–31G level. To take into account van der Waals interactions, the dispersion correction GD32 was used².

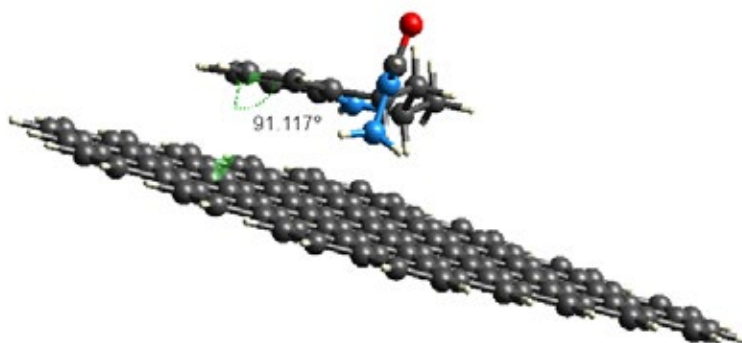


Figure 1. Optimized model of the sorption complex

The influence of the solvent (acetonitrile - water) on the sorption process was taken into account using the PCM model. A comparison of the total energy of the complexes showed that this value for a solution is approximately ~10 kJ/mol lower than in vacuum.

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UNIVERSAL DERIVATIZING REAGENTS FOR GC-MS AND HPLC-MS: FLUORINATED BENZYL BROMIDES IN THE DETECTION OF ALKYLPHOSPHONIC ACIDS

Stepanova V.A., Aleksenko S.S., Kiseleva M.G., Novikova I.V.

*FSUE «State Scientific Research Institute of Organic Chemistry and Technology»
State research center of Russian Federation, 111124 Moscow, shosse Entuziastov, 23.
e-mail: centrallab@gosniiokht.ru*

One of the directions of analytical research in non-targeted analysis, is the unification of methods and approaches of sample preparation in order to cover as many substances as possible in one analysis procedure. At the same time, the reliability of the identification of compounds in the sample is ensured by including a combination of several analytical methods, such as, for example, GC and HPLC with tandem mass spectrometry (MS/MS).

When investigating cases of illegal activities in the field of production, use and storage of toxic chemicals (TC), non-targeted screening is associated with the identification of compounds belonging to the Lists of the Annex on Chemicals of the Convention on the Prohibition of the Development, Production, Stockpiling and Use of Chemical Weapons and on their Destruction. The range of such substances is not limited only to TC, but includes their precursors and degradation products, and in the case of biomedical samples, biotransformation metabolites. Among the markers of organophosphorus TC, alkylphosphonic acids (APA) and their esters are polar and non-volatile compounds. One of the approaches to change the selectivity of their separation, increase the sensitivity of detection and reliability of identification in complex matrices is derivatization reactions. Applying a single sample preparation procedure for different methods allows to reduce the time spent on analysis, as well as correlate the results obtained with each other.

This paper shows the possibility of carrying out an alkylation reaction of a mixture of nine APA and their esters, followed by the determination of the derivatives obtained by GC-MS/MS and HPLC-MS/MS methods at low ppm level in environmental objects. Pentafluorobenzyl bromide, tetrafluorobenzyl bromide (TFB) and tetrafluoro-4-(trifluoromethyl)benzyl bromide (TMFB) were taken as derivatizing agents, among which TFB and TMFB were used for the alkylation of APA and their esters for the first time. Optimal separation and MS/MS conditions have been selected for derivatives detection. The effectiveness of combining two separation methods with one sample preparation for the identification of compounds in non-targeted analysis of TC is shown.

GAS CHROMATOGRAPHIC ANALYSIS OF VOLATILE COMPONENTS OF MEDICINAL PLANTS OF THE FAMILY LAMIACEAE

Tolochilin N.A., Salmanidina O.V., Onuchak L.A.

*Samara National Research University, Moskovskoe highway 34,
Samara, 443086, Russia, e-mail: nitol98@mail.ru*

The aim of this work is to determine volatile and moderately volatile compounds in the equilibrium vapor phase (EVP) of industrial samples of plants «Moldavian dragonhead» (Horst) and «Catnip» (Herbs of the mountainous Crimea), belonging to the Lamiaceae family.

The EVP was obtained by thermostating a dried plant sample in a sealed vessel at a temperature of 120°C for 20 minutes. The experiment was carried out on a gas chromatograph «Crystal 5000.2», using a quartz capillary column RTX-5 (30m×0.32mm, df = 0.25μm) and FID¹. From the obtained experimental data, the Van den Dool and Kratz retention indices (I_i^T) and the relative peak areas ($A_{rel,i}$) of plant volatile components were calculated.

In the EVP of the sample «Moldavian dragonhead» (Horst), 31 components were registered in the range of retention indices $I_i^T = 296 \pm 2 - 1370 \pm 2$. The dominant contents are components with retention indices: 300 (17,96%), 539 (21,92%), 653 (19,42%). In the EVP of the sample «Catnip» (Herbs of the mountainous Crimea), 46 components were registered in the range of retention indices $I_i^T = 296 \pm 2 - 1416 \pm 2$. The dominant contents are components with retention indices: 540 (19,62%), 644 (20,75%).

The headspace-spectrum of the studied plant samples in Fig. 1 demonstrate a specific combination of compounds included in its composition (so-called «fingerprint»), which makes it possible to use this spectrum for the rapid identification.

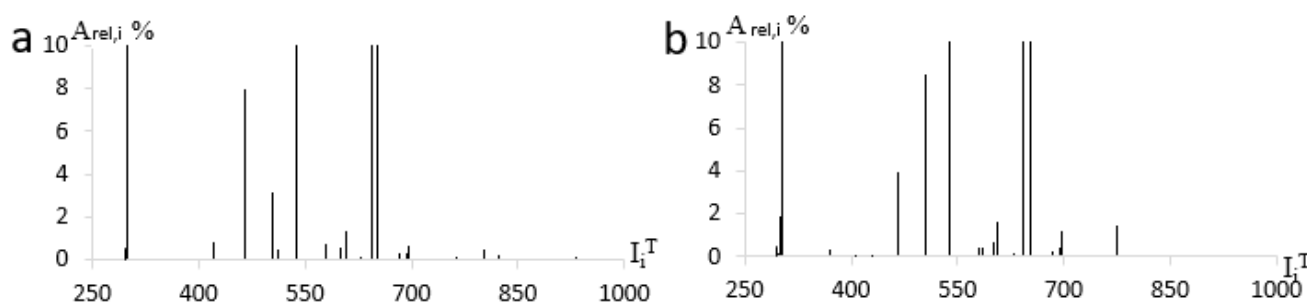


Figure 1. Headspace spectra of plant samples: a – «Moldavian dragonhead» (Horst),
b – «Catnip» (Herbs of the mountainous Crimea).

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SYNTHESIS OF MESOPOROUS SILICA GEL USING SAPONINS AND STUDY OF TEXTURE AND SORPTION CHARACTERISTICS

Ulugboeva G.O., Uzokov Zh.R., Mukhamadiev N.K.

*Samarkand State University named after. Sh. Rashidova,
Uzbekistan, 140104, Samarkand, University Boulevard, 15
e-mail: gulbahorulugboeva95@gmail.com*

The purpose of this work is to synthesize mesoporous silica gel using saponins as surfactants and study its texture and sorption characteristics.

To synthesize mesoporous silica gel, TEOS and saponins isolated from *Acanthophyllum gypsophiloides* Regel plants were used as starting materials. Saponins were dissolved in an aqueous-alcoholic solution, TEOS was added to the solution and acidified to pH 2 with HCl. The resulting mixture was kept at various temperatures for a certain time to form a mesoporous structure. After this, the product was filtered, washed, dried and calcined at 500°C.

Using the sorption isotherm and the linear BET equation, the specific surface area of the sorbent (S_{BET}), pore size (D , nm), capacity of the adsorbent monolayer (a_m), and saturation adsorption (a_s) were calculated.

Table 1. Textural characteristics of mesoporous silica gel

$t, ^\circ\text{C}$	$S_{BET}, \text{m}^2/\text{g}$	$a_m, \text{mol/kg}$	D, nm	$a_s, \text{mol/kg}$
30°C	745,6±10,2	2,3±0,7	0,8±0,05	7,3±1,2
50°C	500,4±6,2	1,6±0,5	6,5±1,18	5,0±0,8
70°C	418,2±20,4	0,9±0,3	32,4±8,24	3,8±0,4
90°C	403,3±100	0,5±0,1	50,5±12,1	1,5±0,5
120°C	253,6±30,4	0,3±0,1	72,5±13,6	1,3±0,5

From these tables it is clear that the synthesis temperature has a significant effect on the textural and sorption properties of silica gel. Low synthesis temperatures promote the formation of mesoporous structures with high specific surface area, small pore sizes, high capacity of the adsorbent monolayer and saturation adsorption. SEM images show that the surface of silica gel is rough and heterogeneous with a large number of porous structures, where the pores have sizes from 2 to 50 nm.

THE ROLE SIZE EFFECTS IN SEPARATION ON MACROCYCLIC SORBENTS IN GAS CHROMATOGRAPHY

Avvakumov L.S.,^a Yashkina E.A.,^a Yashkin S.N.,^{a,b}

*^aSamara Regional Center for Gifted Children,
70 ul. Cheremshanskaya, 443016 Samara, Russian Federation,*

*^bSamara State Technical University,
244 ul. Molodogvardeiskaya, 443100 Samara, Russian Federation
e-mail: snyashkin@mail.ru*

Cyclodextrins have a number of unique physicochemical and structural characteristics that allow them to be used as effective selectors in various versions of gas and liquid-bone chromatography. In the present work, by equilibrium gas-liquid chromatography on columns with α -Dex 120 (SPh: 20% permethylated α -CD immobilized in SPB-35 poly (35% -phenyl/65% -dimethylsiloxane)) and gas-adsorption chromatography (SPh: GTB with a monolayer α -CD) under conditions extremely low concentrations of sorbate in the gas phase, retention parameters and thermodynamic characteristics of sorption of a large group of derivatives of hydrocarbons of flat, linear and frame structure are determined. For the first time, a method has been proposed for determining the size of the internal cavity of α -CD by the difference in the retention of reference molecules, which is in good agreement with the results of molecular modeling methods.

The high structural selectivity of the studied SPh with respect to ortho/meta/para isomers of benzene derivatives, characterized by high values of separation factors, is shown. The reason for the high meta/para selectivity is the possibility of the formation of strong guest-host inclusion complexes between arene molecules and α -CD molecules. The key factor determining the strength of such complexes is the geometric correspondence of the sizes of sorbate molecules and the internal cavity of the α -CD (0.52 nm). The study shows the effect of the nature and number of substituents in the aromatic moiety on the stability of the complexes formed. It was found that, unlike benzene derivatives, molecules of adamantane derivatives that are larger in geometric size practically do not form inclusion complexes on the studied SPh. This is confirmed by the fact that in the SPB-35 phase, adamantane mono-derivatives are held stronger than benzene mono-derivatives with the same functional groups, and in the α phase, α -Dex 120, on the contrary, is weaker. It was established that the retention of adsorbates of linear structure changes non-additive: there is a noticeable «breakthrough» in the retention values for C9-C10 sorbates, which is associated with the dimensional effect of SPh when forming an inclusion complex with a linear C-fragment of sorbate of limited length.

INVERSE GAS CHROMATOGRAPHY IN THE STUDY OF THE PROPERTIES OF CARBON ADSORBENTS

Dmitriev D.N.,^a Yashkina E.A.^b Popov A.S.,^a Yashkin S.N.,^{b,c}

^aLomonosov Moscow State University, 1, Leninskie gory, Moscow, 119991,

^bSamara Regional Center for Gifted Children, 70 ul. Cheremshanskaya, 443016 Samara, Russian Federation,

^cSamara State Technical University, 244 ul. Molodogvardeiskaya, 443100 Samara, Russian Federation

e-mail: yashkina11@mail.ru

The advantage of inversion gas chromatography (IGC) in infinity dilution is the ability to directly study the adsorption properties and characteristics of the most active surface areas in the region of the adsorption isotherm close to zero surface filling (Henry region). In a series of studies performed by us, as model objects with various degrees of energy and geometric heterogeneity of the surface, we considered a number of non-porous carbon adsorbents (soot, fullerenes, nanotubes), for which values of thermodynamic adsorption characteristics (TCA) were determined by IGC in the area of extremely low concentrations of reference adsorbates in the equilibrium gas phase. For the first time, the methodological aspects of achieving the Henry domain on heterogeneous surfaces under IGC conditions were considered. It was found that the concentration boundaries of the chromatographic-graphically reached Henry region significantly narrow as the degree of energy heterogeneity of the surface increases, while the asymmetry of chromatographic peaks increases. It has been shown that graphitized samples of the studied active carbon blacks can act as certain standards that allow comparing adsorbents with different degrees of energy heterogeneity, but with graphite crystallites similar in size, forming the surface of the graphite-like adsorbents considered. In addition, GTB was used as a reference adsorbent in the McReynolds-Rorschneider parameter system to assess the chromatographic polarity of the surface of adsorbents used in chromatography. It is shown that using the values of the thermal component of the entropy of the adsorbed substance, a conclusion can be made about the degree of heterogeneity of the surface of the investigated carbon adsorbents. For the first time, the effect of polar retention on gas-phase graphite was detected.

ISOLATION AND IDENTIFICATION OF RESIDUAL OF POLYMER REAGENTS IN THE PROCESSED WATER OF OIL PRODUCING WELLS

Zadorozhny P.A., Polyakova N.V., Sukhoverkhov S.V.

*Institute of Chemistry Far Eastern Branch of Russian Academy of Science,
prospect 100-letia Vladivostoka, 159, Vladivostok, 690022, Russia
e-mail: zadorozhny@mail.ru*

Nowadays various polymers and their compositions are widely used in drilling and development of oil production wells, as well as in hydraulic fracturing of producing wells. The use of polymers makes it possible to obtain the required technological characteristics of drilling fluids, well-killing and hydraulic fracturing fluids. During mentioned above operations, part of the solutions containing polymers enters the bottomhole zone of the productive formation and later, during the well operation, is carried out by the water phase which leads to complications in the operation of surface equipment: formation of sediments (sludge), gels, emulsions stabilized by polymers. The aim of this work was to develop a methodological approach, including the isolation, identification and determination of the concentration of polymers present in the water phase of well production.

Samples of produced water were studied after the launch of an oil production well and after treating the well with a polymer scale inhibitor. The total mineralization of the samples was 25-190 g/l. Removal of low molecular weight matrix and inorganic salts by dialysis allows the sample to be purified and prepared for further research, that significantly improves the quality of the analysis¹.

The use of IR-spectroscopy, pyrolytic chromatography-mass spectrometry and gel permeation HPLC methods makes it possible to identify and characterize the isolated polymer. Thus, in the studied samples, in one case, a viscosity regulator for drilling fluids - modified starch, and in the other, a scale inhibitor - sulfated polyacrylamide were found. The proposed method allows reliable qualitative and quantitative analysis of samples of highly mineralized waters containing high-molecular polymers of various nature.

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This work was carried out according to state order No FWFN-2022-0002 with use of equipment of Far Eastern Center of Structural Research



**11TH INTERNATIONAL
FRUMKIN SYMPOSIUM ON
ELECTROCHEMISTRY**

FEATURES OF REGISTRATION OF FLUCTUATION- NOISE PHENOMENA IN LOW-RESISTANCE CHEMICAL CURRENT SOURCES

Abaturov M.A., Andreev V.N.

*A.N. Frumkin Institute of Physical Chemistry and Electrochemistry RAS,
Russia, 199071, Moscow, Leninsky prosp., 31, b.4
e-mail: abatur@yandex.ru pan*

Fluctuation-noise processes are usually characterized by extremely low intensity up to the level of fundamental thermal noise. In such cases, in order to reduce interference from the measuring amplifier, it is necessary to observe a certain condition for the consistency of the applied amplifier circuit with the object of study in terms of resistance R and, accordingly, in terms of the level of intrinsic noise e_n , which are interconnected by the well-known Nyquist formula $e_n = \sqrt{4kTRB}$ (k - is the Boltzmann constant, T - is the temperature and B - is the frequency band). Commercially available ultra-low-noise chips cover a wide range of resistances from 400 ohms to 1 Mohm and above ¹. But objects, such as chemical current sources, usually have significantly lower resistance, which creates a matching problem.

In this paper, it is proposed to use a method of parallel switching on two amplifiers with subsequent summation of the signal to solve this problem. At the same time, in order to achieve an optimal amplifier mode, it is necessary to use weighting coefficients, taking into account the intrinsic noise of each of them ². The use of this method, as shown by measurements, allowed to expand the range of matching resistance below the specified limit of 400 ohms and, accordingly, reduce the intrinsic noise of the measuring circuit. Thus, for the AD8597 chip, the intrinsic noise voltage was reduced to 0.88 nV/ $\sqrt{\text{Hz}}$, which made it possible to register the fundamental thermal noise of a chemical current source of type RC2032 at the level of 1.14 nV/ $\sqrt{\text{Hz}}$ with a sufficiently high accuracy of about 1% for random signals. The proposed method has shown its effectiveness and can be used in studies of low-resistance chemical current sources.

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The work was carried out in accordance with the current State Task of the Laboratory of Electrocatalysis (A.N. Frumkin Institute of Physical Chemistry and Electrochemistry RAS).

FEATURES OF ELECTROCHEMICAL REDUCTION OF CHROMIUM FROM FORMATE CR(III) BASED ELECTROLYTIC SOLUTIONS

Arshinova I.S., Kuznetsov V.V.

*D. I. Mendeleev Russian University of Chemical Technology,
125047, Moscow, Miusskaya Ploshchad, 9,
e-mail: arshinova.i.s@muctr.ru*

Aqueous formate solutions based on Cr(III) can become a safe alternative to toxic solutions based on Cr(VI)¹. Their advantages include a wide range of operating pH, stable and uniform weight gain of the coating over the course of electrolysis. However, these baths require to undergo preliminary electrolysis treatment and tend to fail after some time of operation.

The purpose of this work is to determine the ability of formate solutions to electrochemically reduce chromium depending on the holding time of the electrolyte and the presence of development. As part of this work, we studied aqueous electrolytes of the following composition (mol/l): $\text{Cr}_2(\text{SO}_4)_3$ – 0.5, HCOONa – 1.4. The pH of the solutions was maintained at 2.0 ± 0.05 .

Three solutions were chosen for the study: 1) freshly prepared solution; 2) solution after electrochemical treatment for three hours at a current density $i = 12 \text{ A/dm}^2$; 3) solution stored 1 month without work, and then operated in the manner described above.

Cyclic voltammograms were obtained using a copper electrode $S = 2 \text{ cm}^2$ while scanning the electrode potential from the no-current value to the cathodic region at a scanning rate of 5 mV/s .

For solutions 1 and 3, the cyclic voltammograms appear shifted towards more positive potentials, which helps to slow down (or stop) the electrocrystallization of chromium. The equilibrium potential for the release of metallic chromium is not achieved, apparently, due to the facilitation of hydrogen evolution at the copper cathode due to the inability of the polynuclear Cr(III) complexes formed in solutions to undergo electrochemical reduction. Due to the above reasons, it is impossible to obtain high-quality chromium deposits from these electrolytes. In solution 2, metallic chromium deposition potentials are reached in the region of which a nucleation loop is observed. Thus, this solution makes it possible to obtain coatings of satisfactory quality.

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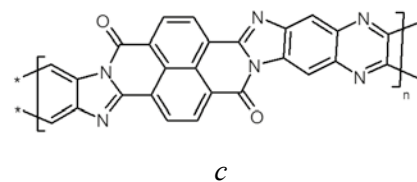
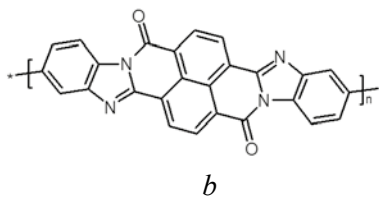
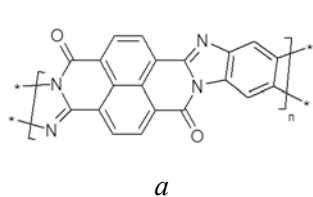
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POLYNAPHTHOYLENEBENZIMIDAZOLES AS CATHODE MATERIALS FOR METAL-ION BATTERIES

Baluda Yu.I., Kraevaya O.A., Troshin P.A.

*Federal Research Center for Chemical Physics and Medicinal Chemistry of RAS,
Academician Semenov av. 1, Chernogolovka, 142432, Russia,
e-mail: yury.baluda@yandex.ru*

Naphthoylenebenzimidazoles represent a class of organic electrode materials (OEMs), which are structurally similar to naphthalene diimides; however, they remain relatively less studied^{1,2}. In the present work we report the synthesis of three redox-active polymers derived from naphthalene dianhydride and 1,2,4,5-tetraaminobenzene (*a*), 3,3'-diaminobenzidine (*b*) or 2,3,7,8-tetraamino-phenazine (*c*), as well as the evaluation of their performance as cathode materials for Li- and K-ion batteries.



The polymers were prepared by the reaction of precursor compounds in 1:1 molar ratio in N-methylpyrrolidone under reflux. Further, the composites of polymers with conductive carbon and binder were studied in the cells with Li anodes using 1M LiTFSI in DOL-DME (2:1) as electrolyte, and K-Na alloy (66:34) anodes on porous nickel using 1M KPF₆ in DME as electrolyte. Optimal cycling ranges were determined using the CV method. In Li⁺ cells, the materials demonstrated the specific discharge capacities up to 110 (*a*), 95 (*b*) and 160 (*c*) mAh/g at current density of 100 mA/g, CEs of 100%, median discharge voltages of 2.1–2.25 V; cyclability reached 500 cycles or more. In K⁺ cells, the initial capacities of all materials reached 110 mAh/g at the same current density; after 300 cycles, the capacities decreased to 50–70 mAh/g. CEs were close to 100% and median discharge voltages reached 2.3–2.45 V.

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This work was supported by the Ministry of Science and Higher Education of the Russian Federation, project № 122111700046-3 (FFSG-2022-0001, "Laboratory of perspective electrode materials for chemical power sources").



SUPPLEMENTED MONITORING OF CORROSION PROCESSES USING PROJECTION-BASED MACHINE LEARNING METHODS – PCA/PLS WITHIN A TEMPORAL APPROACH

**Bashirova Z.A.^a, Bizhanova G.G.^a, Maksyutova E.I.^a, Gareev I.A.^a,
Sidelnikov A.V.^a, Budnikov G.K.^b**

^a*Ufa University of Science and Technology, 450076, Ufa, 32 Zaki Validi St.,
e-mail: Bashirova2903@gmail.com*

^b*Kazan Federal University, 420008, Kazan, 18 Kremlin St.*

Monitoring of reactions and processes is a special activity and approach to the study of chemical macro and micro objects. Its features are associated with the need to obtain real-time high-precision characteristic signals, not only static but also dynamic.

In all known instrumental methods of analysis, the mathematical model type is initially known, and the parameters of the analytical equation are determined empirically. However, it should be noted that such approaches are applicable only when the useful analytical signal is sufficiently intense and not complicated by interfering components. At low signal intensity, it is practically impossible to determine substances, but the intensity is still sufficient for substance detection. In the case of trace amounts, the analytical signal is so small that it is considered statistically insignificant and cannot be characterized by data processing methods.

The proposed approaches are based on the accumulation of signals in the form of voltammetric time series and their quantitative description using percolation theory, fractal approaches, generalized principal component methods, and discrete geometric invariants. This work presents one of the author's approaches that complements known methods for monitoring corrosion processes. It is based on the analysis of temporal electrochemical databases recorded with the participation of the investigated alloy as a working electrode in the measuring cell.

The of projections onto latent structures (PLS) allows for the quick determination of dynamic and kinetic characteristics of processes in a generalized form, both overall and individually for each component. The proposed approaches help complement the knowledge base of monitoring from electrochemical data, particularly using voltammetry, and enable the separate assessment of the contribution of each chemical substance.

THREE-COMPONENT COATINGS BASED ON IRON TRIAD METALS. COMPOSITION AND CORROSION PROPERTIES

Fishgoit L.A., Galiakberova M.R., Andreeva P.P.

*Lomonosov Moscow State University. Chemistry Department,
119991, Moscow, Leninskie Gory, 1, build. 3, GSP-1,
e-mail: ddyyyaq@gmail.com*

Currently, research on the processes of electrodeposition of coatings in the form of amorphous metal-based alloys is actively developing. Triads of iron, which are produced in industrial volumes, are obtained by metallurgical methods. However, amorphous alloys obtained galvanically differ from their metallurgical counterparts both by processes leading to the formation of an amorphous state and by physical properties and have a number of undeniable advantages over similar alloys obtained by metallurgical (spinning, quenching into rolls, pulling from the melt) and physical (magnetron sputtering, chemical vacuum deposition, etc.) methods, namely, the possibility of obtaining a coating with the desired properties directly on the product, without the need for heat treatment, resource saving and the ability to obtain a seamless coating with an amorphous alloy.

The synthesis of electrodeposited coatings of the *Fe-Co-P* system was carried out on an installation consisting of a 50 ml three-electrode cell and a potentiostat galvanostat *Elins P-40X* (Russia) under the control of specialized *ES8* software. A pre-chemically polished copper wire was used as the working electrode.

It is shown that with an increase in *pH* from 1 to 4 and a decrease in the deposition current density, the surface morphology improves (less cracking occurs, the coating becomes dense and homogeneous), the percentage of oxide phases decreases until it disappears, which means maximum deposition of the main elements and complete restoration of all alloy components. It has been established that the corrosion properties of a series of synthesized alloys depend more on the morphology of the surface than on the composition. The higher the surface cracking, the higher the density of the corrosive current. The optimal composition of the alloy was determined (55.6 wt% *Fe*, 38.2 wt % *Co* and 6.2 wt. % *P*) synthesized at a current density of -15 mA/cm^2 for 10 minutes and a *pH* value of 4, according to X-ray phase analysis, the alloy is a phase of the Fe_7Co_3 composition with a lattice period of $a = 0.2840 \text{ nm}$, spatial symmetry *CsCl*.



INVESTIGATION OF THE POSSIBILITIES OF ELECTROCHEMICAL DETERMINATION OF IRON IN HUMAN BLOOD

Fishgoit L.A., Kurakin D.P., Kononenko D. V., Dolov M.S.

*Lomonosov Moscow State University. Chemistry Department.
119991, Moscow, Leninskie Gory, 1, build. 3, GSP-1,
e-mail: ddyyyaq@gmail.com*

In the human body, iron is an important cofactor, being part of hemoglobin, a substance that carries oxygen through the blood. Lack of iron in the body leads to the development of anemia, a dangerous chronic disease. At the same time, a violation of the removal of iron from the body leads to an excess of the norm of iron content and the development of hemochromatosis, fraught with cirrhosis of the liver.

Investigation of serum iron in the blood can help in the prevention of these diseases. We came up with the idea that the iron oxidation reaction could be an accurate analytical signal. The purpose of this work is to establish the possibility of usage of electrochemical analysis methods to determine the iron content in human blood.

The measurements were carried out on a potentiostat *P-40X* combined with a *PC*. The oxidation of *Fe(II)/Fe(III)* under the conditions of our system was previously qualitatively confirmed using a solution of ammonium thiocyanate $NH_4(SCN)$. To compile the calibration schedule, solutions with an iron content with concentrations from 30 μM (the permissible maximum of iron in the blood) to 12 μM (the permissible minimum of iron in the blood) were prepared by dilution. An exponential relationship has been established between the concentration of iron in an isotonic solution and the “effective” charge spent on the *Fe(II)/Fe(III)* oxidation reaction. Iron oxidation in an isotonic solution simulating blood plasma occurs at a potential of 0.6 V. Based on the data of the study, it can be concluded that diseases caused by increased iron content (hemochromatosis) can be accurately determined using electrochemical analysis methods.

BROMATE REDUCTION ON ROTATING DISC ELECTRODE: NUMERICAL SIMULATION OF EXPERIMENTAL DATA

Gordienko D.V.^{a,b,c}, Goncharova O.A.^{b,c}, Konev D.V.^{b,c}, Vorotyntsev M.A.^b

^a*Moscow Institute of Physics and Technology (NRU), Dolgoprudny, RF*

^b*Frumkin Institute of Physical Chemistry and Electrochemistry of RAS, Moscow, RF*

^c*FRC Problems of Chemical Physics and Medical Chemistry of RAS, Chernogolovka, RF,*

e-mail: gordienko.dv@phystech.edu

Search for electrical power sources based on novel chemistries represents now an active area of studies. One of such directions is related to the bromate reduction process which takes place via a combination of electrochemical and chemical steps^{1,2}. The autocatalytic type of this process makes it particularly interesting for its use in various applications, e.g. in hydrogen-bromate flow batteries³.

In this work, experimental chronoamperometric data for the bromate anion reduction process with excessive background acid on a rotating disk electrode under limiting-current conditions after potential step have been interpreted. For this purpose, a system of transport-kinetic equations of the convective-diffusion transport for this process has been solved via a finite-difference numerical method based on an explicit-implicit discretization scheme (second-order precision) over non-uniform and adaptive grids for spatial coordinate or time, respectively. This approach has made it possible to achieve a high accuracy of calculations, while spending a significantly less time for each configuration of the system, in comparison with the traditional approach based on uniform grid. This approach has allowed us to provide an interpretation of experimental data for the non-stationary current via their comparison with calculated results.

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The work was carried out with the financial support of the RSF, project 23-13-00428.



PHOSPHORYLATION OF ACRIDINES UNDER ELECTROCHEMICAL CONDITIONS

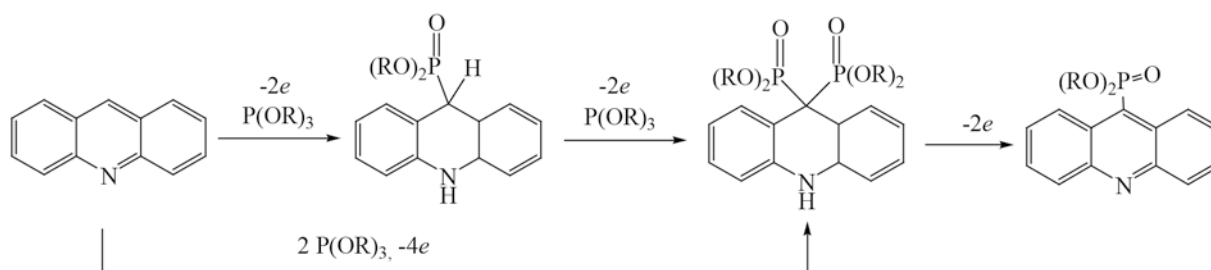
Gryaznova T.B., Tarasov M.V., Fayzullin R.R., Morozov V.I., Budnikova Yu.G.

*Arbuzov Institute of Organic and Physical Chemistry,
FRC Kazan Scientific Center, Russian Academy of Sciences
Arbuzov str. 8, Kazan, 420088 Russian Federation 420008,
e-mail: gryaznovatv@gmail.com*

Polyaromatic heterocyclic systems, especially condensed ones containing a pyridine fragment, are of great importance for both synthetic chemistry and medical chemistry. The presence and position of the heteroatom in the ring electronically activate certain Csp^2 positions, providing substrate control for regioselective C–H functionalization. Acridine derivatives are used as building blocks for heterocyclic systems and are of great importance for biology, pharmacy and material sciences.

However, at the moment, the properties of phosphorylated acridines have been little studied, and the methods for their production require improvement. Organic electrosynthesis is an efficient and environmentally friendly synthetic method.

A mild, effective electrochemical method of direct $C(sp^2)$ –H phosphorylation of acridine by trialkyl phosphites has been developed¹. Joint electrosynthesis without a catalyst or an external oxidising agent leads to selective C9-phosphorylation of acridines with good yields. The reaction mechanism was investigated using voltammetry and EPR spectroscopy.



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The work was carried out with the financial support of the Russian Science Foundation (project No. 22-13-00017).

ELECTROPOLYMERIZATION OF PYROGALLOL RED AT THE ELECTRODE MODIFIED WITH CARBOXYLATED MULTI-WALLED CARBON NANOTUBES

Kalmykova A.D., Ziyatdinova G.K.

*Kazan Federal University,
Kremleyevskaya 18, Kazan, 420008, Russia,
e-mail: alena.kalmykova.pnb.2000@mail.ru*

Electrodes with polymer coverages are actively developed at the moment. Electrochemical methods for polymeric films fabrication are of interest, in particular, potentiodynamic electrolysis, because it excludes the need to use additional chemical reagents and volatile organic solvents, and control of the electrochemical process parameters ensures a coverage of the required thickness and structure. Among monomers, attention is paid to phenolic compounds forming non-conductive coverages. Therefore, various carbon nanomaterials are usually used as a platform for polymer deposition.

The electropolymerization of triphenylmethane dye pyrogallol red has been performed in neutral medium at the glassy carbon electrode (GCE) modified with carboxylated multi-walled carbon nanotubes dispersed in 1% sodium lauryl sulfate. The dye is irreversibly oxidized at 0.28 and 0.59 V. Only a weak-pronounced step is observed at the second oxidation potential. The anodic steps correspond to the oxidation of partially deprotonated molecule of pyrogallol red with the participation of phenolate fragment with formation of phenoxyl radicals that can undergo further reactions of dimerization and polymerization. The oxidation currents are decreased on the second and following cycles that confirm the formation of a non-conducting coverage. Variation of the electropolymerization conditions (the nature and pH of supporting electrolyte, number of cycles, monomer concentration and electrolysis parameters) has shown that polymeric coverage to be obtained from 100 μM monomer solution in Britton-Robinson buffer pH 7.0 by tenfold potential cycling in the range of 0.0 to 1.3 V at a scan rate of 75 mV s^{-1} .

A polymer-modified electrode has been characterized by scanning electron microscopy and the complex of electrochemical methods. The effectivity of electron transfer on the created electrode has been shown (electron transfer rate constants equal to $9.12 \times 10^{-5} \text{ cm s}^{-1}$ vs. $4.12 \times 10^{-5} \text{ cm s}^{-1}$ for bare GCE).



OBTAINING OF PROTECTIVE COATINGS FOR SOFC INTERCONNECT APPLICATIONS USING OF NON-STATIONARY ELECTROLYSIS METHOD

Khramenkova A.V.^a, Finaeva O.A.^a, Pikalov O.V.^b, Demeneva N.V.^b

^a*Federal State Budgetary Educational Institution of Higher Education
“M.I. Platov South Russian State Polytechnic University (NPI)”,
346428, Novocherkassk, 132 Prosveshcheniya St., Russia,
e-mail: anna.vl7@yandex.ru*

^b*Institute of Solid State Physics RAS, 142432, Moscow District,
Chernogolovka, 2 Academician Osipyan St., Russia*

The problem of increasing of service life of solid oxide fuel cells (SOFCs) is the object of study of large number of researchers. The insufficient service life of SOFCs is primarily associated with the failure of their components – interconnects. Interconnects are made of ferritic stainless steels; however, when operating at high temperatures, their characteristics sharply deteriorate due to the formation of poorly conducting chromium oxides. The solution to this problem is to apply protective coatings to their surface.

This paper presents the results of obtaining of protective Co-Mn oxide coatings with spinel structure on the surface of stainless steel using non-stationary electrolysis method. The formation of coatings was carried out on the surface of Crofer 22 APU stainless steel the at a temperature of 60 °C during 60 minutes, the asymmetry coefficient was 1.63. The electrolyte consists of cobalt and nickel nitrates, cobalt chloride, boric acid, manganese sulfate and surfactant.

According to X-ray diffraction data, the main phase of the resulting coatings is CoMn_2O_4 , the chemical composition of the coatings is given in Table 1, and the presence of iron in the composition can be explained by the contribution of the substrate.

Table 1. X-ray photoelectron spectroscopy data

Element	Co	Mn	O	Fe
Concentrations of elements (at.%) in the surface layer	7.5	16.3	61.6	14.7

The research was carried out with the help of a grant Russian Science Foundation № 24-23-00113, <https://rscf.ru/en/project/24-23-00113/>.

SYNTHESIS OF MODIFIED HYBRID ELECTRODE MATERIALS FOR SUPERCAPACITORS USING NON-STATIONARY ELECTROLYSIS METHOD

Khramenkova A.V., Moshchenko V.V., Laptii P.V.

*Federal State Budgetary Educational Institution of Higher Education
«M.I. Platov South-Russian State Polytechnic University (NPI),
132 Prosveshcheniya st., Novocherkassk, 346428, Russia,
e-mail: anna.vl7@yandex.ru*

Supercapacitors are widely used as backup and auxiliary power sources in portable electronic devices, pacemakers, and hybrid vehicles due to their high power density and fast recharge capability.

Electrode materials for supercapacitors can be conventionally divided into double-layer capacitive materials (carbon and its modifications) and materials with Faradaic processes (transition metal oxides, conductive polymers).

The direction associated with the development of modified binder-free electrodes is becoming increasingly developed, which concludes in applying of an active material layer to a substrate.

This paper presents the results of research on electrochemical synthesis and the study of electrochemical properties of hybrid electrode materials, representing carbon fabric modified with metal oxides in combination with polymers, for supercapacitors. The synthesis was carried out with polarization by alternating asymmetric current at a temperature of 60 °C for 40 minutes, the asymmetry coefficient was 1.5. The electrolyte solution consists of cobalt, nickel and iron sulfates, cobalt chloride, boric acid, ammonium heptamolybdate, citric acid. Polyacrylic acid (PAA) or polyethylene glycol (PEG-600) was used as a polymer additive to the electrolyte.

Electrochemical measurements were recorded on a potentiostat/galvanostat P-40X in a three-electrode cell relative to a silver chloride reference electrode (Ag/AgCl, 3.5 M KCl). Pt plates were used as an auxiliary electrode and a current collector for the working electrode. The electrolyte was a 2 M aqueous solution of KOH.

The specific capacity of the hybrid material modified with PAA was 1669 mF/cm² at a current density of 5 mA/cm²; the hybrid material modified with PEG-600 – 911 mF/cm² at a current density of 5 mA/cm², which is comparable to the values of the specific capacitance of similar commercial electrode materials.



DIAPHRAGM AND ANION-EXCHANGE MEMBRANES FOR ALKALINE WATER ELECTROLYSIS

Kuleshov V.N., Kuleshov N.V., Kurochkin S.V., Gavriluk A.A.

*MPEI, 111250, Russia, Moscow, Krasnokazarmennaya street, 14, 1,
e-mail: kurochkinsv@mpei.ru*

Alkaline water electrolysis (AWE) has been used in industry for many years to produce hydrogen. Recently, AWE has been undergoing significant changes, which are aimed at reducing energy costs and increasing the purity of generated gases through the creation of new separating diaphragms and membranes.

At the turn of the 90s, the diaphragm material Zirfon of the Agfa Pearl trademark appeared, which is currently used in many high-performance AWE, while research to improve Zirfon continues. Thus, the Agfa company began producing UTP 220 membrane, the thickness of which was reduced to 220 microns while maintaining gas tightness. Our country has also developed a porous composite polymer diaphragm based on domestic materials¹.

In recent years, interest in the development of a new generation of anion-exchange membranes (AEM) has sharply increased in the world, with the following trends being observed: the attachment of functional groups to the main polymer chain and the creation of ion-solvated or gel-polymer membranes². AEM in alkaline electrolysis make it possible to move on to the technology of forming membrane-electrode assembly, by analogy with proton-exchange membranes.

This work presents data on the synthesis of ion-solvated membranes based on a polysulfone matrix. Of particular interest are alkali-resistant inorganic hydrogels impregnated into the original polymer matrix, which made it possible to impart anion-exchange properties to this membrane.

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The work was carried out with the financial support of the Ministry of Science and Higher Education of the Russian Federation within the framework of State Assignment No. FSWF2023-0014 (Agreement No. 075-03-2023-383 dated January 18, 2023) in the field of scientific activity for 2023-2025.

PROMISING AIR ELECTRODES FOR SOFCS BASED ON MODIFIED BARIUM FERRITES

**Kuznetsova P.S.^a, Tarutina L.R.^{a,b}, Starostina I.A.^{a,b},
Starostin G.N.^{a,b}, Medvedev D.A.^{a,b}**

^a*Ural Federal University named after the First President of Russia B.N. Yeltsin,
620002, Ekaterinburg, st. Mira, 19,
e-mail: lina.kuznetsova.00@list.ru*

^b*Institute of High Temperature Electrochemistry of the Ural Branch,
620066, Ekaterinburg, st. Academic, 20*

Proton-ceramic fuel cells (PCFCs) offer a promising approach for the efficient conversion of chemical energy stored within fuels into electrical energy. One key advantage of PCFCs, in comparison to traditional solid oxide fuel cells (SOFCs), is the ability to operate at low temperatures (400–800 °C). This feature solves the issues related to rapid degradation of functional material properties, the sealing of electrodes comprising porous structures, and chemical interactions between the fuel and the gas components. One of the challenges in the development of PCFCs is the selection of suitable materials for air electrodes. One potential solution lies in the production of mixed ion-electron conductors based on Ce-doped BaFeO_{3-δ}. In this work, the specific features of BaCe_{0.5}Fe_{0.5}O_{3-δ} complex oxide preparation were studied. The influence of different sintering temperatures on the phase formation, sinterability and functional properties of these materials is also investigated.

The synthesis of the complex oxide BaCe_{0.5}Fe_{0.5}O_{3-δ} was carried out via the citrate-nitrate method. The obtained powder was then calcined at 1100 °C for (5 h), followed by grinding the obtained powders in an acetone medium and then pressing into pellets of 20 mm diameter. The sintering of the ceramics was carried out at temperatures of 1100, 1200, 1300 and 1350 °C (5 h). The ceramic samples obtained at these temperatures were re-milled, then pressed again and sintered at 1100 °C (5 h). X-ray diffraction (XRD) analysis revealed the presence of BaCeO₃ and BaFeO₃ phases, across the entire range of sintering temperatures. The X-ray images were refined using the Rietveld method. The surface morphology of the sintered ceramics was investigated using scanning electron microscopy. The data from the study indicated that with the increase in sintering temperature, there was expected densification of the samples. The total conductivity in the temperature range of 100–1000 °C was investigated by the four-probe method under wet air (pH₂O=0.03 atm) conditions.

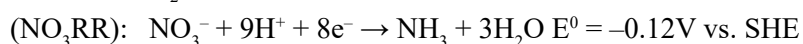
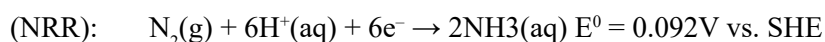
MODIFIED CATALYSTS BASED ON CO-NANOPARTICLES TO INCREASE THE EFFICIENCY OF THE ELECTROCHEMICAL REACTION OF AMMONIA SYNTHESIS

Kuznetsova I.I.^a, Kultin D.Yu.^a, Lebedeva O.K.^a, Kustov L.M.^{a,b}

^a*Department of Chemistry, Lomonosov Moscow State University, 119991 Moscow, Russia,
e-mail: kuznetsowair@yandex.ru*

^b*N.D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences,
Leninsky Prospect 47, 119991 Moscow, Russia*

Along with classical catalytic methods, photo- and electro-catalytic methods can also be used for the same reactions.¹ The group of reactions under the general «aegis» of the nitrogen reduction reaction (NRR) is currently studied almost exclusively in electrocatalytic design.² The reactions have great prospects for replacing the Haber-Bosch ammonia synthesis process and are eco-friendly. The main challenge is to find conditions and catalysts to increase the product yield and Faraday efficiency (FE) selectivity.



The obtained metal nanoparticles were characterized by means of scanning electron microscopy.³ Among the studied nanocatalysts (on the basis of cobalt, iron and copper), the best activity and selectivity were shown by samples containing electrochemically deposited cobalt nanoparticles. Even samples containing trace amounts of cobalt by weight have already shown FE > 40%.

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ELECTROCHEMICAL SEPARATION OF NON-FERROUS METALS FROM PRODUCTION SOLUTIONS PRODUCTION OF COPPER AND ITS ALLOYS

Maksimov I.S., Brodskiy V.A.

*D.I. Mendeleev Russian University of Chemical Technology
Faculty of TIS and HTM, 125047, Moscow, Miusskaya square, 9c1,
e-mail: vanyamaks@mail.ru*

In modern metallurgy, the “liquid extraction-electrolysis” method (SX-EW) for extracting copper from solutions is becoming increasingly popular. The aim of this work is to develop a process for the separation of non-ferrous metals (copper and zinc) from copper and copper alloy production solutions.

The sulfuric acid electrolyte (1 M H_2SO_4), which was studied, was used to return it to the process and obtain pure cathode materials in the first stage of separation ($i_k(Si) = 1.25 \text{ A/dm}^2$, $W = 65\%$; $i_k(Zn) = 1 \text{ A/dm}^2$, $W = 85\%$).

After the sulfuric acid treatment, the copper residue was subjected to copper ammonia and copper chloride treatments (Fig. 2, b). Copper extraction from the leach solutions was performed using the LIX-54 extractant, which has been proven to be the most effective method. The electrical separation of copper from the extracting solutions ($i_k = 0.6 \text{ A/dm}^2$) was carried out.

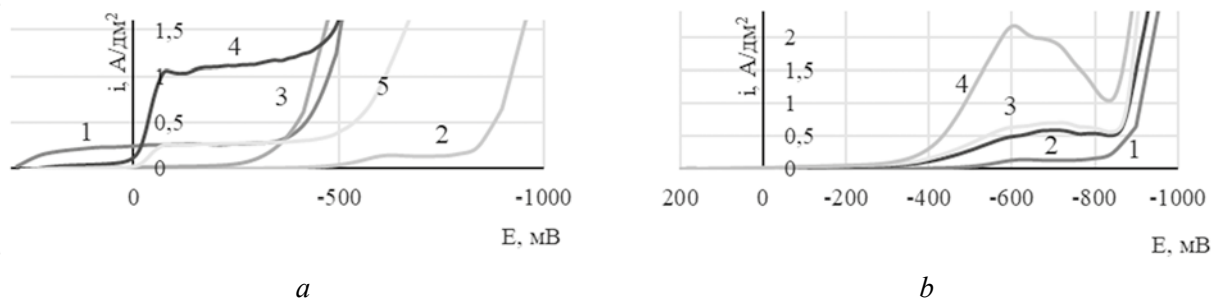


Figure 1. Polarization curves of copper (a) and zinc (b) release

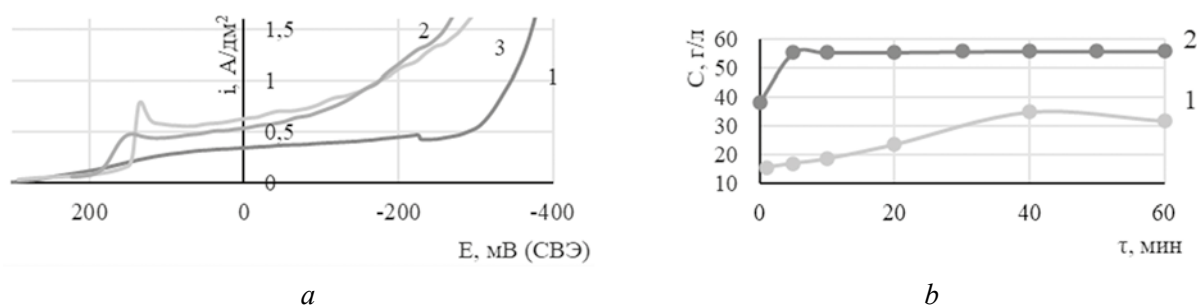


Figure 2. Polarization curves of copper extraction from the reextraction solution (a); Efficiency of copper leaching from the copper cake (b)

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HYDROGEN PERMEABILITY OF PALLADIUM SAMPLES OBTAINED BY DIFFERENT METHODS

Morozova N.B.^{a,b}, Odnokozova Ya.S.^a, Vvedensky A.V.^a, Dontsov A.I.^{a,b}

^a*Voronezh State University, 394018, Voronezh, Universitetskaya pl. 1,*

e-mail: mnb@chem.vsu.ru

^b*Baikova Institute of Metallurgy and Materials Science Russian Academy of Sciences,
119334, Moscow, Leninsky prospect 49*

One of the important areas of hydrogen energy is the production of high-purity hydrogen using palladium-based membranes. Effective palladium membranes must have not only high specific hydrogen permeability and corrosion resistance, but also high ductility. The characteristics of these membranes are largely determined by their thickness. The purpose of this work is to identify the influence of the Pd electrode manufacturing method on the parameters of hydrogen permeability.

The thickness of sample 1, made of compact palladium, is about 7 mm. Sample 2 was obtained by cold rolling followed by annealing at 950 °C. Its thickness is 41 μm. The study of hydrogen permeability was carried out using cyclic voltammetry and cathode-anode chronoamperometry in a deaerated solution of 0.1 M H₂SO₄.

The calculation of hydrogen permeability parameters was carried out using mathematical modeling. As a result, the coefficient of hydrogen permeability K_D , the concentration of atomic hydrogen in the alloy Δc_H , the adsorption equilibrium constant of the phase-boundary exchange stage K , which is expressed through the effective rate constants of injection \bar{k} and extraction \bar{k} , were obtained.

	$K_D \cdot 10^9, \text{mol/cm}^2 \cdot \text{s}^{1/2}$	$\Delta c_H \cdot 10^5, \text{mol/cm}^3$	$K \cdot 10^{-4}, \text{cm}^{-1}$	$\bar{k} \cdot 10^5 \text{ cm/s}$	\bar{k}, s^{-1}
Sample 1	20.6 ± 7.6	3.26 ± 1.31	2.95 ± 1.29	2.43 ± 0.86	8.64 ± 1.97
Sample 2	17.94 ± 2.49	3.28 ± 0.46	2.57 ± 1.45	3.75 ± 0.11	9.64 ± 1.51

The obtained values of the hydrogen permeability parameters of the Pd samples under study are in good agreement and coincide within the error. Therefore, the manufacturing method of the palladium electrode does not have much influence on the permeability characteristics of atomic hydrogen.

The work was carried out with the financial support of the Russian Science Foundation, project №. 23-19-00767.

ELECTROCHEMICAL STUDY OF THE ADSORPTION OF ALIPHATIC ALCOHOLS ON PALLADIUM IN AN ACID MEDIUM

Morozova N.B., Kopalina P.N., Vvedensky A.V.

*Voronezh State University,
394018, Voronezh, Universitetskaya pl.1,
e-mail: mnb@chem.vsu.ru*

The interaction between organic molecules and the metal surface plays an important role in a number of electrochemical systems, from electrocatalysis to the protection of metals from corrosion. This type of interaction may involve direct adsorption of organic molecules on the electrode or its electroadsorption with or without destruction of the molecules. Adsorption of organic compounds on a metal electrode is the initial stage of their interaction and can be assessed by the degree of surface coverage. The purpose of This work was to find the degree of coverage of the palladium surface with aliphatic alcohols in aqueous sulfuric acid solutions using the charging curve method.

The studies were carried out on a smooth palladium electrode in a deaerated aqueous solution of 0.1 M H₂SO₄. Ethanol concentrations *n*-propanol, isopropanol and *n*-butanol in the background solution were varied from 10⁻⁴ to 10⁻² M. The adsorption study was carried out using the method of charging curves in galvanostatic regime.

The values of the degrees of palladium filling with aliphatic alcohols (table), calculated from the hydrogen (Θ(H)) region of the charging curves, increase with increasing concentration of alcohols in the solution. A decrease in adsorption is also observed with increasing length of the hydrocarbon radical. The Θ(O) values have lower values and change in the opposite direction. The adsorption of secondary alcohol differs from primary alcohol throughout the entire concentration range.

<i>c</i> (alcohol), M	1·10 ⁻⁴	5·10 ⁻⁴	1·10 ⁻³	5·10 ⁻³	1·10 ⁻²
Θ(H), %					
C ₂ H ₅ OH	9.49	5.75	10.85	17.91	20.09
<i>n</i> -C ₃ H ₇ OH	6.88	9.35	9.51	14.49	14.58
<i>iso</i> -C ₃ H ₇ OH	12.68	26.77	30.17	30.71	32.12
<i>n</i> -C ₄ H ₉ OH	6.97	8.33	9.33	12.00	14.54
Θ(O), %					
C ₂ H ₅ OH	5.31	2.62	2.02	10.85	4.25
<i>n</i> -C ₃ H ₇ OH	9.36	9.44	6.49	7.09	5.94
<i>iso</i> -C ₃ H ₇ OH	5.32	5.93	3.87	4.20	3.41
<i>n</i> -C ₄ H ₉ OH	10.22	17.79	19.04	18.38	19.68

ELECTROCHEMICAL PREPARATION OF METAL NANOPARTICLES AND THEIR NANOCOMPOSITES IN SOLUTION

Nasretdinova G.R., Fazleeva R.R., Yanilkin V.V.

*Arbuzov Institute of Organic and Physical Chemistry,
FRC Kazan Scientific Center, Russian Academy of Sciences,
Arbuzov St. 8, 420088 Kazan, Russia,
e-mail: nasybullina@iopc.ru*

The unique properties of metal nanoparticles (MNPs) and their nanocomposites, a wide variety of areas of their potential applications motivate researchers to create new ways to obtain these nano-objects. We have developed a new electrochemical method for the preparation of MPs in solution based on the mediated reduction of metal ions (complexes) in the presence of MNP stabilizers. The mediator (Med_{ox}) is reduced directly at the electrode, the reduced form of the mediator (Med_{red}) passes into solution where chemical reduction of metal ions takes place (Fig. 1). Metal ions can be supplied to the solution by anodic dissolution of bulk metal. This variant of electrosynthesis is fully in line with the principles of «green chemistry», since its only result is the transfer of metal from the anode to the solution in the form of NPs.

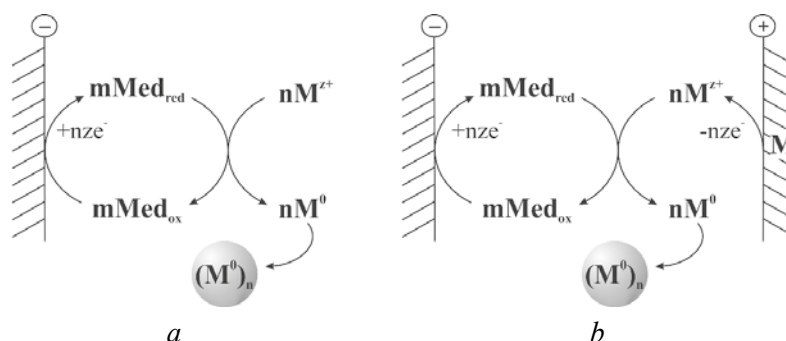


Figure 1. Scheme of the mediated electrosynthesis of MNPs $(\text{M}^0)_n$ in solution volume in (a) divided and (b) undivided (using a sacrificial anode) cell

The method of the mediated electrosynthesis has proven its efficiency in obtaining NPs of such metals as Pd, Ag, Au, Pt, Rh, Co, Cu, as well as bimetallic (Pd+Ag, Pd+Rh) NPs, in aqueous, aqueous-organic and organic media. Nanocomposites of MNPs with silica and polymeric NPs, nanocellulose, fullerenes, oxides and oxide-hydroxides of metals (Cu, Fe, Co, Zn, Ti, Al), macrocyclic compounds (tetraviologen calix[4]resorcinates, cyclobis(paraquat-*p*-phenylene)) were obtained.

INVESTIGATION OF THE CATALYTIC PROPERTIES OF ELECTROLYTIC NICKEL FOAMS IN RELATION TO THE OXYGEN RELEASE REACTION

Nikitin V.S., Ostanina T.N., Sretensky S.D.

*UrFU named after the first President of Russia B.N. Yeltsin, Mira str. 28,
Yekaterinburg, 620002, Russia,
e-mail: v.s.nikitin@urfu.ru*

One of the ways to produce hydrogen is the water electrolysis in an alkali solution, which occurs at very high overvoltages. To reduce energy consumption, porous electrodes are widely used, in particular nickel foams, which can exhibit catalytic properties both in relation to the reaction of hydrogen and oxygen release.

The aim of The work was to study the effect of current density on the catalytic properties of electrolytic nickel deposits in relation to the anodic oxygen release reaction.

The working electrodes with a working surface of 0.84 cm^2 were made of copper plates with a pre-applied layer of nickel. Nickel foams were deposited from a solution of 0.2 M NiCl_2 , $2 \text{ M NH}_4\text{Cl}$ ($\text{pH}=3.2$) at a temperature of 25°C and current densities of 0.3 , 0.6 and 0.9 A cm^2 based on the geometric surface of the electrode. The deposition time was 5 , 10 and 15 minutes for each current density. The anodic polarization curves were registered in a solution of 1 M NaOH using the Solartron 1280C electrochemical station with a potential sweep rate of 3 mV s^{-1} .

As a criterion of catalytic properties, the depolarization value was determined as the difference between potential of a smooth nickel electrode (E_{sm}) and that of an electrode with deposit (E_{dep}): $\Delta E = E_{\text{sm}} - E_{\text{dep}}$ at a current density of 0.3 A cm^2 . It was found that with a short deposition time (5 min), an increase in current density leads to an increase in ΔE , which facilitates the oxygen release reaction on the foam and, as a result, should reduce the anodic overvoltage during water electrolysis. However, with an increase in the deposition time up to 15 minutes, the current density practically ceases to affect the catalytic properties of nickel deposits. This may be due to the formation of a regular pore structure that varies little on deposit thickness. This fact is confirmed by micrographs of the outer surface of the foams.

The research funding from the Ministry of Science and Higher Education of the Russian Federation (Ural Federal University Program of Development within the Priority-2030 Program) is gratefully acknowledged.



LAYERED P2-TYPE $\text{Na}_{2/3}\text{Ni}_{1/3}\text{Mn}_{2/3}\text{O}_2$: CONDUCTIVITY AND ELECTROCHEMICAL CHARACTERISTICS

Novikova S.A., Yaroslavtsev A.B.

*Kurnakov Institute of General and Inorganic Chemistry, Russian Academy of Sciences,
31 Leninsky av., Moscow, 119991, Russia,
e-mail: novikova@igic.ras.ru*

Lithium-ion batteries have been widely used as energy sources for various electronic devices due to their high capacity and efficiency. However, the lithium content in the earth's crust is low and the global distribution of raw materials for LIBs is imbalanced, which limits its application to meet the rapidly growing demand for energy storage devices. The use of compounds of the significantly more abundant and cheaper sodium instead of lithium analogs can help to solve this problem. Layered oxides $\text{Na}_x\text{M}'\text{M}''\text{O}_2$, where $\text{M}=\text{Mn, Fe, Co, Ni, V, Cr, etc.}$ are promising cathode materials for sodium-ion batteries (SIBs).

The cathode material of $\text{Na}_{2/3}\text{Ni}_{1/3}\text{Mn}_{2/3}\text{O}_2$ composition was obtained by the carbonate coprecipitation followed by solid-phase reaction and characterized by XRD analysis, ICP-MS, electron and impedance spectroscopy. $\text{Na}_{2/3}\text{Ni}_{1/3}\text{Mn}_{2/3}\text{O}_2$ crystallizes in a P2-type layered hexagonal structure (sp. gr. P63/mmc), consists of spherical agglomerates of ~1–3 microns in size, formed from the plate-like primary grains. It is shown that the particles have the smallest size in the direction of the crystallographic «c» axis. The $\text{Na}_{2/3}\text{Ni}_{1/3}\text{Mn}_{2/3}\text{O}_2$ ionic conductivity value was $1.8 \cdot 10^{-4}$ and $1.3 \cdot 10^{-4} \text{ S cm}^{-1}$ at room temperature when measured perpendicularly and parallel to the pressing axis, respectively. The calculated value of activation energy was equal to the value of ~21 kJ/mol. The diffusion coefficients of sodium cations (D_{Na^+}) calculated from the Nernst-Einstein equation were of the order of $\sim 10^{-9} \text{ cm}^2 \text{ sec}^{-1}$. The obtained materials were tested as cathodes in a sodium-ion battery cells versus sodium metal. The discharge capacity of $\text{Na}_{2/3}\text{Ni}_{1/3}\text{Mn}_{2/3}\text{O}_2$ was 160 mAh/g and 86 mAh/g in the potential range of 1.5–4.0 V and 2.3–4.0 V, respectively (20 mA/g). $\text{Na}_{2/3}\text{Ni}_{1/3}\text{Mn}_{2/3}\text{O}_2$ was shown to be stable under cycling in the potential range of 2.3–4.0 V and can be used as the cathode of a SIB.

Funding: This work was supported by the Ministry of Science and Higher Education of the Russian Federation as part of the State Assignment of the Kurnakov Institute of General and Inorganic Chemistry of the Russian Academy of Sciences.

OXIDATION OF ZINC-NICKEL COATING COMPONENTS IN CHLORIDE-CONTAINING ELECTROLYTE

Protasova I.V., Khangeldieva A.O., Perevalova O.A.

*Voronezh State University,
University Square, 1, 394018, Voronezh, Russia,
e-mail: protasova@chem.vsu.ru*

One of the main aspects of the development of zinc-based coatings is the creation of composite coatings that contain other substances in addition to zinc.

In this work, zinc-nickel coatings were obtained on a steel electrode at potentials of -0.990 ; -1.020 and -1.100 V and deposition time from 60 to 1800 s. Energy dispersive, X-ray diffraction and electrochemical methods have shown that the composition of the coating varies depending on the time and deposition potential. It was found, that with increasing polarization time, the coating is enriched in phases with a high zinc content. By 180 s a coating is formed, the elemental composition of which does not change with increasing thickness. The ratio of metals in the coating obtained at potentials of -0.990 and -1.020 V coincides with the ratio of metal ions in the deposition solution. Deposition at higher cathodic polarization (-1.100 V) and time 600–1800 s leads to abnormal coating deposition. In this case, the coating contains 3–6 times more zinc than nickel.

In solutions containing 0.1 M chloride ions with $\text{pH } 1 \div 1.7$, the coating applied at -1100 V oxidizes at a faster rate. The corrosion potential decreases and the corrosion current increases as the zinc concentration in the coating increases and the cathodic deposition potential decreases. Anodic polarization of coatings leads to the preferential removal of the zinc component from zinc-containing phases. Under the selected processing conditions, only the high-zinc coating retains zinc-containing phases. From coatings in which zinc and nickel are in a 1:1 ratio, zinc is removed almost completely, and nickel remains on the electrode surface. An increase in the acidity of the solution is accompanied by an increase in the rate of anodic oxidation of the coating, which manifests itself in a decrease in the polarization of the process of local activation of the electrode. Analysis of the partial anodic ionization curves of the coating components showed the dissolution of the nickel component from the coating during anodic and cathodic polarization.

It is expected that the results obtained in this work will be useful in predicting production modes and operating conditions of protective zinc-nickel coatings.



THE ROLE AND SIGNIFICANCE OF A.N. FRUMKIN AND N.A. BACH IN THE CREATION OF A NEW DIRECTION IN SCIENCE – A RADIATION CHEMISTRY

Revina A.A., Danilkina O.P.

*A.N. Frumkin Institute of Physical Chemistry and Electrochemistry RAS,
Russia, 199071, Moscow, Leninsky prosp., 31, b.4,
e-mail: Alex_revina@mail.ru*

The publication is devoted to an important personal role and significance of A.N. Frumkin and N.A. Bach in creation and first stages development of a new science, now called radiation chemistry. Indeed it was created in electrochemistry sector of physical chemistry Institute of RAN in 1946 year by academician A.N. Frumkin in connection with the special governmental tasks fulfilment on atomic energetics, namely, the studies of process mechanisms in the different materials and objects under the various ionizing irradiations action and influence.

Since 1936 year, when he and N.A. Bach, director of Central Chemical Laboratory (later Physical Chemistry Institute after L.Ya. Karpov) had received famous Irene and Frederic Joliot-Curie at All-Union conference on nuclear physics and cosmic rays in Moscow. The French scientists already had known that any the radioactive elements investigation is dangerous and new field studies need the urgent attraction of chemists, physicist and biologists for to work out the new defence means and protection methods.

Professor N. A. Bach was assigned to head a specially organized radiation chemical laboratory in Physical Chemistry Institute of USSR Academy of Sciences, where the studies of the radiolysis mechanism in aqueous and aqueous-organic solutions were initiated. Also (together with P.I. Dolin's group) the problem of explosive mixture formation and its yield reducing in the nuclear reactors aqueous circuits was studied.

For to carry out the radiation investigation programme in IELAN were equipped the special rooms with possible usage of the powerful ionizing irradiation sources: radioactive cobalt GURH-4000, (later GURH-100 000 and the linear accelerators – UELU-10-10-T and 'Elektronika 003 with electrons energy 5 MeV. The accelerators were complected with advanced devices, created in our institute under management of V.I. Zotulovsky and D.M. Zorin. On the initiative of A.N. Frumkin and with the support of a correspondent member of the USSR Academy of Sciences V.A. Legasov was studied the ionizing radiation conversion energy in the nuclear reactor (Ulugbek, Uzbek SSR) using electrochemical cells with electrodes made of semiconductor materials^{1,2}.

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ELECTRODEPOSITION OF TIN-ZINC ALLOYS

Shekhanov R.F., Fryakin A.A.

Ivanovo State University of Chemical Technology

The electrolytic tin-zinc alloy has higher protective properties compared to zinc in conditions of significant humidity and temperature changes¹. Individual tin coating is very porous and since it is cathodic in relation to steel, it can protect steel only if there are no pores in the coating. Individual zinc coating is a protective coating and is anodic to steel, however, due to the activity of zinc, it quickly dissolves to form basic salts. Coating with a zinc-tin alloy makes it possible to maintain the anodic nature of steel protection from atmospheric corrosion, as well as to reduce the porosity of the coating, which leads to increased corrosion resistance of the alloy.

Tin-zinc electrolytic alloys were deposited from ammonium oxalate electrolytes. The coating was anodic to steel. Coatings with tin-zinc alloys with a zinc content of 15–20 at. %, deposited from ammonium oxalate electrolytes, are superior in corrosion resistance to coatings with similar alloys with a zinc content of 20 to 30%, obtained from pyrophosphate electrolytes². The reason for the increased corrosion resistance of coatings deposited from ammonium oxalate electrolytes is their low porosity compared to similar alloys obtained from pyrophosphate electrolytes. The lightest and most uniform coatings from ammonium oxalate electrolytes were obtained at a temperature of 50 °C, in the range of cathode current densities of 0.25–1.0 A/dm². Deposition mode from pyrophosphate electrolytes: temperature 50–65 °C, 0.5–1.0 A/dm². It has been established that with increasing temperature, of all the studied electrolytes, the tin content in the alloy increases. OS-20 was used as an additive to improve the structure of the coating. In addition, the proposed oxalate-ammonium electrolytes are two times less concentrated in the complexing salt compared to pyrophosphate electrolytes and, therefore, have a lower cost when preparing a solution.

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SYNTHESIS AND ELECTROCATALYTIC PROPERTIES OF MAGNETIC $\text{Cu/NiFe}_2\text{O}_4$ COMPOSITES

Soboleva Ye.A., Ivanova N.M., Vissurkhanova Ya.A.

*Institute of Organic Synthesis and Chemistry of Coal of Kazakhstan Republic,
100000, Karaganda, Alikhanov Str. 1,
e-mail: esoboleva-kz@mail.ru*

Catalytic systems made from metal nanoparticles supported on magnetic iron-oxide carries attract close attention of scientists due to their efficiency, chemical stability, and technical convenience of their use.

In this work, composites of copper nanoparticles deposited on nickel ferrite ($\text{Cu/NiFe}_2\text{O}_4$) with different component ratios were prepared through the chemical reduction of copper cations in the presence of magnetic carrier particles treated with ultrasound. The specific surface area of the NiFe_2O_4 sample synthesized by co-precipitation method and treated at 500 °C was $72.7 \pm 1.4 \text{ m}^2/\text{g}$. The structure and morphological features of the synthesized composites were studied by X-ray diffraction spectroscopy and scanning electron microscopy methods. It was shown that copper particles are located on the surface of NiFe_2O_4 both in the form of individual rounded formations with sizes of 120–700 nm consisting of smaller grains, and in the form of their aggregations.

The resulting $\text{Cu/NiFe}_2\text{O}_4$ composites containing 20–80% copper particles were deposited in the form of powders on the surface of a Cu cathode in a diaphragm cell with an external magnet. Electrolysis of an aqueous-alkaline solution was accompanied by excessive release of oxygen, which indicated the occurrence of electrochemical reduction of copper cations from its oxides contained in small quantities in copper particles. After this, all the prepared composites were used as catalysts in the electrohydrogenation of acetophenone (APh).

Experiments on electrocatalytic hydrogenation of APh were carried out in an aqueous-alcohol-alkaline catholyte solution at a current of 2.5 A and a temperature of 30 °C, the anode being a Pt grid. It was found that the electrocatalytic activity of the studied $\text{Cu/NiFe}_2\text{O}_4$ composites, expressed in an increase in the rate of APh hydrogenation compared to its electrochemical reduction on the Cu cathode (without a catalyst), appears when their copper content becomes $\geq 40\%$. The APh conversion using almost all composite-catalysts reaches maximum values. The main hydrogenation product is 1-phenylethanol, which was confirmed by chromatographic analyses.

This research was funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (Project No. AP23487279).

BEHAVIOR OF ELECTRODEPOSITED SILICON THIN FILM DURING LITHIATION

Leonova A.M., Leonova N.M., Koryakin E.A., Suzdaltsev A.V.

Ural Federal University, 620002, Ekaterinburg, Mira st. 19,
e-mail: a.v.suzdaltsev@urfu.ru

Currently, more and more attention is being paid to the development of energy storage devices with improved performance and higher specific energy density. One of such materials is silicon in the form of nanoscale fibers or thin films.

In the present work, the behavior of thin (3–6 μm) silicon films electrodeposited on a carbon substrate in $\text{LiCl-KCl-CsCl-K}_2\text{SiF}_6$ melt at 550 $^\circ\text{C}$ was studied by cyclic voltammetry, galvanostatic cycling with different currents, electrochemical impedance, and scanning microscopy.

Fig. 1 shows the dependencies of the change in the charging and discharging capacity of the silicon film in the anode half-cell of a lithium-ion current source during the first charge-discharge cycle with a constant current of 0.1C. During charging, the anode potential changed smoothly from 0.6 to 0.05 V (the specified final value), and during discharging, respectively, from 0.05 to 0.9 V, after which it shifted sharply to the region of values more positive than 1.5 V. The discharge capacity was more than 25000 at the first cycle, and during multiple cycling with different currents it decreased to values from 300 to 3795 mAh/g depending on the current (from 0.1C to 2C) with Coulomb efficiency of 99.6–99.8%. This indicates that the lithium-ion current source can be operated even at high charge rates.

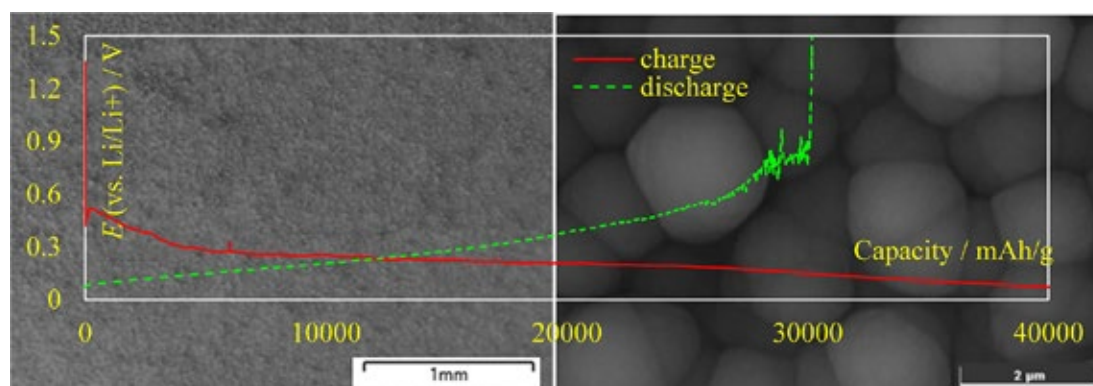


Figure 1. SEM-images and charge-discharge dependencies of the first forming cycle of silicon thin film

This work is performed in the frame of the theme number FEUZ-2020-0037



CATHODE PROCESS IN THE $\text{KF-AlF}_3\text{-Al}_2\text{O}_3\text{-Y}_2\text{O}_3$ MELT

Diallo A.Ou.^a, Suzdaltsev A.V.^{a,b}, Zaikov Yu.P.^{a,b}

^aUral Federal University, 620002, Ekaterinburg, Mira st. 19,
e-mail: a.v.suzdaltsev@urfu.ru

^bInstitute of High-Temperature Electrochemistry UB RAS,
620066, Ekaterinburg, Akademicheskaya st. 20

Aluminium master alloys with rare earth metals (REM) are increasingly used in various fields. One of the promising methods of their production includes electrolysis of oxide-fluoride melt $\text{KF-AlF}_3\text{-Al}_2\text{O}_3$ with the addition of REM oxide. During electrolysis, oxygen or CO_2 is released at the anode, and aluminium and REM at the liquid-metal aluminium cathode.

To determine the parameters of master alloy production by electrolysis, data on the kinetics of the cathodic process in the investigated melt with the addition of REM oxide are required. Such data were obtained in this work at the molybdenum electrode using the cyclic chronovoltammetry method.

Fig. 1 shows typical voltametric dependencies on molybdenum for $\text{KF-AlF}_3\text{-(0.5 wt\%)}\text{Al}_2\text{O}_3$ melt containing 0, 0.5 and 1.0 wt% Y_2O_3 at 790 °C and potential sweep rate of 0.1 V/s. It follows that the addition of Y_2O_3 practically does not affect the mechanism of the investigated process, while it leads to an increase in the cathodic current density. This is due to the more negative potential of yttrium release, as well as the formation of Al_2O_3 during the dissolution of Y_2O_3 in the melt.

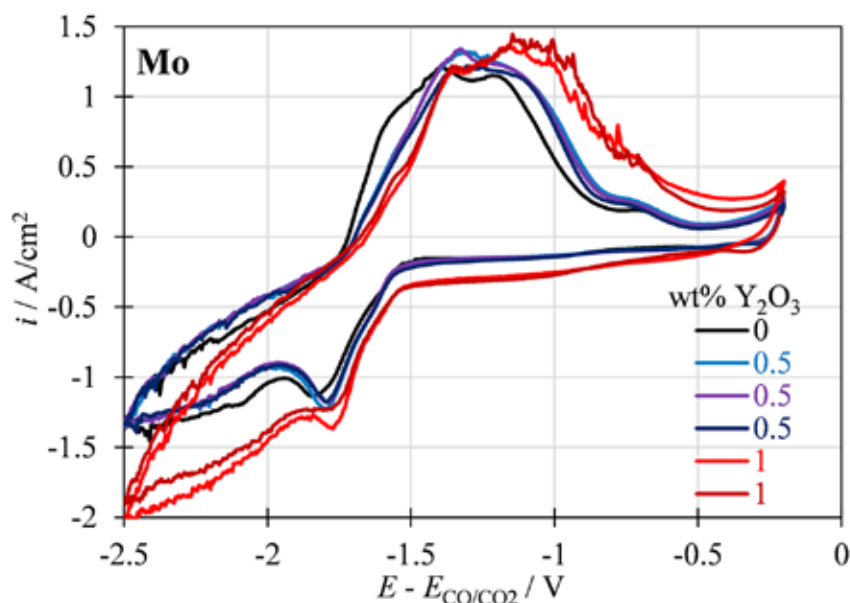


Figure 1. Voltametric dependencies on molybdenum in $\text{KF-AlF}_3\text{-Al}_2\text{O}_3\text{-Y}_2\text{O}_3$ melts at 790 °C and potential sweep rate of 0.1 V/s. Reference electrode – CO/CO_2

IZATINE ELECTROSORPTION ONTO CARBON FIBER

Tsvetnov M.A., Morgun N.P., Kondrikov N.B.

*Far Eastern Federal university,
690922, Russia, city Vladivostok, tn. Ayaks, 10,
e-mail: tsvetnov.ma@dyfu.ru*

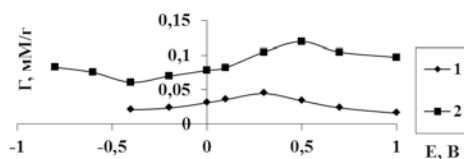
Carbon activated fibers (CAF) more preference at granulated activated carbon (GAC): biggest adsorption capacitance, extension surface, heist kinetic parameters, fasted and uniformly charged.

As adsorbent we use carbon fiber “Aktilen – B”, structural parameters in table.

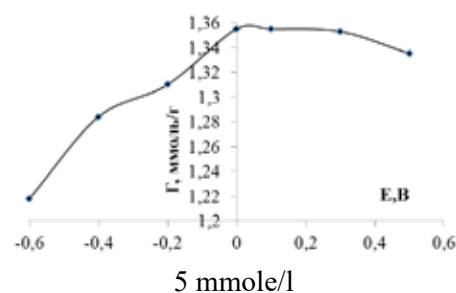
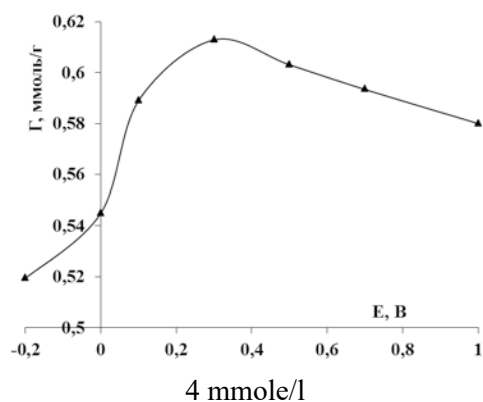
Pore volume, cm ³ /g				r, nm	S _{BET} , m ² /g
V _Σ	V _{mi}	V _{me}	V _{ma}		
0,400	0,400	—	—	0,40	700

As adsorbate was izatine – lactone of izatinic (o-aminephenylglyocsalene) acid.

In picture are relationships: izatine adsorption vs. electric potential of carbon fiber “Aktilen – B” for variety adsorbate concentrations.



1 – 0,2; 2 – 0,5 mmole/l



Electrosorption dependence izatine in dilute solutions are cupola-forms, as theoretic prediction for solid electrode adsorption. With concentration increase sorption maximum become express-less and disappear at concentration solution.

ELECTROCHEMICAL STUDY OF ANTI-CORROSION PROPERTIES OF EXPIRED DRUGS

Tsygankova I.E.^a, Bryksina V.A.^a, Shel N.V.^b, Alekhina O.V.^a

^a*Derzhavin State University,
ul. Internatsyonalnaya, 33, Tambov, 392000,
e-mail: vits21@mail.ru*

^b*Tambov State Technical University,
ul. Sovetskaya, 106, Tambov, 392000*

Indiscriminate disposal of expired and unused drugs, leading to their release into the environment from landfills, wastewater treatment plants, waste from medical institutions and pharmaceutical production, poses a threat to public health and the environment. This leads to contamination of drinking water, destruction of beneficial bacteria and other aquatic organisms. One method to address the problem of inappropriate drug disposal is the possibility of using them to inhibit the corrosion of metals, since their structure is similar to that of target organic corrosion inhibitors. We have studied the anti-corrosion properties of expired omeprazole ((RS)-5-methoxy-2-[(4-methoxy-3,5-dimethylpyridin-2-yl)methylsulfanyl]-1H-benzimidazole) and anaprilin ((RS)-1-isopropylamino-3-(1-naphthoxy)-2-propanol hydrochloride) in relation to St3 steel in 1 N solutions of HCl and H₂SO₄ using impedance spectroscopy and potentiodynamic polarization methods.

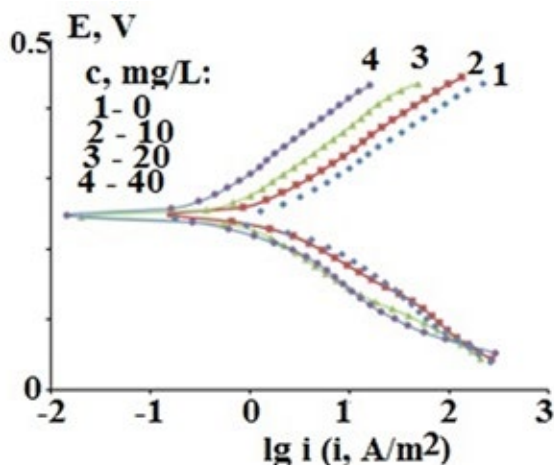


Figure 1

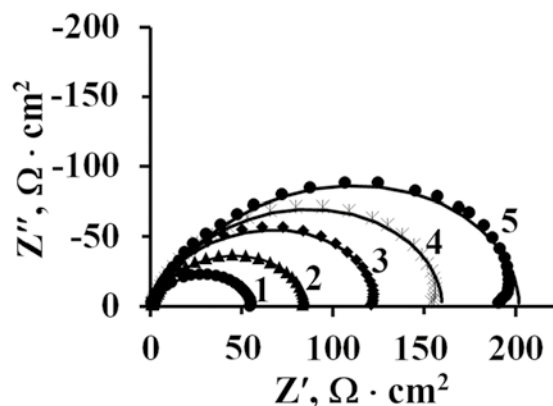


Figure 2

Omeprazole (10–40 mg/L) in HCl solution (Fig. 1) leads to inhibition of anodic and cathodic partial electrode reactions and a decrease in corrosion current. In the Nyquist diagram measured on St3 steel in H₂SO₄ solution, the increase in the diameter of semicircles with increasing concentration of anaprilin (20–80 mg/L) (Fig. 2) indicates an increase in polarization resistance and a decrease in corrosion current. The inhibition coefficient at the maximum concentration of drugs in the solutions of HCl and H₂SO₄ is 12.

ELECTROCHEMICAL PROPERTIES OF RARE EARTH METAL CARBOXYLATES CONTAINING A 2,6-DI-TERT-BUTYL-PHENOL FRAGMENT AND THEIR RELATIONSHIP TO RADIOPROTECTIVE ACTIVITY

Tyurin V.Yu., Nikitin E.A., Moiseeva A.A.

*Lomonosov Moscow State University, Department of Chemistry,
119991, Moscow, Leninskii gory, 1-3,
e-mail: olivecc@mail.ru*

It is known that about 80% of the damage caused by ionizing radiation is due to the indirect effect of radiation and radical processes induced by it. In this regard, the use of antioxidants to protect organs and tissues from damage is a promising strategy. The combination of a redox-active protective organic fragment and a metal with its own physiological activity in one molecule will make it possible to increase the effectiveness of the drug. Lanthanum and cerium carboxylates with a fragment of 2,6-di-*tert*-butylphenol were synthesized, the compounds were characterized by IR spectroscopy, ^1H NMR, ^{13}C and thermogravimetry.

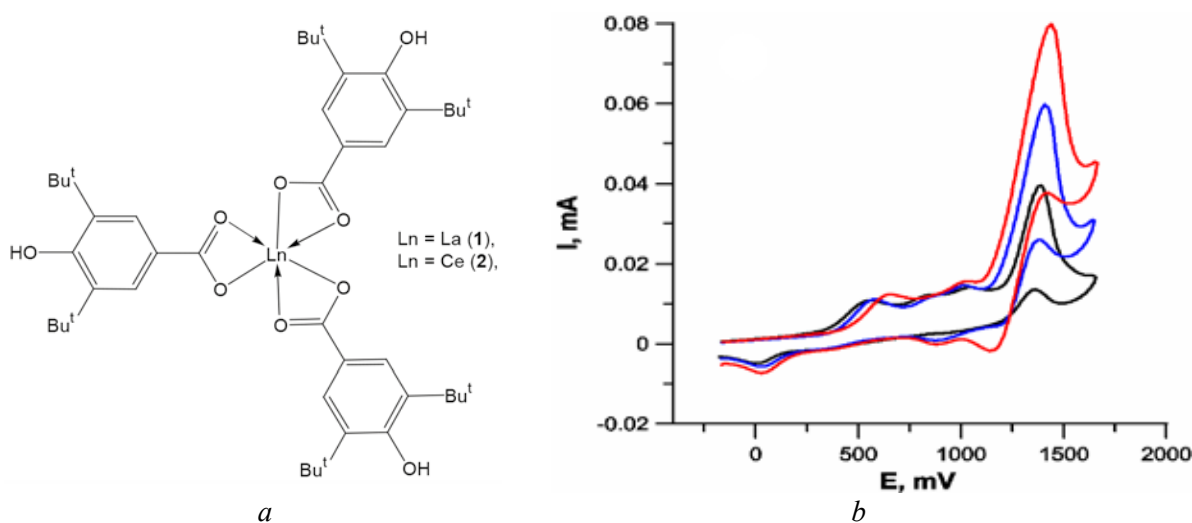


Figure 1. *a* – structural formulas of synthesized compounds,
b – CVA of complex 2 in the presence of *n* mol equivalents of Ce(NO₃)₃,
(*n*=0 – black, *n*=1 – blue, *n*=2 – red)

The electrochemical properties of the complexes were studied using the CVA and RDE methods. Compounds **1** and **2** have been shown to have antioxidant and radioprotective activity, as well as exhibit unusual redox behavior. The proposed scheme of redox transitions allows us to propose a potential mechanism of their activity.

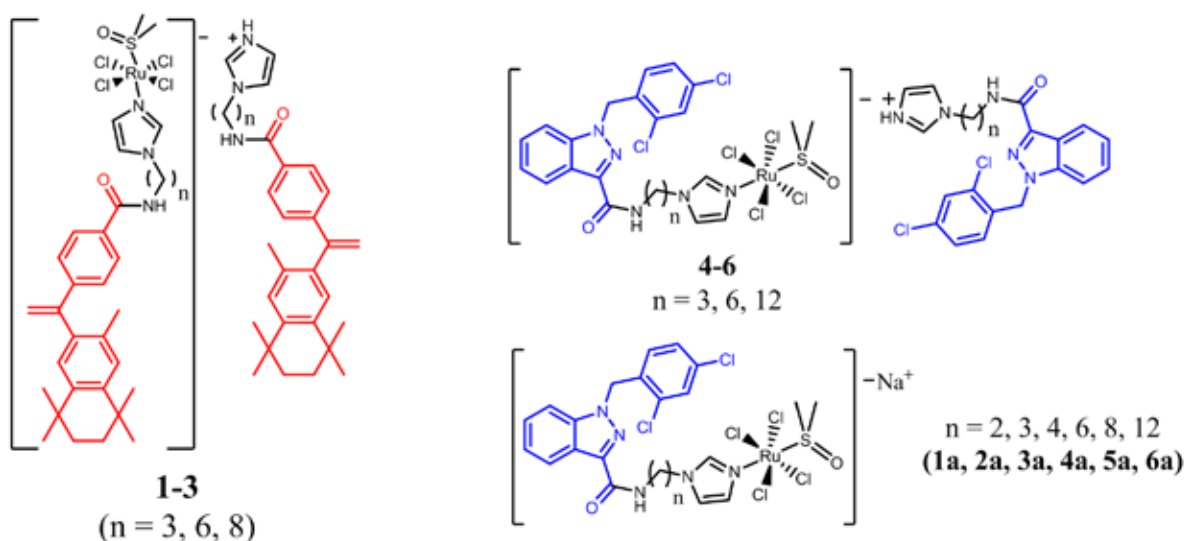
This study was carried out with the financial support of the Russian Science Foundation, project 23-23-10030.

STUDY OF ELECTROCHEMICAL PROPERTIES OF NEW RU(III) COMPLEXES WITH BIOLOGICALLY ACTIVE LIGANDS AND THEIR RELATION TO ANTIPROLIFERATIVE ACTIVITY

Tyurin V.Yu., Shutkov I.A., Antonets A.A., Nazarov A.A., Milaeva E.R.

*Lomonosov Moscow State University, Department of Chemistry,
119991, Moscow, Leninskii gory, 1-3,
e-mail: olivecc@mail.ru*

Ru(III) complexes are promising antitumor agents, the mechanism of action of which is based on the activation process by reducing Ru(III) to Ru(II). The study of the redox properties of ruthenium complexes makes it possible to more accurately assess their potential as anti-cancer drugs. We synthesized new Ru(III) complexes **1–6** and **1a–6a** with biologically active ligands lonidamine, bexarotene and abiraterone. The combination of a cytotoxic metal ion and biologically active fragments in one molecule opens the way to the creation of multitargeted compounds with low overall toxicity.



The electrochemical behavior of complexes **1–6** and **1a–6a** was studied by the CBA method. Schemes of redox transitions are proposed, and potentials for the reduction of Ru(III) to Ru(II) are determined. The obtained data are analyzed on the basis of the Lever equation. The data obtained were compared with the results of biological tests and cytotoxicity data, which allowed us to conclude that the use of these complexes as antiproliferative agents is promising.

ATMOSPHERIC STABILITY OF NANOSTRUCTURED PRODUCTS OF NON-EQUILIBRIUM ELECTROCHEMICAL OXIDATION OF METALS

Usoltseva N.V.

*Tomsk Polytechnic University, Lenin avenue 30, Tomsk, 634050, Russia,
e-mail: usoltseva@tpu.ru*

The increased reactivity of nanomaterials results in their intense interaction with the environment through both physical sorption and chemical transformations at low concentrations of active compounds.

The joint electrochemical oxidation of metals under non-equilibrium conditions is a appropriate way to create some conditions for the formation of dispersed products consisting of several nanostructured phases. Coprecipitation of different metal compounds provides the stabilization of these compounds and intense chemical transformations.

The study of the products of such interaction provides the better understand the patterns of phase formation processes during the electrochemical oxidation of metals. It should be considered that the change in the electrochemical characteristics of the non-equilibrium electrolysis process was identified.

Using the products of joint oxidation of copper and aluminum, it is shown that interaction with atmospheric carbon dioxide leads to the formation of new phases. It is confirmed by X-ray diffraction, thermal analysis and IR spectroscopy.

It has been confirmed that the low content of carbon dioxide in the air (300–450 ppm)¹ provides a sufficient concentration of carbonic acid ions for the formation of compounds containing carbonate ions. This contributes to a shift in the equilibrium of the CO₂ dissolution reaction due to the formation of new phases. Depending on the structure of the electrolysis products, along with layered double hydroxide Cu-Al/LDH², it is possible to form copper hydroxycarbonates – malachite Cu₂(OH)₂CO₃ and azurite Cu₃(OH)₂(-CO₃)₂. In atmospheric conditions malachite is more stable copper hydroxycarbonates and is formed at a lower partial pressure.

The results obtained allow us to consider the products of the joint electrochemical oxidation of copper and aluminum as sorbents both for the identification of compounds and for their removal from gaseous media.

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VOLTAMMETRY OF HYDROXYCINNAMIC ACIDS AT THE ELECTRODES MODIFIED WITH ELECTROPOLYMERIZED DYES

Ziyatdinova G.K., Zhupanova A.S.

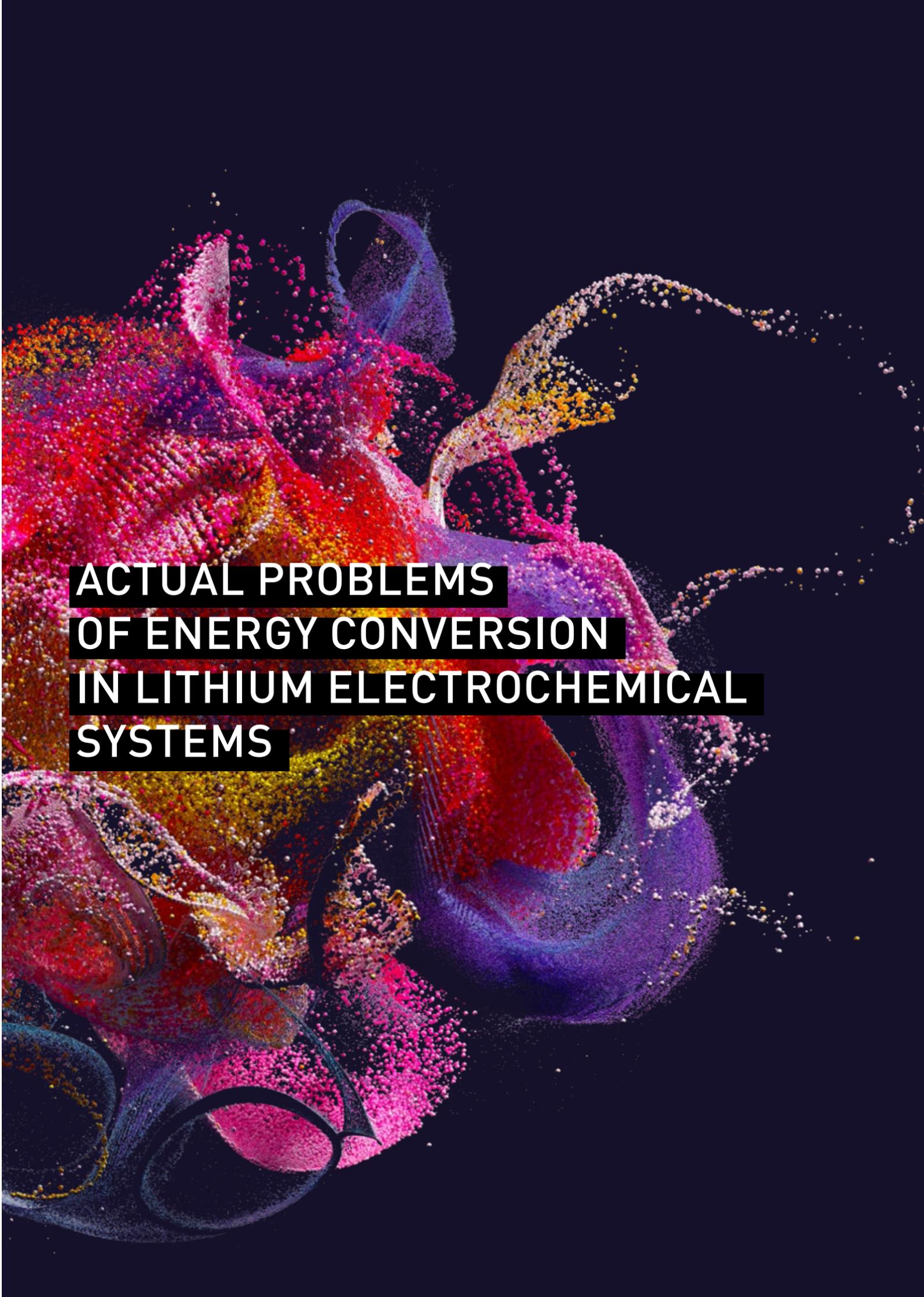
*Kazan Federal University,
Kremleyevskaya 18, Kazan, 420008, Russia,
e-mail: Ziyatdinovag@mail.ru*

Hydroxycinnamic acids (chlorogenic, caffeic, ferulic, and *p*-coumaric) are secondary metabolites of plant origin and the major antioxidants of coffee. Therefore, they are of interest as research objects in electroanalytical chemistry. The voltammetric behavior of chlorogenic, caffeic, ferulic, and *p*-coumaric acids has been studied at glassy carbon electrodes (GCE) modified with carbon nanotubes and electropolymerized dyes.

GCE modification with multi-walled carbon nanotubes and potentiostatically electropolymerized Sunset Yellow FCF provides oxidation potential separation of 190 mV for the chlorogenic and ferulic acids as well as statistically significant increase of the oxidation currents that make possible their simultaneous voltammetric determination. GCE modified with polyaminobenzene sulfonic acid functionalized single-walled carbon nanotubes and potentiodynamically electropolymerized phenol red allows to get sensitive response of caffeic, ferulic, and *p*-coumaric acids when presented simultaneously. The oxidation potential separation of 191 mV has been achieved for both caffeic and ferulic acids, as well as for ferulic and *p*-coumaric acids. The oxidation currents are 4.0–6.6-fold increased compared to those at bare GCE.

Cyclic voltammetry and electrochemical impedance spectroscopy data confirm the increase in the electroactive surface area and electron transfer rate for the polymer-modified electrodes.

The variation of supporting electrolyte pH and potential scan rate has shown that electrooxidation of hydroxycinnamic acids is a diffusion-controlled process involving participation of two electrons and two protons at both modified electrodes. The corresponding *o*-quinones are formed as an oxidation product. Anodic transfer and diffusion coefficients as well as heterogeneous electron transfer rate constants have been calculated.



**ACTUAL PROBLEMS
OF ENERGY CONVERSION
IN LITHIUM ELECTROCHEMICAL
SYSTEMS**

NON-FLAMMABLE GEL ELECTROLYTES BASED ON TRIMETHYL PHOSPHATE FOR POTASSIUM-ION BATTERIES WITH ORGANIC ELECTRODES

Baymuratova G.R.^a, Yarmolenko O.V.^a, Troshin P.A.^{a,b}, Kraevaya O.A.^a

^a *Federal Research Center of Problems of Chemical Physics and Medicinal Chemistry, Russian Academy of Sciences
Academician Semenov avenue, Chernogolovka, Moscow region, 142432 Russian Federation*

e-mail: guzalia.rb@yandex.ru

^b *Zhengzhou Research Institute, Harbin Institute of Technology, Longyuan East 7th 26, Jinshui District, Zhengzhou
450003, China*

This work is aimed at creating gel electrolytes that are highly safe gel electrolytes for potassium-ion batteries that use organic electrodes. The work proposes to use a simple approach to obtain gel electrolytes based on 1 M KPF₆ in a mixture of 1,3-dioxolane/1,2-dimethoxyethane (1:2 by weight) with the introduction of a polymerization initiator of LiPF₆ salt at a concentration of 0.7 M and the addition of trimethyl phosphate (TMP), which increases the safety of batteries.

At the first stage of the work, the physical and chemical properties of gel electrolytes were studied. Using electrochemical impedance spectroscopy, it was shown that the addition of TMF to the electrolyte has virtually no effect on the conductivity - $6 \div 8$ mS/cm at 20°C. It was shown by voltammetry that the upper limit of the window of electrochemical stability of electrolytes is in the range of 4.1-4.5 V.

Thermal analysis showed that the addition of TMF increases the thermal stability of electrolytes. The self-extinguishing time of the electrolytes was assessed using the ignition test. Significant fire-retardant properties were achieved with a gel electrolyte containing 20 vol.% TMF.

At the second stage, testing was carried out on prototype batteries. The use of non-flammable electrolytes made it possible to obtain a high and stable discharge capacity for organic electrode materials (~140-115 mAh/g for 200 cycles at a current density of 35 mA/g). The resulting new fire-resistant gel electrolytes will be able to increase the safety and service life of potassium-ion batteries.

This work was supported by the Ministry of Science and Higher Education of Russian Federation, project no. 122111700046-3 (FFSG-2022-0001, "Laboratory of perspective electrode materials for chemical power sources")

ANODE MATERIAL BASED ON LITHIUM TITANATE DOPED WITH EUROPIUM FOR LITHIUM-ION BATTERIES

Chirkova E.V.,* Kornev P.V., Kulova T.L.

*A.N. Frumkin Institute of Physical Chemistry and Electrochemistry, RAS, Leninsky prospekt 31-4,
Moscow, 119071, Russia,
e-mail: kate.chirkova@yandex.ru*

One of the promising anode materials for lithium-ion batteries is $\text{Li}_4\text{Ti}_5\text{O}_{12}$ with a spinel structure: it provides flat discharge characteristics at an average potential of 1,5 V, while in the processes of intercalation and deintercalation of lithium ions there is practically no deformation of the crystal lattice, which allows the material to withstand tens of thousands of cycles charge-discharge without loss of capacity. One of the disadvantages of lithium titanate is the relatively low theoretical specific capacity (about 175 mAh/g) when cycling in the potential range from 3 to 1,0 V. In this case, with the intercalation of three lithium ions, the average oxidation state of titanium changes from +4 to +3,4. Theoretically, lithium titanate can be reduced to the oxidation state of titanium +3, i.e. it is possible to introduce at least two more lithium ions. In this case, the theoretical specific capacity of lithium titanate will be 290 mAh/g. However, during lithiation in the potential range from 3 to approximately 0,01 V, irreversible structural changes can occur, which will lead to degradation of $\text{Li}_4\text{Ti}_5\text{O}_{12}$ during cycling. Doping $\text{Li}_4\text{Ti}_5\text{O}_{12}$ in certain cases leads to the possibility of reversible intercalation of five lithium ions without irreversible structural changes.

In this work, the processes of lithium insertion/extraction into $\text{Li}_4\text{Ti}_5\text{O}_{12}$ doped with europium at doping degrees from 0,2 to 2,0 wt.% were studied using chronopotentiometry, cyclic voltammetry and impedance spectroscopy. It has been established that the doping of europium helps to accelerate the electrode process and makes it possible to operate such electrodes at loads up to 3200 mA/g (20 C). The optimal range of europium content in $\text{Li}_4\text{Ti}_5\text{O}_{12}$ was determined to be 1,0 – 1,6 wt. %, at which the specific discharge capacity is maximum and is 214 mAh/g at a current density of 20 mA/g and about 50 mAh/g at a current density of 3200 mA/g. It has been established that lithium titanate samples with an optimal degree of doping are characterized by the least degradation during cycling.

This work was supported by the RF Ministry of Science and Higher Education.

TRANSPORT AND ELECTROCHEMICAL PROPERTIES OF SOLVATE IONIC LIQUIDS BASED ON LITHIUM SALTS, LITHIUM POLYSULFIDES AND SULFOLANE

**Savvina A.A., Sheina L.V., Khasanova R.V., Ionina A.M.,
Karaseva E.V., Kolosnitsyn V.S.**

*Ufa Institute of Chemistry Ufa Federal Research Centre
of the Russian Academy of Sciences, 450054, Ufa, Oktyabrya Avenue, 69
e-mail: asavvina@gmail.com*

Solvate ionic liquids (SILs) based on aprotic dipolar solvents (ADSs) and lithium salts are a new type of electrolyte systems for high energy electrochemical energy storage devices. By their chemical nature, SILs are solvate complexes of lithium salts. Unlike solutions of lithium salts in ADSs, solvate ionic liquids have higher electrochemical stability and safety, which allows their application in high energy batteries with lithium metal electrode and active materials of positive electrodes based on elemental sulfur¹ and high-potential transition metal oxides². Sulfolane-based solvate ionic liquids are of particular interest. Sulfolane is a highly polar solvent, dissolves lithium salts well and forms solutions with high mobility of lithium cation.

The report summarizes the results of studies of composition, physico-chemical and electrochemical properties (ion conductivity, lithium cation transfer numbers, lithium metal electrode and lithium-sulfur cell cyclability) of lithium polysulfide solutions with various length in solvate complexes of sulfolane with lithium perchlorate and lithium bis(trifluoromethanesulfonyl)imide. It is shown that sulfolane-based SILs are promising electrolytes for lithium-sulfur batteries.

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The work was financially supported by the Russian Foundation for Basic Research, project No. 21-53-46005 and within the framework of the state assignment on topic No. 122031400252-2 "Electrode materials and electrolyte systems for advanced energy storage devices".

ANODE MATERIAL BASED ON Ge-Co-In NANOSTRUCTURES FOR LITHIUM-ION BATTERIES

Kovtushenko E.V.,* Gavrilin I.M., Kudryashova Y.O., Li S.A., Kulova T.L.

*A.N. Frumkin Institute of Physical Chemistry and Electrochemistry,
RAS, Leninsky prospekt 31-4, Moscow, 119071, Russia,
e-mail: jeny4880523@gmail.com*

Lithium-ion batteries are currently the most versatile current sources, the modernization of which is mainly aimed at increasing practical energy consumption, reducing irreversible capacity losses, improving cyclic stability and the ability to operate at low temperatures.

In this paper, the electrochemical behavior over a wide temperature range of Ge-Co-In nanostructures obtained by electrochemical cathode deposition from an aqueous solution with the addition of germanium dioxide and cobalt sulfate will be considered. The morphology and elemental composition of the obtained samples were characterized by SEM, TEM, energy-dispersive X-ray and X-ray diffraction analysis¹.

Measurements of the specific capacity of the samples were carried out in galvanostatic and potentiodynamic modes in three-electrode cells containing a working electrode (Ge-Co-In), an auxiliary electrode and a reference electrode (lithium metal rolled onto a stainless-steel grid). ¹ M LiClO₄ in a propylene carbonate – dimethoxyethane mixture (7:3) was used as the electrolyte. The amount of water in the electrolyte did not exceed 20 ppm. The average loading of the nanostructures was about 0.1 mg/cm².

The Ge-Co-In electrode (theoretical specific capacity is equal to 1440 mAh/g) demonstrated a specific capacity reaching 1360 mAh/g at +20 °C and 826 mAh/g at -35 °C at a current density of 180 mA/g (C/8), as well as good cyclic stability with degradation of no more than 0.04% per cycle. The material based is promising for negative electrodes of lithium-ion batteries.

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This work was supported by a grant from Russian Science Foundation No 20-79-10312, <https://rscf.ru/en/project/20-79-10312/>

FEATURES OF SOLID ELECTROLYTES POWDERS CONSOLIDATION WITH LITHIUM-ION CONDUCTIVITY BY SPARK PLASMA SINTERING

Kunshina G.B., Bocharova I.V., Tananaev I.G.

*Tananaev Institute of Chemistry - Subdivision of the Federal Research
Centre "Kola Science Centre of the Russian Academy of Sciences",
184209, Apatity, Akademgorodok 26a
e-mail: g.kunshina@ksc.ru*

The spark plasma sintering (SPS) method is a global trend in the field of creating modern ceramic materials for functional purposes. The advantages of the SPS method can be used in the manufacture of solid-electrolyte membrane separators, composite electrodes and in the assembly of prototypes of all solid-state lithium-ion batteries¹.

Monophase powders of lithium-conducting solid electrolytes of the composition $\text{Li}_{1.3}\text{Al}_{0.3}\text{Ti}_{1.7}(\text{PO}_4)_3$ with NASICON structure, as well as Al and Ta-substituted $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ with the garnet structure, were synthesized in accordance with previous works²⁻³. The subsequent consolidation of powders by SPS method was carried out at the Spark Plasma Sintering System SPS-515S installation (Dr.Sinter-LABTM, Japan). Powders and sintered ceramics were studied by X-ray phase analysis, scanning electron microscopy, electrochemical impedance spectroscopy and potentiostatic chronoamperometry.

It was found that during the SPS process there is no change in the phase composition of the samples and the formation of non-conductive impurity phases. The lattice parameters of cubic Al-substituted $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ ($a = b = c = 12.96052\text{\AA}$ and $\alpha = \beta = \gamma = 90.00^\circ$) with the symmetry of the $Ia\bar{3}d$ space group were calculated by the method of full-profile analysis of radiographs. The values of the WPPF parameters, usually used to assess the quality of the profile fit ($R_p = 3.04\%$, $R_{wp} = 4.13\%$ and $\chi^2 = 2.1934$), confirm the good quality of the results obtained. A distinctive feature of the pellets of Al and Ta-substituted $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ consolidated by the SPS method is increased stability in air. High total ionic conductivity ($\sigma_{\text{total}} = 4 \cdot 10^{-4} \text{ S/cm}$) and negligibly electron conductivity ($\sim 2 \cdot 10^{-9} \text{ S/cm}$) is achieved for samples with a maximum density (97-98%).

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STUDY OF ELECTROCHEMICAL PROPERTIES OF SOLID ELECTROLYTES BY ELECTROCHEMICAL IMPEDANCE SPECTROSCOPY METHODS

Kuzmina E.V., Kolosnitsyn D.V., Pilyugina Yu.A., Kolosnitsyn V.S.

*Ufa Institute of Chemistry
Ufa Federal Research Centre RAS, Ufa,
e-mail: kuzmina@anrb.ru , dkolosnitsyn@gmail.com ,*

An actual task in the field of creating a new generation of electrochemical energy storage devices is the development of all-solid-state batteries. One of the most promising solid electrolytes are solid sulfide electrolytes, since they have high ionic conductivity and the ability to operate at high current in a wide temperature range.

The most informative method for studying the structure of an electrochemical system is spectroscopy of electrochemical impedance (SEI). Using functions of Distribution of Relaxation Times (DRT) allows to objectively estimate the number of phase separations present in the electrochemical system and evaluate their parameters.

In the presented work, symmetrical lithium-lithium cells with a solid sulfide electrolyte were studied using the SEI method. SEI analysis was performed using DRT functions.

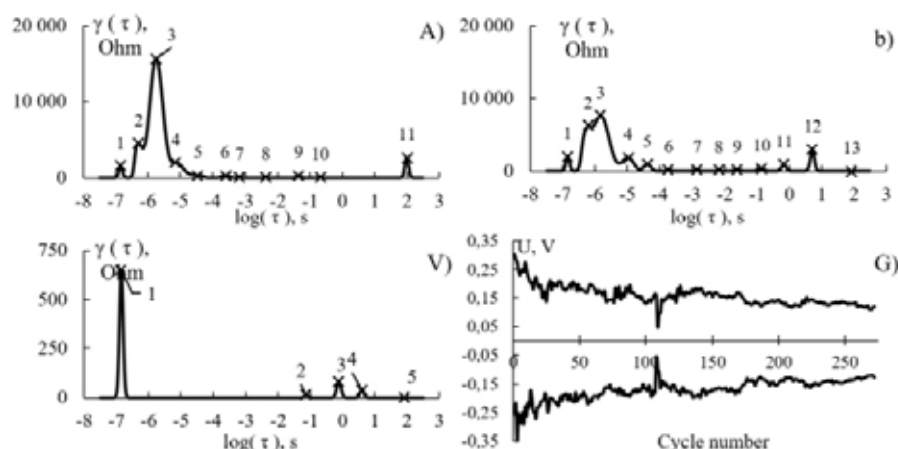


Fig. 1. Evolution of the DRT functions of a symmetrical Li - Li cell with a solid sulfide electrolyte during storage (a - after assembly and b - after 2 months' storage), and after 20 cycles of cathode-anode polarization (c), the average overvoltage on the cell during the polarization process (d)

COMPOSITE CATHODE BASED ON SULFUR AND MICROPOROUS CARBON FOR LI-S BATTERIES

Novikova S.A., Voropaeva D. Y., Stenina I.A., Yaroslavtsev A.B.

*Kurnakov Institute of General and Inorganic Chemistry, Russian Academy of Sciences,
31 Leninsky av., Moscow, 119991, Russia
e-mail: novikova@igic.ras.ru*

Li-S batteries are considered as a promising alternative for lithium-ion batteries due to their high specific energy and low cost of sulfur-based cathodes. The practical application of Li-S batteries is limited by several issues including the safety, low electrical conductivity of sulfur and the discharge products, a significant volume change of the cathode during the charge/discharge processes, formation of polysulfides (Li_2S_n , $n = 4-8$) soluble in the electrolyte and their migration towards the anode (shuttling) with subsequent irreversible reactions leading to the loss of active material. One of the main challenge is to eliminate shuttling of polysulfides. A promising approach is to obtain composites based on sulfur and meso- and/or microporous carbons with a hierarchical porous structure capable of both providing electron transfer and encapsulating sulfur, suppressing the dissolution and migration of polysulfides¹.

In this work, a new cathode material for lithium-sulfur (Li-S) batteries was developed. Microporous carbon (with predominant pore size ≤ 1.2 nm) served as both a matrix for sulfur retention and conductive additive. Microporous carbon was shown to be capable of adsorbing lithium polysulfides thereby suppressing their migration toward lithium anode. The discharge capacity of the S/C composite at the 1st and 20th cycles in Li-S battery operation was 513 and 421 $\text{mAh}\cdot\text{g}^{-1}$ at a scan rate of 0.1 mV s^{-1} .

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Funding: This work was financially supported by the Russian Science Foundation, grant No 23-19-00642, <https://rscf.ru/project/23-19-00642/>.

A NEW APPROACH TO THE SYNTHESIS OF HIGHLY EFFICIENT CATHODE MATERIALS FOR LITHIUM-ION BATTERIES

Zharov N.V., Maslova M.V.

*I.V. Tananaev Institute of Chemistry and Technology of Rare Elements and Mineral Raw Materials of the Russian Academy of Sciences Kola Science Center, 184209, Apatity, Akademgorodok 26a,
e-mail: n.zharov@ksc.ru*

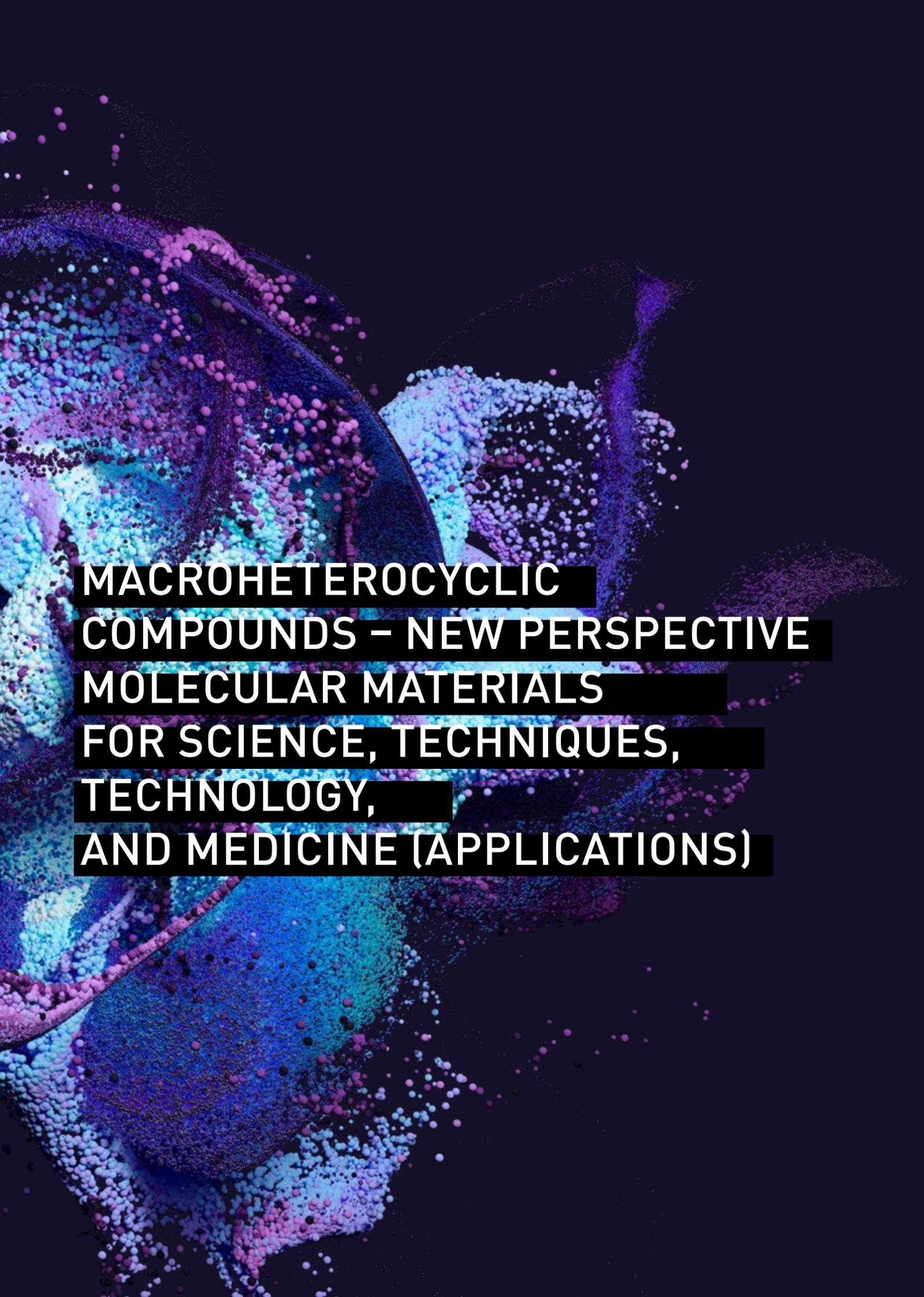
An industrially scalable technology for producing high-quality cathode materials of lithium-ion batteries in a low-temperature salt melt has been developed at ICT KSC RAS1. The developed methodology includes two stages. At the first stage, the synthesis of the $\text{NH}_4\text{MPO}_4 \cdot n\text{H}_2\text{O}$ precursor ($\text{M} = \text{Mn}, \text{Co}, \text{Ni}$, etc.) with controlled morphology and dispersion is carried out. At the second stage, the synthesis of the target LiMPO_4 material is carried out by ion exchange substitution of $\text{NH}_4\text{-Li}$ in a salt melt of lithium nitrate with intensive stirring. In this case, the morphology of the precursor used determines the morphology of the target material¹.

The proposed approach makes it possible to obtain a wide range of cathode materials based on lithium double phosphates and LiMPO_4 transition metal with improved electrochemical characteristics in a short time without the use of expensive precursors and complex hardware design². The advantages of the technology include: low waste, fast synthesis, energy efficiency, environmental friendliness.

The high quality of the resulting product is ensured by the possibility of obtaining both individual and doped highly dispersed composite materials with a core/shell structure with a designed morphology³ and a near-zero degree of cationic disordering. The LiCoPO_4 thus obtained exhibits electrochemical characteristics exceeding most of the world's known analogues (discharge capacity of the first and fiftieth 142 mAh/g and 120 mAh/g, respectively, at a charge/discharge rate of 1C).

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**MACROHETEROCYCLIC
COMPOUNDS – NEW PERSPECTIVE
MOLECULAR MATERIALS
FOR SCIENCE, TECHNIQUES,
TECHNOLOGY,
AND MEDICINE (APPLICATIONS)**

OXIDATION OF 4-METHYLPYRIDINE ON VANADIUM-IRON-OXIDE CATALYST: EFFICIENCY AND KINETICS

Buzayev N.A.,^{a,b} Kadirbekov K.A.^{a,b}

^a *A.B. Bekturov Institute of Chemical Sciences, Sh. Ualikhanov str., 106, Almaty, 050010, Kazakhstan,
e-mail: buzayev.n@gmail.com*

^b *Al-Farabi Kazakh National University, 71 al-Farabi Ave., Almaty, 050040, Kazakhstan*

The vapour-phase oxidation of organic compounds is a pivotal industrial process for synthesizing valuable chemical products such as aldehydes, ketones, and carboxylic acids.¹ Transition metal-based catalysts, particularly those containing vanadium and iron, have emerged as effective agents in facilitating this reaction.² Among these, the V_2O_5 - Fe_2O_3 catalyst stands out for its high activity and stability, especially in the oxidation of aromatic amines.³

Despite these extensive studies, there remains a lack of consensus on the reaction mechanism, the active centers of the catalyst, the interaction between 4-picoline and the catalyst, and the factors determining the selectivity of formation of different products.⁴⁻⁵ In light of this, the present work aims to study the effect of temperature and air feed rate on the vapour-phase oxidation of 4-methylpyridine over V_2O_5 - Fe_2O_3 . The findings of this study will contribute to the existing body of knowledge and potentially provide insights into the optimization of the vapour-phase oxidation process. This could lead to more efficient production of valuable products, thereby having significant implications for the chemical industry.

A series of experiments have been carried out to observe the effects of varying temperature and air feed rates on the catalytic process. Preliminary findings suggest that both temperature and air feed rate significantly impact the oxidation process, influencing the selectivity and yield of desired products. The data indicate potential pathways for optimizing the reaction conditions to enhance the efficiency and selectivity of the V_2O_5 - Fe_2O_3 catalyst.

PTF “Innovative methods of synthesis and technologies for obtaining functional inorganic and organic substances and materials from natural and man-made raw materials” BR18574042 (2022-2024)

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CHLOROPHYLL POLYMERIC FORMS OBTAINING AND STUDY OF THEIR ANTIMICROBIAL PROPERTIES

**Chesnokova I.P.^{a,b}, Gruznova O.A.^b, Gruznov D.V.^c, Popov N.I.^c, Shcherbakova G.S.^c,
Shuteeva E.N.^c, Konyashkina A.V.^c, Lobanov A.V.^{b,d}**

^a MIREA – Russian Technological University, Vernadsky avenue 86, Moscow, 119454, Russia,
e-mail: chesnokkova-irishka@mail.ru

^b Semenov Federal Research Center for Chemical Physics, RAS, Kosygina street 4, Moscow, 119991, Russia

^c All-Russian Research Institute of Veterinary Sanitation, Hygiene and Ecology – Branch of Federal State Budget Scientific Institution “Federal Scientific Center – K.I. Skryabin, Ya.R. Kovalenko All-Russian Research Institute of Experimental Veterinary Medicine”, RAS, Zvenigorodskoe highway 5, Moscow, 123022, Russia

^d Moscow Pedagogical State University, Vernadsky avenue 88, Moscow, 119991, Russia

Due to the increasing number of antimicrobial-resistant microorganism strains, both the development of new drugs and the use of alternative approaches, such as photodynamic and light-independent therapy, are urgent tasks.¹ Metalloporphyrins, in particular chlorophyll, have found wide application in these areas.^{2,3} Incorporation of metalloporphyrins into polymeric matrices is able to increase the bioavailability of these compounds.⁴

This work presents the results of evaluation of the antibacterial activity of chlorophyll aggregated into polymeric matrices of poly-N-vinylpyrrolidone (PVP) and polylactide (PLA) against Gram-positive microorganisms (*S. aureus*, strain 209-P). To prepare polymeric forms, 10% (wt.%) solutions of polymers and chlorophyll solutions with concentration of 0.1 to 0.5% relative to the weight of the polymers were used. The resulting solutions were mixed in a ratio of 1:1 (v/v).

According to the study results, both free and polymeric forms of chlorophyll had antibacterial effect on the growth of *S. aureus* at a dosage of 15 µg, and dosages up to 75 µg showed bacteriostatic action, and 75 µg – bactericidal action. In addition, the polymeric forms had a prolonged effect. The data obtained can be used in the development of antibacterial agents against staphylococcal infections.

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PHTHALOCYANINATOCLATHROCHELATES AS NOVEL AND EFFECTIVE (PHOTO)CATALYSTS OF OXIDATION AND POLYMERIZATION PROCESSES

**Dudkin S.V.,^a Polivanovskaya D.A.,^b Belova S.A.,^a Birin K.P.,^b
Tsivadze A.Yu.,^b Voloshin Y.Z.^{a,c}**

^a A.N. Nesmeyanov Institute of Organoelement Compounds, RAS, Vavilova str. 28, bld. 1, Moscow, 119334, Russia,
e-mail: sdudkin@ineos.ac.ru

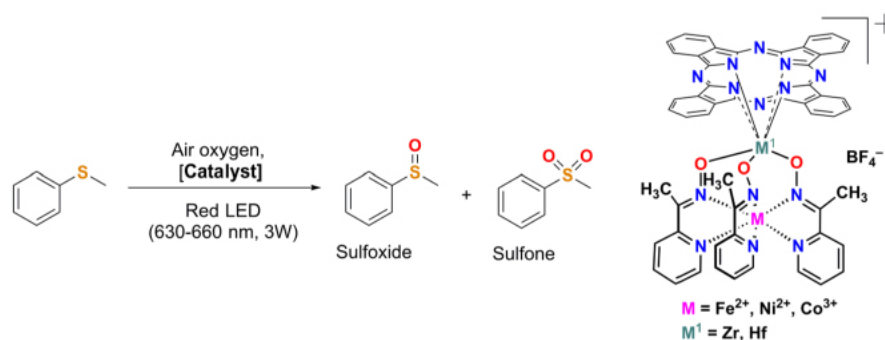
^b A.N. Frumkin Institute of Physical Chemistry and Electrochemistry, RAS,
Leninsky prospect 31, bld. 4, Moscow, 119071, Russia

^c N.S. Kurnakov Institute of General and Inorganic Chemistry, RAS, Leninsky prospect 31,
Moscow, 119071, Russia

Cage metal complexes and their tetrapyrrolic-containing derivatives are prospective, chemically robust, three-dimensional molecular platforms and macrobicyclic building blocks for the design of new types of (photo)catalysts, modern functional materials and prodrugs as well.^{1,2}

Earlier³ we found that the metal(IV)-phthalocyaninato-capped iron, nickel(II) and cobalt(III) clathrochelates are effective catalysts of the radical polymerization of vinyl monomers allowing to regulate a course of their reaction and to affect the properties of thus obtained polymer products. They are also effective catalysts of cyclohexane oxidation into KA-oil.⁴

There we report a photocatalytic oxidation of thioanisole in the presence of the phthalocyaninato-capped iron, nickel(II) and cobalt(III) tris-pyridineoximates (Scheme 1).



Scheme 1

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This work was supported by the Russian Science Foundation (project 24-23-00323)



INHIBITORY EFFECT OF HEMIN IN FREE AND POLYMERIC FORMS AGAINST GRAM-POSITIVE AND GRAM-NEGATIVE MICROORGANISMS

Plaksina L.F.,^a Gruznova O.A.,^b Zhdanova K.A.,^a Gruznov D.V.,^c Popov N.I.,^c
Shcherbakova G.Sh.,^c Shuteeva E.N.,^c Konyashkina A.V.,^c Lobanov A.V.^{b,d}

^a MIREA – Russian Technological University, Vernadsky avenue 86, Moscow, 119454, Russia,
e-mail: plaksinaliliaf@mail.ru

^b Semenov Federal Research Center for Chemical Physics, RAS, Kosygina street 4, Moscow, 119991, Russia

^c All-Russian Research Institute of Veterinary Sanitation, Hygiene and Ecology – Branch of Federal State Budget Scientific Institution “Federal Scientific Center – K.I. Skryabin, Ya.R. Kovalenko All-Russian Research Institute of Experimental Veterinary Medicine”, RAS, Zvenigorodskoe highway 5, Moscow, 123022, Russia

^d Moscow Pedagogical State University, Vernadsky avenue 88, Moscow, 119991, Russia

Compounds of natural and synthetic porphyrins have been successfully used in pharmacology for many years.¹ Hemin is one of the best known representatives of this class.² To increase the effectiveness of porphyrins, they are included in the matrix of a polymeric carrier, for example, poly-*N*-vinylpyrrolidone (PVP).³ The purpose of this work is to study the inhibitory effect of hemin, both in free and polymeric form.

The polymeric form was prepared by mixing (1:1 v/v) 6% aqueous solution of PVP (wt%) and hemin solutions prepared in DMSO at concentrations ranging from 40 to 320 µg/mL. Microbiological studies were carried out on gram-positive (*S. aureus*, strain 209-P) and gram-negative (*E. coli*, strain 1257) microorganisms in accordance with generally accepted methods.

It was found that hemin in free form and polymeric form had an inhibitory effect on the growth of *S. aureus*, starting from a dosage of 20 µg, and on the growth of *E. coli* – from 40 µg. At the same time, hemin-PVP had higher activity and duration of action compared to the free substance. Thus, hemin-PVP has potential for use as an alternative antimicrobial agent.

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SYNTHESIS OF PHENYL(METHYL)OLIGOSILOXANES

Klimova N.V., Ivanov A.G., Natsyuk S.N.

State Scientific Center of the Russian Federation JSC "GNIChTEOS"

Moscow, sh. Entuziastov highway, 38

e-mail: nk20160412@gmail.com

A low-cost, technologically simple method, meeting the requirements of “green chemistry,” has been developed for the production of di-, tri- and oligo-phenyl(methyl)siloxanes by reacting phenyl(methyl)hydridesilanes with alkoxy- and hydroxyphenyl(methyl)silanes and -siloxanes using tris(pentafluorophenyl)borane as a catalyst¹ according to the scheme:



Previously used hydrolytic polycondensation in the presence of strong bases and a solvent made it possible to obtain oligosiloxanes in low yield. In the case of tris(pentafluorophenyl)borane, the yield of the target products according to equation (1) was 90-98%. The composition and structure of the obtained compounds were confirmed by ¹H and ²⁹Si NMR spectroscopy.

The catalyst did not undergo any changes and, after being precipitated from the reaction mass with cold hexane, it can be used repeatedly.

Using the above method, products such as methyl (phenyl) disiloxanes, PhM-1, PhM-2, PPhMS liquids with different lengths of the siloxane chain, etc. were prepared.

The main areas of application of phenylmethylsiloxane liquids are determined due to their qualities such as high resistance and low vapor pressure at high temperatures. Therefore, they are used as, for example, working fluids of steam-oil diffusion pumps to create a deep vacuum (residual pressure 10⁻¹⁰÷10⁻¹³ mm Hg), in microelectronics and as the main coolant of planetary megawatt nuclear reactors.

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PHOTOCYCLOADDITION OF STYRYL DYES IN SOLUTION, SOLID AND GELS. PRE-ORGANIZATION WITH CAVITANDS

**Lobova N.A.,^{a,b} Kondratenko A.D.,^{a,b} Medvedeva A.A.,^{a,b} Aleksandrova N.A.,^a
Vedernikov A.I.^a**

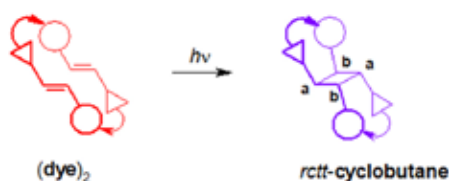
^a NRC "Kurchatov Institute," Moscow, Russia

^b Moscow Institute of Physics and Technology (MIPT), Dolgoprudny, Russia

e-mail: lobova_n_a@mail.ru

The PCA reaction is one of the most interesting reactions in photochemistry and has great potential for the creation of new materials. Styryl dyes have a D- π -A structure and are capable of entering into the PCA-reaction with the formation of cyclobutane derivatives. This reaction can be conveniently observed by electron spectroscopy and NMR.^{1,2}

The aim of our work was to identify the structural factors affecting the control of the [2+2] PCA- reaction of styryl dyes in organic solvents and water, in the presence of cavitands, in the solid phase and in gels.



Multiple non-covalent interactions in a non-competitive environment, a cavitand molecule in a competitive environment, a molecular crystal cell or a biocompatible gel can be used as a pre-organizing factor. The type of photoproduct obtained depends on the preorganizing factor and the type of intermolecular dimer, respectively. During the photoreaction process, interesting phenomena are observed: the preservation of a single crystal cell during the transformation of the molecular structure, the catalytic effect of the presence of cavitand. Reaction yields can reach quantitative values.

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ИНГИБИРУЮЩЕЕ ДЕЙСТВИЕ ГЕМИНА В СВОБОДНОЙ И ПОЛИМЕРНОЙ ФОРМАХ В ОТНОШЕНИИ ГРАМПОЛОЖИТЕЛЬНЫХ И ГРАМОТРИЦАТЕЛЬНЫХ МИКРООРГАНИЗМОВ

**Плаксына Л.Ф.,^а Грузнова О.А.,^б Жданова К.А.,^а Грузнов Д.В.,^в
Попов Н.И.,^в Щербакова Г.Ш.,^в Шутеева Е.Н.,^в Коняшкина А.В.,^в
Лобанов А.В.^{б,г}**

^а ФГБОУ ВО «МИРЭА – Российский технологический университет», 119454, Москва, пр. Вернадского, 86
e-mail: plaksinaliliaf@mail.ru

^б ФГБУН ФИЦ химической физики им. Н.Н. Семенова Российской Академии наук,
119991, Москва, ул. Косыгина, 4

^в ВНИИВСГЭ – филиал ФГБНУ ФНЦ ВИЭВ Российской Академии наук,
123022, Москва, Звенигородское ш., 5

^г ФГБОУ ВО «Московский педагогический государственный университет»,
119991, Москва, пр. Вернадского, 88

Соединения природных и синтетических порфиринов на протяжении многих лет успешно применяются в фармакологии¹. Один из наиболее известных представителей этого класса – гемин². Для повышения эффективности порфиринов используют включение их в матрицу полимерного носителя, например – поли-*N*-винилпирролидона (ПВП)³. Цель работы – изучение ингибирующего действия гемина, как в свободной форме, так и в составе полимерной матрицы ПВП.

Полимерную форму получали путем смешивания (1:1 об./об.) 6% водного раствора ПВП (мас.%) и растворов гемина, приготовленных в ДМСО в концентрациях от 40 до 320 мкг/мл. Микробиологические исследования проводили на грамположительных (*S. aureus*, штамм 209-P) и грамотрицательных (*E. coli*, штамм 1257) микроорганизмах в соответствии с общепринятыми методиками.

Было установлено, что гемин в свободной форме и в составе ПВП оказывал ингибирующее действие на рост *S. aureus*, начиная с дозировки 20 мкг, а на рост *E. coli* – с 40 мкг. При этом, гемин-ПВП обладал более высокой активностью и продолжительностью действия по сравнению со свободной субстанцией. Таким образом, гемин-ПВП имеет перспективу использования в качестве альтернативного антимикробного средства.

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ПОЛУЧЕНИЕ ПОЛИМЕРНЫХ ФОРМ ХЛОРОФИЛЛА И ИЗУЧЕНИЕ ИХ АНТИМИКРОБНЫХ СВОЙСТВ

**Чеснокова И.П.,^{а,б} Грузнова О.А.,^б Грузнов Д.В.,^в Попов Н.И.,^в
Щербакова Г.Ш.,^в Шутеева Е.Н.,^в Коняшкина А.В.,^в Лобанов А.В.^{б,г}**

^а ФГБОУ ВО «МИРЭА – Российский технологический университет»,

119454, Москва, пр. Вернадского, 86, e-mail: chesnokkova-irishka@mail.ru

^б ФГБУН ФИЦ химической физики им. Н.Н. Семенова Российской Академии наук,

119991, Москва, ул. Косыгина, 4

^в ВНИИВСГЭ – филиал ФГБНУ ФНЦ ВИЭВ Российской Академии наук,

123022, Москва, Звенигородское ш., 5

^г ФГБОУ ВО «Московский педагогический государственный университет»,

119991, Москва, пр. Вернадского, 88

В связи с увеличением числа штаммов микроорганизмов, устойчивых к антимикробным препаратам, актуальными задачами являются как разработка новых лекарственных средств, так и использование альтернативных подходов, таких как фотодинамическая и светонезависимая терапии¹. Широкое применение в этих областях нашли металлопорфирины, в частности, – хлорофилл^{2,3}. Включение металлопорфиринов в полимерные матрицы способно повышать биодоступность этих соединений⁴. В работе представлены результаты оценки антибактериальной активности хлорофилла, агрегированного в полимерные матрицы поли-*N*-винилпирролидона (ПВП) и полилактида (ПЛА), в отношении грамположительных микроорганизмов (*S. aureus*, штамм 209-P). Для приготовления полимерных форм использовали 10% (мас.%) растворы полимеров и растворы хлорофилла с концентрацией от 0.1 до 0.5% относительно массы полимеров. Полученные растворы смешивали в соотношении 1:1 (об./об.).

По результатам исследования, как свободная, так и полимерные формы хлорофилла, оказывали антибактериальное действие на рост *S. aureus* в дозировке от 15 мкг, причем дозировки до 75 мкг проявили бактериостатическое, а 75 мкг – бактерицидное действие. Кроме того, полимерные формы обладали пролонгированным действием. Полученные данные могут быть использованы при разработке антибактериальных средств против стафилококковых инфекций.

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SYMPOSIUM ON NUCLEAR CHEMISTRY (BRICS+)

SORPTION CONCENTRATION AND DETERMINATION OF RADIONUCLIDES IN THE MARINE ENVIRONMENT

**Bezhin N.A.^a, Kozlovskaya O.N.^a, Shibetskaia I.G.^a,
Razina V.A.^a, Tananaev I.G.^{a,b}**

^a*Sevastopol State University,
Universitetskaya Street 33, Sevastopol, 299053, Russia,
e-mail: nickbezhin@yandex.ru*

^b*I.V. Tananaev Institute of Chemistry and Technology of Rare Elements
and Mineral Raw Materials, Kola Science Centre, RAS,
Akademgorodok 26a, Apatity, 184209, Russia*

Determination of radionuclide activity values in seawater and suspended matter is used for radioecological monitoring (¹³⁷Cs, ⁹⁰Sr), study of vertical transport processes (⁷Be), determination of sedimentation parameters and suspended matter fluxes (²¹⁰Pb, ²¹⁰Po, ²³⁴Th), assessment of phosphorus biodynamics parameters (³²P, ³³P) and submarine groundwater discharge (²²⁶Ra, ²²⁸Ra). Therefore, we have developed a set of methodological solutions for determining artificial, natural and cosmogenic radionuclides in the marine environment to solve practical problems.

Using the developed approaches, a number of important problems were solved: for the first time, the vertical profiles of ³²P, ³³P and ²²⁸Ra activity and the spatial variability of ²¹⁰Pb and ²²⁸Ra concentrations in the Black Sea were determined;¹ the fluxes of submarine groundwater discharge at Cape Aya were also first assessed using ²²⁶Ra and ²²⁸Ra, and the possibility of using this source as a potential source of fresh water was established;² indicators of sedimentation of suspended matter from the surface layer of the Black Sea were determined based on the imbalance of ²¹⁰Pb/²¹⁰Po and ²³⁸U/²³⁴Th pairs, and the possibility of their use as indicators of the ecological state of the region under study was shown; the seasonal variability of phosphorus biodynamic parameters in the waters of the Heracleon Peninsula was first studied using ³²P and ³³P, and an increased anthropogenic load in the study region was established.³

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The work was carried out with the financial support of Sevastopol State University, project 42-01-09/253/2023-2.



HYDROTHERMAL DECOMPOSITION OF “KU 2-8” ION EXCHANGE RESIN

Golub A.V., Matskevich A.I., Egorin A.M.

*Institute of Chemistry, Far Eastern Branch, Russian Academy of Sciences,
159, Prosp. 100-letiya Vladivostoka, Vladivostok 690022, Russia,
e-mail: mysmatskevich@mail.ru*

Ion exchange resins are widely used as part of systems at nuclear power plants that regulate the water-chemical regime of the first and second circuits, aftertreatment of condensate from evaporation plants and other additional water systems. Spent ion exchange resins (SIER), represent a significant part of the accumulated radioactive waste, which is due to the lack of generally accepted and safe processing methods. To solve the problem of processing accumulated SIER, the development of new technological solutions with high efficiency and safety continues. One of such technological solutions is the destruction of the ionites polymer matrices by the liquid-phase oxidation under hydrothermal conditions (HTO). The decomposition of ionites under hydrothermal conditions proceeds at relatively low temperatures (150–350 °C), without the formation of toxic gaseous products and the removal of radionuclides into the gas phase. Such features make HTO the most preferred among the known technological approaches such as: combustion, pyrolysis, supercritical aqueous oxidation and the Fenton process. Currently, the prospects for the practical application of HTO are limited by the insufficient number of published works demonstrating the possibilities for SIER processing.

The experiments were carried out using batch autoclaves and cation exchange resin of the “KU 2-8” brand (H⁺-form) in the temperature range of 100–150 °C and a pressure of 17–21 atm, a solution of hydrogen peroxide was chosen as the oxidizer. It was determined that the weight reduction coefficient of resin “KU 2-8”, in terms of dry matter, exceeds 100. Growing in the process temperature from 100 to 150 °C increases the rate of ionite decomposition by more than 2 times. The results obtained demonstrate the prospects of the HTO method for solving the problem of processing accumulated SIER.

The work was carried out within the framework of the State Order of the Institute of Chemistry of the Far Eastern Branch of the Russian Academy of Sciences, project No. FWFN (0205)-2022-0002.

THE DEVELOPMENT OF THE NEW MELTER FOR HLW VITRIFICATION AT FSUE “PA ‘MAYAK’”

**Bendasov D.I., Verbitsky K.V., Zubrilovski E.N., Melentev A.B.,
Kozlov P.V., Remizov M.B., Shaidullin S.M.**

*FSUE “PA ‘Mayak’”,
456784, Ozyorsk, Lenin st. 31, Russia,
e-mail: cpl@po-mayak.ru*

Vitrification is the method of choice for immobilization of the liquid high-level waste from the NPP SNF reprocessing. The FSUE “PA ‘Mayak’” started to use the non-removable large scale joule-heat EP-500 type melters for radiochemical facility’s HLW treatment since 1987. Up to now, the EP type melters have processed 28900 m³ of HLW effluent producing 8600 m³ of aluminum-phosphate glass with total incorporated activity of 841 mln. Ci.

The new vitrification facility (NVF) is scheduled for commissioning at “PA ‘Mayak’” in 2027. The concept of the NVF implies the use of two updated EP type melters, and the new melter for borosilicate glass with greater capacity for fission products, that will facilitate the immobilization of HLW generated by ongoing SNF reprocessing. This will provide the means for vitrified glass transfer to the National Operator for Radioactive Waste management or return of glass canisters to the foreign customers.

Unlike the EP melters, the new small-scale melter is a cylindrical joule heated furnace with electrical power of 100 Kw, feed HLW capacity of up to 25 l/h and glass melt output of up to 15 kg/h. The melter’s crucible has a funnel shape and is made of ceramic blocks with additional heat insulation. Remote service, replacement and disassembly of such melters will be provided within the NVF.

In 2018–2020 Mayak had completed tests of two full-scale prototypes of the borosilicate glass melters. The duration of the first prototype’s operation was 200 days, the second – 185 days. The vitrification process control, melter cooling, glass frit and HLW feed, glass melt drain systems and different auxiliary systems were developed during this period.

The completion of the third prototype of new melter, fully compatible with the NVF facility, and the start of the throughout testing is scheduled for 2024.

SORPTION PROPERTIES OF BENTONITE MODIFIED WITH SILVER CHLORIDE TOWARDS IODIDE IONS IN VARIOUS MEDIA

Tyupina E.A., Pryadko A.V.

*Mendeleev University of Chemical Technology of Russia,
125047, 9, Miusskaya square, Moscow, Russia,
e-mail: tk1972@mail.ru*

Disposal of high-level radioactive waste (HLRW) containing ^{129}I is expected to be in geological disposal facilities (GDF). Leaching of radioiodine as iodide ions from solid matrices is possible in GDF conditions under impact of media with various pH and ionic strength: groundwaters, concrete constructions and HLRW matrix leachates etc. Adding of the sorbent for iodide-anions, among which AgCl-containing bentonites are proved the most effective, to the composition of bentonite clay-based engineering safety barriers (ESB) is necessary to prevent migration of ^{129}I to the environment.

The purpose of current work is to investigate sorption properties of bentonites with AgCl deposited onto the surface in environments corresponding to various possible operating conditions of ESB in GDF.

Samples of bentonite of the 10th Khutor deposit with AgCl deposited onto the surface in amount of 0.5; 1; 3; 5; 7% Ag from clay weight were obtained via the previously developed technique¹. Investigation of iodide ions sorption at initial iodine concentration 10^{-3} M, at room temperature and solid-to-liquid ratio 1:100 indicated the equilibrium sorption yield of I^- on bentonite with AgCl in amount of 0.5% Ag from clay weight was 92% in the synthetic Nizhnetskanskiy rock massif groundwater solution, 96 and 91% in 0.01M KCl and K_2SO_4 solutions respectively, 96% in H_2SO_4 solution with pH=2 and 84% in $\text{Ca}(\text{OH})_2$ solution with pH=9. Equilibrium sorption yield of iodine on other AgCl-containing samples (1–7%) was 97–100% in every media listed above.

Thus, high sorption properties of the obtained sorbents towards iodide ions in wide range of aqueous phase ionic strength and pH values have been confirmed. Consequently, the developed sorbent as the ESB constituent will prevent ^{129}I migration outwards the GDF under various aggressive media impact.

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This research was funded by Russian Science Foundation, project number 22-29-0067.

EXPERIENCE IN THE IMPLEMENTATION AND PROSPECTS FOR THE APPLICATION OF THE CROSS-FLOW FILTRATION METHOD IN CHEMICAL-METALLURGICAL AND RADIOCHEMICAL FACILITIES OF FSUE PA “MAYAK”

**Samarina N.S., Konnikov A.V., Lagunova N.Yu., Logunov M.V.,
Lukin S.A., Lyzlova E.V., Melentev A.B.**

*FSUE “PA ‘Mayak’”,
456784, Ozyorsk, Lenin st. 31, Russia,
e-mail: cpl@po-mayak.ru*

Currently, membrane technologies are widely used in various industries. The advantages of this method are relative simplicity, reliability of equipment, and low specific energy consumption. For the nuclear industry, the cross-flow membrane filtration is perhaps of the greatest interest, where the flow of the filtered slurry continuously moves longitudinally through the filter channel, on the inner surface of which a ceramic membrane layer is applied, and the permeate flow is diverted through the membrane to the outer surface of the filter perpendicular to the slurry flow. At the same time, sediment accumulation does not occur on the membrane layer.

At FSUE PA “Mayak” for more than 10 years the research has been conducted on the cross-flow filtration process in relation to solving a number of production tasks. Significant results were achieved in the field of processing low- and medium-active LRW, where it is not required to use remote handling equipment.

A large installation for special sewerage water purification, as well as a small unit for cleaning alkaline technological waste from alpha-active nuclides, has been installed and is successfully operated at the chemical – metallurgical facility. At the radiochemical plant, cross-flow filtration has been introduced to purify and transfer to a lower category (in terms of activity) the mother liquor from the precipitation of ammonium polyuranate. In general, the creation and use of the industrial cross-flow filtration units had reduced the number of secondary processing operations, as well as the final volume of LRW, and significantly increased the environmental safety of production operations.

The use of the cross-flow filtration for clarification of highly active SNF solutions requires remotely serviced equipment. The development of canyon-type pulp pumps made it possible to create a full-scale test stand. The model solution tests had showed the possibility of using the cross-flow filtration to clarify SNF solutions. The technology is now ready for testing on real “hot” solutions.



WAYS OF BRIGHTNESS AMPLIFICATION FOR TRITIUM SOLID-STATE RADIOLUMINESCENT LIGHT SOURCES

Shvindin M.A.^{a,b}, Bakhmetyev V.V.^a, Zelenina E.V.^{a,b}

^a*Saint-Petersburg State Institute of Technology,
Moskovsky prospect 24-26, St. Petersburg, 190013, Russia,
e-mail: shvindin2012@yandex.ru*

^b*Khlopin Radium Institute,
2-nd Murinsky prospekt 28, St. Petersburg, 194021, Russia*

Nowdays gaseous tritium is the only commercial radioisotope for the radioluminescent light sources (RLS). And the breakability of the tritium-filled glass tubes creates the potential radiohazard of releasing the radioactivity. Developing the effective RLS without radioactive gaseous phase where tritium is bounded as titanium tritide (TiT_2) is the relevant objective to make RLS more safe and bright.

Bounding tritium in solid matrix decreases the brightness of RLS and the task of improving brightness without rising the included tritium activity can be solved by developing the more powerful radiophosphors. Copper-activated Zinc Sulfide ($ZnS:Cu$) is the most famous and effective radiophosphor. For improving its radioluminescent brightness at 0.4 Ci solid-state tritium source excitation in our work we have tested the various ways of energetic treatment of ZnS crystal structure. There were plasmochemical treatment in low-temperature nitrogen plasma at 1500 V., electron-beam treatment at 900 keV with 60 Mrad absorbed dose and ultra-high-frequency irradiation at 2400 MHz.

Each method of treatment of the initial ZnS charge has different impact on structure of synthesized phosphors and their spectral-brightness characteristics of radioluminescence. All types of treatment leads to the phase changes in the phosphors and in most cases results the increasing of the wurtzite phase content for ZnS -phosphors synthesized below the phase transition temperature. UHF and plasma treatment causes the blue shift of the radioluminescence spectra and decreasing of “green” luminescence intensity at 524 nm. In fact, the electron-beam treatment intensifies green intensity in spectra and allows the brightness rising upto 75% after double treatment.¹

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SPECTROPHOTOMETRIC METHOD OF PRECISE DETERMINATION OF URANIUM, PLUTONIUM AND OTHER RADIONUCLIDES IN SOLUTIONS BY SERIAL EQUIPMENT

Shvindin M.A., Mialochkin D.L.

*Khlopin Radium Institute,
2-nd Murinsky prospekt 28, St. Petersburg, 194021, Russia,
e-mail: shvindin2012@yandex.ru*

Precise determination of radioactive elements, such as uranium and plutonium, with repeatability standard deviation (relative form) $S_r < 0.1\%$ can guarantee non-proliferation of nuclear materials. Along with generally accepted methods, this task may be accomplished by using a spectrophotometric method in photometric mode of operation on serial spectrophotometric equipment, in particular Shimadzu UV.

In our recent studies we pointed out that, besides multiple repeated scan spectra, applying of internal standardization principle is alternative way to increase spectrophotometric measurements precision.¹⁻³ Auto-zero function, that usually exists at serial equipment, permanently keeps the track of baseline (100% light transmission) This provides internal standardization in spectra and optical density measurement of solutions. Multiple photometric measurements (1 to 300 times per operation) of the optical density at selected wavelengths allows to determine concentration of elements in solutions with relative repeatability standard deviation $< 0.1\%$.

Precise determination results for uranium, plutonium, ruthenium, erbium, gadolinium, samarium, rhenium and technetium in pure solutions by spectrophotometry in photometric mode of operation were obtained with $S_r = 0.02 - 0.1\%$. Serial equipment also provides more precise control of spectrophotometric analysis optimal conditions, such as temperature and acidity of solutions.

Precise spectrophotometric method allows to accomplish tasks, mainly related to manufacturing and (or) certification of standard samples – radioactive tracer solutions of U-233 or Pu-242 with specified mass fraction. Also this method can be applied for accounting and control of nuclear materials.

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COMPLEXES OF COPPER AND LEAD RADIONUCLIDES WITH BENZOAZACROWN ETHERS

Zamurueva L.S.,^a Egorova B.V.,^a Ikonnikova I.S.,^a Zubenko A.D.^b

^a*Lomonosov Moscow State University, Leninskie Gory, 119991, 1, Moscow, Russia,
lyubovzam@mail.ru*

²*A.N.Nesmeyanov Institute of Organoelement Compounds of Russian Academy of Sciences,
Vavilova St. 28, 119991, Moscow, Russia*

Nowadays many studies in radiopharmacy are devoted to copper radioisotopes ^{67}Cu and ^{64}Cu , which can be used for theranostics, and ^{212}Pb isotope, which can be applied in radiopharmaceuticals as an *in vivo* generator of short-lived therapeutic alpha-emitter ^{212}Bi . These radionuclides bind to biological vectors via bifunctional ligands. In our study, complexes of lead and copper cations with new benzoazacrown ethers were investigated with regard to possible applications in nuclear medicine.

The ligand protonation constants and stability constants of complexes were determined by potentiometric titration. Radioisotopes ^{64}Cu , ^{212}Pb and the long-lived ^{210}Pb was used to radiolabel the complexes. Complexation with these ligands occurs instantaneously at room temperature. The stability of the complexes was studied in biologically relevant media. To analyze the stability of complexes *in vivo*, a biodistribution of complex in mice was studied in comparison with copper free solution.

It has been established that tripicolinate, tetrapicolinate and tetraacetate benzoazacrown esters form complexes with copper with the highest stability constants ($\log\beta(\text{CuL})$: 19.3, 20.4 and 24.8, respectively) and formation of binuclear complexes with these ligands was also shown. For the Pb^{2+} cation, the largest constants are observed for complexes with the tetrapicolinate ligand ($\log\beta(\text{PbL})=21.3$) and with the tetraacetate ligand ($\log\beta(\text{PbL})=21.6$), only with the first of them the form $\text{Pb/L } 2/1$ is observed.

The tetrapicolinate ligand coordinates copper cations outside the macrocycle, resulting in an inert complex *in vitro* that does not release copper *in vitro*. The biodistribution profile of this complex with Cu^{2+} *in vivo* shows accumulation in the liver, which may indicate partial release of the cation.

All studied lead complexes are stable *in vitro*. In the case of ^{212}Pb , less than 10% of the daughter ^{212}Bi is released from the complex with the tetraacetate ligand. This complex is inert *in vivo* and is almost completely eliminated within 6 hours, so this complex is of interest for the production of radiopharmaceuticals based on ^{203}Pb and $^{212}\text{Pb}/^{212}\text{Bi}$.

This study is supported by state assignment of Lomonosov Moscow State University "Obtaining and application of radionuclides and labeled compounds for the purposes of nuclear medicine, the study of biologically significant processes and the inter-action of living organisms with ionizing radiation" (Project Reg. No. 122012600116-4)



**RUSSIAN-CHINESE SYMPOSIUM
ON SELECTIVE TECHNOLOGIES
FOR SEPARATION OF SUBSTANCES
WITH SIMILAR PROPERTIES**

SORPTION MATERIALS FOR RADIONUCLIDES SELECTIVE RECOVERY: SYNTHESIS, PROPERTIES, APPLICATION

**Bezhin N.A.^a, Shibetskaia I.G.^a, Razina V.A.^a, Kozlovskaya O.N.^a,
Milyutin V.V.^b, Tananaev I.G.^{a,c}**

^a Sevastopol State University, Universitetskaya Street 33, Sevastopol, 299053, Russia,
e-mail: nickbezhin@yandex.ru

^b Frumkin Institute of Physical Chemistry and Electrochemistry, RAS,
Leninsky Prospekt, 31, building 4, Moscow, 119071, Russia;

^c I.V. Tananaev Institute of Chemistry and Technology of Rare Elements and Mineral Raw Materials,
Kola Science Centre, RAS, Akademgorodok 26a, Apatity, 184209, Russia

Synthesis and research of sorption materials for the radionuclide's concentration is a relevant task. It is widely used in the isotope industry, nuclear medicine and radioecology.

We have obtained several selective sorbents for the radionuclide's recovery ($^{137}\text{Cs}^1$, $^{90}\text{Sr}^{2,3}$, ^{210}Pb and $^{210}\text{Po}^{3,4}$, $^{198,199}\text{Au}^5$) from technological solutions and natural environments. The obtained sorbents were studied in detail under static and dynamic conditions. The distribution coefficients, DEC and TDEC were determined, the output sorption curves were plotted, and the physical and chemical regularities (isotherms, kinetics, selectivity) of sorption were studied. The obtained dependences of sorption parameters on time are described using intraparticle diffusion model, pseudo-first and pseudo-second order models, and the dependence of sorption parameters on the equilibrium concentration of the element in solution using Langmuir and Freundlich sorption isotherms. The obtained sorbents were tested in practice.

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The work was carried out with the financial support of Sevastopol State University, project 42-01-09/253/2023-2.

COPPER(II) COMPLEXES WITH 2-HYDROXYPHENYLPHOSPHONIC ACIDS. SYNTHESIS, STRUCTURE AND BIOLOGICAL ACTIVITY

**Rogacheva Yu.I.,^a Baulin V.E.,^a Lapshina M.A.,^a Tsebrikova G.S.,^b Ivanova I.S.,^c
Ilyukhin A.B.,^c Solov'ev V.P.,^b Pyatova E.N.,^c Tsivadze A.Yu.^b**

^a Federal Research Center of Problems of Chemical Physics and Medicinal Chemistry,
Russian Academy of Sciences, Severny proezd, 1, Moscow region, Chernogolovka, 1142432, Russia,
e-mail: ximik1988200811@rambler.ru

^b Frumkin Institute of Physical Chemistry and Electrochemistry, Russian Academy of Sciences,
Leninsky prospekt, 31/4, Moscow, 119071, Russia

^c Kurnakov Institute of General and Inorganic Chemistry, Russian Academy of Sciences,
Leninsky Prospekt, 31, Moscow, 119991, Russia

Copper(II) complexes with 2-hydroxyphenylphosphonic acids, which are phosphoryl analogues of salicylic acid, are able to accumulate in HeLa cells, have low toxicity and higher analgesic activity than free acids.¹ In this work, acids $H_3L-H_3L_6$ and their copper(II) complexes were obtained for the first time.

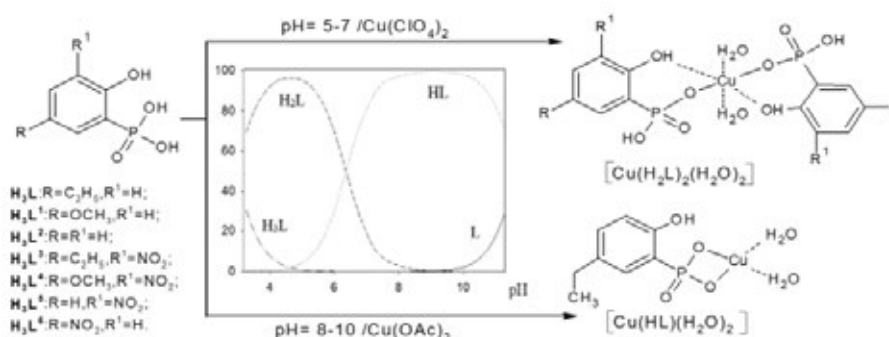


Figure 1. Structural formulae of synthesized 2-hydroxyphenylphosphonic acids and their Cu(II) complexes.
Distribution diagram of chemical forms of acid H_3L in water.

The composition and structure of the obtained complexes were determined by DFT, X-ray, IR, UV-Vis, TGA, DSC and elemental analysis. The protonation constants of acids and stability constants of their complexes in water were determined by potentiometric titration. It was found that the prevailed structure of the complexes depends on the pH of the medium.

The work was financially supported by the Russian Science Foundation, project No. 22-13-00051.

COPPER EXTRACTION FROM LEACHING SOLUTIONS OF COPPER PRODUCTION DUST BY MEXTRAL EXTRACTANTS

Sokolov A.Y.^a, Kasikov A.G.^a, Dvornikova A.M.^a, Fuxiang Y.^b

^a *Tananaev Institute of Chemistry, 184209, Russia, Apatity, Akademgorodok str., 26a,
e-mail: cobaltag@yandex.ru*

^b *Richem Holding Limited, 999077, Hong Kong, Kowloon, Fa Yuen str., 75*

One of the options for processing copper raw materials is copper concentrate roasting with subsequent leaching of the cinder by copper electrolyte and copper electroextraction. During roasting metallurgical dust is produced, which enriches with iron and a number of impurities, which make it difficult to obtain copper from dust and requires it independent processing¹. Selective copper solvent extraction by oxime-type extractants is usually used for copper refining.

A wide range of such extractants are currently available in China under the brand name Mextral, which consist of aldoximes and ketoximes or mixtures thereof. Depending on the composition of the extractant, its properties differ in copper extraction and stripping ability. It was found that the studied extractants can be arranged in a series in terms of extraction capacity: Mextral 84H < Mextral 5910 < Mextral 5910 < Mextral 984 < Mextral 5640. Copper stripping is significantly easier when using Mextral 84H (Fig.), which made it possible to strip copper from the extract by electrolyte with sulfuric acid concentration of 140 g/L. The results obtained were used to improve the copper concentrate processing technology at Kola MMC.

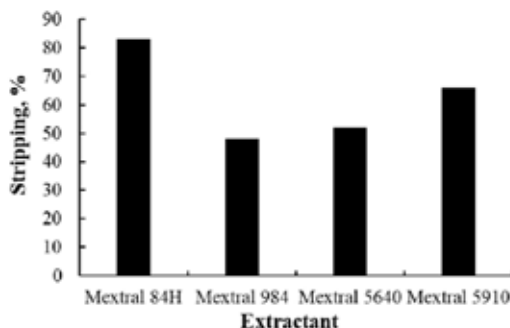


Figure. Copper stripping by sulfuric acid solution from Mextral extractants

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DEVELOPMENT OF THE MINERAL RESOURCES FOR RUSSIA'S TECHNOLOGICAL SOVEREIGNTY

ACIDOPHILIC CHEMOLITHOTROPHIC MICROORGANISMS OF ACID SULFATE THERMAL SPRINGS OF KAMCHATKA AND THE KURIL ISLANDS: PROSPECTS OF APPLICATION IN BIO-LEACHING PROCESSES

[Averyanova V.E.](#)

*Scientific Research Geotechnological Center of the Far Eastern Branch of the Russian Academy of Sciences, 683002,
Petropavlovsk-Kamchatsky, North-Eastern highway, 30, a/yu 56
e-mail: purlac@inbox.ru*

Thermoacidophilic chemolithotrophic bacteria are of great interest for the biohydrometallurgy of poor ores. Their use, due to high temperatures, can contribute to a more complete bio-leaching of such resistant minerals as chalcopyrite^{1,2}.

Microorganisms for biological leaching must be adapted to acidic conditions (pH below 3), the presence of certain heavy metals and other factors. Therefore, the search for these microorganisms must be conducted at mining sites, in drainage systems of acid mines and geothermally active zones, where such conditions exist. Promising habitats for the isolation and use of such strains as *Acidithiobacillus*, *Sulfolobus*, *Leptospirillum*, *Acidianus*, *Sulfobacillus* are the areas of thermal fields and hydrotherms of Kamchatka and the Kuril Islands.

The Kamchatka Peninsula and the Kuril Islands are areas of active volcanic activity and have geothermal zones. The temperature of the thermal outlets is 15-96 °C, pH 3.45-4.62. Deep hydrothermal waters contain high concentrations of reduced iron, which, upon reaching the surface, undergoes a chemical and biological oxidative reaction leading to the formation of insoluble iron oxides³.

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STUDY AND PROSPECTS FOR DEVELOPMENT OF ORE MINERAL RESOURCES IN THE SEA OF THE EAST OF RUSSIA

**Astakhov A.S., Akseptov K.I., Astakhova N.V., Kolesnik A.N.,
Kolesnik O.N., Sattarova V.V.**

*V.I. Il'ichev Pacific Oceanological Institute Far Eastern Branch Russian Academy of Science.
43, Baltiiskaya St., Vladivostok, 690041 Russia,
e-mail: astakhov@poi.dvo.ru*

The study of ore mineral resources of the Far Eastern and Eastern Arctic seas of the Russia began in the mid-20th century. Flooded alluvial and coastal-marine placers of gold and cassiterite have been most studied including with an assessment of predicted resources, whereas placers of platinum group metals, monazite, and zircon have been studied to a lesser degree. Metalliferous sediments of various types and ferromanganese diagenetic and hydrothermal sedimentary ores are also known. These formations haven't received practical importance due to small reserves, difficult mining and geological conditions, the presence of undeveloped similar deposits on the coast, as well as the priority importance of biological resources over mineral ones in certain areas.

Nevertheless, some of these types of mineral raw materials could be in demand due to the emerging demand for individual metals, changes in market conditions and external conditions. The Laboratory of Geochemistry of Sedimentary Processes of the POI FEB RAS (Marine ore formation until 2018) has identified at least two types of promising mineral occurrences that require priority study.

Monazite-zircon metal-bearing deposits and coastal marine placers of the Laptev Sea and the western part of the East Siberian Sea with relatively low contents [1, 2], in response to the relative availability and simplicity of mining and enrichment technologies considered as a possible source of strategic metals (REE, Nb, Sc, Zr...). Rich hydrothermal-sedimentary manganese ores of the seamounts of the Sea of Japan are a source of manganese and some rare metals [3, 4]. The average manganese content in manganese ores varies within 30-50% on various volcanoes; in pure pyrolusite ores is 63% [3], that is two to three times higher than, for example, on the guyots from the central part of the Pacific Ocean.

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This study was supported by the Russian Science Foundation (RSF), projects 23-27-00004, 24-17-00028 and 24-17-00159.

PROBLEMS OF THE DEVELOPMENT OF SMALL-SCALE PLACER DEPOSITS AND TECHNOGENIC FORMATIONS OF GOLD IN THE ARCTIC ZONE OF YAKUTIA

Batugina N.S.,^a Gavrilov V.L.^{a, b}

^a *Chersky Institute of Mining of the North, Siberian Branch, Russian Academy of Sciences,
Lenina av., Yakutsk, 677980 Russia*

^b *Chinakal Institute of Mining, Siberian Branch, Russian Academy of Sciences,
Krasniy av., Novosibirsk, 630091 Russia
e-mail: gylugorsk@mail.ru*

In the Arctic zone of Yakutia placer deposits of gold, tin and diamonds have been developed for decades. A large number of small deposits of alluvial gold and technogenic formations are located in the region, including those that are currently off-balance in terms of quality and mining conditions, or are not accounted for. These facilities, as a rule, are not of commercial interest for large and medium-sized subsoil users, but can be attractive for small businesses.

Involvement in economic turnover of such deposits and sites in the Far North, which are often characterized by the presence of other metals important for high technology, is possible by introducing the category «small-scale placer deposits and technogenic formations» with regard to their potentially effective development. This should take into account the impact on the efficiency of exploration, assessment and development of physical-geographical and geological conditions of placement and occurrence; simplification of the licensing and taxation system; changing the social and economic and legal status of this category with the introduction of adjustable quantitative criteria for the assignment of an object to it (table 1).

Table 1. Classification criteria for small-scale placer deposits and technogenic formations of Arctic regions of Yakutia

Criteria	Deposit	Technogenic formation
Reserves (resources), kg	< 30-50	< 60-80
Average content, g/m ³	< 0,1-0,12	< 0,05-0,09
Occurrence conditions	Simple, depth ≤ 5-7 m	volume < 300 thousand m ³

The compilation of an inventory of small-scale placer deposits and technogenic gold formations, which are usually characterized by cluster distribution of useful components, allows them to rank in importance with the unification of approaches to the choice of technical means, technologies for mining operations and enrichment of extracted minerals.

The work was supported by RSF, project № 24-28-20376



ALGORITHM FOR SELECTION OF REAGENTS FOR FLOTATION EXTRACTION OF NON-FERROUS METALS FROM DIFFICULT ORES

Fedotov K.V., Sarapulova G.I.

National Research Technical University, Russia, 664074, Irkutsk, Lermontov-st., 83. E-mail: sara131@mail.ru

Copper-zinc ores are difficult to process because they are a complex structural conglomerate consisting of sulfide complexes of copper, zinc, iron, host rock minerals, as well as gold, silver, cadmium, indium, tellurium, arsenic, etc.

The similarity of the flotation properties of copper sulfides and zinc sulfides (activated with copper ions) constitutes the main difficulty in the beneficiation of such ores. In this regard, much attention is paid to methods of conditioning low-grade concentrates obtained from the processing of copper-zinc ores, as well as testing new reagent regimes, selecting compositions of collectors and depressants, and studying the mechanism of their action. An active search is underway for parameters for effective selective flotation of sulfide ores based on combinations of collectors of various classes of compounds in order to improve technological indicators and scale them into the production process.

We have carried out a series of laboratory experiments using a model charge characterizing a copper-zinc mixed type of difficult-to-process ore. The use of empirical simulation modeling has been substantiated and tested to assess the effectiveness of collective selective flotation of copper-zinc ores of multicomponent composition in order to obtain a collective concentrate.

It was established that controlled dosing of the flow of supplied reagents in flotation operations made it possible to empirically substantiate the variable dynamic parameters of flotation enrichment. On this basis, a clear algorithm for the process of enrichment of mineral copper-zinc raw materials of complex composition has been developed, which allows you to control the enrichment process and regulate the optimal ratios of reagents for the effective yield of target products: copper and zinc concentrate.

The effectiveness of two-stage flotation enrichment using a direct selective scheme has been demonstrated.

ESTIMATION OF CONTENT OF ASSOCIATED VALUABLE ELEMENTS IN LOW-GRADE RAW MATERIALS AND ANTHROPOGENIC WASTES BY INAA METHOD WITH CALIFORNIUM NEUTRON SOURCE

Ivannikov S.I., Markin N.S., Zemskova L.A.

*Institute of Chemistry of the Far Eastern Branch of the Russian Academy of Sciences,
690022, Vladivostok, 100th Anniversary of Vladivostok Avenue, 159
e-mail: fyajkfqn@mail.ru*

As ore deposits are depleted and the quality of ores in the mining industry declines, the involvement of alternative sources in processing becomes relevant. Anthropogenic raw materials, such as wastes from subsoil use, metallurgical, chemical and energy industries, are becoming sources of valuable metals in the leading industrialized countries. And in some places these sources are already a traditional source of certain metals^{1,2}. The development of such raw materials requires both efficient recovery technologies and high-precision analytical techniques.

Along with modern analytical methods, the use of instrumental neutron activation analysis (INAA) as one of the most highly sensitive non-destructive methods of analysis remains relevant. The INAA facility with neutron source Cf-252 at the Institute of Chemistry of the Far East Branch of the Russian Academy of Sciences has carried out a number of works to evaluate anthropogenic waste as a source of strategic elements.

The study of the content of critical metals (Sc and Au) in ash and slag wastes and their separation products was carried out for some Primorsky CHPPs. Wastes of tin enrichment of mining and processing plants were examined. The study of accumulation of valuable metals Sc and In - tin satellites in carrier minerals (cassiterite, wolframite, chalcopyrite) was carried out. The content of valuable metals in a number of black shale samples was determined. Methods for the determination of strategic metals (Au, Sc, In, REE) in the studied samples were developed. The correctness of the obtained results was confirmed by the En-score statistical criterion.

In the conditions of the Russian Far East region in the absence of research reactors and particle gas pedals, INAA with californium neutron source is an effective alternative for solving a wide range of analytical problems.

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The work was carried out within the framework of the state assignment of Institute of Chemistry FEB RAS, project № FWFN (0205)-2023-0002

MODERN PROBLEMS OF DEVELOPMENT OF PLACER MINERAL DEPOSITS OF STRATEGIC METALS

[Lalomov A.V.](#)

*Institute of Geology of Ore Deposits, Petrography, Mineralogy and Geochemistry of Russian Academy of Sciences,
119017, Moscow, Staromonetny 35
e-mail: lalomov@mail.ru*

Placer mineral deposits are important source for providing strategic types of mineral resource base for both Russia and the world as a whole. Placers have a number of advantages that make them in demand by the mining industry: relatively shallow occurrence, disintegrated state of productive deposits, simplicity of enrichment processes (mainly gravitational and gravitational –magnetic systems), as well as the possibility of rapid involvement in exploitation, which significantly reduces payback period for investments. All this is even more relevant for present-day Russia, when, in the shortest possible time, in conditions of a shortage of credit resources, it is necessary to implement a program of import substitution and provide the country with scarce types of strategic mineral feedstock, such as tin, rare metals (including zirconium and rare earth elements), titanium, chromium.

The analysis performed (in terms of import substitution) for priority development allows us to recommend the following objects: Sn – Tirekhtyakh, Chokurdakh and Valkumey placers (Yakutia and Chukotka); Nb, Ta, REE – loparite placers of the Revdinsky group and man-made deposits in the tailings of Lovozersky GOK (Kola Peninsula); Ti and Zr – Tugan (Siberia) and Beshpagir (Pre-Caucasus region) deposits, Itmanov site of the Lukoyanov placer deposit (Central Russia region) (Zr, Cr)¹.

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The research was carried out at the expense of a grant from Russian Science Foundation № 24-27-00109, <https://rscf.ru/project/24-27-00109/>

CONCENTRATIONS AND MINERAL FORMS OF AS, TE, SE, SB IN THE PRODUCTS OF AVACHA VOLCANO ACTIVITY (KAMCHATKA, RUSSIA)

Plutakhina E.Yu., Malik N.A., Skilskaya E.D.

*Institute of Volcanology and Seismology, Far Eastern Branch of the Russian Academy of Sciences,
Piipa b. 9, 683006, Petropavlovsk-Kamchatsky, Russia
e-mail: e.plutakhina@gmail.com*

Volcanic gases consist of H₂O, CO₂, SO₂, H₂S, HCl, HF and various trace element compounds. The trace element composition of the products of fumarolic activity of each volcano is unique (the data scatter can exceed four orders of magnitude for a particular element under the same degassing conditions). New types of minerals are often found in fumarolic systems of volcanoes¹.

At Avacha volcano (since 2013), not only gases and natural exhalations are studied, but also “sublimates”. Sublimates are mineral aggregates formed from fumarolic gases (T>500°C) in quartz tubes². Realgar, auripigment and arsenosulfurite are common in the exhalates, but X-ray amorphous (As,S)-glass predominates by mass in the sublimates of each tube. According to ICP and SEM analyses - Te, Se and Sb concentrations are directly correlated with the As-phase. Se and Te are diagnosed as spherical phases of variable composition (Se,Te) in exhalations and sublimates; no nugget minerals were found for Sb. In all As-minerals and (As,S)-glasses impurities of Te, Se and Sb in amounts up to 6 wt.% were determined. For example, in (As,S)-glass in quartz tube No. 12 the concentrations of As 60069 ppm, Te 3386 ppm, Se 5016 ppm, Sb 55 ppm were determined. Local concentrations in (As,S)-glass are Se <7 weight %, Te <9 weight %, Sb <2 weight %.

The study of distribution and forms of Se, Te and Sb concentrations is part of the assessment of potential metalliferousness of volcanic gases of Avacha volcano.

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The study was supported by RSF, grant No. 23-27-00156.



MOLYBDENUM, TUNGSTEN AND RHENIUM MINERALS IN PRODUCTS OF THE HIGH-TEMPERATURE FUMAROLIC SYSTEM OF AVACHINSKY VOLCANO

Plutakhina E.Yu., Malik N.A.

*Institute of Volcanology and Seismology, Far Eastern Branch of the Russian Academy of Sciences,
Piipa b. 9, 683006, Petropavlovsk-Kamchatsky, Russia
e-mail: e.plutakhina@gmail.com*

Exhalation ore mineralization is often observed in the fumarole fields of World volcanoes. Contents of rare metals in fumarolic deposits can reach concentrations comparable to ore deposits 1. Within the Kurilo-Kamchatka island arc, rhenium mineralization in exhalations was found on volcanoes Tolbachik², Avachinsky³, and Kudryavy¹.

Regular mineralogical and geochemical monitoring of fumarolic activity of the Avacha volcano has been carried out since 2013. The maximum concentrations of Mo, W, Re in bulk samples of natural exhalations and sublimates (mineral phases deposited in quartz tubes from fumarolic gases) are shown in Table 1.

Table 1. Maximum concentrations of Mo, W, Re at Avacha volcano in mineral samples, in ppm.

Elements	Samples		
	Exhalations	Sublimates, 2014.	Sublimates, 2018.
Mo	460	17366	1049
W	6	9	4
Re	52	8256	114

The authors diagnosed molybdenite MoS_2 (with admixture of Re up to 6 weight.%), ferberite FeWO_4 , rhenite ReS_2 and also phase KReO_4 in exhalations and sublimates; only in sublimates - molybdenite MoO_3 and powellite $\text{Ca}(\text{MoO}_4)$.

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The study was supported by RSF, grant No. 23-27-00156.1.

RARE METAL MINERALIZATION IN ORES OF EPITHERMAL AU-AG DEPOSITS OF VOLCANIC-PLUTONIC BELTS OF KAMCHATKA

Skilskaya E.D., Shishkanova K.O., Zobenko O.A., Sergeeva A.V.

*Institute of Volcanology and Seismology, Far East Branch of the Russian
Academy of Sciences, Piipa b. 9, 683006, Petropavlovsk-Kamchatsky, Russia,
E-mail: wideworldscience@gmail.com*

Rare and disseminated elements – Cd, In, Bi, Se, Te, Sb are typical impurities in the ore minerals in the Au-Ag ore deposits in the volcanic-plutonic belts of Kamchatka. In bonanza ores of quartz veins their concentrations reach >1000 ppm. In nature they rarely form their own minerals; more often they are concentrated in the form of impurities in other ore minerals.

Tellurium occurs as kalaverite, sylvanite, hessite, altaite, and is also found as an impurity in other ore minerals. Tellurides are widely distributed in the gold deposits in central Kamchatka (Aginskoye, Oganchinskoye). As impurities tellurium with concentration of about 16,69 -18,79 % is often found in goldfieldite in the deposits from southern Kamchatka (Mutnovskoye, Vilyuchinskoye). Tolstykh N.D. reported about new gold seleno-telluride – maletoyvayamite $\text{Au}_3\text{Te}_6\text{Se}_4$ found in ore deposit in north Kamchatka.

Selenium is generally found as impurities in ore minerals. The gold-bearing ores of the Asachinskoye in the South Kamchatka consist of Se-enriched galena, argentite, stibiopyrseite-arsenopolybasite, and uytenbogaardtite, in which the amount of Se is up to 4-5 %. As impurities in argentite (13,57 %) and pyrargyrite (7,00 %) is found in the northern ore deposits in Kamchatka. Sulfoselenides are found at the Asachinskoye deposit and selenides in ore from the Ozernovskoye deposit.

Rare Bi-bearing minerals – chodrusite ($\text{Cu}_8\text{Bi}_{12}\text{S}_{22}$), bismuthine (Bi_2S_3), Bi sulfoselenides, berryite ($\text{Cu}_3\text{Ag}_2\text{Pb}_3\text{Bi}_7\text{S}_{16}$) are found in ores of the Vilyuchinskoye mineral prospect and Mutnovskoye Au-Ag-polymetallic deposit in south of Kamchatka.

Antimony is most often included in tetrahedrite group minerals, which are widely distributed in ore deposits in Kamchatka.

Indium and cadmium are typical impurity elements in sphalerite of Mutnovskoye, which is the largest Au-Ag-polymetallic deposit in the south of Kamchatka. Indium content reaches up to 9,1 %, cadmium – 7,8 %.

The above described elements are concentrated in the zones of mineral growth, causing zonal heterogeneous structure, caused by sharp fluctuations of physical and chemical parameters of ore-forming environment.



ACCUMULATION OF LITHIUM IN CLAY MINERALS OF MODERN THERMAL FIELDS OF KAMCHATKA

Sergeeva A.V., Kiryukhin A.V., Kartasheva E.V., Nazarova M.A.,
Kuzmina A.A., Martynenko D.O., Pozolotina L.A.

*Institute of Volcanology and Seismology, FEB RAS, Piipa Blvd. 9, 683006, Petropavlovsk-Kamchatsky, Russia,
E-mail: anastavalers@gmail.com*

In Kamchatka, in the areas of modern volcanism, natural hydrothermal systems are developed, realized as discharges of vapor-hydrotherms to the day surface. As a result, thermal fields are formed, which are heated areas of tens to hundreds of meters in length, where heated deep solutions flow to the surface, and the rocks in contact with the flows are transformed into clay layers, up to several meters in thickness

The upper part of clay formations is mainly composed of kaolinite, montmorillonite, jarosite and alunite minerals, pore solutions have mainly slightly acidic environment. Deeper horizons of thermal fields are composed of zeolite minerals. Since the main secondary minerals are typical cation exchangers, they naturally accumulate cations carried by thermal waters to the surface.

In the present work, lithium extraction from clayey soil samples of a number of thermal fields in Kamchatka: Valley of Geysers, Uzon caldera, Mutnovskoye vapor-hydrothermal field, Pauzhetsko-Kambal-Koshelevsky area was investigated. For lithium extraction, aqueous extracts from air-dry clay samples were obtained with distilled water and in a 2% NaCl solution, assuming that due to ionic exchange there will be sodium substitution of all cations accumulated in the newly formed cation-exchangers. It was found that the concentration of lithium in solutions in contact with clays, in the case of using sodium chloride solution increases by 2 - 20 times - depending on the mineral composition of a particular sample - compared to the extraction with distilled water. Apparently, natural cation-exchange minerals - mainly montmorillonite - are natural accumulators of a number of elements, including lithium. It is possible to consider these minerals as a sorbent for extraction of lithium and other cations, or as a raw material.

LEACHING OF METALS FROM WASTES OF FLOTATION ENRICHMENT OF SULPHIDE PLATINUM-COPPER-NICKEL ORES

Starostina S.I.,^{a,b} Yurkevich N.V.^a

^a Trofimuk Institute of Petroleum Geology and Geophysics Siberian Branch of the Russian Academy of Sciences,
630090, Novosibirsk, 3, Koptug Avenue,
e-mail: starostinasi@ipgg.sbras.ru

^b Novosibirsk State University, 630090, Novosibirsk, 1, Pirogova str.

Tailings dumps are modern alternative sources of raw materials. This paper shows the results of studying the mineral and elemental composition of waste from flotation enrichment of sulfide platinum-copper-nickel ores. Among the ore minerals in the tailings chalcopyrite CuFeS_2 , pentlandite $(\text{Fe,Ni,Co})_9\text{S}_8$ (incl. silver-containing), pyrrhotite Fe_{1-x}S , pyrite FeS_2 , cubanite CuFe_2S_3 , as well as sphalerite ZnS , galena PbS and wurtzite $(\text{Zn,Fe})\text{S}$ predominate. Au occurs as alloys with Ag and Pd. Pt forms its own minerals. The concentration of Ni in waste is on average 1700 g/t, Cu – 1060 g/t. Co and Pt contents are at the level of modern developed deposits (110 g/t and 0,31 g/t respectively).

Oxidative leaching experiments carried out with a 30 % solution H_2O_2 (NAG-test¹) and ammonium acetate buffer solution² showed the advantage of the latter. The mobility of Fe and Pb increased by one and a half times compared to peroxide extracts, Zn – by 8 %. Ni, Cu, Co and Pt became more mobile in slightly acidic extracts by 20-30 %.

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This research was supported by Basic research project of Ministry of Science and Higher Education of the Russian Federation FWZZ-2022-0029.



SYMPOSIUM ON MEDICINAL CHEMISTRY

SYNTHESIS OF CARBENEPLATINUM (II) COMPLEXES OF ARYLBIPYRIDINES WITH ANTITUMOR ACTIVITY

Abramov V.M., Tokhtueva M.D., Melekhin V.V., El'tsov O.S.

*Ural Federal University, Institute of Chemical Engineering,
620002, Russia, Yekaterinburg, Mira, 28,
e-mail: vladislav.abramov@urfu.ru*

Organoplatinum complexes are unique functional materials with significant potential in chemotherapy of cancer¹. This work is a continuation of our earlier studies².

We synthesized carbeneplatinum (II) complexes **2**, the structure of which was proved by NMR and IR spectroscopy, mass spectrometry, and elemental analysis (Fig. 1).

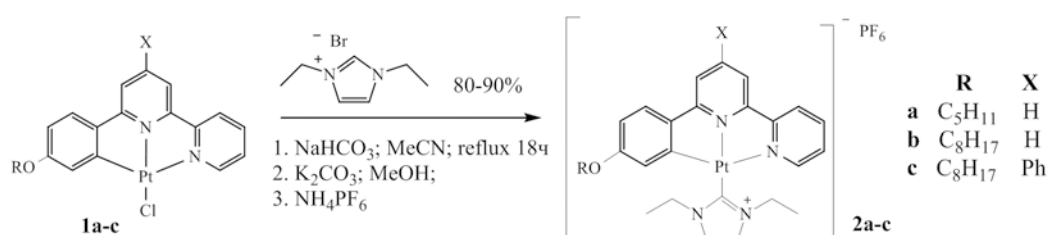


Figure 1. Scheme of synthesis of Pt(II) complexes

The cytotoxicity index (IC₅₀) values were determined using the MTT test. The drug cisplatin (Cpt) was chosen as the object of comparison (Fig. 2).

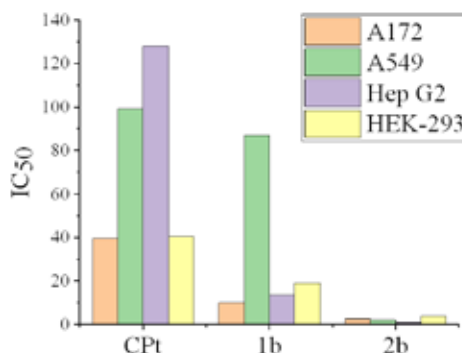


Figure 2. Comparative MTT test data for complexes **1b**, **2b** and Cpt

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The work was financially supported by RNF, grant 23-23-00375.

SEARCH FOR ANTIMICROBIAL/FUNGICIDAL PREPARATIONS IN A RANGE OF NEW N-ARYLALKYLPYPERIDINE DERIVATIVES

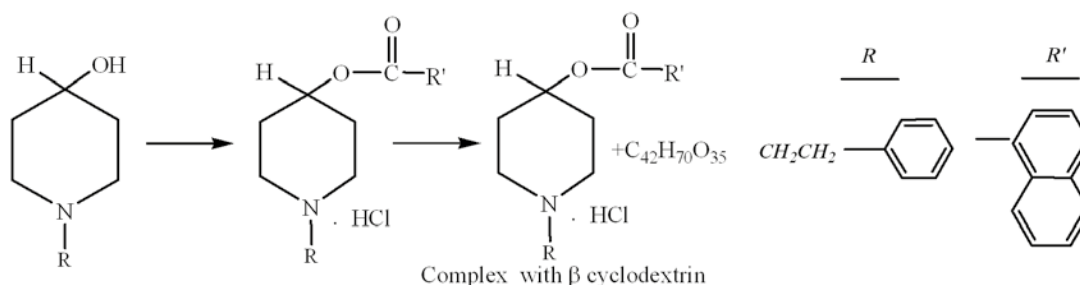
Akhmetova G.S.^a, Praliyev K.D.^a, Maksatova A.M.^b

^a*A.B. Bekturov Institute of Chemical Sciences JSC,
106 Sh. Ualikhanov str., 050010, Almaty,
e-mail: gulgakhmet@mail.ru*

^b*National Medical University JSC,
88 Tole bi str., 050012, Almaty*

Substances with an antibacterial activity are of great value for medicine. Despite the large number of drugs, the search for new antimycobacterial preparations is an urgent task, primarily due to the high adaptability of pathogenic organisms to various antibiotics.

In continuation of the targeted research for anti-infective agents, with the aim of introducing a naphthoyloxy group into the structures of piperidines, elucidating the effect on the anti-infective activity of the compounds, the corresponding naphthoic acid ester hydrochloride has been obtained by the acylation of N-phenylethyl-4-hydroxypiperidine with naphthoyl chloride with the yield of 89.6%. The acylation has been carried out in chloroform, the ratio of piperidol: acylating agent is 1:2. Based on the hydrochloride, an inclusion complex with β -cyclodextrin has been obtained.



The synthesized new derivatives of N-arylalkylpiperidines have an antimicrobial activity *in vitro* against the museum strains of microorganisms: *Staphylococcus aureus* ATCC 6538-P, *Candida albicans* ATCC 10231, *Aspergillus brasiliensis* (*niger*) ATCC 16404, as well as multidrug-resistant *Staphylococcus aureus* ATCC BAA-39. They have significant advantages over the reference preparations used in practical medicine, such as ampicillin, nystatin, which are recommended for the further in-depth studies.

The work has been carried out within the frames of the PCF KN MNE RK No. BR21882220

SEARCH FOR ANTIMICROBIAL PREPARATIONS IN A RANGE OF FLUOBENZOIC ESTERS OF N-BENZYL-PIPERIDINEKETOXIMES

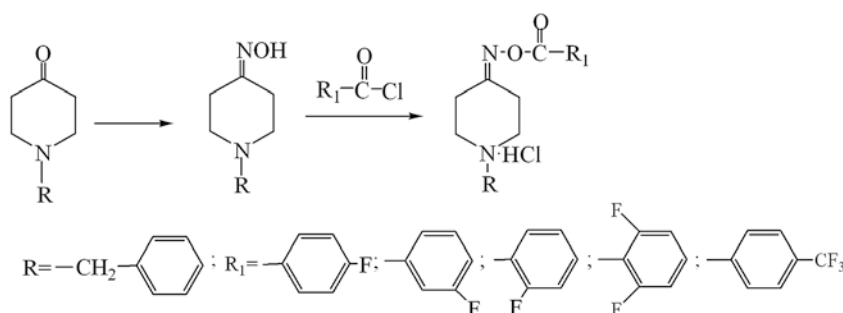
Praliyev K.D.^a, Akhmetova G.S.^a, Issayeva U.B.^b

^a*A.B. Bekturov Institute of Chemical Sciences JSC,
106 Sh. Ualikhanov str., 050010, Almaty,
e-mail: gulgakhmet@mail.ru*

^b*Republican Training Resource Center for Civil Protection JSC, MIA RK,
300 Baizakov str., 050040 Almaty*

Today, the most important group of antibacterial preparations includes nitrogenous heterocycles, in particular quinolones. And, as it has turned out, the introduction of fluorine into the quinolone molecule has led to the preparations, which are superior in their level of activity and spectrum of an antibacterial activity to many antibiotics, including the third-generation cephalosporins, and other chemotherapeutic agents.

In continuation of the targeted research for anti-infective/antimicrobial agents, as well as in order to clarify the effect of the introduction of a fluorine atom in the aromatic ring upon the antibacterial activity based on the ketoxime 1-(benzyl-)piperidin-4-one, an acylation by *para*-, *meta*-, *ortho*- fluorobenzoyl chlorides, as well as by 2,6-difluoro-, *p*-(trifluoromethyl)-benzoyl chlorides has been carried out.



The synthesized fluorine derivatives have an antimicrobial activity *in vitro* against the museum strains of microorganisms: *Escherichia coli* ATCC 8739, *Staphylococcus aureus* ATCC 6538-P, *Candida albicans* ATCC 10231, as well as multidrug-resistant *Staphylococcus aureus* ATCC BAA-39. They have significant advantages over the reference preparations used in practice medicine, such as fluconazole and ampicillin, which are recommended for the further in-depth studies.

The work has been carried out within the frames of the PCF KN MNE RK No. BR18574042

Artamonova Y.S., Sultanova R.M.

The concept of hybridisation, based on the combination of several pharmacophore groups in one molecule, is actively used in the development of new biologically active compounds. Combining structural fragments of 1,3-dioxane and oxime group in the molecule is a promising option for obtaining new compounds with potential biological activity^{1,2}.

[illegible]

References

- The work was carried out within the framework of the state assignment of the Ministry of Education and Science of Russia in the field of scientific activity. FEUR publication number – 2022-0007 “Petrochemical reagents, oils and materials for thermal power engineering”*

PHOTOREGULATED TRANSPORT OF BIOLOGICALLY ACTIVE AND NATURAL OCCURING MOLECULES USING HETEROCYCLIC FLUOROPHORES

Belskaya N.P.^a, Gagarin A.A.^a, Minin A.S.^a, Shevyrin V.A.^a, Benassi E.^b

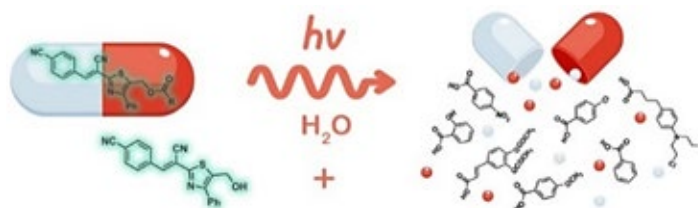
^a*Ural Federal University, 19 Mira Str., Yekaterinburg, 620002, Russia,
e-mail: n.p.belskaya@urfu.ru*

^b*University of Modena and Reggio Emilia, Modena, 41125, Italy*

Photocleavable protecting groups (PPGs) (photocages, photocouriers, photocontainer) are photoactive compounds used as safeguard for a temporal masking of the functional (either chemical or biological) activity of a molecule.¹ PPGs were object of intensive investigations in a plethora of domains of applications in organic syntheses and in the study of processes in chemistry, in materials science, in biological and medical research fields, diagnostic and for temporally and spatially controlled delivery of bioagents.

Exposure to light induces the breaking of the covalent bond between PPG and the caged biomolecule (cargo), leading to the restoration of the biomolecule's activity. In this way, a spatial and temporal control of the substrate bioactivity can be achieved, making PPGs powerful tools for the study of small molecules, short-living particles, or therapeutic agents, such as pharmaceuticals, signaling agents, neurotransmitters, ions in living organisms.

We have synthesized a series of new fluorophores based on an arylidenethiazole framework and studied the prospects for their use as a photocontainer for the targeted delivery of drugs, diagnostic agents, or natural compounds containing a carboxyl group.



The mechanism of photorelease of biomolecules was studied using spectral studies, HPLC-HRMS and quantum mechanical calculations. Biological experiments have shown the biocompatibility of the hybrids and the selectivity of their intracellular localization in the endoplasmic reticulum, lipid droplets and mitochondria.

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THE STUDY OF SYNTHETIC APPROACHES FOR REGIOSELECTIVE PRODUCTION OF 3,5-DISUBSTITUTED ISOXAZOLES AND THEIR DERIVATIVES

Demina O.V., Belikov N.E., Safinova A.Ya., Varfolomeev S.D., Khodonov A.A.

*N.M Emanuel Institute of Biochemical Physics of Russian Academy of Sciences,
Kosygina st., bl. 4, Moscow, 119334, Russian Federation,
ovd@sky.chph.ras.ru*

For the regioselective preparation of 5-substituted 3-pyridyl isoxazoles the following approaches were studied: a) the classical reaction of [3+2] Huisgen cycloaddition of terminal alkynes and alkenes with pyridyl hydroxymoyl chloride hydrochlorides; b) phase transfer catalysis method¹. An alternative approach consisted in the preparation of 5-substituted 3-pyridylisoxazoles with sufficiently high yields via the syntheses of their 4,5-dihydro derivatives with the followed transformation by the dehydrogenation. Using these schemes, a library of compounds possessed the antiaggregatory activity was synthesized^{1,2}.

We have developed the methods for the introduction of photochromic and/or fluorescent labels into the pharmacophore fragment of 3,5-disubstituted isoxazoles molecules³.

The structures of all compounds were proved by ¹H and ¹³C NMR spectroscopy and mass spectrometry. The purity of the substances was confirmed by HPLC and ¹H NMR spectroscopy.

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The work was partially supported by the framework of the State Assignment of N.M Emanuel Institute of Biochemical Physics of Russian Academy of Sciences in 2022–2024 (Project No. 122041300210-2) and partially supported by the Russian Foundation for Basic Research (grant No. 20-03-00139).

MOLECULAR COMPLEXES OF TRITERPENE GLYCOSIDES WITH 5-FLUOROURACIL SODIUM SALT: SYNTHESIS AND PHYSIOLOGICAL ACTIVITY

Dokichev V.A.^a, Yakovishin L.A.^b, Grishkovets V.I.^c, Gibadullina N.N.^a

^a*Ufa Institute of Chemistry, Ufa Federal Research Centre,
Russian Academy of Sciences, 69 prosp. Oktyabrya, 450054, Ufa,
e-mail: dokichev_vl@mail.ru*

^b*Sevastopol State University,
33 ul. Universitetskaya, 299053, Sevastopol*

^c*V. I. Vernadsky Crimean Federal University,
4 prosp. Vernadskogo, 295007, Simferopol*

The creation of combination drugs based on natural compounds – triterpene glycosides – makes it possible to reduce therapeutic doses, expand the spectrum of pharmacological activity and reduce the general toxic effect of chemotherapeutic drugs^{1,2}.

In this work, molecular complexes of triterpene glycosides α -hederin, hederasaponin C and monoammonium salt of glycyrrhizic acid with the chemotherapeutic drug sodium salt of 5-fluorouracil (5FU) in a molar ratio of 1:1 were obtained, their cytotoxic properties and the synergistic effect of the initial components were studied³. To confirm complex formation and determine functional groups and fragments, as a result of non-covalent interaction of which complexes are formed, methods of IR spectroscopy, as well as ¹³C and ¹⁹F NMR spectroscopy were used with analysis of changes in the values of chemical shifts of the signals of the corresponding atoms ($\Delta\delta$) and the spin-spin coupling constants. The complexation of 5FU with glycosidic molecules is of the same nature for all selected triterpene saponins and occurs predominantly due to the formation of intermolecular hydrogen bonds of the C(2)-N(1)-C(6) fragment of the 5FU molecule with hydroxyl groups of carbohydrate cycles. In complexes with α -hederin and hederasaponin C, the interaction of the N(1) 5FU nitrogen atom with the hydroxyl groups of carbohydrate fragments is observed, and in the case of the monoammonium salt of glycyrrhizic acid with carbonyl and carboxyl groups.

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ANTIBACTERIAL ACTIVITY OF COMPLEX COMPOUNDS SYNTHESIZED ON THE BASIS OF GLUTAMINE AND N, O, S – CONTAINING LIGANDS

Ganiyev B.Sh., Mardonov U.M., Jumayeva Z.R., Avezov K.G.

*Bukhara State University,
M. Ikbol str., 11, Bukhara, 200117, Uzbekistan,
e-mail: b.sh.ganiyev@buxdu.uz*

Development of methods for the synthesis of new compounds with effective biological pharmaceuticals has been and remains an active part of modern preparative chemistry. For this purpose, the most appropriate production after organic compounds containing various products with a set of N,O,S-atoms and metal ions with nd^{1-10} electronic configuration.

One of these compounds with different reactivity and coordination methods is glutamine, which contains the same (C,H,N,O) atoms, but they have different functionality, such as: α -aminocarboxylic– $CH(NH_2)COOH$ and γ -carboxamide–in the form of $C(O)NH_2$, and due to this effect, glutamine (GlnH) as one of the two amide-amino acids is involved in many biochemical processes, like other vital analogues.

According to the results of the analysis of the above properties of glutamine, synthesized of various Cu(II), Ni(II), Zn(II), VO(II), Co(II), Cr(III) ion complex compounds with homo- and heteroligands. Studied by IR, UV and EPR spectroscopy and powder XRD methods.¹ Dimer composition of heteroligand complexes of Cu^{+2} ion with glutamine and amides was determined by EPR spectroscopy and antibacterial properties of the document were studied.

According to the results of studying the activity of complex compounds synthesized on the basis of glutamine and N, O, S-containing ligands against the pathogenic fungus *Candida albicans* and the bacterium *Pseudomonas aeruginosa*, the antibacterial properties of glutamine and thiosemicarbazide complexes. It was found to increase in the row of $Cr^{+3} < Cu^{+2} < Co^{+2}$.

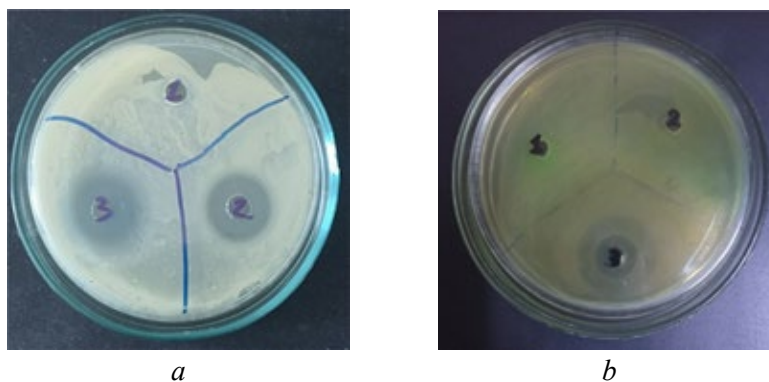


Figure 1. Activity of complexes against pathogenic *Candida albicans* fungus (a) and *Pseudomonas aeruginosa* bacterium (b)

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ORGANOTIN COMPLEXES WITH ABIRATERONE ACETATE AND ABIRATERONE: ANTIPROLIFERATIVE ACTIVITY AND MECHANISM OF CELL DEATH

Gracheva Yu.A., Zazdravnykh A.V., Antonenko T.A., Milaeva E.R.

*Lomonosov Moscow State University,
Leninskie Gory, 1/3, Moscow, 119991, Russia,
e-mail: jullina74@mail.ru*

Organotin compounds possess high antiproliferative activity, the main mechanisms of which are based on the ability of the Sn atom to bind to the SH groups of proteins, as well as to promote cellular oxidative stress. Abiraterone (AbOH) is a well-known anticancer drug that can specifically bind to the active site of CYP17A1 in certain types of cancer cells, preventing androgen production. Its prodrug is abiraterone acetate (AbOAc).

For new organotin complexes with abiraterone acetate and abiraterone of the composition $\text{Bu}_2\text{SnCl}_2 \cdot 2\text{AbOAc}$ (**1**), $\text{Ph}_2\text{SnCl}_2 \cdot 2\text{AbOAc}$ (**2**), $\text{Bu}_2\text{SnCl}_2 \cdot 2\text{AbOH}$ (**3**) and $\text{Ph}_2\text{SnCl}_2 \cdot 2\text{AbOH}$ (**4**) their antiproliferative activity against colon cancer HCT-116 and the diploid human fibroblast cell line WI-38 was studied in comparison with cisplatin. The compounds were found to be highly active; they also significantly induce apoptosis (Fig. 1).

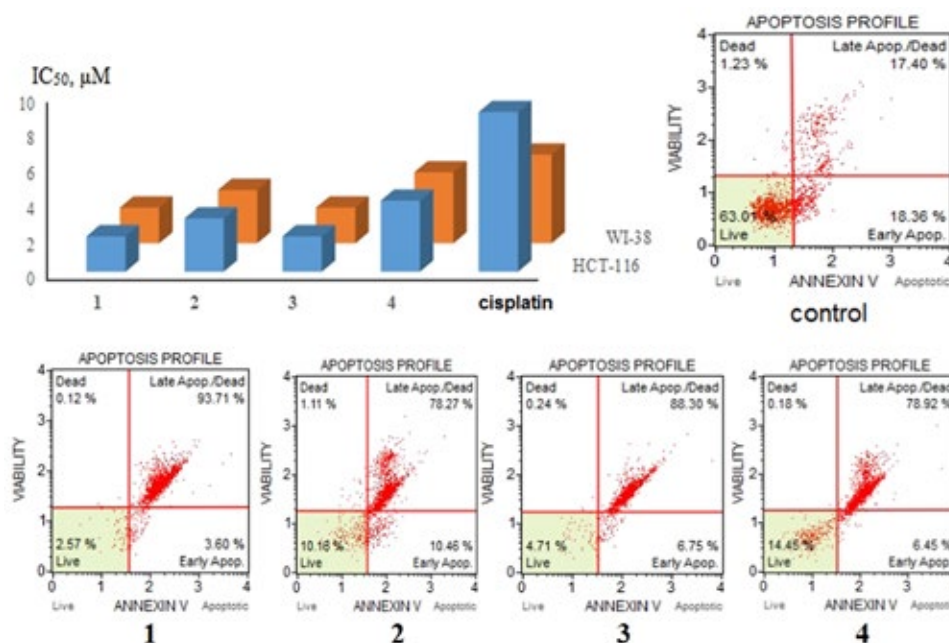


Figure 1. IC₅₀ values for compounds **1–4**, as well as apoptotic profile analysis by flow cytometry on the HCT-116 line after treatment with compounds **1–4** after 48 h

The work was carried out with the financial support of the Russian Science Foundation, grant No. 22-63-00016.

TOTAL ANTIOXIDANT CAPACITY OF ORIGANUM VULGARE

Kraynik V.V., Romanova E.V., Melnik M.V., Samoylenko Z.A.

*Surgut State University,
628403, Surgut, 1 Lenin Avenue,
e-mail: kraynik_vv@surgu.ru*

For many years, aromatic plants have been used for a large number of purposes including medicine, nutrition, cosmetics and industrial uses¹⁻².

The studied species were *Origanum vulgare* spp. (*Origanum vulgare* subsp. *Hirtum*, *Origanum vulgare* subsp. *Italian*).

Species were planted on a different conditions: (1) on vertical hydroponic ebb and flow system with mineral wool substrate with different lighting regimes: lighting with colorful diodes; lighting with white diodes; (2) in open ground³.

The Spectrophotometric Folin–Ciocalteu method was used for the determination of total phenolic content (TPC). Total antioxidant capacities of the selected aromatic plant extracts were determined by using ferric reducing antioxidant power (FRAP).

The results of this study demonstrated that the different *Origanum* species contained similar levels of TPC and antioxidant properties. Total phenol content and FRAP values ranged from 8,4 to 10,6 mg GAE/g, from 1,6 to 2,0 mmol Fe²⁺/g respectively. The results of the investigated plants are in agreement with studies that have been conducted with regard the total phenolic and FRAP of many aromatic plants belonging to this family¹⁻². It was found that their total phenolic content and FRAP values decreased in the following order: lighting with colorful diodes > lighting with white diodes ≥ in open ground.

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A GROUP OF NEMP PEPTIDASES ACTING IN THE ENVIRONMENT OF THE MAMMALIAN BRAIN AND THE PROTECTION OF MEDICINAL PEPTIDES FROM THEM

Kropotova E.S.^a, Ivleva I.S.^b, Karpenko M.N.^b, Mosevitsky M.I.^a

^a*Institute of macromolecular compounds RAS,
V. O. Bolshoy prospect 31, St. Petersburg, 199004, Russia,
e-mail: ekono@mail.ru*

^b*Institute of experimental medicine, Acad. Pavlov Street 12, St. Petersburg, 197022, Russia*

We found that in the mammalian brain (rat, cow), a group of metallopeptidases acting in the extracellular environment, called NEMP (Neuron bound Extracellular MetalloPeptidases), is associated with the axonal endings of neurons. A total of four NEMP enzymes have been found¹. Presumably, the physiological function of NEMP is the control (catabolism) of peptide neurotransmitters (neuropeptides). However, NEMP peptidases can also destroy peptides introduced into the brain from the outside for medicinal purposes. We have shown that the exopeptidases present in the NEMP group are unable to degrade the peptide if the terminal amino acid is beta-alanine. Created by us modification of the endogenous analgesic peptide enkephalin, called ModEnk2 (β Ala-Tyr-Gly-Gly-Phe-NH₂), in experiments on animals (rats) with intranasal administration provides effective prolonged analgesia². ModEnk2 is an agonist (ligand) of μ -opioid receptors. Morphine and other narcotic painkillers acting on the same receptors cause side effects harmful to the body: respiratory disorders, addiction and etc. In appropriate animal tests, we have shown that even at higher doses of ModEnk2 there are no side effects. These results mean that the analgesic peptide ModEnk2 may be a safe alternative to narcotic drugs.

We used the same method of protecting peptides to obtain a stable modification of the antimicrobial peptide LPRDA. This peptide prevents infection of cells by staphylococcus aureus, but when introduced into the body it is quickly destroyed. The modifications we created are much more stable. Their use will significantly reduce therapeutic doses. These experiments are ongoing.

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ONE-POT HPLC DETERMINATION OF GLYCINE AND HISTIDINE WITH PRE-COLUMN DERIVATIZATION WITH PHENYL ISOTHIOCYANATE

Kalmykova A.A.^{a,b}, Kustova T.P.^b, Kalmykov P.A.^a, Kustov S.O.^b

^a*GENERIUM, Zavodskaya street, p. 273, Vladimir region, Volginsky, 601125, Russia,
e-mail: a.kalmykova@generium.ru*

^b*Ivanovo State University, Ermaka street, 39, Ivanovo, 153025, Russia*

Free amino acids (histidine, glycine, arginine, etc.) are widely used as stabilizers of protein molecules, which are used to treat various orphan diseases. When producing such drugs, it is necessary to control the number of excipients, so the development of a method for determining amino acids in drugs is an urgent task.

The paper presents the results of the determination of two amino acids – glycine and histidine – in the drug of protein origin Innonafactor® by reverse-phase HPLC with pre-column derivatization with phenyl isothiocyanate (PITC).

The technique involves *one-pot* sample preparation for analysis, which, unlike multi-stage sample preparation, reduces the loss of analytes. The available equipment from the standard quality control department is used as testing equipment. An HPLC system with an ultraviolet detector and a C18 column with a grain size of 4.6 µm allows you to obtain accurate and reproducible results for the determination of glycine and histidine in the drug solution under study. A mixture of acetate buffer with pH = 3.5 and 80% acetonitrile solution are used as mobile phases, and a solution of PITC in acetonitrile is used as a derivatizing agent. The stability of the studied solutions is noted during 24 hours of storage in a thermostat at temperatures from 2 to 8 °C, which is an advantage compared to similar methods for determining amino acids, for example, derivatives with *ortho*-phthalaldehyde, the stability of which does not exceed several minutes¹.

The proposed method is universal for a wide range of amino acids due to their characteristic feature of forming a bond with PITC at the *N*-terminal amino group.

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SYNTHESIS OF NEW INDOLE-2-CARBOXYLIC ACID DERIVATIVES

Țiuleanu P., Marenin I.Y., Shchekotikhin A.E.

Department of organic chemistry, Mendeleev University of Chemical Technology of Russia,
125047, Moscow, Myusskaya sq. 9,
e-mail: iv.marenin@yandex.ru

As part of the study of the structure-activity relationships, several new indole-2-carboxylic acid derivatives promising for the development of new drugs were synthesized¹.

Indole-2-carboxylic acid ethyl ester **1** was obtained according to the Japp-Klingemann method². Subsequent hydrolysis of ester **1** led to the indole-2-carboxylic acid **2**. Obtained acid was used for the synthesis of the following compounds: esters **3** and **4** and further glycine derivatives **8**, **9**; indole-2-hydroxamic acid derivatives **5–7**. Hydrazinolysis of ester **1** yielded as hydrazide **10**. Obtained hydrazide was used for the synthesis of the following compounds: thiosemicarbazide **11** and further 2-azolilindoles **12–14**; series of arylhydrazones with main structure as **15**.

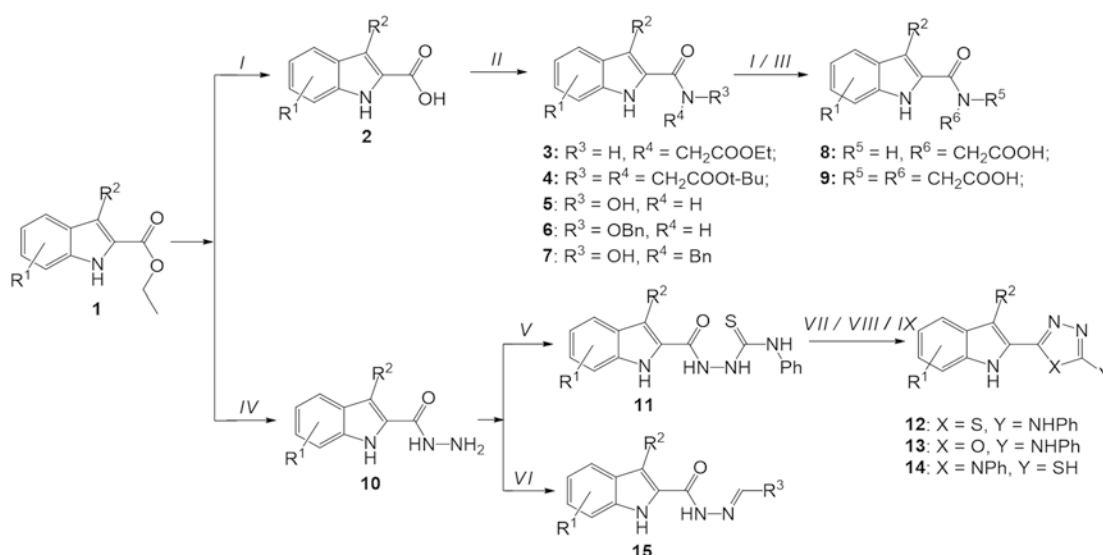


Figure 1. Synthesis procedure of indole-2-carboxylic acid derivatives.

I – THF, EtOH, 2M NaOH (**8**); II – PyBOP, DIPEA, amine or hydroxylamine, DMF;
 III – TFA, DCM (**9**); IV – N₂H₄ (51%), EtOH, 80 °C; V – PhNCS, EtOH, 80 °C; VI – ArCHO, EtOH, 80 °C;
 VII – POCl₃, PhCl, 130 °C (**12**); VIII – DCC, PhH, DMF (**13**), 80 °C; IX – 5% NaOH, 100 °C (**14**)

The structure of the compounds was confirmed using ¹H NMR, HRMS-ESI, purity (>90%) was determined by HPLC. Studies of biological properties have revealed important structure-activity relationships.

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SYNTHESIS OF WATER-SOLUBLE ADDUCTS OF DIHYDROQUERCITIN WITH AMINO ACIDS

**Tatarinov G.G.^a, Koroteev M.P.^a, Pozdeev A.O.^a, Koroteev A.M.^a,
Kaziev G.Z.^a, Stepnova A.F.^{a,b}**

*Federal State Budgetary Educational Institution of Higher Education “MPGU”,
Institute of Biology and Chemistry, Moscow, Russia,
e-mail: gavril_tatarinov@mail.ru
Peoples’ Friendship University of Russia, Faculty of Physics,
Mathematics and Natural Sciences., Moscow, Russia*

In this study, a method was developed for the synthesis of water-soluble adducts of dihydroquercitin (DHQ) with the amino acids lysine, arginine, ornithine and histidine. Their solubility is more than an order of magnitude higher than the original DHQ at 20 °C. It has been shown that the adduct of DHQ with arginine exhibits antioxidant activity 20 times higher comparatively with the original flavonoid^{1,2}.

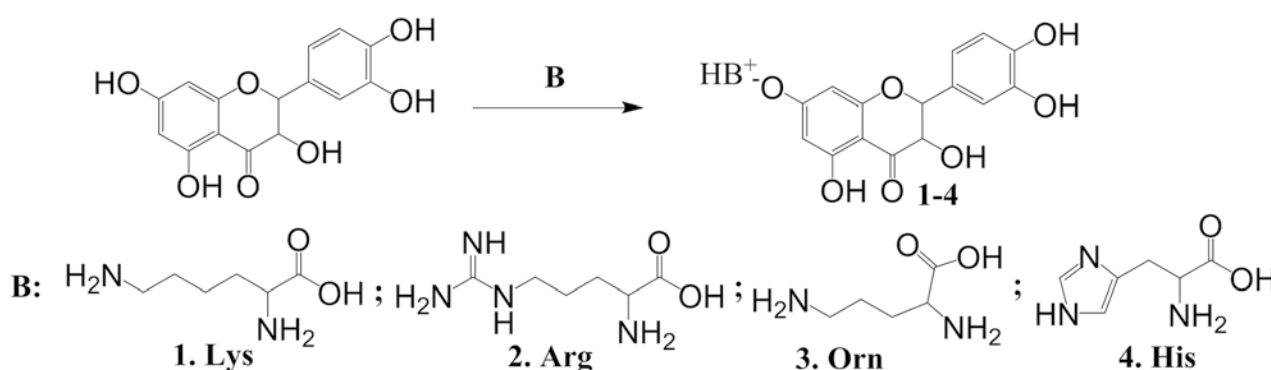


Table 1. Water solubility of derivatives 1–4 at 20 °C

Compound, №	DHQ	1	2	3	4
Solubility χ , %	0,02	54,0	33,0	16,0	1,8

The water solubility of the resulting adducts significantly exceeds the solubility of the original DHQ, which makes it possible for their wider use in the medicinal aspect.

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The work was carried out within the framework of the project “Research on the problems of recycling natural waste for the purpose of practical use of the resulting products” (122122600056-9).



LIVER MICROSOMES AS A TOOL FOR ISOTOPE-LABELED COMPOUNDS SYNTHESIS

**Tupertsev B.S.^{a,b}, Osipenko S.V.^a, Ikonnikova T.A.^a,
Nikolaev E.N.^a, Kostyukevich Y.I.^a**

^a*Skolkovo Institute of Science and Technology,
121205, Moscow, Bolshoy blvd., 30, str 1,*

^b*Moscow Institute of Physics and Technology (NRU),
141701, Dolgoprudny, Moscow Region, 9 Institutsky Lane,
e-mail: tupertsev.bs@phystech.edu*

HPLC-MS systems in preclinical and clinical studies is the gold standard in pharmacology. Despite the development of sample preparation methods, the use of wide classes of mobile and stationary chromatographic phases, the development of an instrument base, drug metabolism HPLC-MS analysis is still a challenging task. One of the main limiting factors is the matrix effect in complex biological samples. To minimize this issue, internal stable isotope labeled standards may be used: ^2H , ^{13}C , ^{15}N , ^{18}O , etc. However, their use is limited due to the synthetic difficulties of introducing isotope labels. This study aims to propose a method for the production of isotopically labeled compounds under the action of a liver microsomes (LM) in the presence of heavy water, both H_2^{18}O and D_2O .

For incubation of progestogens in heavy water, the initial phosphate buffer saline was prepared in H_2^{18}O and D_2O in accordance with the experiment. On the one hand, during incubation of compounds in the presence of H_2^{18}O heavy water, it was found that LM catalyze the $^{16}\text{O}/^{18}\text{O}$ isotope exchange reaction up to 30 times compared with the control sample of drugs in excess of H_2^{18}O without LM.

On the other hand, during the incubation of progestogens with LM in the presence of heavy water D_2O , it was found that LM also catalyze the H/D isotope exchange reaction. However, in the control sample of drugs in excess of D_2O without ML, exchange reactions in the progestogen molecules were not detected.

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The work was carried out with the financial support of the Umnik Innovation Promotion Fund, project 17643GU/2022.

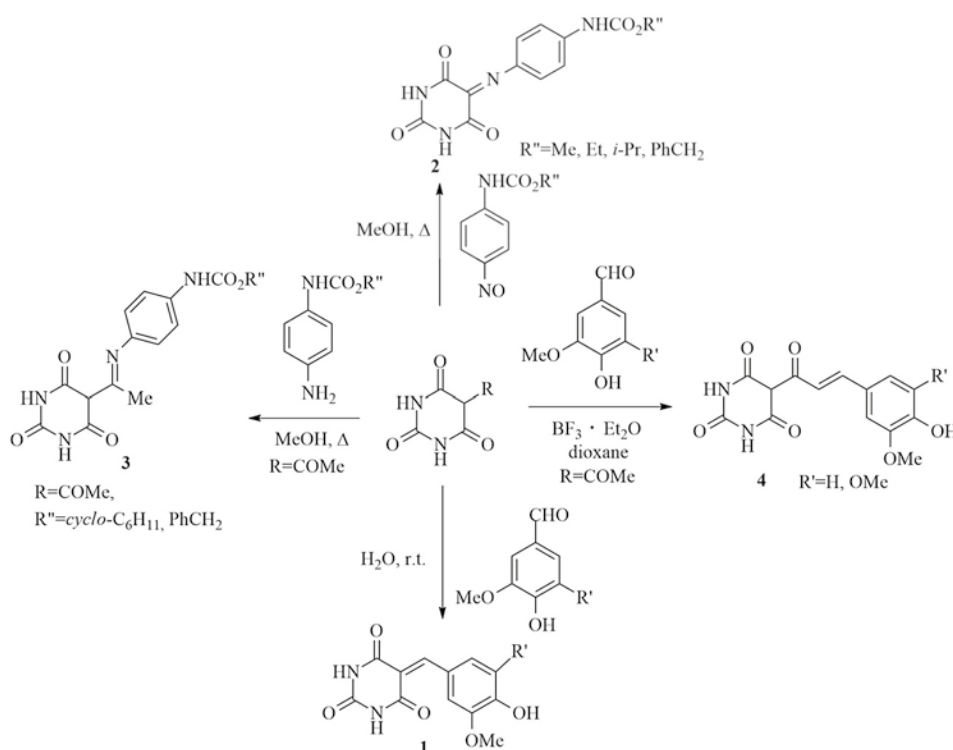
SYNTHESIS OF NEW BARBITURIC ACID DERIVATIVES

Velikorodov A.V.^a, Kutlalieva E.N.^{a,b}, Shustova E.A.^b, Kotova V.Yu.^b

^a*Astrakhan Tatishchev State University,
Shaumyan pl. 1, Astrakhan, 414000, Russia,
e-mail: avelikorodov@mail.ru*

^b*Astrakhan State Medical University, Astrakhan, 414000, Russia*

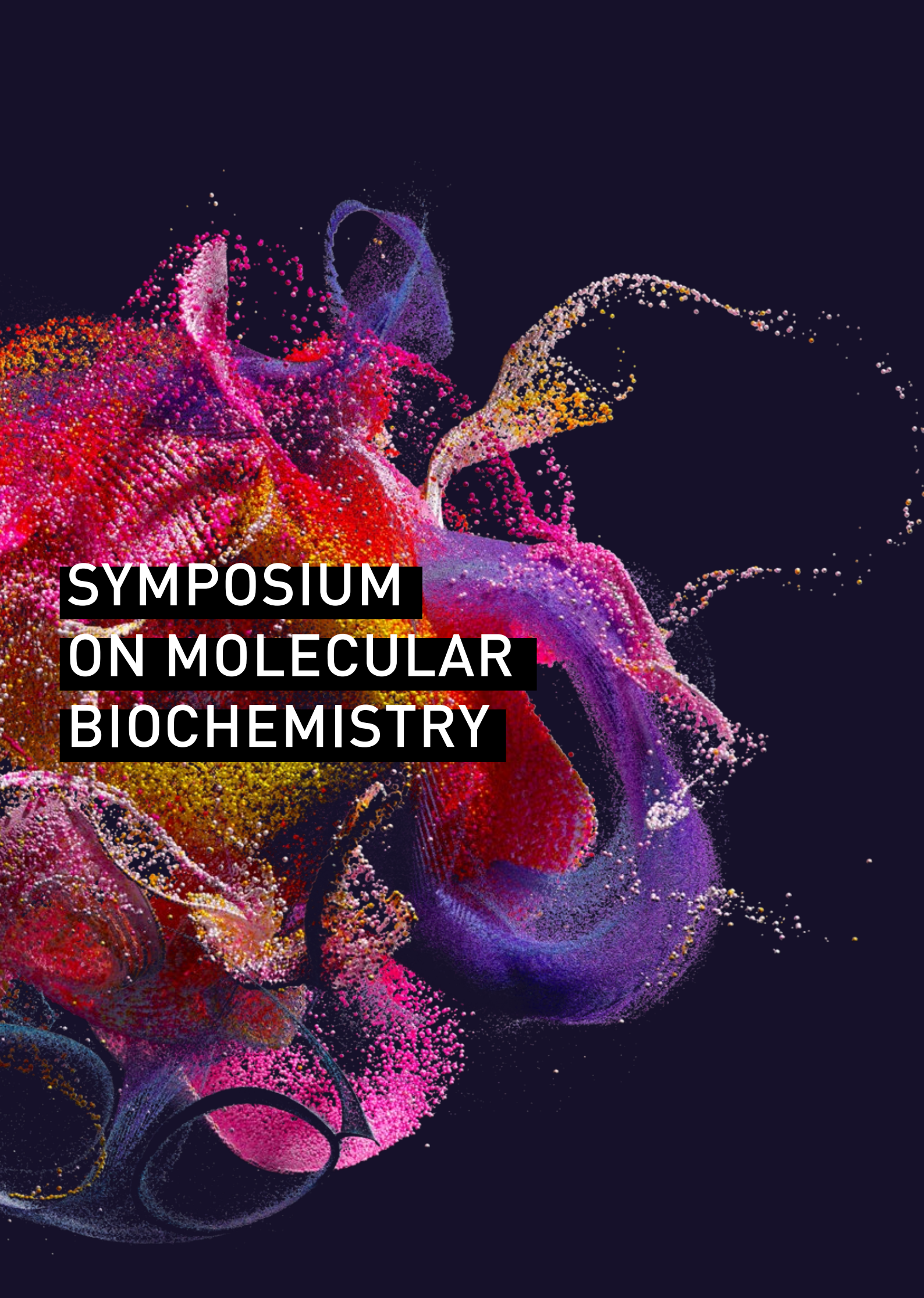
Derivatives of barbituric acid have a wide spectrum of antimicrobial activity¹. By condensation of barbituric acid (R=H) with aromatic aldehydes, as well as with alkyl N-(4-nitrosophenyl)carbamates, 5-arylidene derivatives **1** and imines **2** were obtained, respectively. Imines **3** and chalcones **4** were obtained by condensation of 5-acetylbarbituric acid² (R=COMe) with aldehydes and alkyl N-(4-aminophenyl)carbamates.



The structure of the new compounds was confirmed by IR, ¹H NMR, and ¹³C spectroscopy.

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**SYMPOSIUM
ON MOLECULAR
BIOCHEMISTRY**

FEATURES OF MOLECULES OF INORGANIC FORMS OF LIFE CAPABLE OF SELF-GENERATION BY POLYCONDENSATION

Dudenzkov I.V.

*A.A. Baikov Institute of Metallurgy and Materials Science of the RAS, 119334, Moscow, Leninsky Prospekt 49,
e-mail: idudenzkoff@mail.ru*

In the first proposed versions of informational inorganic polymers¹, the information carrier is either (a) the position of the hydrogen bond proton in a complementary pair of monomer units, or (b) the ring size of the monomer unit. For method (a), the monomer unit must also contain at least one ring so that the conformation of the unit is sufficiently rigid for reliable mutual recognition of the components of a complementary pair of units. In this case, the position of the proton, up to mutations, is predetermined by the position of O atoms or NH₂ groups in the terminal positions of the (MN)₃ rings (M = C^{+IV}, P^{+V}, S^{+VI}); local variations in oxidation states or As^{+V} impurities are also possible, Se^{+VI} or Cr^{+VI} to perform any enzymatic functions. For method (b), the proton oscillates between two positions, and the information carrier is the ring size of the monomer unit, usually (MO)₃ or (MO)₄ (M = sp³-B^{+III}, Si), but with two possible isomeric variants of the dimer structure. For the structure of bridge groups connecting such monomer units into a polymer chain, a greater variety of options is possible. Of all these variants of electropositive M atoms, only C^{+IV} is trigonal-coordinated; in other cases, M is tetrahedrally coordinated. Therefore, for boron-based life (if we do not consider purely boron-hydrogen cases, since a suitable method of complementary pairing of units is unknown for them), a pressure of at least several thousand atmospheres is required, at which H₃BO₃ will cyclically trimerize like the HBO₂-III fragment or tetramerize. Si-based life requires the presence of terminal H or SiH₃ substituents to avoid cross-linking of polymers, which can only form in extreme reducing environments. For possible Be-based life, only prototypes with (BeO)₃ cycles are known so far. The most likely inorganic life is based on (PN)₃, (SN)₃ units or their hybrids, which are sufficiently stable in liquid ammonia - the most suitable environment for inorganic life.

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INVESTIGATION OF PLASMID DNA DELIVERY BY CATIONIC LIPOSOMES BASED ON LIPID 2X3 AND HELPER LIPID DOPE ON VARIOUS CELL LINES

Mikheev A.A., Shmendel E.V., Maslov M.A.

*Lomonosov Institute of Fine Chemical Technologies, MIREA – Russian Technological University Technology,
Vernadsky Avenue 78, Moscow, 119454 Russia,
e-mail: aa-mixeev@mail.ru*

Gene therapy is one of the effective methods of treating a wide range of diseases, implemented by introducing nucleic acids (NC) into patients' cells in order to directly change gene defects or give cells new functions.

In order to find more efficient NC delivery systems, cationic liposomes (CL) based on 2X3 lipid and DOPE helper lipid prepared in various ratios have been developed.

To determine the most promising composition of CL for NC delivery, we investigated the effect of the ratio of liposome components on transfection efficiency for various cell cultures: A549, HeLa, CL-16, NIH 3T3, 4T1.

The transfecting activity of the CL series was evaluated at a different N/P ratio. The efficiency of NC CL delivery was assessed by the intensity of luminescence in the cell culture fluid due to the expression of the *pGLuc* reporter gene.

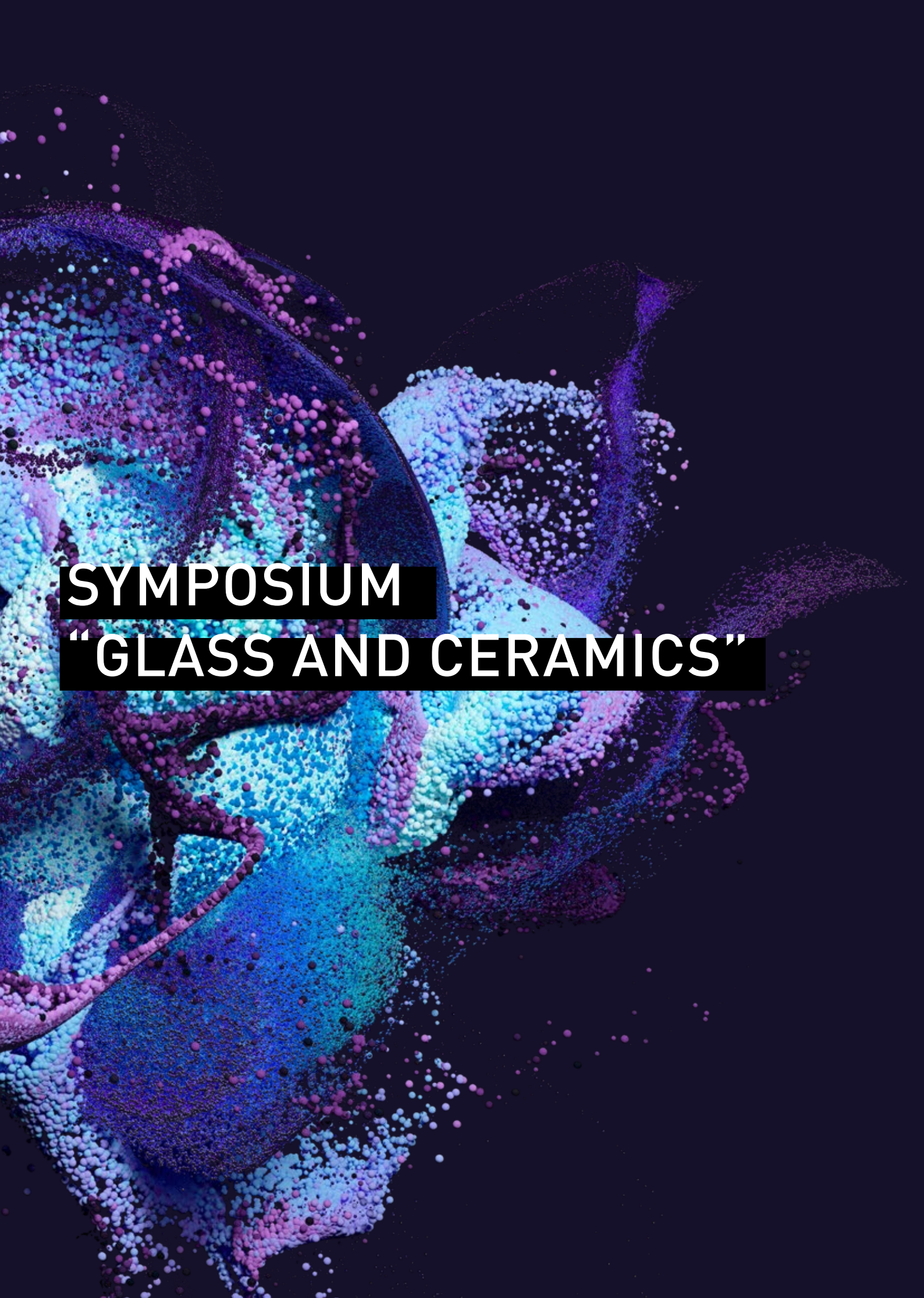
It was shown that the greatest efficiency is shown by an experimental CL sample with a ratio of lipid 2X3 to helper lipid DOPE 1:2.5 in complex with pDNA at a ratio N/P = 8/1 for all cell types studied. On cell lines CL-16, NIH 3T3, HeLa, the CL series was higher in transfection efficiency than the commercial drug Lipofectamine® 2000.

In the future, CL based on 2X3 lipid and DOPE helper lipid can be used as an alternative to commercial in vitro NC delivery systems due to their high transfecting activity and low cost.

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The research was carried out at the expense of a grant from the Russian Science Foundation No. 23-73-10168, <https://rscf.ru/project/23-73-10168>.



SYMPOSIUM “GLASS AND CERAMICS”

OLD GLASSES – NEW CHALLENGES

Sigaev V.N.

Mendeleev University of Chemical Technology, Moscow, Russia

e-mail: sigaev.v.n@muctr.ru

Glass is one of the oldest materials. By the middle of the last century, the glass-forming ability was discovered for a huge set of silicate, borate and phosphate systems, and the basic ratios "composition-conditions of production-structure-properties" were revealed in them. By the same time, basic concepts on the structure of glass were developed, and this time is quite appropriately attributed to the golden age of glass science. These concepts were formed in the era of very limited experimental possibilities of physical methods, and nevertheless, according to the X-ray scattering curves obtained in a very narrow range of scattering vector changes ($Q_{\max} \sim 5 \text{ \AA}^{-1}$) Zahariasen, Porai-Koshits et al. managed to create models of glass structure that have changed little over the past half century, despite the fact that the capabilities of diffraction methods (neutron diffraction and synchrotron radiation) - have increased immeasurably ($Q_{\max} \sim 30 \text{ \AA}^{-1}$ and more). They made it possible to significantly increase the accuracy of determining interatomic distances in a glass-forming polyhedron but the interpretation of the functions of the radial distribution of electron and nuclear density beyond the first two or three coordination spheres half a century ago and today is (and it can't be otherwise) very conditional in nature.

Therefore, the efforts of scientists are noticeably reoriented today to research the initial stages of phase separation in glasses, volumetric, surface or local micro- and nanomodification. New possibilities of physical methods have ensured the transition from the golden age of glass science to the golden age of applications, as the challenges arising from the needs of optical instrumentation, opto- and microelectronics, photonics, laser technology, medicine extremely quickly initiate new and new directions for the development of high-tech glass technologies.

The report provides a brief excursus into the history of structural glass research and, using the example of the work of the Department of Glass and Glass-ceramics of the Mendeleev University of Chemical Technology, discusses new glass-based materials and new approaches to their functionalization: - formation of birefringent polarization-dependent microstructures by a femtosecond laser beam in heat-resistant materials (silica and nanoporous glasses, transparent glass ceramics with a near-zero value of thermal expansion coefficient) and the development of a technology for super-stable (not requiring rewriting) archival optical memory on glass; direct laser writing of nonlinear optical crystalline waveguide structures of complex architecture in a glass volume; optically homogeneous glasses with a low content of a glass-forming agent (highly refractive, magneto-optical, laser); glasses nanostructured with nonlinear optical crystals with high second-order optical nonlinearity; new laser glassy media; UV and X-ray visualizers, etc.

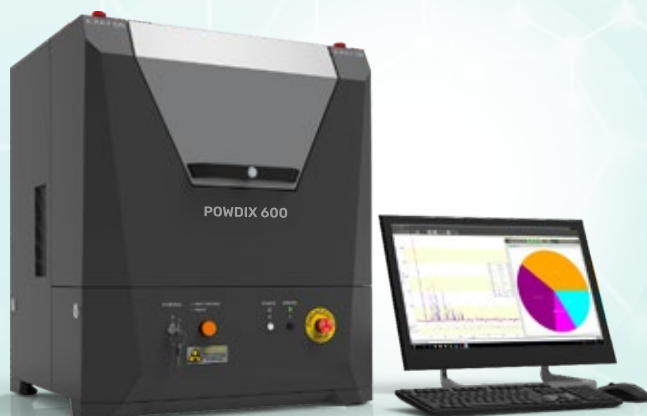
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Экологические проблемы планеты становятся все более значимыми и тревожащими, поэтому инновации, которые помогали бы эти проблемы решить, не просто привлекают интерес, а приобретают поистине глобальную актуальность. Сохранение окружающей среды и природных ресурсов для будущих поколений – суть новой этики прогресса.

ПРОГРЕСС, БЕЗОПАСНЫЙ ДЛЯ ПРИРОДЫ

Компания «ФосАгро» – лидер российской химической промышленности выступила с инициативой создания фонда для финансовой и научной поддержки перспективных ученых-химиков, в сферу интересов которых попадают охрана окружающей среды, здравоохранение, продовольствие, повышение энергоэффективности и рациональное использование природных ресурсов.

В 2013 году между ЮНЕСКО, Международным союзом теоретической и прикладной химии (IUPAC) и компанией «ФосАгро» было подписано соглашение о партнерстве в создании программы грантов для ученых, занимающихся так называемой «зеленой химией». Предметом этого направления в науке является создание производственных технологий и материалов, безопасных для природы и человека.

Так родился проект «Зеленая химия для жизни», помогающий талантливой молодежи не только материальными средствами для

продолжения исследовательской работы и реализации проектов, но и плодотворным общением со старшими коллегами – видными современными химиками, и организацией информационного обмена в научной среде. Это первый проект в истории ЮНЕСКО и ООН, реализуемый за счет средств российского бизнеса. ФосАгро выделила более \$2,5 млн на развитие и реализацию проекта.

ТРИНАДЦАТЬ МУДРЕЦОВ

Отбор заявок на участие в проекте – обязанность компетентного жюри, в которое входят 13 ученых из 11 стран. Проект-победитель должен соответствовать нескольким критериям. Оцениваются его научная новизна, глобальная и локальная значимость, соответствие принципам «зеленой химии», компетентность молодого ученого и его команды, оснащенность института и лабораторий, в которых предполагается вести проект. Качество работ очень высокое, и членам жюри приходится порой вступать в длительные диспуты по той или иной кандидатуре.

НАУЧНЫЙ ПОИСК БЕЗ ГРАНИЦ

В 2016 году был учрежден специальный грант за исследования в области применения фосфогипса. В 2019 году в штаб-квартире ЮНЕСКО в Париже в рамках открытия Года Периодической таблицы химических элементов было принято решение продлить грантовую программу «Зеленая химия для жизни».

Проблемы экологического характера, к сожалению, есть во всем мире, и во всем мире есть ученые, которые предлагают решения для многих из этих проблем методами и технологиями «зеленой химии». Это наглядно демонстрирует география проекта «Зеленая химия для жизни». За время реализации программы на рассмотрение жюри поступило более 1000 заявок, 55 грантов было присуждено молодым ученым из 33 стран. Самый главный результат грантовой программы – практическое применение разработок молодых исследователей.



ЖИЗНЬ ПОСЛЕ ГРАНТА

Дважды за первые 10 лет существования проекта победителями конкурса становились ученые из России. Одна из них – Галина Калашникова, заведующая лабораторией синтеза и исследования минералоподобных функциональных материалов Центра наноматериаловедения ФИЦ КНЦ РАН. В 2019 году грант «Зеленая химия для жизни» был присужден проекту «Разработка универсального и экологичного метода гранулирования синтетических титаносиликатных материалов (сорбентов, катализаторов, регенерируемых матриц), полученных на основе отходов региональных горно-обогатительных и металлургических производств».

Галина Калашникова:

– В рамках проекта удалось опробовать 5 разных методов грануляции для новых материалов с широким функционалом свойств (сорбенты, катализаторы для органического синтеза, керамические матрицы), которые мы синтезируем именно в нашей лаборатории. Мы смогли выбрать наиболее подходящий метод получения гранул для каждого из них, а также приоритетные нетоксичные связующие. Полученные гранулы были опробованы в качестве сорбентов для очистки жидких радиоактивных отходов от радиоизотопов 137-цезия и 90-стронция совместно с лабораторией хроматографии радиоактивных элементов и станцией переработки радиоактивных отходов Института физической химии и электрохимии им. А. Н. Фрумкина РАН.

Работа по проекту продолжается, несмотря на окончание действия гранта. Все полученные средства были потрачены только на выполнение основной задачи, благодаря чему мы приобрели необходимое оборудование, получили хороший опыт в работе с зарубежными коллегами и выстроили приоритетные направления дальнейшей совместной работы со многими научно-исследовательскими организациями.

Хочется пожелать организаторам конкурса еще больше новых проектов, которые были бы направлены на самые острые вопросы взаимосвязи экологии и современной промышленности.





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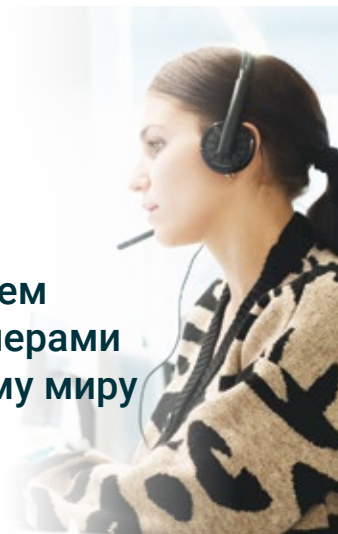
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BOOK OF ABSTRACTS

Published in the author's edition and proofreading.

Signed for printing on __.10.2024.
Format 60×90/8.
Offset paper. Digital printing.

Circulation 20 copies.
Order No.
Printed in "BukiVedi" LLC
www.bukivedi.com



7 — 12.10.2024

Federal Territory “Sirius”, Russia