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Abstracts are devoted to chemistry of solid micro- and nanostructured, thin film and molecular systems on the base of inorganic and organic substances, metals and metal complexes as well as methods of their synthesis and investigation of their chemical and phase composition, microstructure and properties. The problems of chemical education, chemistry teaching and training in schools and universities are discussed.

Тезисы докладов, посвященных проблемам химии твердотельных, микро- и наноструктурированных, тонкопленочных и молекулярных систем на основе органических и неорганических соединений, металлов и металлокомплексов, а также методам их синтеза, исследованию химического и фазового состава, микроструктуры и свойств. Обсуждаются проблемы химического образования и организации учебного процесса и преподавания химии в высшей школе.

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SYNTHESIS, PROPERTIES AND STRUCTURE OF INORGANIC COMPOUNDS. KINETICS AND MECHANISM

Sensory properties of solid solutions based on cobaltites of rare earth elements and bismuth ferrite

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The paper summarizes the results of the study of sensory properties of solid solutions based on rare-earth elements cobaltites LnCoO_3 (where $\text{Ln} = \text{La}$ and rare-earth elements), and bismuth ferrite BiFeO_3 . Cobaltites LnCoO_3 and their solid solutions undergo semiconductor – metal phase transition accompanied by the change in spin state of cobalt ions. Bismuth ferrite BiFeO_3 and its derivatives are the multiferroics and their Neel and Curie temperatures are above the room temperature ($T_N \gg 643 \text{ K}$, $T_C \gg 1083 \text{ K}$).

The investigated samples were prepared by a conventional ceramic method from the respective oxides of high purity [1] and specially developed sol-gel method [2, 3] using citric acid as the complexing agent. XRD analysis confirmed the individuality of the prepared samples. Sensory properties were investigated on thick film samples with silver contacts by means of the formula: $S = \frac{R_{\text{gas}} - R_{\text{air}}}{R_{\text{air}}} \cdot 100\%$, where S – the response (%), R_{air} – resistance of the film in the air, R_{gas} – resistance of the film in the gas-containing atmosphere.

We studied the sensitivity of the above films to the vapors of ethanol, butanol, acetone, diethyl ether, benzene, ammonia, etc. in the air.

It was shown that in all cases the dependence of S on T is nonmonotonic and had maximum lying in the region of the phase transition semiconductor–metal (in the case of solid solutions based on LnCoO_3) and between the Neel and Curie temperatures (in the case of solid solutions based on BiFeO_3).

It was also shown that the sensitivity of $\text{Bi}_{1-x}\text{Ln}_x\text{Fe}_{1-x}\text{Me}_x\text{O}_3$ films has been significantly higher than that of the films based on LnCoO_3 .

We also obtained calibration dependencies of the response of the corresponding thick films on the vapor content of the test substances (in ppm) in the air. For a number of substances they were close to the straight lines in a wide range of concentrations. The data obtained allowed us to fix quickly the achievement of lower and / or upper concentration limit of the vapors inflammation for combustible substances in the air and can be used in the development of the ecologically safe technologies.

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Thermal behaviour of the system $\text{H}_3\text{BO}_3\text{--NH}_4\text{PO}_3$

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It was shown earlier that ammonium polyphosphate NH_4PO_3 (APP) was a convenient reagent for preparation of normal and double ammonium-containing condensed phosphates [1]. The use of APP as phosphate-containing reagent allows to synthesize well-known compounds as well as new condensed phosphates which cannot be prepared by other techniques. In this way more than 20 well-known double ammonium-containing phosphates were synthesized in the systems $\text{MO--NH}_4\text{PO}_3$ and $\text{MO}_2\text{--NH}_4\text{PO}_3$: polyphosphates $\text{M}^{\text{II}}\text{NH}_4(\text{PO}_3)_3$ ($\text{M}^{\text{II}} = \text{Mg, Co, Ni, Cu, Zn, Pb}$), cyclotriphosphates $\text{M}^{\text{II}}\text{NH}_4\text{P}_3\text{O}_9$ ($\text{M}^{\text{II}} = \text{Mg, Ca, Mn, Cd}$), polyphosphates $\text{M}^{\text{II}}(\text{NH}_4)_2(\text{PO}_3)_4$ ($\text{M}^{\text{II}} = \text{Mn, Co, Zn, Cd}$), cyclotetraphosphates $\text{M}^{\text{II}}(\text{NH}_4)_2\text{P}_4\text{O}_{12}$ ($\text{M}^{\text{II}} = \text{Sr, Pb}$), cyclooctaphosphate $\text{Cu}_3(\text{NH}_4)_2\text{P}_8\text{O}_{24}$, tetraphosphates $\text{M}^{\text{IV}}(\text{NH}_4)_2\text{P}_4\text{O}_{13}$ ($\text{M}^{\text{IV}} = \text{Si, Ge}$). Furthermore, 10 new compounds were also obtained in these systems. They are orthorhombic cyclotriphosphate $\text{MnNH}_4\text{P}_3\text{O}_9$, polyphosphates $\text{M}^{\text{II}}(\text{NH}_4)_2(\text{PO}_3)_4$ ($\text{M}^{\text{II}} = \text{Mg, Ca, Ni}$) and $\text{Ni}(\text{NH}_4)_2(\text{PO}_3)_4 \cdot 2\text{H}_2\text{O}$, polyphosphates $\text{Ba}_2\text{NH}_4(\text{PO}_3)_5$ and $\text{Ba}(\text{NH}_4)_4(\text{PO}_3)_6$, tetraphosphates $\text{M}^{\text{IV}}(\text{NH}_4)_2\text{P}_4\text{O}_{13}$ ($\text{M}^{\text{IV}} = \text{Sn, Ti}$) [2, 3].

Double metal-ammonium condensed phosphates are of practical interest because they reveal flame retardant properties in polyamides [4, 5]. An advantage of these compounds for this application is their high thermal stability. In fact, polyamides are processed at high temperatures limiting the use of flame-retardants having low thermal stability. Unfortunately, the fire retardant properties of the majority of well-known double ammonium-containing phosphates are still deficient for real applications. Therefore, a search for new compounds of this family demonstrating higher efficiency is topical.

This work continues our systematic investigation of synthesis of trivalent metal phosphates in the systems $\text{M}_2\text{O}_3\text{--NH}_4\text{PO}_3$ in a wide range of temperatures and reactant ratios covering the crystallization fields of phosphates of various condensation of the anion [6–8]. The aim of this study was to establish regularities of formation of boron phosphates in the APP flux, to develop a convenient technique for synthesis of detected compounds.

Thermal behavior of the $\text{H}_3\text{BO}_3\text{--NH}_4\text{PO}_3$ system within the temperature range of 30–800 °C at the molar ratio $\text{H}_3\text{BO}_3 : \text{NH}_4\text{PO}_3 = 1 : (1\div 10)$ using STA was studied. As a result, formation of only one boron phosphate BPO_4 was determined. It was shown by XRD that this compound was a tetragonal polymorph of BPO_4 [9]. No double ammonium-containing boron phosphates were detected. Finally, the “poorness” of boron phosphate chemistry is considered.

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Particular features of crystallization and chemical nature of diphosphates in the system $\text{MnSO}_4 - \text{CoSO}_4 - \text{K}_4\text{P}_2\text{O}_7 - \text{H}_2\text{O}$

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Individual cobalt(II) and manganese(II) diphosphates are used as a basis of various modern materials such as catalysts in organic synthesis, corrosion-resistant coatings, components of lubricating fluids etc. It is perspective to synthesize solid solution based on Co(II) and Mn(II) diphosphates with a variable Co : Mn ratio on purpose to improve physico-chemical and production characteristics of the materials. The aim of this work was to find out the conditions of synthesis of solid solutions based on hydrated manganese(II) and cobalt(II) diphosphates and to determine their chemical nature.

$\text{Mn}_{2-x}\text{Co}_x\text{P}_2\text{O}_7 \cdot 5\text{H}_2\text{O}$ and $\text{Co}_{2-x}\text{Mn}_x\text{P}_2\text{O}_7 \cdot 6\text{H}_2\text{O}$ diphosphates were synthesized by interaction of the mixture of manganese(II) and cobalt(II) sulfates in the water solutions with potassium diphosphate solution, taken in a certain ratio. The most significant parameters of their synthesis has been established that appeared to be the atomic ratio of components in initial solutions $n = \text{P}_2\text{O}_7^{4-} : \Sigma\text{Me}^{2+} = 0.25$; $K = \text{Mn} : \text{Co} = 9,00,0,02$; concentration of solutions equal to 0.1 mole/l; duration of contact between a solid phase and a parent solution enough to achieve the equilibrium; temperature of 293–298 K. Using a complex of chemical and physico-chemical methods of research it was established that $\text{Mn}_{2-x}\text{Co}_x\text{P}_2\text{O}_7 \cdot 5\text{H}_2\text{O}$ and $\text{Co}_{2-x}\text{Mn}_x\text{P}_2\text{O}_7 \cdot 6\text{H}_2\text{O}$ present solid solutions of substitution with limited solubility on the basis of diphosphate-matrixes of $\text{Mn}_2\text{P}_2\text{O}_7 \cdot 5\text{H}_2\text{O}$ and $\text{Co}_2\text{P}_2\text{O}_7 \cdot 6\text{H}_2\text{O}$, which have different structure. The limits of homogeneity of solid solutions was defined as $0 < x \leq 0,83$ and $0 < x \leq 0,23$, respectively.

By X-ray diffraction method it was established that $\text{Mn}_{2-x}\text{Co}_x\text{P}_2\text{O}_7 \cdot 5\text{H}_2\text{O}$ sol-

id solutions crystallize in orthorhombic system and they were structural analogs of $\text{Mn}_2\text{P}_2\text{O}_7 \cdot 5\text{H}_2\text{O}$. $\text{Co}_{2-x}\text{Mn}_x\text{P}_2\text{O}_7 \cdot 6\text{H}_2\text{O}$ solid solutions crystallize in monoclinic system and they are structural analogs of $\text{Co}_2\text{P}_2\text{O}_7 \cdot 6\text{H}_2\text{O}$. Parameters and the volume of primary cell of the synthesized diphosphates crystalline lattice together with correlation between their values and cationic composition of diphosphates were determined.

Detailed analysis of the IR spectra of synthesized diphosphates allowed us to estimate the cation nature effect on the energy of hydrogen bonds which is realized in the structure of diphosphates. For example, the values of H-bonds energy in $\text{Mn}_{2-x}\text{Co}_x\text{P}_2\text{O}_7 \cdot 5\text{H}_2\text{O}$ vary depending on the composition of diphosphates within 9.5–40.8 kJ/mole. With the increase in cobalt(II) content in diphosphates the energy of H-bonds increases, causing an increase in the strength of the whole system of H-bonds at the transition from $\text{Mn}_2\text{P}_2\text{O}_7 \cdot 5\text{H}_2\text{O}$ to $\text{Mn}_{1,17}\text{Co}_{0,83}\text{P}_2\text{O}_7 \cdot 5\text{H}_2\text{O}$. The influence of the cation nature on diphosphate anion was appreciated. It was displayed in the change in the angle of P–O–P bridge bond. For example, the Δ values (where $\Delta = [v_{\text{as}} - v_{\text{s}}(\text{POP})] : [v_{\text{as}} + v_{\text{s}}(\text{POP})]$) for $\text{Co}_2\text{P}_2\text{O}_7 \cdot 6\text{H}_2\text{O}$, $\text{Co}_{1,80}\text{Mn}_{0,20}\text{P}_2\text{O}_7 \cdot 6\text{H}_2\text{O}$ and $\text{Co}_{1,77}\text{Mn}_{0,23}\text{P}_2\text{O}_7 \cdot 6\text{H}_2\text{O}$ are 10.94, 11.02 and 11.08 %. These changes in the Δ value characterize the gradual increase in the P–O–P bond angle and in the symmetry of unsymmetrical $\text{P}_2\text{O}_7^{4-}$ anions. Thus, for the first time the hydrated diphosphates of $\text{Mn}_{2-x}\text{Co}_x\text{P}_2\text{O}_7 \cdot 5\text{H}_2\text{O}$ ($0 < x \leq 0,83$) and $\text{Co}_{2-x}\text{Mn}_x\text{P}_2\text{O}_7 \cdot 6\text{H}_2\text{O}$ ($0 < x \leq 0,23$) composition were synthesized by the interaction in the system $\text{CoSO}_4 - \text{MnSO}_4 - \text{K}_4\text{P}_2\text{O}_7 - \text{H}_2\text{O}$. They present solid solutions of substitution with the limited solubility, which are formed owing to substitutability of isomorphic Mn(II) and Co(II) cations in the structures of $\text{Mn}_2\text{P}_2\text{O}_7 \cdot 5\text{H}_2\text{O}$ and $\text{Co}_2\text{P}_2\text{O}_7 \cdot 6\text{H}_2\text{O}$ diphosphate-matrixes. Peculiarities of diphosphates crystalline structure and their possible effect on physical and chemical properties of substituted diphosphates are discussed in the report.

Ammonium compounds as objectionable impurities in inorganic building materials made from concrete

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The presence of ammonia compounds in inorganic building materials made from cement concrete was investigated. The emission of ammonia from the building structures in the air of the building spaces leads to undesirable health hazard. The main possible reasons of ammonia accumulation in concrete are the following: cement transportation in unpurified wagons; the presence of heightened content of grinding intensifiers that are injected during cement milling; the presence of ammonia in fly ashes that are used as mineral admixture in cements and concretes; chemical modifying additive agents that are injected in concrete mixture. The aim of this work was to study the possibility of determination of free ammonia in water solu-

tions of the chemical modifying additive agents used in inorganic building concrete materials as of the main source of ammonia in concrete. The process of preparation of the solutions for potentiometric method and its applicability was analyzed. Since the range of sensitivity of ion-selective electrodes for ammonia analysis requires very diluted solutions and they do not work in any organic solutions, optimal dilutions and conditions have been determined. The Table contains the results of determination of free ammonia in pure water solutions of concrete admixtures. It was shown, the working solutions of chemical modifying additive agents had to be diluted for 100 times, their operating pH was applicable for potentiometric determination. As contrasted to pure admixtures, the water extracts from concrete dust containing different types of chemical modifying additive agents are not always applicable for potentiometric determination and in most cases require the decrease in pH values.

Table – Potentiometric determination of free ammonia in the solutions of chemical modifying additive agents

Chemical modifying additive agent	pH	Temperature, °C	Concentration, mol/dm ³	pC
Sample 1	7,22	20,2	$1,462 \cdot 10^{-4}$	3,835
Sample 2	6,77	19,8	Not found	Not found
Sample 3	6,97	19,9	Not found	Not found
Sample 4	7,13	19,8	Not found	Not found

As it was mentioned above concrete dust from inorganic building materials was also investigated. It was determined that ammonia content in inorganic cement concrete building materials strongly depends on the content of a cement including the quantity and the type of admixture and conditions of hardening of concrete as a final product. It was determined that thermomoiest treatment of hardening concrete in most cases provokes the decrease in water-soluble ammoniac compounds content.

Stability of sulphide-fucntionalized SBA-15 in aqueous medium

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The stability of mesoporous mesostructured MCM-41 and SBA-15 materials has been previously investigated [1]. In [2] the sulfide-functionalized sorbents (Fig.) based on these materials have been obtained and their potential availability for selective sequestration of heavy and noble metals from aqueous solutions was proved. The questions arise: How stable these sorbents are? How long can they function as a sorbent in solutions processing. The preliminary results on stability of sul-

fide-functionalized SBA-15 sorbents in aggressive media have been obtained. The R-S-R' type materials have been treated with water, hydrochloric, nitric and sulfuric acids, ammonia. The pickling has been carried out by processing the materials for one hour in 1 M acids and 0.1 M ammonia solutions. The solid / liquid ratio was equal to 1: 100. Similar experiments have been performed on silica gel to compare.

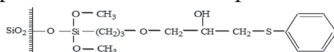


Fig. The sulfide-functionalized SBA-15 sorbent [2].

The control of pored silicate structure, organic part content and sorption ability has been realized during the pickling process. For that process the mass loss of samples has been observed. The mass loss for the functionalized silica-gel samples was greater than that for functionalized SBA-15 samples, especially in case of acidic media. We also observed an increase in the specific surface areas and pore volume during the pickling process. However, the materials have a high degree of structural order before and after the pickling process that was confirmed by accurate X-ray diffraction. The silicate framework does not degrade according to IR-spectroscopy data as well. We can observe three bands in the region 400-1200 cm^{-1} that respond to Si-O-Si vibrations in tetrahedron SiO_4 . These bands stay invariable after treatment in all aggressive media.

Nevertheless the part of organic component insignificantly decreases. This is due to the decomposition process of the surface graft layer. The graft layer decomposition leads to decreasing sulfur content and as a consequence to decreasing the sorption ability of materials. However, in these experiments we have used a very harsh environments than it is needed for practical sorption processes. Thus, these materials can be employed in different technological solutions for a long time.

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Sonochemical surface modification of galvanic nickel in the presence of vanadium acid

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The sonication of nickel films in the aqueous solution of vanadium acid results in the immobilization of vanadium oxo-compounds at the nickel surface in the form of hydrated V_2O_5 as evidenced by EDX and IR spectroscopy. The sonochemically derived epitaxial films of V_2O_5 are chemically bound to the nickel surface, with the amount of the sonodeposited V_2O_5 saturating at the level of 0.35 mmol cm^{-2} . The sonochemical

deposition involves the following stages: (i) binding of vanadates with nickel and (ii) sonoinduced polycondensation of anchored oxo(hydroxo)-species that ensure filling of nickel surface with vanadium oxide as demonstrated in the insertion in Fig.

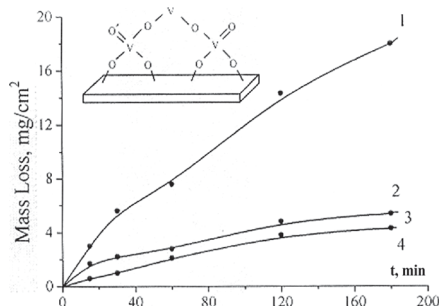


Fig. Mass loss during mechanical wearing for (1) bare nickel, (2) V_2O_5 -modified nickel, (3) benzotriazole: V_2O_5 -modified nickel. The scheme of sonochemical modification of nickel surface by vanadium oxide is given in the insert

The sonochemical modification of nickel improves the corrosion stability of nickel film (by 50%). The corrosion susceptibility exhibits 3-fold decrease after sonochemical modification in the presence of benzotriazole. IR spectroscopy points to the incorporation of benzotriazole (known to behave as a corrosion inhibitor) into the sonochemically derived film of hydrated V_2O_5 which thus plays a role of the depot for inhibiting agent.

The ultrasound-assisted deposition of surface films of V_2O_5 leads to radical (3-fold) enhancement of wear resistance of nickel coatings (most probably due to antifriction properties imparted to nickel surface by deposition of V_2O_5 of lamellar structure [1]). Further enhancement of wear resistance is observed in case of V_2O_5 films grown in the presence of benzotriazole which ensures 5-fold increase of wear resistance as compared to bare nickel. High mechanic stability of nickel coatings modified with benzotriazole-doped V_2O_5 films can be attributed to the suppression of the tribocorrosion processes.

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New hydrophosphates $MH_3(PO_4)_2 \cdot 0.5H_2O$ ($M = Er, Y$)

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Hydrogen phosphates(V) of rare earth metals are perspective as catalysts in organic synthesis, being also promising precursors in preparation of condensed

phosphates of rare earth metals. However, very scant information has appeared in the literature about these salts, because there are difficulties in their synthesis.

Here we present two new hydrophosphates of rare earth metals, namely $\text{ErH}_3(\text{PO}_4)_2 \cdot 0.5\text{H}_2\text{O}$ and $\text{YH}_3(\text{PO}_4)_2 \cdot 0.5\text{H}_2\text{O}$. Thin-layer technique, developed previously [1, 2], was used for preparation of the compounds. The crystal structures of these salts were obtained from X-ray powder diffraction data at room temperature.

Both compounds are monoclinic (S.G. $\text{P}2_1/\text{c}$) and were found to be isotypic. They reveal layered crystal structure, with metal-phosphate polymeric layers and water molecules, located in interlayer space. The atoms O2, O6, and O8 of POH groups lie to the outside of the layer near the water molecules with oxygen atom O9 (see Fig.). The hydrogen atoms of POH groups form hydrogen bonds $\text{O}-\text{H} \cdots \text{O}$ with water molecules and also intra- and interlayer hydrogen bonds with neighboring phosphate anions.

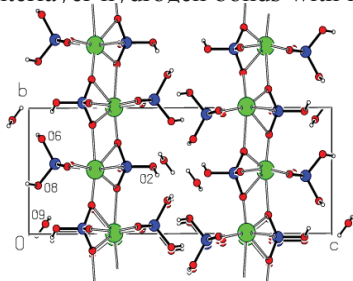


Fig. The crystal structure of $\text{ErH}_3(\text{PO}_4)_2 \cdot 0.5\text{H}_2\text{O}$ viewed along the a axis. The oxygen atoms of POH groups and water molecule are indicated.

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Crystallization of chromium condensed phosphates in the system $\text{CrO}_3 - \text{NH}_4\text{PO}_3$

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The aim of this work was to study the possibility to obtain double ammonium-containing condensed phosphates in the system $\text{CrO}_3 - \text{NH}_4\text{PO}_3$. Thermal behaviour of the system $\text{CrO}_3 - \text{NH}_4\text{PO}_3$ at the temperatures of 300 and 350 °C and molar ratio of $\text{CrO}_3 : \text{NH}_4\text{PO}_3 = 1 : 6, 1 : 12$ and $1 : 20$ has been investigated. As a result, optimal conditions for synthesis of double ammonium-containing Cr(III) triphosphate $\text{CrN}-\text{H}_4\text{HP}_3\text{O}_{10}$ (form I), cyclododekaphosphate $\text{Cr}_3(\text{NH}_4)_3\text{P}_{12}\text{O}_{36}$, cyclooctaphosphate $\text{Cr}_2(\text{NH}_4)_2\text{P}_8\text{O}_{24}$ and polyphosphate $\text{Cr}(\text{PO}_3)_3$ (form C) have been determined. For

the first time these compounds were synthesized earlier [1–3]. It has been found that an increase in temperature and/or duration of reaction causes a consecutive crystallization of chromium phosphates in the following order:



Formation of other Cr(III) phosphates was not detected during experiment.

Thermal behavior of the compound has been investigated within the temperature range of 30–800°C. It was found that both $\text{Cr}_2(\text{NH}_4)_2\text{P}_8\text{O}_{24}$ and $\text{Cr}_3(\text{NH}_4)_3\text{P}_{12}\text{O}_{36}$ demonstrate high thermal stability. They decompose at the temperature of about 500 °C.

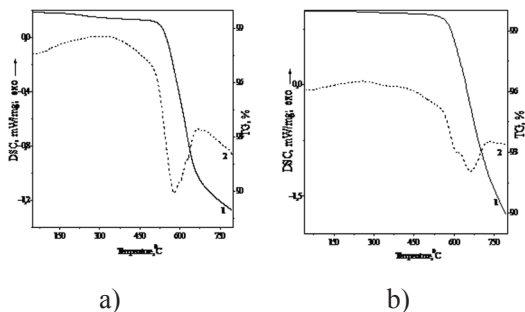


Fig. Curves TG (1) and DSC (2) of $\text{Cr}_2(\text{NH}_4)_2\text{P}_8\text{O}_{24}$ (a) and $\text{Cr}_3(\text{NH}_4)_3\text{P}_{12}\text{O}_{36}$ (b). Final crystal products of thermal decomposition of the compounds are $\text{Cr}(\text{PO}_3)_3\text{-D}$ and $\text{Cr}(\text{PO}_3)_3\text{-C}$, respectively.

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Composite materials on the base of the SiO_2 - TiO_2 , TiO_2 - Al_2O_3 systems modified by macrocyclic endorreceptors

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Composite materials based on heterocyclic endoreceptors functionalized by benzo-crown ethers, fixed on the surface or incorporated into the polymer matrix, belong to relatively new class of sorbents and catalysts that permits to resolve a number of problems in the phase transfer catalysis, organic synthesis, analytical chemistry, biology and medicine [1]. The consumption of endoreceptors can be reduced by directional change of the effective surface and other properties of the sorbent. Binary $\text{SiO}_2\text{-TiO}_2$, $\text{TiO}_2\text{-Al}_2\text{O}_3$ oxides nanoparticles. Dual Si-Ti, Ti-Al nanooxides used as macrocycle substrate are of par-

ticular interest, because they combine the positive properties of individual oxides and have certain specific characteristics, due to components interference or interaction effects [2].

Preparation of composite materials was carried out by sol-gel and co-precipitation methods using as precursors inorganic titanium, silicon and aluminum components. Introduction of dibenzo-18-crown-6, dibenzo-21-crown-7, dibenzo-24-crown-8 crown ethers was performed by two methods: 1) by stair-step sol-gel transition from dimethylformamide solution into oxide sols without side-holding components; 2) by injection into hybrid xerogels or coprecipitated powders with high specific surface area. The final step was a drying to a constant weight at 120–150°C. Method of chemical grafting of aminosubstituted dibenzo-ester as a mixture of isomers to the surface of the nanocomposites $\text{SiO}_2\text{-TiO}_2$ was used.

Targeted modification of the properties of composites was carried out by variation of the components ratio, processing temperatures, introduction of templates, structure modifiers and macrocyclic endoreceptors into sols of the oxides under mixing. For the first time using IR spectroscopy method it was shown that three benzo-crown-ethers, asymmetric dibenzo-21-crown-7 provided the strongest interaction with the surface of mixed $\text{SiO}_2\text{-TiO}_2$ nanoparticles, resulting in a distortion in the structure of the macrocycle that can affect the material sorption properties.

The results of differential-thermal analysis of the organic–mineral composite revealed that physically adsorbed water was removed at the temperatures up to 100°C. The amount of this water rose with an increase in the titanium-containing component and a reduction of an amount of the crown ether. Noticeable weight loss of the samples (10–45 %) in the temperature range 100–200°C was caused by the removal of residual solvent (DMF). It was especially typical for composites based on titanium and aluminum oxides that characterized surface properties of these composites. In the temperature range 300–500°C crown ethers and products of their thermal destruction were removed. Common weight loss amounted to 27–40 % for $\text{SiO}_2\text{-TiO}_2$ composites and to 70–75 % for $\text{TiO}_2\text{-Al}_2\text{O}_3$ composites depending on a content of crown ethers which increased from 3 to 50% in dibenzo-18-crown-6, dibenzo-21-crown-7, dibenzo-24-crown-8 crown ethers row.

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The solidphase synthesis of solid solution $(\text{Mg}_{1-x}\text{Co}_x)_2\text{P}_4\text{O}_{12}$

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Individual cobalt(II) and manganese(II) diphosphates are used as a basis of various modern materials such as catalysts in organic synthesis, corrosion-resistant coatings, components of lubricating fluids etc. It is perspective to synthesize solid solution

based on Co(II) and Mn(II) diphosphates with a variable Co : Mn ratio on purpose to improve physico-chemical and production characteristics of the materials. The aim of this work was to find out the conditions of synthesis of solid solutions based on hydrated manganese(II) and cobalt(II) diphosphates and to determine their chemical nature.

$\text{Mn}_{2-x}\text{Co}_x\text{P}_2\text{O}_7 \cdot 5\text{H}_2\text{O}$ and $\text{Co}_{2-x}\text{Mn}_x\text{P}_2\text{O}_7 \cdot 6\text{H}_2\text{O}$ diphosphates were synthesized by interaction of the mixture of manganese(II) and cobalt(II) sulfates in the water solutions with potassium diphosphate solution, taken in a certain ratio. The most significant parameters of their synthesis has been established that appeared to be the atomic ratio of components in initial solutions $n = \text{P}_2\text{O}_7^{4-} : \Sigma\text{Me}^{2+} = 0.25$; $K = \text{Mn} : \text{Co} = 9,00, 0,02$; concentration of solutions equal to 0.1 mole/l; duration of contact between a solid phase and a parent solution enough to achieve the equilibrium; temperature of 293–298 K. Using a complex of chemical and physico-chemical methods of research it was established that $\text{Mn}_{2-x}\text{Co}_x\text{P}_2\text{O}_7 \cdot 5\text{H}_2\text{O}$ and $\text{Co}_{2-x}\text{Mn}_x\text{P}_2\text{O}_7 \cdot 6\text{H}_2\text{O}$ present solid solutions of substitution with limited solubility on the basis of diphosphate-matrixes of $\text{Mn}_2\text{P}_2\text{O}_7 \cdot 5\text{H}_2\text{O}$ and $\text{Co}_2\text{P}_2\text{O}_7 \cdot 6\text{H}_2\text{O}$, which have different structure. The limits of homogeneity of solid solutions was defined as $0 < x \leq 0,83$ and $0 < x \leq 0,23$, respectively.

By X-ray diffraction method it was established that $\text{Mn}_{2-x}\text{Co}_x\text{P}_2\text{O}_7 \cdot 5\text{H}_2\text{O}$ solid solutions crystallize in orthorhombic system and they were structural analogs of $\text{Mn}_2\text{P}_2\text{O}_7 \cdot 5\text{H}_2\text{O}$. $\text{Co}_{2-x}\text{Mn}_x\text{P}_2\text{O}_7 \cdot 6\text{H}_2\text{O}$ solid solutions crystallize in monoclinic system and they are structural analogs of $\text{Co}_2\text{P}_2\text{O}_7 \cdot 6\text{H}_2\text{O}$. Parameters and the volume of primary cell of the synthesized diphosphates crystalline lattice together with correlation between their values and cationic composition of diphosphates were determined.

Detailed analysis of the IR spectra of synthesized diphosphates allowed us to estimate the cation nature effect on the energy of hydrogen bonds which is realized in the structure of diphosphates. For example, the values of H-bonds energy in $\text{Mn}_{2-x}\text{Co}_x\text{P}_2\text{O}_7 \cdot 5\text{H}_2\text{O}$ vary depending on the composition of diphosphates within 9.5–40.8 kJ/mole. With the increase in cobalt(II) content in diphosphates the energy of H-bonds increases, causing an increase in the strength of the whole system of H-bonds at the transition from $\text{Mn}_2\text{P}_2\text{O}_7 \cdot 5\text{H}_2\text{O}$ to $\text{Mn}_{1,17}\text{Co}_{0,83}\text{P}_2\text{O}_7 \cdot 5\text{H}_2\text{O}$. The influence of the cation nature on diphosphate anion was appreciated. It was displayed in the change in the angle of P–O–P bridge bond. For example, the Δ values (where $\Delta = [v_{\text{as}} - v_{\text{s}}(\text{POP})] : [v_{\text{as}} + v_{\text{s}}(\text{POP})]$) for $\text{Co}_2\text{P}_2\text{O}_7 \cdot 6\text{H}_2\text{O}$, $\text{Co}_{1,80}\text{Mn}_{0,20}\text{P}_2\text{O}_7 \cdot 6\text{H}_2\text{O}$ and $\text{Co}_{1,77}\text{Mn}_{0,23}\text{P}_2\text{O}_7 \cdot 6\text{H}_2\text{O}$ are 10.94, 11.02 and 11.08 %. These changes in the Δ value characterize the gradual increase in the P–O–P bond angle and in the symmetry of unsymmetrical $\text{P}_2\text{O}_7^{4-}$ anions.

Thus, for the first time the hydrated diphosphates of $\text{Mn}_{2-x}\text{Co}_x\text{P}_2\text{O}_7 \cdot 5\text{H}_2\text{O}$ ($0 < x \leq 0,83$) and $\text{Co}_{2-x}\text{Mn}_x\text{P}_2\text{O}_7 \cdot 6\text{H}_2\text{O}$ ($0 < x \leq 0,23$) composition were synthesized by the interaction in the system $\text{CoSO}_4 - \text{MnSO}_4 - \text{K}_4\text{P}_2\text{O}_7 - \text{H}_2\text{O}$. They present solid solutions of substitution with the limited solubility, which are formed owing to substitutability of isomorphic Mn(II) and Co(II) cations in the structures of $\text{Mn}_2\text{P}_2\text{O}_7 \cdot 5\text{H}_2\text{O}$ and $\text{Co}_2\text{P}_2\text{O}_7 \cdot 6\text{H}_2\text{O}$ diphosphate-matrixes. Peculiarities of diphosphates crystalline structure and their possible effect on physical and chemical properties of substituted diphosphates are discussed in the report.

Influence of aggressive environment and temperature on the mordenite of the Nakhchivan Autonomous Republic

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Open more than two hundred years ago natural minerals zeolites in recent years have aroused increased interest of scientists around the world. To assess the quality of the zeolite materials and to identify possible areas of their use it is necessary to know their physical-chemical properties. Thermal stability, resistance to aggressive substances are most important properties. This shows the relevance of Nakhchivan zeolites research. These zeolites consist mainly of mordenite which is of great practical importance.

The purpose of this work was the creation of physical-chemical foundation of Nakhchivan zeolites study and investigation of the influence of the aggressive media and temperature on the structure of the zeolite.

The composition of Nakhchivan zeolites and the influence of aggressive environments and temperature were investigated by methods of differential thermal analysis (NETZSCHSTA 449F3), X-ray diffraction (2DPHASER «Bruker» CuK_α , 2θ , 20–80 degrees) and microstructural (Hitachi-3000) analysis.

Effect of the aggressive environment on the Nakhchivan zeolite was investigated in concentrated sulfuric, hydrochloric and nitric acids. Zeolite was placed into three flasks with concentrated sulfuric, nitric and hydrochloric acids and treated for 10 days. After ten days it was filtered, washed with distilled water and dried for analysis. According to X-ray diffraction and microstructural analysis (Fig.) no changes in the structure of the zeolite occur, that demonstrates the resistance of zeolite to aggressive (acidic environment).

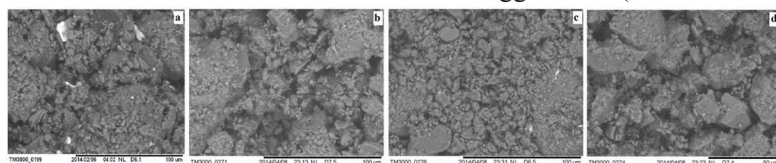


Fig. SEM photographs of zeolite surface: a – initial mordenite, b – mordenite treated with hydrochloric, c – nitric, d –sulfuric acid

The thermal stability of mordenite was studied by thermographic analysis. At 1000 °C mordenite structure does not change as shown by X-ray diffraction analysis, that shows Nakhchivan mordenite is resistant up to this temperatures. At the raising the temperature up to 1300 °C according to X-ray diffraction analysis, the structure of mordenite is destroyed.

The above confirms that Nakhchivan zeolite is resistant to aggressive environments and high temperatures (up to 1000 °C and more).

Synthesis and thermal stability of lanthanum chloride and sulfate lowest hydrates

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Different methods are used for drying air, other gases and organic liquids. Certain advantages give the methods based on the use of chemical water absorbents, especially anhydrous salts, such as chlorides and sulfates often having high hygroscopic properties. It was shown [1] that the drying power of these salts depends on their lowest hydrates thermal stability; thus the temperature dependence of these hydrates water pressure is necessary to describe the desiccant properties of anhydrous salts. The aim of this work was to obtain this information for lanthanum chloride and sulfate lowest hydrates. A derivatographic method with a special vessel having a thin capillary was used to determine the decomposition temperature of the lowest hydrates at the atmospheric pressure. Then the temperature dependence of water vapor was derived [2] by use of the approximate decomposition entropy ($146,8 \pm 4 \text{ J/mol} \cdot \text{K}$ [3]). This functional dependence (Fig.) is not very precise, but it is sufficient for the evaluation of drying power of the salts concerned.

The highest hydrates of these salts ($\text{LaCl}_3 \cdot 7\text{H}_2\text{O}$ and $\text{La}_2(\text{SO}_4)_3 \cdot 5\text{H}_2\text{O}$) were obtained by crystallization from their water solutions. The latter does not liquefy on heating in our conditions, but the chloride melts incongruently at about 90°C to give a sintered product showing too high decomposition temperatures of trihydrate and monohydrate. Therefore the lower hydrate $\text{LaCl}_3 \cdot 3\text{H}_2\text{O}$ was obtained with a method of controlled isothermal drying at the temperature 80°C . This intermediate hydrate shows no liquefying on heating and thus the minimal kinetic inhibition of the decomposition process is achieved.

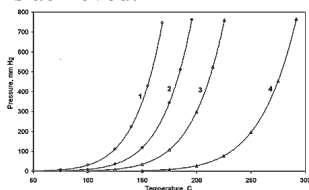


Fig. Water pressure of hydrates: LaCl_3 tri- (1) and mono- (2), $\text{La}_2(\text{SO}_4)_3$ penta- (3) and mono- (4)

Fig. Water pressure of hydrates: LaCl_3 tri- (1) and mono- (2), $\text{La}_2(\text{SO}_4)_3$ penta- (3) and mono- (4)

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Fire-retardant and weatherproof properties of nitrogen–phosphorus-containing suspensions based on dolomite and tripoli

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Fire-retardant phosphate suspensions (FRS) for wood and peat with the use of local natural mineral raw materials were developed [1]. The conditions of FRS synthesis were optimized in order to reduce the FRS cost with providing their effectiveness at the level of well-known fire-retarding agents. Acid and alkaline decomposition methods of aluminosilicate (tripoli) and calciferous-magnesium (dolomite) natural minerals with further neutralization of the reaction mixture by alkaline and acidic agents were used in the synthesis.

Studies of flame retardant, fire extinguishing properties and running ability (aggregate stability, weatherability) of synthesized suspensions were carried out. Then, the obtained data were compared with those of well-known specialized FRS. So, it was found that the flame retardant properties and storage stability of tripoli-containing suspensions increase, if a natural mineral decomposition was carried out in an alkaline solution. In the case of dolomite-containing suspensions, in contrast with tripoli-containing systems, maximum fire-resistant, fire-extinguishing efficiency to wood and peat and aggregate stability was observed for FRS synthesized by acid decomposition of the mineral.

It was found experimentally that the nature of the mineral and the amount of HCl used during the synthesis has an effect on aggregate stability of suspensions. So, P_2O_5 : HCl molar ratio should be at least 1–1.3 for suspensions with dolomite, and more than 1.7 for tripoli-containing FRS.

The dependence of suspensions' weatherability (ability of FRS to keep fire tests after water treatment of flame-retarded wood) on the content of dispersed components and the degree of their dispersion was revealed. Thus, maximum weatherability was shown for suspensions in which content of the dispersed components was not less than 30 %. 70–80 % of the particles were smaller than 5 μm when 30–37 % of them were smaller than 2 μm . It has been suggested that the fine-dispersed component of FRS provides deep penetration of fire retardants into the surface layer of wood, that allows them keeping steadily on the surface without their washing away under moisture impact. These factors have to be considered in the synthesis of weatherproof FRS.

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Properties of lead sulfide films deposited from $[\text{Pb}(\text{CH}_3\text{COO})_2(\text{N}_2\text{H}_4\text{CS})_2]$ complex compound

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Lead sulfide is one of main materials used as detectors of infrared radiation in semiconductor optoelectronics. The infrared sensors and transducers used in night vision instruments and thermal systems for missile targeting are created on its basis. So, developing technologies for creating lead sulfide films with specific optical and photoelectric properties and crystal structures is of great interest. The pyrolysis of aerosols of thiourea coordination compounds (TCC) is one of the simplest and cheapest ways of accomplishing this, and it allows us to obtain high quality samples with specific properties [1, 2]. The aim of this work was to study the optical properties and structure of lead sulfide films deposited from $[\text{Pb}(\text{CH}_3\text{COO})_2(\text{N}_2\text{H}_4\text{CS})_2]$ complex compound.

Lead sulfide films were prepared via pyrolysis of an aerosol from water solutions of thiourea coordination compounds $[\text{Pb}(\text{CH}_3\text{COO})_2(\text{N}_2\text{H}_4\text{CS})_2]$ formed during interaction between lead acetate ($C_{\text{Me}} = 0.1 \text{ mol/l}$) and thiourea ($C_{\text{thio}} = 0.1\text{--}0.5 \text{ mol/l}$). For complexation we used $\text{Pb}(\text{CH}_3\text{COO})_2 \cdot 4\text{H}_2\text{O}$ salt of chemically pure grade and thiourea $\text{N}_2\text{H}_4\text{CS}$ of extra pure (9–5) grade. Melt quartz plates $0.3 \mu\text{m}$ thick were used as substrates. The substrate temperature during pyrolysis was ranged from 250 to 450°C . The time of film deposition varied from 1.5 to 2.5 min. The films had a high degree of continuity and shiny surface. Studies of surface properties via atomic force microscopy (AFM) showed that the size of the conglomerates surface varies from 110 to 120 nm depending on the deposition temperature. XRD analysis showed that the films were structured lead sulfide. The crystallite size determined from the broadening of a specific diffraction peak (200) was changing with the deposition temperature increase at close to a linear law between 11 and 52 nm. Intrinsic absorption spectrum as measured by Fourier spectrometer in the wavelength range of $0.7\text{--}1.5 \mu\text{m}$ showed that the main mechanism of absorption in this area is indirect allowed transitions, the energy of which varies little depending on the technological parameters of the production of films ($E_{\text{gid}} = 0,47 \pm 0,2 \text{ eV}$).

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The obtained nanoparticles AgInS_2 in $\text{AgNO}_3\text{--In}_2\text{S}_3\text{--C}_2\text{H}_4(\text{NH}_2)_2$ systems

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Ternary $\text{A}^{\text{I}}\text{B}^{\text{III}}\text{C}_2^{\text{VI}}$ compounds are among the important functional materials of modern technology. Most of this class of compounds are widely used or are considered as promising materials with valuable semiconductor, photo-, ferro- and thermoelectric properties. This shows the relevance of research the preparation of nanoparticles of AgInS_2 in $\text{AgNO}_3\text{--In}_2\text{S}_3\text{--C}_2\text{H}_4(\text{NH}_2)_2$ systems.

The purpose of this work was to study of physical-chemical foundations of nanoparticles of AgInS_2 preparation in ethylenediamine environment.

To investigate the conditions for obtaining, structure and properties of the AgInS_2 compound differential thermal (DTA), X-ray diffraction (XRD) and microstructural (MSA) analysis methods were used.

As precursors for AgInS_2 compounds synthesis in the ethylenediamine medium silver nitrate (AgNO_3) and indium sulfide (In_2S_3) were used. At first In_2S_3 was obtained by the interaction of InCl_3 with $\text{CH}_3\text{CS}(\text{NH}_2)$. Then In_2S_3 with AgNO_3 in an environment of ethylenediamine at molar ratio 3: 2, respectively, were mixed for synthesis of AgInS_2 compound and it was transferred into an autoclave. The resulting precipitate was washed several times with distilled water and ethanol, then dried at 353 K in a vacuum oven for 2 hours. The results of microstructural analysis (HITACHI TM3000) have shown that the synthesized compound consists of nanoparticles. Depending on the concentrations of the components and the temperatures particle of different size and shape were obtained.

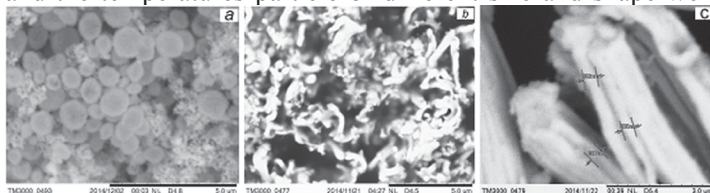


Fig. Micrographs of AgInS_2 nanoparticles obtained: a – 383 K, b – 410 K, c – 450 K

By the DTA and XRD methods the individuality of the resulting compound was proved. Crystallographic studies of the samples have been conducted with X-ray diffractometers 2D PHASER “Bruker” (CuK_α , 2 θ , 20–80 deg.). According to XRD data it was revealed that at 383–450 K AgInS_2 is mainly in the amorphous state. The intensity of the diffraction lines of AgInS_2 after thermal treatment corresponds to the literature data [1, 2].

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Synthesis and chemical nature of the products of Co(II) and Mg phosphates coprecipitation

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The work carried out in terms of diversification of hydrated phosphates that contain two different cations in their composition the contents of which can be purposely changed. Thereby their physico-chemical and exploitation properties could be changed in the wide limits.

The aim of this work was to determine the composition and chemical nature of the products of cobalt(II) and magnesium phosphate coprecipitation.

The joint precipitation of Co^{2+} and Mg^{2+} cations was carried out under conditions that provide the formation of the secondary hydrated phosphates. Specific conditions of precipitation were chosen for separate series of experiments depending on the composition of the solid phase from the main process parameters. pH of the reaction solutions was changed using aqueous solutions of Na_2HPO_4 , Na_3PO_4 or their mixture $\text{Na}_2\text{HPO}_4 : \text{Na}_3\text{PO}_4 = 2 : 1$ and $\text{Na}_2\text{HPO}_4 : \text{Na}_3\text{PO}_4 = 1 : 1$ as precipitator. Correlation in the initial solutions $n = \text{P} / \sum \text{Co}^{2+}, \text{Mg}^{2+}$ was maintained equal to 0.67 that was stoichiometric and it was necessary for the formation of secondary phosphates of divalent metals. Correlation of cations $K = \text{Co}^{2+} / \text{Mg}^{2+}$ was varied within the range from 25.0 to 1.5. Concentration of the solutions was changed in the range of 0.05–0.25 mol/l, the deposition temperature was maintained in the range of 50–75 °C.

The results of complex analyzes of the solid phase showed that at the values $K = \text{Co}^{2+} / \text{Mg}^{2+} = 25.0$ –1.6 octahydrate secondary phosphates were formed. They contained both Co^{2+} and Mg^{2+} cations. The ratio of cations could be changed within wide limits by the variation of composition of the initial reagents (Table).

Correlation $K = \text{Co}/\text{Mg}$, mol	The composition of the solid phase				
	Chemical, wt. %				Phase
	Co	Mg	P	H ₂ O	
25.0	41.77	0.54	13.62	15.86	$\text{Co}_{2.9}\text{Mg}_{0.1}(\text{PO}_4)_2 \cdot 8\text{H}_2\text{O}$
9.0	40.15	1.35	13.50	15.92	$\text{Co}_{2.75}\text{Mg}_{0.25}(\text{PO}_4)_2 \cdot 8\text{H}_2\text{O}$
4.0	37.48	2.74	14.22	16.23	$\text{Co}_{2.51}\text{Mg}_{0.49}(\text{PO}_4)_2 \cdot 8\text{H}_2\text{O}$
2.5	34.70	4.13	14.31	16.63	$\text{Co}_{2.27}\text{Mg}_{0.73}(\text{PO}_4)_2 \cdot 8\text{H}_2\text{O}$
1.6	31.36	5.83	14.87	17.26	$\text{Co}_{2.0}\text{Mg}_{1.0}(\text{PO}_4)_2 \cdot 8\text{H}_2\text{O}$
1.5	28.49	8.36	15.79	17.02	The mechanical mixture of two phases: $\text{Co}_{2.9}\text{Mg}(\text{PO}_4)_2 \cdot 8\text{H}_2\text{O} + \text{MgHPO}_4 \cdot 3\text{H}_2\text{O}$

Table – The dependence of $\text{Co}_{3-x}\text{Mg}_x(\text{PO}_4)_2 \cdot 8\text{H}_2\text{O}$ ($0 < x \leq 1.00$) phosphates composition on the ratio $K = \text{Co}/\text{Mg}$ in the initial solutions (precipitator was $\text{Na}_2\text{HPO}_4 : \text{Na}_3\text{PO}_4 = 1 : 1$)

The general formula of precipitated phosphates was $\text{Co}_{3-x}\text{Mg}_x(\text{PO}_4)_2 \cdot 8\text{H}_2\text{O}$. The synthesized phosphates presented themselves solid solution of substitution. The re-

gion of homogeneity at the use of $\text{Na}_2\text{HPO}_4 : \text{Na}_3\text{PO}_4 = 1 : 1$ as a precipitator was maximal and could be varied in the limits $0 < x \leq 1.00$. The saturated solid solution what formed under these conditions which had the composition of $\text{Co}_{2.0}\text{Mg}_{1.0}(\text{PO}_4)_2 \cdot 8\text{H}_2\text{O}$.

If an aqueous Na_2HPO_4 solution was used as a precipitator the range of homogeneity of $\text{Co}_{3-x}\text{Mg}_x(\text{PO}_4)_2 \cdot 8\text{H}_2\text{O}$ solid solution was $0 < x \leq 0.54$ or at $\text{Na}_2\text{HPO}_4 : \text{Na}_3\text{PO}_4 = 2 : 1$ it was varied in the limits of $0 < x \leq 0.70$. Trying to obtain octahydrate $\text{Co(II)}\text{--Mg}$ phosphate with magnesium content larger than 5.83 wt. % ($K = \text{Co}^{2+}/\text{Mg}^{2+} < 1.6$) the precipitation of mechanical mixture of two crystalline phases occurred.

Instruments and chemical sensors for the control of gases leaks on the enterprises of “Belneftekhim” concern for oil and chemistry

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Among important analytical tasks one should concern the task of sensing devices development for the systems of anti-wreck automatic protection, technical processes automatic control, and local detection of under explosive concentrations of burning gases and vapors of volatile flammable liquids on the enterprises for gas, oil and chemical industry, and also on other enterprises, where formation of dangerously explosive mediums is possible.

Enterprise INNOVATSENSOR starting from 1998 solves the tasks of such kind and develops devices on the basis of the sensors worked out jointly with the researchers of the Belarusian State University. The goal of these investigations is to ensure import substitution on the enterprises of “Belneftekhim” concern. INNOVATSENSOR enterprise possesses the special permission (licence) of the Department for work safety supervision in industry of the Emergency Situations Ministry of the Republic of Belarus for the activities in the area of industrial security. All the types of sensing devices are included into the list of state registration of the State Committee for Standardization of the Republic of Belarus.

At the present time INNOVATSENSOR enterprise produces sensors and gas analyzers on their basis for the following purposes.

1. Control of the under explosive concentrations of dimethylformamide with its content in the air in the range from 0 to 50% (“Polimir” plant, OJSC “Naftan”, Novopolotsk).
2. Control of the under explosive concentrations of carbon disulfide in the air of working area and storage rooms (OJSC “SvetlogorskKhimvolokno”, Svetlogorsk).
3. Persistent automatic measurement of methane volume concentration in air in the salt mines (JSC “Belaruskali”, Soligorsk).
4. Control of the under explosive concentrations of methane on the compressor stations of gas transmittal pipelines of JSC “Beltransgas”, and in the closed stalls of garage

for compressed gas transport (Gas Transmittal Pipelines Administration, Neswizh).

5. Control of the under explosive concentrations of ethyl alcohol in the working areas of JSC “Dionis Grape Wines Factory” (Minsk region).

6. Control of the under explosive concentrations on paint and varnish manufacturing line of PUE “Ruzhansk furniture factory” (Ruzhany, Brest region).

7. Control of the under explosive concentrations of fatty acids methyl ethers on the fabrication system of Organic Synthesis Plant, OJSC “Mogilevkhimvolokno”.

In the report scientific approaches to development of the existent and prospective types of sensors, which find or can find application for the above mentioned purposes, are discussed.

Electrochemical deposition of calcium phosphates in polyvinyl alcohol

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Synthesis of calcium phosphates in aqueous-polymeric media is one of the methods for regulation of their phase composition, structure and physiochemical properties [1–5]. The aim of this work is to obtain calcium phosphates in polyvinyl alcohol (PVA) media by a chemical interaction of Ca^{2+} with HPO_4^{2-} ions and to deposited calcium phosphates with electrochemical methods on the titanium substrate from aqueous solutions containing PVA, Ca^{2+} and H_2PO_4^- ions. Composite films based on brushite and PVA were prepared by the treatment of PVA– CaCl_2 film with $(\text{NH}_4)_2\text{HPO}_4$ solution at a ratio of $\text{Ca} : \text{P} = 1.67$ and pH 7–8 (Fig. a). Treatment of brushite / PVA films by ammonia solution (pH 10–11) leads to the transformation of brushite to amorphous calcium phosphate. Electrochemical deposition on a titanium substrate in $\text{CaCl}_2 / \text{NH}_4\text{H}_2\text{PO}_4 / \text{PVA}$ electrolyte with a ratio of $\text{Ca} : \text{P} = 1.67$ and pH 3–5 was used for the preparation of composite coatings consisting of brushite and basic calcium phosphate particles distributed in PVA film (Fig. b). Brushite and portlandite particles were deposited in PVA films under constant current (20 mA/ cm^2) during 10–20 min. Brushite, octacalcium-phosphate and hydroxyapatite particles were prepared at a constant voltage (20 V) during 10–30 min. The films enriched with basic calcium phosphates can be used as bio-coatings on implants for improving their degree of osseointegration.

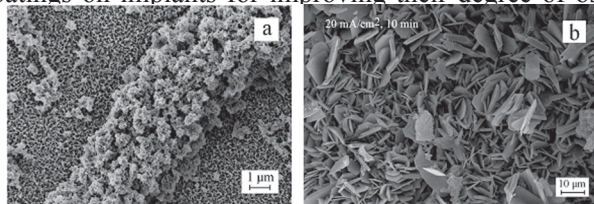


Fig. SEM images of calcium phosphates composite films (a) and coatings (b) in PVA media

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The composition of the products of Co (II) -Zn dihyphosphates heat treatment under isothermal conditions

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Polymeric phosphates of bivalent metals are widely used as the basis for creating various inorganic materials. For practical realization of their synthesis by heat treatment of hydrated salts the data on their composition, formation temperature and thermal stability of the products of partial and complete dehydration are needed. Such data on the products of Co(II) –Zn dihydrogen phosphates heat treatment under isothermal conditions are absent in the literature. Their preparation is the aim of this work.

Heat treatment of $\text{Co}_{1-x}\text{Zn}_x(\text{H}_2\text{PO}_4)_2 \cdot 2\text{H}_2\text{O}$ ($0 < x < 1.0$) was performed in the range of 100–350 °C (± 5 °C). The sample was held at a predetermined temperature for 0.5, 1.5, 3.0, 5.0 and 7.0 hours. The total phosphorus content and anionic composition were determined with quantifying the percentage of each of the polymeric phosphates in the dehydration products.

According to our data, at the heat treatment of $\text{Co}_{0.5}\text{Zn}_{0.5}(\text{H}_2\text{PO}_4)_2 \cdot 2\text{H}_2\text{O}$ at 100 °C for 0.5–7 hours a heterophase mixture of solid and liquid phases containing only monophosphate anion is formed. Condensation of the anion in the solid phase begins upon heating up to 150 °C starting a crystalline hydrate. Its treatment at this temperature for 0.5 hours leads to the formation of 12.6 wt. % diphosphate and 1.2 wt. % triphosphate. At the increase in the calcination time to 7 hours the degree of polycondensation of the phosphate anion (n) rose to 4. The most complex mixture of polymeric phosphates with linear structure of the anion (the n value reaches 9) is formed on calcining $\text{Co}_{0.5}\text{Zn}_{0.5}(\text{H}_2\text{PO}_4)_2 \cdot 2\text{H}_2\text{O}$ for 7 hours at 225 °C.

Phosphate with cyclic anion structure, cyclotetraphosphate (up to 5.8 wt. % in terms of P_2O_5), has been identified in the products of $\text{Co}_{0.5}\text{Zn}_{0.5}(\text{H}_2\text{PO}_4)_2 \cdot 2\text{H}_2\text{O}$ heat treatment at 275 °C for 3 hours. An increase in the calcination time at this temperature to 7 hours results in the simplification of the anionic composition of the heat treatment product. It consists of cyclotetraphosphate up to 86 % of the total

P₂O₅ content. The solid phase obtained at 350 °C practically completely is formed by the condensed phosphate which is CoZnP₄O₁₂ anhydrous cyclotetraphosphate.

The total percentage of free phosphoric acids in the heat treatment products of Co_{0.5}Zn_{0.5}(H₂PO₄)₂·2H₂O is maximal, when it is heated for 0.5 hour at 150°C. It presents 8.8 wt.% of P₂O₅ in the form of monophosphate acid. Anionic condensation processes begin at prolonging the heat treatment to 1.5 hours.

Besides monophosphate acid, diphosphate acid (up to 6 % of the total P₂O₅) is formed. The similar changes in the anionic composition of the acid component occur at heat treatment in the range of 150–185 °C. When the temperature rises to 350 °C the percentage of free phosphoric acids decreases. They are absent in the products of thermal treatment of Co_{0.5}Zn_{0.5}(H₂PO₄)₂·2H₂O at 350 °C.

The results obtained make it possible to select the optimum conditions for the synthesis of dihydrophosphates Co_{1-x}Zn_x(H₂PO₄)₂·2H₂O with different composition and structure of the anion polymeric products of heat treatment. Changing the value of x in the range 0 < x < 1.0 does not almost affect on their composition. When increasing the percentage of cobalt(II), the temperature ranges of polymeric products formation shifts by 10–15 °C to higher temperatures.

On the participation of crystalline hydrate water in the solid phase Mn₂P₂O₇ · 5H₂O hydrolysis

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Dehydration of hydrated salts is often accompanied by their solid-phase hydrolysis. It causes significant complications of thermal and structural transformations of crystalline hydrates, in particular the phenomenon of polycondensation of phosphate anion. However, it is not insufficiently studied.

The purpose of this work is to establish the sequence of thermal and structural transformations accompanying thermolysis of Mn₂P₂O₇ · 5H₂O and the participation of crystalline hydrate water in its solid phase hydrolysis.

Thermolysis of Mn₂P₂O₇ · 5H₂O was studied in the range of 298–1273 K under dynamic and quasi-isothermal heating conditions (derivatograph Q-1500D). Heat treatment products were obtained at temperatures of thermal effects on DTA curves and identified using methods of analysis: chemical, X-ray phase analysis, infrared spectroscopy.

According to thermoanalytical experiment, the removal of 1.44 moles of H₂O from Mn₂P₂O₇ · 5H₂O (first stage of dehydration) occurs by the molecular mechanism. The main structural motif of the original crystalline hydrate is retained. Structural changes are recorded by removing 3.96 moles of H₂O (second stage

of dehydration). Heating $\text{Mn}_2\text{P}_2\text{O}_7 \cdot 5\text{H}_2\text{O}$ to 463 K results in the formation of a mixture of two solid phases: $\text{Mn}_2\text{P}_2\text{O}_7 \cdot 2\text{H}_2\text{O}$ (38.2 wt. % in terms of P_2O_5) and X-ray amorphous monophosphate (8.7 wt.%). Its formation is due to the hydrolytic breaking of P–O–P bonds with the participation of crystalline hydrate water.

The composition of the products of $\text{Mn}_2\text{P}_2\text{O}_7 \cdot 5\text{H}_2\text{O}$ heating to 573 K is the most complex. In addition to mono- (11.5 wt. %) and diphosphate anion (32.1 wt. %), they contain phosphate with higher degree of polycondensation that is triphosphate (4.3 wt.%). Interpretation of the results shows the realization of a dissociative mechanism of water removal, which leads to solid-phase hydrolysis of the salt. The first step of this process is the formation of the groups of P–OH and M–OH type. They are capable to polycondensation at higher temperatures.

Using the maximum degree of polycondensation (n) as a measure of the solid-phase hydrolysis degree, it was found that in case of $\text{Mn}_2\text{P}_2\text{O}_7 \cdot 5\text{H}_2\text{O}$ thermolysis $n = 3$ that is 2.0–2.5 times lower than in case of $\text{Co}_2\text{P}_2\text{O}_7 \cdot 6\text{H}_2\text{O}$ thermolysis when $n = 7$. The obtained data are correlating with the energy state of crystalline hydrate water in these diphosphates. The energy of H-bonds in the structure of $\text{Mn}_2\text{P}_2\text{O}_7 \cdot 5\text{H}_2\text{O}$ is 40 kJ/mol, and in that of $\text{Co}_2\text{P}_2\text{O}_7 \cdot 6\text{H}_2\text{O}$ it makes 45 kJ/mol. This leads to a stronger phosphate anion polymerization.

The removal of another portion of crystalline hydrate water from $\text{Mn}_2\text{P}_2\text{O}_7 \cdot 5\text{H}_2\text{O}$ in the range of 573–603 K leads to a simplification of the anionic composition of the thermolysis products. Owing to their solid-state interaction, the final product, anhydrous crystalline diphosphate $\text{Mn}_2\text{P}_2\text{O}_7$, is formed.

The formation of $\text{Mn}_2\text{P}_2\text{O}_7$ takes place by two routes at the same time. The first route involves the classical thermal dehydration of $\text{Mn}_2\text{P}_2\text{O}_7 \cdot 5\text{H}_2\text{O}$ (it is realized at 70 %). According to the second route, up to 30 % $\text{Mn}_2\text{P}_2\text{O}_7$ is formed as a result of solid-phase hydrolysis of $\text{Mn}_2\text{P}_2\text{O}_7 \cdot 5\text{H}_2\text{O}$ involving crystalline hydrate water.

Microwave synthesis of YFeO_3

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Microwave radiation acting directly on the reaction mixture leads to higher rate of the chemical reaction as compared with the thermal heating. Sodium hydroxide NaOH (20 %, analytical grade, Russian State Standard GOST 432877), yttrium nitrate $\text{Y}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$ (analytical grade, CAS 13494-98) and iron nitrate (III) $\text{Fe}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$ (pure, TU 6-09-02-553-96) were used as precursors for the synthesis of YFeO_3 .

The reaction of yttrium ferrite precipitating was carried out under microwave irradiation on the precursors solution at 700 W during 26 min. After cooling to room temperature, yttrium ferrite precipitate was separated from the solution by filtration, air dried and annealed in a muffle oven for two hours

at 800 °C. According to the XRD the sample is almost pure YFeO_3 with minor inclusions of Y_2O_3 and Fe_2O_3 . The average particle size is about 40 nm.

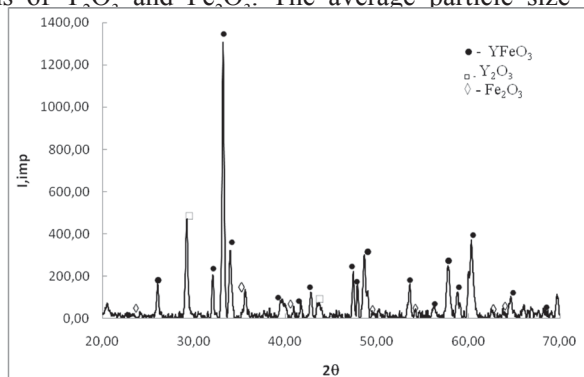


Fig. The diffractogram of YFeO_3 , synthesized under microwave irradiation.

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Study of synthesis condition of silver antimony selenide by hydrothermal method

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Analysis of literary material shows that for AgSbSe_2 , only thin films by vacuum thermal evaporation have been obtained. With regard to the production of nano- and microparticles of AgSbSe_2 , data are not available in the literature. The influence of the deposition conditions of amorphous-crystalline nano- and microparticles of AgSbSe_2 from ethylene glycol solutions on their morphology is investigated in the present work.

The mixture of potassium antimonyl tartrate with silver chloride (1) was mixed with ethylene glycol; then sodium selenosulfate was added to the mixture as a selenizing reactant. Experimental glassware in a teflon cell was placed in a microwave electric oven Speedwave four BERGHOF (Germany). The sample was stored in the oven for 10 h at a temperature of 433 K. The resulting precipitate was filtered through a glass filter, washed with diluted solution of hydrochloric acid, ultrapure water, finally, with ethyl alcohol, dried at 333–343 K in vacuum. The output was 90–92 %. At the temperature of 453–473 K resulting precipitate of AgSbSe_2 was partially dissolved in ethylene glycol. Experiments have been carried out with fine chemical reagents. Composition of the obtained compound (ratio Ag : Sb : Se) was determined by derivatograph NETZSCH STA 449F349F3 (Germany) and by chemical analysis. Phase analysis of nano- and microparticles

of AgSbSe_2 was studied using the X-diffractometer D2 PHASER “Bruker” (CuK_α radiation 2θ , ($\lambda = 1.54056 \text{ \AA}$), 10–70 degrees) and chemical analysis. Morphological investigations have been performed using scanning electron microscopy TM 3000 (Hitachi, Japan). Chemical, thermographic, X-ray and morphological analyses were performed. Optical absorption was measured using a spectrophotometer U-5100 (Hitachi), the value of the band gap on the basis of the spectrum obtained from the dispersed AgSbSe_2 solution in ethyl alcohol was calculated.

Analyses of the samples synthesized by hydrothermal method (silver antimony selenide), were carried out by thermogravimetric and differential calorimetric methods. The analysis results have shown that when the sample was heated to the temperature of 20–750 °C the weight loss of 10–11 % occurred. Calculations according the graph (the melting point) have shown that the ratio by mass (weight) of silver and antimony to selenium corresponds to 53.42 : 45.57. The data obtained correspond to the formula of AgSbSe_2 . Differential calorimetric analysis of the sample showed that at the melting point (862 K) the peak area was 9,5781 $\mu\text{Vs/mg}$.

The results of X-ray analysis of silver antimony selenide by the intensities and positions of the exhibiting peaks fully correspond to the standard data (PDF 00:012:0379). The effect of temperature on the production, growth and formation of nano- and microparticles synthesized by solvothermal method was investigated; the images of these particles using an electron microscope were recorded. Composition of AgSbSe_2 compound was also confirmed by chemical methods.

Alteration of paramagnetic centers in MoO_3 and TiO_2 : MoO_3 composites after heating under reducing atmosphere

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Individual MoO_3 as well as TiO_2 : MoO_3 composites find wide application as catalysts in dehydration processes and as sensing materials for detection of under explosive concentrations of hydrogen. Investigation of paramagnetic centers that can act as H_2 adsorption sites in MoO_3 and TiO_2 : MoO_3 composites is an urgent scientific task.

In the work MoO_3 was synthesized by precipitation with HNO_3 from $(\text{NH}_4)_6\text{Mo}_7\text{O}_{24}$ saturated solution. TiO_2 : MoO_3 nanocomposites with MoO_3 content under 5 mol.% were synthesized by sol-gel method. The oxide materials were heated at 450 °C. Paramagnetic centers in the materials were investigated by ESR spectroscopy (room temperature, air, radiation power 200 mW).

It was established, that ESR spectrum of individual MoO_3 (Fig. a) contains eight resonance lines corresponding to six paramagnetic centers: $(\text{Mo-O})^{5+}$ (resonance line 1) and O^- hole centers (line 2), adsorbed O_2^- radicals (line 3), F-centers (line 4), 6-fold coordinated Mo^{5+} in axially distorted oxygen environment (lines 5, 6, 8), $[(\text{Mo=O})^{3+}-(\text{O}^{2-})_3]$ molybdenyl centers (line 7). In case of TiO_2 : MoO_3 composite in the ESR spectrum (Fig. c) only three resonance lines can be regis-

tered, which correspond to two types of paramagnetic centers – 6-fold coordinated Mo^{5+} in axially distorted oxygen environment (lines 9, 11), and $[(\text{Mo}=\text{O})^{3+}-(\text{O}^{2-})_3]$ molybdenyl centers (line 10). Reduction of the quantity of resonance lines in ESR spectra of multioxide material can be explained by the presence of intense dipole-dipole interaction between Ti^{3+} paramagnetic centers that leads to the hard broadening of these resonance lines in the spectrum up to complete disappearance of all possible resonance lines in the spectrum of individual TiO_2 .

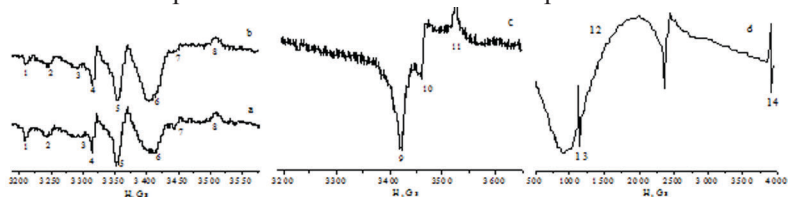


Fig. ESR spectra of MoO_3 before hydrogen treatment (a), immediately after H_2 treatment (b); $\text{TiO}_2 : \text{MoO}_3$ composite before H_2 treatment (c) and after prolonged H_2 treatment (d)

Heating under reducing atmosphere was lead at 300 °C in hydrogen. The following ESR investigation of the materials (Fig. b) revealed a decrease in the intensity and the amplitude of $(\text{Mo}-\text{O})^{5+}$ centers and $[(\text{Mo}=\text{O})^{3+}-(\text{O}^{2-})_3]$ molybdenyl centers both in individual MoO_3 and $\text{TiO}_2 : \text{MoO}_3$ composites. Such alteration can be due to the processes of hydrogen adsorption on these paramagnetic centers. Moreover intensity of Mo^{5+} paramagnetic centers line sharply increases after heating in H_2 with subsequent gradual lowering to the initial values in air both in MoO_3 and $\text{TiO}_2 : \text{MoO}_3$ composite. This fact indicates that Mo^{6+} to Mo^{5+} reduction in the hydrogen atmosphere takes place with the following reverse oxidation by the atmospheric oxygen. When heating time is increased, the quantity of Mo^{5+} centers in $\text{TiO}_2 : \text{MoO}_3$ composite enhances so, that in the ESR spectra ferromagnetic component can be observed (Fig. d, broad line 12) (lines 13, 14 – calibrating $\text{Al}_2\text{O}_3 : \text{Cr}$ crystal). Under these conditions $\text{TiO}_2 : \text{MoO}_3$ composite can be treated as substitutional solution of Mo^{5+} ions in diamagnetic TiO_2 matrix, where paramagnetic Mo^{5+} centers form a sort of regularized structure.

Synthesis and properties of $\text{Tb}_x\text{La}_{1-x}\text{InO}_3$ ($x \leq 0.15$) indates

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In present work $\text{Tb}_x\text{La}_{1-x}\text{InO}_3$ solid solutions with $x = 0.03, 0.05, 0.07, 0.15$ were synthesized by the ceramic method and their crystal struc-

ture, thermal expansion and thermal stability, magnetic susceptibility, IR-spectra, excitation and photoluminescence spectra were investigated.

It was found that in $\text{TbInO}_3 - \text{LaInO}_3$ binary system with $x \leq 0.15$ there was a continuous range of $\text{Tb}_x\text{La}_{1-x}\text{InO}_3$ solid solutions with the structure of orthorhombically distorted perovskite.

IR-spectra of the samples investigated were found to be almost coequal.

Average coefficients of linear thermal expansion for the ceramic samples of $\text{Tb}_x\text{La}_{1-x}\text{InO}_3$ solid solutions depend insignificantly on the substitution degree of Tb^{3+} ions by La^{3+} ions and vary without certain dependence from $8.11 \cdot 10^{-6} \text{ K}^{-1}$, to $10.53 \cdot 10^{-6} \text{ K}^{-1}$. When heating $\text{Tb}_x\text{La}_{1-x}\text{InO}_3$ samples up to 1273 K no thermal effects were observed, total weight loss varied from 0.1325 to 0.3254 wt. % without a certain dependence on substitution degree x

It was found that significant magnetic dilution of paramagnetic Tb^{3+} ions by diamagnetic La^{3+} ions leads to a decrease in effective spin-orbital magnetic moment of Tb^{3+} ions. This could be explained by an increase in «partial freezing» of orbital magnetic by crystal field of orthorhombically distorted perovskite.

It was found that $\text{Tb}_{0.07}\text{La}_{0.93}\text{InO}_3$ and $\text{Tb}_{0.15}\text{La}_{0.85}\text{InO}_3$ samples possess the highest photoluminescence intensity among all the $\text{Tb}_x\text{La}_{1-x}\text{InO}_3$ solid solutions investigated (unlike it had been stated in [1]) and so they are established to be effective phosphors with visible green emission, hence, prospective for white LEDs (Fig.).

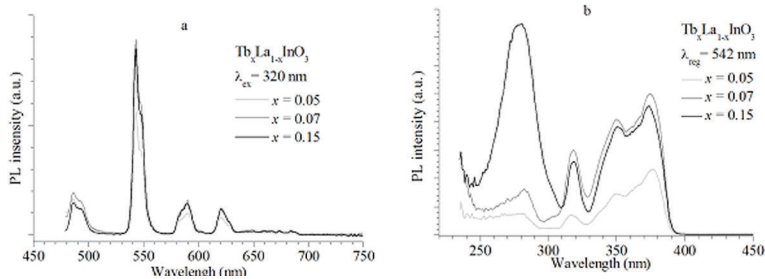


Fig. Excitation (a) and emission (b) spectra of $\text{Tb}_x\text{La}_{1-x}\text{InO}_3$ solid solutions with $x = 0.05, 0.07, 0.15$

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Magnetic and photoluminescent properties of $\text{La}_{1-x}\text{Nd}_x\text{InO}_3$ solid solutions ($0.007 \leq x \leq 0.05$) with perovskite structure

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For $\text{La}_{1-x}\text{Nd}_x\text{InO}_3$ ($x = 0.007, 0.02, 0.05$), $\text{La}_{1-x}\text{Nd}_x\text{In}_{1-y}\text{Cr}_y\text{O}_3$, $\text{La}_{1-x}\text{Nd}_x\text{In}_{1-y}\text{Mn}_y\text{O}_3$ ($x = 0.05, y = 0.005$) solid solutions magnetic susceptibility in the temperature range of 5–300 K in a magnetic field of 0.86 T was measured and effective magnetic moment of Nd^{3+} ions was calculated (Fig. a). Magnetization dependences of these solid solutions on the magnetic field up to 14 T were investigated at 5 K and 300 K. X-ray diffraction patterns showed that the samples were single-phase and had the structure of orthorhombically distorted perovskite.

$x = 0.007$ (1); 0.02 (2); 0.05 (3)

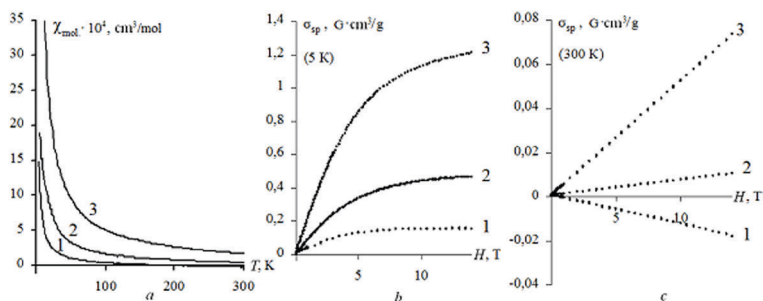


Fig. 1 Magnetic properties of $\text{La}_{1-x}\text{Nd}_x\text{InO}_3$ solid solutions: a – the temperature dependence of the molar magnetic susceptibility, b, c – the field dependence of the specific magnetization at 5 K and 300 K

The effective magnetic moment of the Nd^{3+} ion for $\text{La}_{1-x}\text{Nd}_x\text{InO}_3$ solid solutions with $x = 0.007, 0.02, 0.05$ was significantly smaller than its theoretical value ($3.62 \mu_B$). The magnetic moments of Nd^{3+} ions for $\text{La}_{1-x}\text{Nd}_x\text{InO}_3$ solid solutions with $x = 0.007, 0.02, 0.05$ calculated from their magnetization value at 5 K in a field of 14 T (Fig. b) were equal to $1.18 \mu_B, 1.26 \mu_B, 1.31 \mu_B$, respectively.

With an increase in Nd^{3+} ions content in $\text{La}_{1-x}\text{Nd}_x\text{InO}_3$ from $x = 0.007$ to 0.05 there was a significant increase in photoluminescence intensity at infrared wavelengths. The intensity of the photoluminescence band at $\lambda = 860\text{--}960$ nm for $\text{La}_{0.95}\text{Nd}_{0.05}\text{In}_{0.995}\text{Cr}_{0.005}\text{O}_3$ sample was higher than that for $\text{La}_{0.95}\text{Nd}_{0.05}\text{InO}_3$ sample due to the superposition of Nd^{3+} and Cr^{3+} ions photoluminescence bands.

Thermal properties of manganese(II) dihydrophosphate tetrahydrate

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Heat treatment of crystal hydrates is one of the ways to obtain anhydrous salts. This process in many respects is defined by an extent of hydration of crystalline hydrate. The thermal transformation of manganese(II) dihydrophosphate dihydrate $\text{Mn}(\text{H}_2\text{PO}_4)_2 \cdot 2\text{H}_2\text{O}$ have been determined [1]. Thermal properties of $\text{Mn}(\text{H}_2\text{PO}_4)_2 \cdot 4\text{H}_2\text{O}$ tetrahydrate are studied insufficiently.

The aim of this work was to study thermal behaviour of $\text{Mn}(\text{H}_2\text{PO}_4)_2 \cdot 4\text{H}_2\text{O}$ to determine the sequence of thermal and structural transformations and how the extent of hydration affects these transformations.

Thermal transformations were studied, as in [1], using Q-1500D derivatograph. According to the results of the differential and thermal analysis, $\text{Mn}(\text{H}_2\text{PO}_4)_2 \cdot 4\text{H}_2\text{O}$ is resistant when heating in air with a rate of 2.5 K/min to 50 °C. Further temperature increase is followed by a loss of weight. It is registered by four accurate steps on TG curve.

Interpreting the results of the complex characterization of the products of partial and complete dehydration of $\text{Mn}(\text{H}_2\text{PO}_4)_2 \cdot 4\text{H}_2\text{O}$, we found the following. Heat treatment of $\text{Mn}(\text{H}_2\text{PO}_4)_2 \cdot 4\text{H}_2\text{O}$ in the range of 50–110 °C is followed by the removal of two molecules of water by the molecular mechanism and the formation of $\text{Mn}(\text{H}_2\text{PO}_4)_2 \cdot 2\text{H}_2\text{O}$. At the same time partly the process of the anion disproportionation is realized with the formation of $\text{MnHPO}_4 \cdot 3\text{H}_2\text{O}$ and H_3PO_4 .

The second stage of dehydration ends up in the range of 110–160 °C with the formation of two mixed crystalline phases which are $\text{Mn}(\text{H}_2\text{PO}_4)_2$ and $\text{Mn}_5(\text{HPO}_4)_2(\text{PO}_4)_2 \cdot 4\text{H}_2\text{O}$. The quantity of free H_3PO_4 in the thermolysis products of $\text{Mn}(\text{H}_2\text{PO}_4)_2 \cdot 4\text{H}_2\text{O}$ increases and at 160 °C it makes 2.12 wt % (based on P_2O_5).

The process of the anion condensation begins at the third stage of $\text{Mn}(\text{H}_2\text{PO}_4)_2 \cdot 4\text{H}_2\text{O}$ thermolysis. At 185 °C the losses of the weight correspond to a removal of 4.55 mol of H_2O . The salt component includes the condensed phosphate with $n = 2-5$. The acid component includes polyphosphoric acids of the general formula $\text{H}_{n+2}\text{P}_n\text{O}_{3n+1}$ ($n = 2-4$).

Most difficult it is to determine the composition of the products at heating of $\text{Mn}(\text{H}_2\text{PO}_4)_2 \cdot 4\text{H}_2\text{O}$ to 275 °C. It is presented by a mixture of condensed phosphates and polyphosphoric acids with $2 \leq n \leq 7$. The condensed phosphates with $n = 3-8$ are X-ray amorphous.

At heating of $\text{Mn}(\text{H}_2\text{PO}_4)_2 \cdot 4\text{H}_2\text{O}$ to 300 °C the anion composition of thermolysis products is simplified. The finish products of dehydration appear. It is identified as cyclotetraphosphate with composition of $\text{Mn}_2\text{P}_4\text{O}_{12}$. Its crystallization ends up at 335 °C.

Thus, the sequence of thermal solid-phase transformations accompanying $\text{Mn}(\text{H}_2\text{PO}_4)_2 \cdot 4\text{H}_2\text{O}$ thermolysis was established. The composition of the products of its partial and full dehydration was identified; the temperature intervals of their formation and thermal stability were concretized. It was shown that the final product of thermolysis is $\text{Mn}_2\text{P}_4\text{O}_{12}$ (monoclinic system, sp. gr. C2/c, $Z = 4$; $a = 1.2084$, $b =$

0.8471, $c = 1.0171$ nm; $\beta = 119.29^\circ$) is formed by two directions. The first direction provides thermal dehydration of the protonated condensed phosphates (up to 65 %). According to the second direction, up to 35 % of $\text{Mn}_2\text{P}_4\text{O}_{12}$ is formed as a result of solid-phase interactions of thermolysis intermediate products. The general scheme of thermal solid-phase transformations of $\text{Mn}(\text{H}_2\text{PO}_4)_2 \cdot 4\text{H}_2\text{O}$ was proposed.

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On the chemical transport of some binary sulfides

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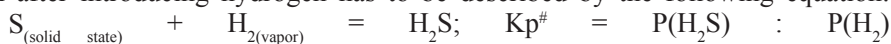
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The present work is concerned with the investigation of the phase diagrams for the systems In–S and Fe–S. It is known that some of these sulphides are promising materials for new technologies, however there are considerable discrepancies concerning the types and temperatures of the solid phase transformations and homogeneity regions of these phases. These discrepancies can be caused by the very low volatility of metal-enriched iron and indium sulphides as well as ambiguous interpretation of the results of electrical measurements. For the scanning of P–T–x-diagram of the sulphides systems (In–S and Fe–S) the spectrophotometric technique is elaborated. We suggested studying the equilibria of indium and sulfides with hydrogen as an auxiliary component. It is proved that the equilibrium in this system after introducing hydrogen has to be described by the following equation:



So, there is no noticeable vaporization of chemically bounded indium to the vapor. When the shift of equilibrium (1) takes place, this element should be accumulated (consumed) in the condensed part of the system and cause transformations of some sulfides into other sulfides or changes in their non-stoichiometry.

Vast thermodynamic information about phases of sulphide systems can be received if it is possible to determine $K_p^\#$, which relates pressures of hydrogen and hydrogen sulfide (see eq. 1).

To find the value of $K_p^\#$, one needs to know partial pressure of, at least, one of two molecular forms - H_2 or H_2S . Then the equilibrium pressure of another form (for example, P_{H_2}) can be determined if the pressure of initially introduced hydrogen (P°) is known. Hydrogen sulfide is known to have an electronic absorption spectrum in the “air” ultraviolet spectral region ($\lambda_{\text{max}} = 196$ nm). This enables quantitative determination of H_2S in the vapor phase by spectrophotometry. The fulfilled

experiments give the opportunity of obtaining data about the In-S phase diagram.

The objective of this work is the refinement of the phase diagram of the In-S system within the composition field of 50–60 mol. % and analysis of homogeneity region of the phase $\text{In}_{3-x}\text{S}_4$. Analyzing the $K_p^{\#}$ -T – dependences we assume that the $\text{In}_{3-x}\text{S}_4$, a phase with a broad homogeneity range, has a tendency to decompose into two separate phases in a wide temperature range. Moreover, our results confirm the existence of a narrow two phase field between $\text{In}_{3-x}\text{S}_4$ and In_2S_3 at low temperature region.

For the Fe-S system iron(III) chloride can be used as an auxiliary component also. We report initial results from our spectrophotometric study of the equilibrium «solid – vapor» for iron(III) chloride in a wide range of temperatures (150–800 °C). The purpose of this part of the work was to determine (at least qualitatively) the composition of unsaturated vapor of iron(III) chloride. The experiment consisted in scanning in situ the absorption spectra of the vapor (wavelength interval 200–800 nm) in two temperature regimes: incremental increasing and decreasing. The presence of some species in unsaturated vapor has been discussed. As metal halides are often used as transport agents for growing sulfides, current results together with some future investigations in this field can find their application, for example, as a base for pyrite production for the needs of technology and energetics.

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Synthesis, properties and structure of solid solutions on the basis of $\text{Bi}_2\text{Fe}_4\text{O}_9$

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The solid solutions based on ferrite $\text{Bi}_2\text{Fe}_4\text{O}_9$ were prepared by a solid-state reactions method. According to the results of X-ray phase analysis it was revealed that $\text{Bi}_2\text{Fe}_4\text{O}_9$ had an orthorhombic structure (sp. gr. Pbam) of mullite with lattice parameters $a = 7.9595 \text{ \AA}$, $b = 8.4297 \text{ \AA}$, $c = 5.9912 \text{ \AA}$, $V = 401.987 \text{ \AA}^3$. At partial isovalent substitution of Bi^{3+} ions by La^{3+} ions, as well as at heterovalent substitution of Fe^{3+} ions simultaneously by Ti^{4+} and Co^{2+} ions in $\text{Bi}_2\text{Fe}_4\text{O}_9$, corresponding solid solutions $\text{Bi}_{2-x}\text{La}_x\text{Fe}_4\text{O}_9$, $\text{Bi}_2\text{Fe}_{4-2x}\text{Ti}_x\text{Co}_x\text{O}_9$ are formed. The formation of solid solutions is indicated not only by the results of X-ray diffraction (changing the parameters a , b , c , c/a и V), but also by the data of IR spectroscopy. At substitution of Bi^{3+} ions by La^{3+} ions in $\text{Bi}_2\text{Fe}_4\text{O}_9$, a shift of the absorption bands to the high-frequency region takes place, which is a consequence of a reduction in the bond lengths Fe–O in the octahedra FeO_6 and decreasing O–Fe–O angles. Analysis of the temperature dependence of the specific magnetization showed that $\text{Bi}_2\text{Fe}_4\text{O}_9$ was an antiferromagnet with $T_N = 258 \text{ K}$, and the introduction of La^{3+} ions in the $\text{Bi}_2\text{Fe}_4\text{O}_9$ crystal structure shifts T_N to the low temperature region, and

T_N becomes equal to 246 K for $\text{Bi}_{1.95}\text{La}_{0.05}\text{Fe}_4\text{O}_9$ and 243 K for $\text{Bi}_{1.8}\text{La}_{0.2}\text{Fe}_4\text{O}_9$.

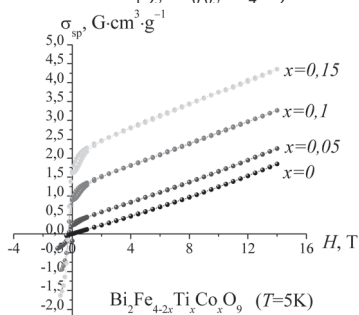


Fig. The field dependence of the specific magnetization (σ_{sp}) of the $\text{Bi}_2\text{Fe}_{4-2x}\text{Ti}_x\text{Co}_x\text{O}_9$ solid solutions at 5 K

The field dependencies of the specific magnetization for solid solutions based on $\text{Bi}_2\text{Fe}_4\text{O}_9$ were studied at 300 K and 5 K (Figure). The results obtained show the presence of negative exchange interaction in the samples, which leads to an antiferromagnetic arrangement of the magnetic moments of the two sublattices (octahedral and tetrahedral), in which Fe^{3+} ions are placed. The temperature dependencies of the thermoelectric power and thermal expansion were also studied at 300–1000 K.

Synthesis and structure of $\text{Bi}_{0.95}\text{La}_{0.05}\text{FeO}_3$ solid solutions using $\text{Bi}_{1.8}\text{La}_{0.2}\text{Fe}_4\text{O}_9$ as a precursor

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Synthesis of polycrystalline ferrite $\text{Bi}_{1.8}\text{La}_{0.2}\text{Fe}_4\text{O}_9$, which is a precursor in the preparation of ferroelectric $\text{Bi}_{0.95}\text{La}_{0.05}\text{FeO}_3$, was carried out by solid-state method using Bi_2O_3 , Fe_2O_3 , La_2O_3 oxides calcined in the air at $T = 800^\circ\text{C}$ for 8 hours. Prepared solid solution $\text{Bi}_{1.8}\text{La}_{0.2}\text{Fe}_4\text{O}_9$ with the structure of the orthorhombically distorted perovskite contained extremely small amount of impurity phase BiFeO_3 . This may be due to the fact that in the range 25–800°C $\text{Bi}_2\text{Fe}_4\text{O}_9$ formation from oxides is thermodynamically more favorable than BiFeO_3 formation, but these processes are competing. For the synthesis of $\text{Bi}_{0.95}\text{La}_{0.05}\text{FeO}_3$ ferrite powders of $\text{Bi}_{1.8}\text{La}_{0.2}\text{Fe}_4\text{O}_9$ precursor and Bi_2O_3 oxide were mixed in a stoichiometric ratio according to the reaction: $\text{Bi}_{1.8}\text{La}_{0.2}\text{Fe}_4\text{O}_9 + \text{Bi}_2\text{O}_3 = 4\text{Bi}_{0.95}\text{La}_{0.05}\text{FeO}_3$ and calcined at three different regimes: I – $T = 830^\circ\text{C}$, 30 min; II – $T = 900^\circ\text{C}$, 30 min; III – $T = 900^\circ\text{C}$, 4 h. At the selection of the synthesis temperature we took into account the temperatures of the incongruent melting of the compounds $\text{Bi}_2\text{Fe}_4\text{O}_9$ (960°C) and BiFeO_3 (930°C), which limited the upper limit value of the annealing temperature (900°C). The figure shows the diffraction patterns of the $\text{Bi}_{0.95}\text{La}_{0.05}\text{FeO}_3$ and BiFeO_3 samples. $\text{Bi}_{0.95}\text{La}_{0.05}\text{FeO}_3$ solid solutions were prepared under different heat treatment conditions, as well as non-substi-

tuted ferrite BiFeO_3 , was synthesized by the reaction: $\text{Bi}_2\text{O}_3 + \text{Fe}_2\text{O}_3 = 2\text{BiFeO}_3$ [1].

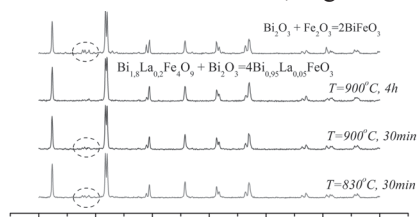


Fig. X-ray diffraction patterns of ferrites $\text{Bi}_{0.95}\text{La}_{0.05}\text{FeO}_3$ prepared using regimes (I – III) and BiFeO_3

Analysis of the diffraction patterns showed that $\text{Bi}_{0.95}\text{La}_{0.05}\text{FeO}_3$ samples had crystal structure of rhombohedrally distorted perovskite, unit cell parameters of which were in a good agreement with the literature data. Note, that diffractograms of the $\text{Bi}_{0.95}\text{La}_{0.05}\text{FeO}_3$, heated at $T = 830^\circ\text{C}$ for 30 min and at $T = 900^\circ\text{C}$ for 30 min, contained trace amounts of impurity phases such as antiferromagnetic $\text{Bi}_2\text{Fe}_4\text{O}_9$ of mullite phase and paramagnetic $\text{Bi}_{25}\text{FeO}_{39}$ of sillenite phase. The regions of existence of these impurity phases are marked by dotted lines in the diffraction patterns. Synthesis conducted at longer heating time (4 h at $T = 900^\circ\text{C}$) led to the production of the practically single-phase $\text{Bi}_{0.95}\text{La}_{0.05}\text{FeO}_3$ samples. Thus we can conclude that this time-temperature regime is the best for preparation of substituted ferroelectric $\text{Bi}_{0.95}\text{La}_{0.05}\text{FeO}_3$ using $\text{Bi}_{1.8}\text{La}_{0.2}\text{Fe}_4\text{O}_9$ as precursor.

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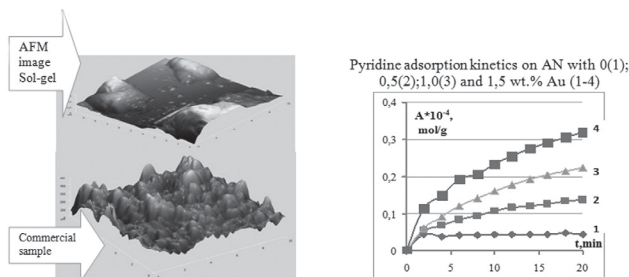
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The effect of UV treatment on the properties of TiO_2 with gold additives

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Ultrafine TiO_2 powders were prepared after crystallization of organogels at 500°C . All samples, synthesized in various precursors ratio, were monophased of anatase (AN) type only and showed the augmentation of paramagnetic centers number (ESR data) and changes of surface morphology (AFS) after UV irradiation not more than 3 minutes. The gold introduction increased the surface acidity, tested by pyridine adsorption (PyA). The linear correlations between Au content and the rate of PyA, as well as total PyA were obtained. After UVT the adsorption capacity decreased.

If during the adsorption experiment the Py solution in octane with Au-doped TiO_2 is exposed in UV light the rate of PyA augments in 2 times in compared with dark conditions. This effect is not observed for samples without Au and with 1.5 % wt. of Au. So, photoactivated Py adsorption depends on the surface composition of oxide, that is confirmed by our previous results. For supported Ag, Cu, Au additives the highest stimulation for adsorption of donor molecule was obtained for $\text{Au/TiO}_2(\text{AN})$.



As in case of photocatalysis the reason of such stimulation is connected with holes (h^+) formation that react with adsorbing molecules. The influence of UV-treatment of Ag, Cu, Au/TiO₂ was studied for catalytic reactions of ethanol in flow conditions [1]. After UV irradiation of TiO₂ and Ag/TiO₂ the yields of acetaldehyde and ethylene respectively increase, but for Cu/TiO₂ catalyst, on the contrary, decrease.

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AFM-investigations of the surface morphology of V₂O₅ / A^{III}B^V heterostructures

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Vanadium pentoxide deposited on the surface of A^{III}B^V by different methods is an effective chemostimulator of the semiconductors thermal oxidation. The purpose of this research is Atomic Force Microscopy investigation of the dependence of the V₂O₅ / A^{III}B^V heterostructures surface morphology on the method of vanadium pentoxide thin films deposition and conditions of heterostructures thermal oxidation.

The objects of the study were mechanically carved wafers of GaP (100) and GaAs (111) with chemically polished surface. V₂O₅ thin films were deposited by magnetron sputtering (hard method, film thickness 30 nm) and by deposition of vanadium pentoxide gel through aerosol phase followed by thermal annealing (soft method, film thickness 8 nm [1]).

The surface of V₂O₅ / GaP heterostructures formed by magnetron sputtering before the thermal oxidation was smooth, the film had a pronounced grain structure with an anisotropic shape of the grains. The relief height did not exceed 20 nm. After 60 minutes of thermal oxidation in oxygen at 650 °C the surface of films changed due to interactions between the film and semiconductor substrate. The relief height increased to 30–40 nm (Figure 1, a), wherein the surface roughness became equal

to 9.07 nm against 2.34 nm for non-oxidate structure (the area scan 3x3 nm²).

The surface of V_xO_y / GaAs heterostructure formed by the soft method before oxidation had the relief with a height about 10–12 nm, the film had a grain structure with a grain size of about 40–80 nm. As a result of thermal oxidation at 530 °C for 60 min the height of the relief slightly varied (Fig. 1, b), the film remained smooth and the grain structure became less pronounced. The roughness was reduced from 1.60 nm to 0.78 nm (the scan area 3x3 nm²). Thus, differences in the surface morphology of V₂O₅ thin film deposited on the surface of GaAs and GaP wafers by magnetron sputtering and deposition throw aerosol phase were determined by AFM method. It was shown that the mild method of V₂O₅ deposition provides the formation of more smooth surfaces, both before and after thermal oxidation of V₂O₅ / A^{III}B^V heterostructures.

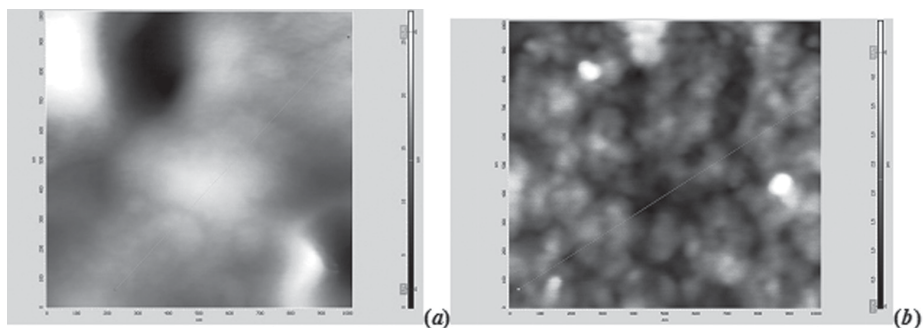


Fig. 1 AFM-images of the V₂O₅ / GaP surface (650 °C) (a) and V_xO_y / GaAs (530 °C) (b) heterostructures oxidized during 60 min (scanning region 1x1 μm)

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CATALYSIS, PHOTOCATALYSIS

The application of perovskite-type ferrites in the catalytic hydrogenation of carbon monoxide

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Studied in this paper layered oxides and solid solutions were synthesized by the high temperature solid-state reactions and by sol-gel technology. Among synthesized ferrites there are three-dimensional perovskites GdFeO_3 , SrFeO_{3+x} and two-dimensional perovskite-type layered structures GdSrFeO_4 , $\text{Gd}_2\text{SrFe}_2\text{O}_7$, $\text{Gd}_{2-x}\text{Sr}_{1+x}\text{Fe}_2\text{O}_7$ ($x = 0.1-0.6$), belonging to Ruddlesden-Popper phases $\text{A}_{n+1}\text{B}_n\text{O}_{3n+1}$ ($n = 1, 2$) that are built up from the blocks of perovskite layers with different thickness. X-ray powder diffraction confirmed the presence of single phase for samples obtained both by high temperature solid state reactions and by sol-gel technology as well. Scanning electron microscopy demonstrated a decrease in size of complex ferrite particles from 10 μm , obtained by ceramic technology, up to 200 nm, obtained by the sol-gel technology. Mössbauer spectroscopy showed the difference of electronic state of complex ferrite, prepared by ceramic technology (Fe^{+3}) and oxides obtained by sol-gel technology (Fe^{+3} in the three different surrounding and Fe^{+4}).

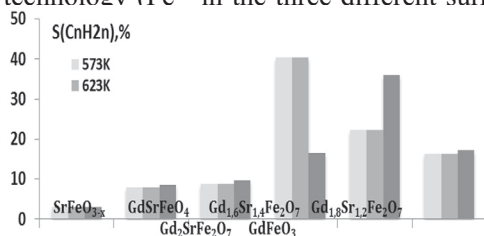


Fig. Total olefin selectivity during the reaction in a ratio of $\text{CO} : \text{H}_2 = 1 : 2$

Reaction products of carbon monoxide hydrogenation are hydrocarbons $\text{C}_1 - \text{C}_5$, the main of them are methane, ethylene, propylene. The greatest amount of olefins formed in the reaction was observed at the stoichiometric $\text{CO} : \text{H}_2$ ratio. It was found that perovskite catalytic activity (rate of product formation) in the catalytic hydrogenation of carbon monoxide increases in the series: $\text{SrFeO}_{3-x} < \text{GdSrFeO}_4 < \text{Gd}_{1.6}\text{Sr}_{1.4}\text{Fe}_2\text{O}_7 < \text{Gd}_{1.8}\text{Sr}_{1.2}\text{Fe}_2\text{O}_7 < \text{Gd}_2\text{SrFe}_2\text{O}_7 < \text{GdFeO}_3$, that is in correlation with the number of alternating perovskite layers in the ferrites structure varying from 1, 2 to ∞ . However, samples with $n = 2$ showed the highest selectivity for ethylene and propylene (Fig).

The increase in strontium content in the layered $Gd_{2-x}Sr_{1+x}Fe_2O_7$ oxides to $x = 0.6$ decreases the symmetry of Fe^{3+} ions and increases the number of oxygen vacancies, which affect the selectivity (its maximum value was observed at $x = 0.3$). It was suggested that heterovalent state of iron (Fe^{3+} , Fe^{4+}) favors the CO activation, which leads to C^\cdot and CH_x^\cdot radicals formation. It was shown that under the influence of the reaction medium and the temperature a change in the active centers state occurs. Probably this change consists in partial iron reduction.

Higher catalytic performance of perovskite-like ferrites synthesized by sol-gel method can be related to their nanocrystalline state with a porous structure, as well as to iron heterovalent state.

Acknowledgment. This work was supported by the Russian Foundation for Basic Research (№ 14-03-00940).

The effect of Co(II) cations and their position in $NaZr_2(PO_4)_3$ lattice on catalytic conversion of 2-propanol

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Complex phosphates are solid electrolytes of the Na-Super-Ionic CONductor (NASICON) [1]. The basic phosphate is sodium-zirconium phosphate $NaZr_2(PO_4)_3$ (NZP). The composition of NZP can be varied by full or partial replacing of sodium(a) or zirconium (b) ions [2] without substantial changes in the crystal structure (Figure). The introduction of various ions into NZP offers promise for use it as active and selective catalysts with a micro porous structure formed by ionic conductivity channels. The purpose of this work is to study the role of Co+2 doping ion position in cationic (a) or in anionic (b) parts of complex phosphate on its catalytic activity in dehydrogenation reaction of 2-propanol. Note that in case a Co+2 ions can undergo the transfer from M1 to M2 at a temperature T^* , that influences the Co+2 surrounding.

Catalysts were prepared by the sol-gel method. The X-ray data substantiated the structure of NZP. The surface layer composition of NZP was characterized by X-ray photoelectron spectroscopy (XPS). The conversion of alcohol was performed in continuous-flow reactor at atmospheric pressure and 200-400 °C. The reaction mixture was analyzed chromatographically with a flame-ionization detector. In table NC=O is the yield of aldehyde in $\mu\text{mol}/(\text{g}\cdot\text{h})$.

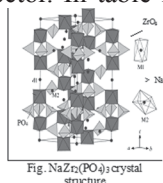


Table. The yield and selectivity of aldehyde			
		a $Na_2Co_{0.5}Zr_{1.5}(PO_4)_3$	b $Na_2ZrCo(PO_4)_3$
Ratio Na : Co		2:1	3:1
Ratio Co : Zr		1:8	1:1
N^{CO}	1) 300 °C	37	58
	2) 350 °C	181	135
$S^{CO} \%$	350 °C	100	90
E_a^{CO} , kJ/mol		1) 93; 2) 60	11
$\ln V_0^{CO}$		1) 16.2; 2) 9.7	2.0

Fig. $NaZr_2(PO_4)_3$ crystal structure

We see that the content and the position a or b of the ion-dopant has little effect on the yield NC=O when the selectivity does not change sufficiently SC=O (Table). In a series of a cobalt cation transition is observed at $T^* = 330^\circ\text{C}$. The dehydrogenation reaction senses the change in the cobalt ions' position, due to the transition of some cobalt ions from the M1 to M2 position leading to a new catalytically active center (M1–M2) on which interaction with the OH group of alcohol occurs. These centers have higher bond energy with alcohol than the adsorption on the M1 center at low temperatures, so the value of apparent activation energy E_a is lowering in 1.5 times. The pre-factor $\ln N_0$ is also decreasing.

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Catalytic properties features of perovskite-type ferrites in dry (carbon dioxide) methane reforming

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The perovskite-type ferrites GdSrFeO_4 , $\text{Gd}_2\text{SrFe}_2\text{O}_7$, GdFeO_3 and solid solutions $\text{Gd}_{2-x}\text{Sr}_{1+x}\text{Fe}_2\text{O}_7$ ($x = 0.1\text{--}0.6$) were synthesized by the high temperature solid-state reactions and by sol-gel technology.

The complex physico-chemical investigations showed that synthesized catalysts are well-crystalline homogenous perovskite-type ferrites with different number of perovskite layers GdSrFeO_4 ($n = 1$), $\text{Gd}_2\text{SrFe}_2\text{O}_7$ ($n = 2$), GdFeO_3 ($n = \infty$) and solid solutions $\text{Gd}_{2-x}\text{Sr}_{1+x}\text{Fe}_2\text{O}_7$. Samples obtained by ceramic technology are in microcrystalline state and the iron atoms are found in Fe^{3+} state, which is magnetically ordered; oxides prepared by sol-gel technology are in nanocrystalline state and iron atoms are in a heterovalent state (Fe^{3+} coexists with Fe^{4+}) in three different symmetry fields.

The maximum conversion ($\alpha_{\text{CH}_4} = 37\%$, $\alpha_{\text{CO}_2} = 57\%$) and products formation rate ($\text{WH}_2 = 0.07 \text{ mol}/(\text{h}\cdot\text{g})$, $\text{WCO} = 0.16 \text{ mol}/(\text{h}\cdot\text{g})$) were achieved by performing the reaction at an equimolar ratio of CH_4 and CO_2 . In spite of high temperatures the catalytic activity did not decrease during 40 hours. The catalyst demonstrated the high resistance to coke formation.

Among the reaction products the water was detected in almost all investigated ferrites, the quantity of generated carbon monoxide was 2–4 times greater than the quantity of hydrogen and carbon dioxide conversion was almost two times higher than methane conversion. Activation energies of CO formation and the corresponding values of $\ln k_0$ were less than the similar values of E_a and $\ln k_0$ for hydrogen. On the base of these data it was suggested that the DRM reaction was complicated by the reverse steam reforming of CO.

It was shown that an increase in the number of perovskite layers (n) in the com-

plex oxides structure led to an increase in the catalytic activity. A partial substitution or complete replacement of Gd^{3+} ions by Sr^{2+} ions led to some reduction of activity. Among the systems of variable composition $Gd_{2-x}Sr_{1+x}Fe_2O_7$ obtained by the sol-gel technology samples had the highest activity at $x = 0.3$. The increase in strontium content led to lowering the symmetry of the surroundings of Fe^{3+} atoms and to occurrence of heterovalent state of iron atoms (Fe^{3+} , Fe^{4+}) with oxygen vacancies. It influenced an increase in the total surface acidity and catalytic activity in terms of CO_2 conversion. The catalytic activity increased in the row $SrFeO_{3-x}$ ($n = \infty$) \approx $GdSrFeO_4$ ($n = 1$) \approx $Gd_{2-x}Sr_{1+x}Fe_2O_7$ ($n = 2$) $<$ $GdFeO_3$ (ceramic) ($n = \infty$) $<$ $GdFeO_3$ (sol-gel) ($n = \infty$). Higher catalytic properties of perovskite-type ferrites synthesized by sol-gel technology can be associated with their nanocrystalline state, a porous structure, as well as with heterovalent iron state and oxygen vacancies, which probably are favorable for the surface oxidation-reduction reactions and the process of CO_2 activation.

Acknowledgment. The reported study was supported by the Russian Foundation for Basic Research grant 14-03-00940.

New catalysts for cross-coupling reactions based on Pd(II) complexes with substituted isoxazoles and isothiazoles

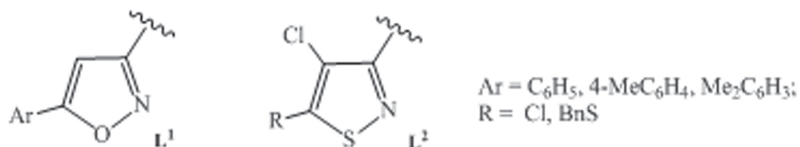
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Pd(II) complexes are effective catalysts for cross-coupling reactions awarded the Nobel Prize in Chemistry in 2010. We have recently demonstrated that isoxazole (L1) and isothiazole (L2) derivatives can form complexes with palladium(II) exhibiting high catalytic activity in cross-coupling reactions in aqueous and aqueous-alcohol media (Green Chemistry) [1, 2].



Immobilization of Pd(II) complexes on different carriers opens the path to refillable catalytic systems. In this work we carried out a targeted modification of isoxazoles and isothiazoles, synthesized their Pd(II) complexes, obtained catalytic systems on silica and carbon carriers and studied their catalytic activity in model cross-coupling reactions. We also synthesized activated esters of isoxazole and isothiazole series for conjugation with reactive polymers and obtaining catalysts on the polymer matrix. Obtained catalytic systems exhibited high catalytic activity in the model Su-

zuki reaction of 4-methoxyphenyl boronic acid with 3-bromobenzoic acid in aqueous and aqueous-methanol media. With the usage of 0.05–0.1 ml.% of the catalyst, the process was completed in 15–30 min and led to the target cross-coupling product with 93–100 % yield without formation of byproducts in case of some isothiazolic Pd(II) complexes. All tested azole-based Pd(II) catalytic systems were characterized by extremely low residual Pd contamination. The capabilities of new catalysts were demonstrated in the synthesis of nonsteroidal antiinflammatory drug Diflunisal.

Acknowledgment. The work was supported by the BRFFR (project X14P-003) and RFFR (project 14-08-90012-Бел_a)

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PHYSICAL CHEMISTRY OF NANOSTRUCTURED SYSTEMS. SOLS, GELS, XEROGELS

The supramolecular system with Nonreversible Resonance Energy Transfer based on the toroidal nanocluster Mo138 and xanthene dye – Rhodamine B

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The new supramolecular system based on the toroid nanoclustered giant polyoxomolybdate (POM) Mo138 and the xanthene dye Rhodamine B (RhB) was produced by the self-assembly method in solution and solid state. For the first time it was characterized by different physicochemical methods. The composition of Mo138 nanocluster is presented by the formula: $(\text{NH}_4)_{32}[\text{MoV}_{110}\text{MoV}_{28}\text{O}_{416}\text{H}_6(\text{H}_2\text{O})_{58}(\text{CH}_3\text{COO})_6] \cdot x\text{H}_2\text{O}$ ($x \approx 250$). In aqueous solution the Mo138 forms multicharged anion. In turn they spontaneously aggregate to hollow, single-wall, spherical globules (diameter is ~300 nm depending on POM concentration and pH) which are stabilized by the NH_4^+ cations and hydrogen bonds. The interaction between positively charged RhB and globular surface is conditioned by the electrostatic force, as a result the ion-associates $\text{Mo138}-(\text{RhB})_n$ are formed. That leads to a decrease in

the zeta-potential value of the supramolecular system from minus 45 mV (for pure Mo138) to zero at the isoelectric point which corresponds to the ratio of components Mo138 : RhB = 1 : 35 in solution (Mo138 concentration is $4.26 \cdot 10^{-6}$ mol/l). At this conditions the average diameter of the supramolecular globular structure passes through minimum from 116 nm (globular diameter in pure Mo138 solution) to 82 nm (minimum point) that is conditioned by compression of the electric double layer due to addition of RhB. By the consecutive washing (ethanol/water) and centrifugation, the produced supramolecular system (at Mo138 : RhB = 1 : 35) was deposited and dried in air. As a result the FTIR-spectrum analysis of this sample revealed the planar arrangement of RhB molecules on the POM surface. The UV-Vis spectrums showed the significant long-wavelength shift of the RhB absorbance bands (from 522 and 558 nm to 533 and 568 nm respectively) for ion-associates in solution. These bands are characteristic for fluorescent part of dye molecule (rigidly connected aromatic rings) and it points to strong interaction between this molecule part and POM surface. Furthermore, this interaction leads to very effective fluorescence resonance energy transfer (FRIP) from RhB molecules (donor) to nanocluster Mo138 (acceptor) by both radiative and nonradiative ways. That was confirmed by the reduction of luminescence intensity (at 592 nm) in ~ 100 times. Moreover, the excitation in the POM absorbance band at 750 nm, which corresponds to the presence of MoV centers in POM structure, does not show the reversible energy transfer from POM to RhB. It is very important to effective promotion of the potential catalytic activities of POM Mo138 conditioned by the presence of molybdenum in variable valency. The analysis of the Raman-spectra of pure RhB and produced ion associates revealed the differences of the xanthene conjugated aromatic system behavior at excitation by the laser with wavelength 488 nm. Thus new supramolecular system with the nonreversible resonance energy transfer possesses the potential ability to use for light-controlled catalysis.

Novel microscopic and spectroscopic imaging solutions in nanoparticles and surfaces characterization

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Recently a new approach has emerged in the field of fundamental and applied materials and surfaces analysis: direct express imaging in place of laborious point-by-point analysis with subsequent image generation. Imaging has become a useful tool for chemistry, composition and physical properties characterization. The new direct imaging approach, which involves

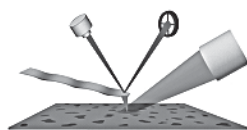


Fig. The principle of nano-IR illustrated

special technical solutions and novel data treatment options, in addition to its rapidity, also allows retrieving the “classical” form of information from the images (spectra or data for each point of the obtained images), if required. Among such novel express imaging systems, several new instruments that were presented in 2014–2015 are of special interest. They are nano-IR systems nano-IR2 and nano-IR2-s (Anasys Instruments), new XPS systems (K-Alpha+, Escalab 250Xi, Theta Probe) and the latest Raman imaging system (DXRxi) manufactured by Thermo Fisher Scientific.

The revolutionary nano-IR method is a combination of IR-microscopy and AFM, which is basically an atomic force microscope combined with a custom-made optical system. The IR source (tunable pulse IR laser) can be adjusted in order to focus on the sample surface close to the AFM tip (Fig). Due to radiation absorption, a short-term local surface heating and reversible deformation take place. This process causes damped oscillations of an AFM tip, which is in contact with the surface. By analyzing the amplitude and frequency of these oscillations, one can obtain an IR absorption spectrum close to the AFM tip, as well as investigate the viscoelastic properties of the surface. The resulting IR spectra are in very good agreement with those obtained using classical FTIR, while the analysis is performed for very small areas down to 10–15 nm. This makes the new imaging nano-IR approach as a great candidate for nanotechnologies, biomaterials studies and reverse engineering.

Another interesting imaging technique has been developed using XPS, which has become one of the most widely applied materials characterization technique due to its versatility, high surface sensitivity, possibility to conduct quantitative analysis, determine the chemical state of the elements, as well as electronic structure information. The versatility is determined by the possibility to use XPS for virtually any solid materials, including dielectrics, polymers, nanomaterials, etc. The imaging techniques allow researchers to study distribution of different elements in various chemical states across the surface. By combining the XPS imaging with other surface analysis techniques (e.g. ISS, AES, REELS and the corresponding imaging options), one can obtain the most comprehensive surface chemistry description with spatial resolution.

The report will focus on the theory and practice of the aforementioned methods for various materials, including nanoparticles, thin films, surfaces, catalysts and other functional materials.

Synthesis of metal nanoparticles and their influence on optical properties of organic dyes

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Recently, silver nanoparticles (AgNP) have attracted much attention because of their unique size and shape dependent optical [1], electrical and magnetic properties. Possible manipulations of these properties lead to various applications of AgNP in optoelectronics, biosensing, catalysis, enhanced optical spectroscopies [2], as antimicrobials [3] and other [4]. For practical use it is crucial to understand the influence of size, shape, aggregation, stability [5] and other features of nanoparticles on their optical properties.

In this work, the influence of spherical and triangular AgNP on optical properties of highly fluorescent organic dyes (rhodamine 6G (R6G), sulforhodamine 640 (SR640)) was investigated. Spherical AgNP were prepared using wet-chemistry techniques: reduction of silver salt ($\text{AgNO}_3 + \text{NaBH}_4 \rightarrow \text{Ag} + \text{H}_2 + \text{B}_2\text{H}_6 + \text{NaNO}_3$), Turkevich method ($4\text{Ag}^+ + \text{Na}_3\text{C}_6\text{H}_5\text{O}_7 + 2\text{H}_2\text{O} \rightarrow 4\text{Ag}^0 + \text{C}_6\text{H}_5\text{O}_7\text{H}_3 + 3\text{Na}^+ + \text{H}^+ + \text{O}_2$). Three different in size triangular AgNP were synthesized using different concentrations of AgNO_3 , NaBH_4 , $\text{Na}_3\text{C}_6\text{H}_5\text{O}_7$ and H_2O_2 . Solutions of nanoparticles and organic dyes were investigated by using steady-state and ultrafast time-resolved absorption and fluorescence spectroscopy (Fig).

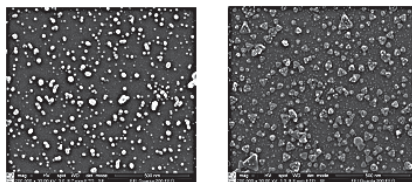


Fig. SEM images of spherical (left) and triangular (right) silver nanoparticles

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Behavior of different models of graphene under tension. Quantum chemical and finite element method calculations

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There are a number of physical models of graphene proposed in the various scientific disciplines that provide calculation of the mechanical properties. They correspond to different mathematical models, which, of course, often lead to discordant results. In this work the Young's modulus and Poisson's ratio for graphene sheet models have been calculated in the framework of the finite element method as well as using semi-empirical PM6 and DFT approaches.

We considered regular graphene sheets of different sizes and started from 3x3 cell. The next graphene sheet was obtained by increasing that cell on one hexagonal cell horizontally and on two cells vertically.

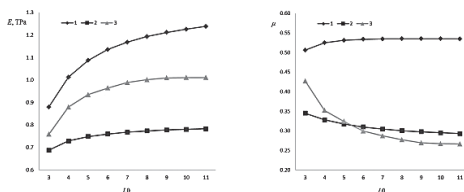


Fig. The calculated values of Young's modulus (E) and Poisson's ratio (μ) depending of the number of cells (L_0) along the horizontal axis
1 – central force field (CFF), 2 – valence force field (VFF), 3 – PM6

All three methods of calculations predict a monotonic increase in the Young's modulus with the rise of sample size with turning curves to asymptote for a bulk samples (Figure). Young's modulus value, calculated using quantum-chemical method PM6, lies between the values obtained using CFF and VFF methods. The results of DFT calculations of small graphene sheets are in a good agreement with those obtained using PM6 method.

The curves showing the dependence of the Poisson ratio of the size of the sample, calculated by different methods, differ significantly (Figure). The Poisson ratio, calculated using a CFF approximation, increases slightly with the rise of a sample size. However VFF and PM6 calculations predict a monotonic decrease of the Poisson ratio with the sample size increasing. Apparently, results of calculations using VFF approximation are not correct.

Thus, the usage of the approaches of classical and quantum mechanics allows to increase the reliability of the results and adjust their input parameters. For example, it becomes possible to use general harmonic force field approximation in the finite element method, which will improve the results.

Colloidal synthesis and optical properties of two-dimensional semiconductor AIBVI heteronanostructures

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Preparation of various heterostructured semiconductor nanoparticles (SNPs) attracted considerable attention, since it provides fabrication of nanomaterials that exhibit intriguing optical and electronic properties which could be altered to the large extent [1]. To day a lot of methods for the colloidal synthesis of various SNPs and heteronanostructures on their basis were developed. At the same time, flat 2D nanocrystals or nanoplatelets (NPLs) composed of cadmium chalcogenides that were introduced in 2008 gained less attention [2].

Recently we introduced 2D heteronanoplatelets with “core-wings” architecture (Figure 1, C) that could be manufactured by selective lateral overgrowth of core CdSe nanoplatelets with the wide gap CdS “wings” [3]. In the current study we demonstrate that similar approach allowed us to prepare heterostructured CdSe–CdTe NPLs with type-II band offset (see Figure 1, B). Elemental and phase composition of the obtained NPLs were confirmed by XRD, EDX and HAADF STEM-images. Optical properties were examined by means of UV-Vis spectroscopy, PL, PLE and PL lifetime measurements. It was found that NPLs exhibit extremely narrow and intensive bands in absorption and at the same time their PL bands are considerably red-shifted for up to 150 nm (Figure 1, A). Time-resolved PL decay measurements showed that due to spatial charge separation average excited state lifetimes are increased by a factor of 10–40.

Owing to anisotropic separation of electrons and holes coupled with high surface area, flat 2D CdSe–CdTe NPLs are believed to be highly promising materials for photocatalytic and photovoltaic applications. At the same time large Stokes shift along with giant oscillator strength effect and high absorption in the visible region makes such NPLs of high interest for efficient optical down-converters.

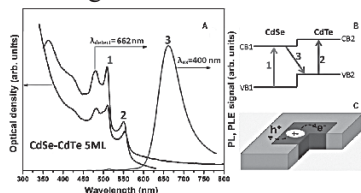


Fig. Absorption, PL and PLE spectra of 5 ML-thick “core-wings”CdSe–CdTe NPLs (A), band level diagram (B) and schematic image of “core-shell” NPLs (C)

Fig. Absorption, PL and PLE spectra of 5 ML-thick “core-wings”CdSe–CdTe NPLs (A),

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Langmuir films of gold sol in reverse micelles of Aerosol OT

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Aerosol OT (AOT) is widely used in the microemulsion synthesis of nanoparticles (NPs) in the nonpolar medium. It was assumed that AOT can be used for the langmuir films formation, since it is slightly soluble in a water (14 g/l, 25 °C). A method for producing gold sol in reversed micelles of AOT in a mixture of chloroform – DMSO in the presence of thiol has been developed, and langmuir films were formed on its basis.

Gold sol in a mixture of chloroform – DMSO (1 : 1) containing 30–200 mM AOT, 0.5 mM thiol, 0.7 mM HAuCl₄ and 7.0 mM NaBH₄ was prepared. Gold NPs were functionalized by 4-mercapto-1-butanol (MB), 1-hexadecanthiol (HDT), 2-aminoethanethiol (AET), mercaptoundecanoic acid (MUA). If AOT concentration in the synthesis medium was less than 200 mM, gold NPs aggregated during storage. Thiols affect the aggregative stability of gold sol in the micellar medium which decreases in the series MB > AET > without thiol > HDT ~ MUA

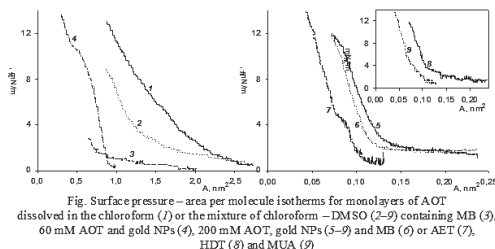


Fig. Surface pressure – area per molecule isotherms for monolayers of AOT dissolved in the chloroform (1) or the mixture of chloroform – DMSO (2–9) containing MB (5), 60 mM AOT and gold NPs (6), 200 mM AOT, gold NPs (5–9) and MB (6) or AET (7), HDT (8) and MUA (9)

Monolayer of AOT formed as in the presence of DMSO (Figure, isotherm 2) and thiol (isotherm 3) so without it (isotherm 1) is unstable because most of AOT molecules dissolve in the aqueous subphase. In this case compressibility of langmuir films does not depend on the amount of the AOT deposited on the subphase and is equal to 0.042 0.004 mN/m. The presence of gold NPs in the AOT monolayer (isotherms 4–9) decreases its compressibility indicating more dense packing of the molecules in the monolayer. Thus in the presence of gold NPs functionalized by MB (isotherm 6) the compressibility of AOT monolayer decreases to 0.031 m/mN.

Quantum ordering of protons in cold solid hydrogen

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A combination of state-of-the-art theoretical methods has been used to obtain an atomic-level picture of classical and quantum ordering of protons in cold high-pressure solid hydrogen. We focus mostly on phases II and III of hydrogen, exploring the effects of quantum nuclear motion on certain features of these phases (through a number of *ab initio* path integral molecular dynamics (PIMD) simulations at particular points on the phase diagram). We also examine the importance of van der Waals forces in this system by performing calculations using the optB88-vdW density functional, which accounts for non-local correlations.

Our calculations reveal that the transition between phases I and II is strongly quantum in nature, resulting from a competition between anisotropic inter-molecular interactions that restrict molecular rotation and thermal plus quantum fluctuations of the nuclear positions that facilitate it. The transition from phase II to III is more classical because quantum nuclear motion plays only a secondary role and the transition is determined primarily by the underlying potential energy surface.

A structure of P21/c symmetry with 24 atoms in the primitive unit cell is found to be stable when anharmonic quantum nuclear vibrational motion is included at finite temperatures using the PIMD method. This structure gives a good account of the infra-red and Raman vibron frequencies of phase II. We found additional support for a C2/c structure as a strong candidate for phase III, since it remained transparent up to 300 GPa, even when quantum nuclear effects were included. Finally, we found that accounting for van der Waals forces improved the agreement between experiment and theory for the parts of the phase diagram considered, when compared to previous work which employed the widely-used Perdew–Burke–Ernzerhof exchange–correlation functional.

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The morphology of silver nanoparticles in sols synthesized in the presence of nitrilotriacetic acid

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Previously we established the possibility of the formation of silver sols in the presence of ligands of aminopolycarboxylic acids family such as EDTA, NTA and DTPA, without a reducing agent and polymer stabilizers [1, 2]. Prospects of these sols for use in the Raman spectra of organic molecules was shown [3]. It was found that silver nanoparticles formed in the presence of EDTA and DTPA are similar in size and morphology. Conversely, sols synthesized in the presence of NTA are distinctly different in morphology. A significant effect of synthesis conditions of silver sols on the morphology of the formed nanoparticles was investigated. It was established that faceted particles and rods were formed in the presence of NTA. The formation of stretched structures (rods) was contributed by some factors (Figure) which are the following.

1) The order of mixing of the initial components: adding AgNO_3 solution to an alkaline solution of the ligand (standard method) or adding an alkali to the mixture of AgNO_3 and the ligand (non-standard method).

2) The ratio of $\text{Ag}^+ : \text{L}$: at a ratio of $\text{Ag}^+ : \text{L} \geq 1$ the formation of stretched structures is not observed. Increment of the synthesis time leads to the formation of longer (by 20–40 percent) stretched structures. Broadening of the spectra and the shift of λ_{max} to longer wavelengths is accompanied by an increase in silver particles size, widening of size distribution and alteration of their morphology, as it is shown by TEM investigations (Figure). Besides, in addition to rounded particles nanorods appear up to 100 nm in length and 20–25 nm in thickness together with well-defined particles.

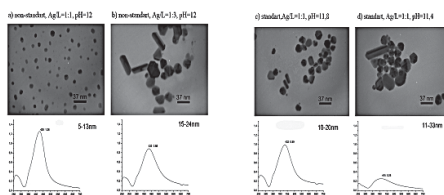


Fig. TEM images and optical spectra of silver sols at different synthesis conditions

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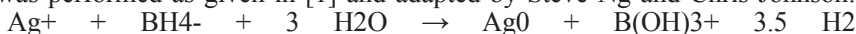
Synthesis, computational studies and characterization of polydiphenylamine nanocomposite with embedded silver nanoparticles

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A promising research area is the development of methods for obtaining hybrid materials and nanocomposites which are based on the introduction of the nanoscale objects into the polymeric matrix. Of particular interest are thin films of conducting polymers with incorporated palladium or silver nanoparticles, as well as bimetallic core-shell objects. At the same time obtaining of such materials with desired functional properties requires the precise control over the polymers conductivity and the coating morphology. In present study, hybrid polymeric PDPA-Ag coatings were obtained via in situ oxidizing polymerization of diphenylamine involving Fe³⁺ cations as catalyst in stationary conditions directly on substrate. Synthesis of silver nanoparticles was performed as given in [1] and adapted by Steve Ng and Chris Johnson:



PDPA and PDPA-Ag coatings characterization was carried out using SEM, AFM and FTIR methods. Quantum-chemical calculations were performed on MP2 level of theory with the cc-pVTZ basis set using the NWChem 6.5 computational chemistry package [2].

It was found, that the introduction of silver nanoparticles suspension during formation of polydiphenylamine film leads to a marked decrease in polymerization rate that can be caused by the suppression of the iron catalyst redox system. Morphology of PDPA-Ag coating (Figure b) has irregular domain structure compared to pure PDPA. It should also be noted that the presence of silver NPs has a significant influence on the PDPA-Ag nanocomposite conductivity due to electron delocalization during the redistribution of electron density or the interfacial electronic interaction. According to the performed simulations, obtained materials can show better stability and improved electrocatalytic performance. In situ synthesis of hybrid polymeric materials provides rich capabilities to control the deposition process and provides fine tuning the characteristics of functional coatings that is essential for fuel cell applications.

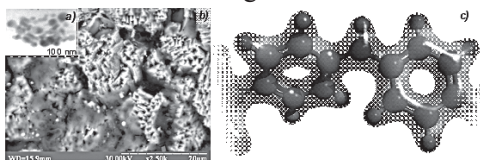


Fig. TEM image of silver NPs (a), SEM image of PDPA-Ag coating (b) and PDPA electron density distribution (c)

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Thermodynamic similarity of stacked-cup multiwall carbon nanotubes and graphite

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This work presents the results of the investigation of physico-chemical properties for stacked-cup multiwall carbon nanotubes (MCNT) supplied by Vision Development (Japan) and synthesized by the gas-phase catalytic pyrolysis of hydrocarbons according to the method [1]. It was shown in [2] that the apparent density of MCNT (2210 ± 22) kg·m⁻³ at $T = 293$ K determined in water, toluene, and [C4mim]PF₆ and the distance between the layers of 0.36 nm are close to the corresponding values for hexagonal graphite being 2260 kg·m⁻³ and 0.3635 nm, respectively.

The heat capacities of MCNT samples in the temperature range of (5 to 370) K have been measured and their energies of combustion have been determined. The thermodynamic parameters of pure (without encapsulated Ni) MCNT were evaluated. The average energy of combustion for pure MCNT is close to the corresponding value for graphite (Table). The difference between their energies of combustion is only ~ 170 J·g⁻¹. Thus, we can conclude that MCNT and graphite are similar not only geometrically, but also thermodynamically. From the Table, it also follows that graphite and MCNT are much more thermochemically stable (about 3 kJ·g⁻¹) forms of carbon compared to fullerenes C₆₀ and C₇₀.

It was found that the heat capacities of MCNT, graphite and fullerenes C₆₀ and C₇₀ per one mole of carbon atoms are consistent within ± 3 % in the temperature interval of (300 to 350) K. Taking into account this fact the extrapolation of the heat capacity of MCNT was carried out up to $T = 2000$ K and thermodynamic properties of nanotubes in the temperature range of (0 to 2000) K were calculated.

The energy of combustion for some carbon materials at $T = 298.15$ K

Compound	Graphite	MCNT*	C ₆₀	C ₇₀
$-\gamma_c U_{298}^0, \text{ J}\cdot\text{g}^{-1}$	32764 ± 4 [3]	32595 ± 13	36017 ± 17 [4]	35802 ± 26 [4]

Thermodynamic analysis of reactions for the synthesis of graphite and MCNT by pyrolysis of carbon-containing gases (CO, CO₂, CH₄, C₃H₈, C₄H₁₀) was performed. The following results were obtained.

1. Hydrogen H₂ (~ 82 mol·kg₋₁) and solid graphite and MCNT (~ 65 mol·kg₋₁) are the main components of the equilibrium mixtures obtained by the pyrolysis of hydrocarbons C_nH_{2n+2} at $T \geq 1300$ K ($P = 1$ bar).

2. The equilibrium of the reaction $2\text{CO}(\text{gas}) - \text{CO}_2(\text{gas}) + \text{C}(\text{graphite}) (\text{C}(\text{MCNT}))$ is almost completely shifted to the right side of the equation in the range of (298 to 900) K.

3. The synthesis of fullerenes C₆₀ and C₇₀ from graphite is thermodynamically

possible only through the high temperature ($T > 3000$ K) sublimation of carbon.

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The rheological characteristics of the solutions containing nanocluster polyoxometalates and polyvinylpyrrolidone

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Spherical nanocluster polyoxometalates based on molybdenum attract the attention by the uniqueness of the structure and the ease of synthesis. They are promising as sorbents, catalysts for fine organic synthesis. Due to the presence of internal cavities and pores on the surface different substances, including drugs can enter inside nanoclusters. It makes them prospective from the point of view of creation of nanocapsules for targeted drug delivery into the body. We found that the nanoclusters are able to stabilize polymers under ultraviolet and X-ray irradiation.

We continued the study of the interaction of nanoclusters with polymers. The effect of nanoclusters on the kinematic viscosity of polyvinylpyrrolidone solution was investigated for $(\text{NH}_4)_{42}[\text{MoVI}_{72}\text{MoV}_{60}\text{O}_{372}(\text{CH}_3\text{COO})_{30}(\text{H}_2\text{O})_{72}]\cdot 300\text{H}_2\text{O}\cdot 10\text{CH}_3\text{COONH}_4$ (Mo132), $(\text{NH}_4)_{32}[\text{MoVII}_{110}\text{MoV}_{28}\text{O}_{416}\text{H}_6(\text{H}_2\text{O})_{58}(\text{CH}_3\text{CO}_2)_6]\cdot x\text{H}_2\text{O}$ ($x\sim 250$) (Mo138), $[\text{Mo}_{72}\text{Fe}_{30}\text{O}_{252}(\text{CH}_3\text{COO})_{12}\{\text{Mo}_{20}\text{O}_7(\text{H}_2\text{O})\}_2\{\text{H}_2\text{Mo}_{20}\text{O}_8(\text{H}_2\text{O})\}(\text{H}_2\text{O})_{91}]\cdot 150\text{H}_2\text{O}$ (Mo72Fe30).

The experimental results showed that the introduction of nanoclusters into the solution of polyvinylpyrrolidone reduces the viscosity of the system. The decrease in viscosity indicates the presence of interaction between components, partial bonding of the active centers of the polymer, which prevents the interaction of polymer molecules with each other. Additional measurements of viscosity for aqueous solutions of polyvinylpyrrolidone with Mo132 were performed after 7 days. In specified conditions nanoclusters were not decomposed. The resulting viscosity was less than that of freshly prepared solutions. It indicated the duration of processes in solutions.

0.042 ± 0.004 mN/m.² of rheological properties of the studied solutions with the processes of interaction between polymer macromolecules and ions of polyoxometalates was also confirmed by the following calculations. For the solutions of polyvinylpyrrolidone with Mo132 and Mo138 the dependence of the ratio of the pure polymer viscosity and its viscosity in the presence of polyoxometalate was derived. The curves illustrating such dependencies (Figure) had a maximum in the region corresponding to the

ratio of the components in nanocluster-polyvinylpyrrolidone associates defined earlier.

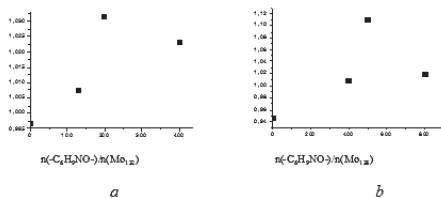


Fig. Dependence of the ratio of pure polymer aqueous solutions viscosity per viscosity of nanoclusters in polyvinylpyrrolidone solution on the number of monomer units per nanocluster:

a – Mo132, b – Mo138, concentration of nanoclusters $4.5 \cdot 10^{-4}$ mol/l, 25 °C

Superparamagnetic composite particles for extraction and purification of genomic DNA

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Silica-coated superparamagnetic iron oxide nanoparticles (SPION) are widely used for a number of biomedical applications [1, 2], including extraction and purification of genomic DNA from biological samples. The method is based on selective adsorption of DNA on γ -Fe₂O₃/SiO₂ silica surface followed by a magnetic separation [3]. Highly pure and concentrated sample of desorbed DNA can be used for real-time polymerase chain reaction (RT-PCR) analysis in clinical diagnostics. In this work, we represent a facile synthesis of γ -Fe₂O₃/SiO₂ composite particles using cheap and environmentally acceptable inorganic chemicals. The synthesis is based on a combined hydrolysis of Fe²⁺ and Fe³⁺ salts with ammonia water solution followed by a hydrolysis of Na₂SiO₃ with hydrochloric acid in the presence of the obtained Fe₃O₄ nanoparticles [1]. The final stage is an oxidation of Fe₃O₄/SiO₂ (35 wt.% SiO₂) into γ -Fe₂O₃/SiO₂ using 9% H₂O₂ water solutions since γ -Fe₂O₃ phase possesses a better thermal and chemical stability. The γ -Fe₂O₃/SiO₂ nanoparticles were dispersed in physiological saline

(NaCl 10 mg·ml⁻¹) to obtain a water suspension with the solid phase concentration of 40 mg·ml⁻¹. The influence of the γ -Fe₂O₃/SiO₂ synthesis conditions on the DNA adsorption, colloidal stability and magnetic properties of the obtained particles were studied.

The diameter of the γ -Fe₂O₃/SiO₂ spherical nanoparticles was estimated by TEM to vary from 40 to 80 nm. The composite particles consist of crystalline γ -Fe₂O₃ grains (8–15 nm) distributed over an amorphous SiO₂ matrix (XRD, TEM, SEM). However, the hydrodynamic size of the nanocomposite, determined by dynamic laser scattering (DLS) measurement was significantly greater (4500–4700 nm). This indicated to a tendency of the particles to form agglomerates in water solution. The powdered nanocomposite shows a superparamagnetic behavior, with the saturation magnetization of about 35–40 A·m²·kg⁻¹. The specific surface area of the powder was measured by BET method and appeared to be 160–170 m²·g⁻¹. The presence of functional silica film on the surface of composite particles was confirmed by IR spectroscopy.

In order to estimate the functional properties of the synthesized sorbent suspen-

sion, a model DNA isolation kit was proposed. It was composed of γ -Fe₂O₃/SiO₂ particles saline dispersion, lysis solution (guanidine hydrochloride), TE buffer (Tris, EDTA, pH~8,0), ethanol and acetone. The nucleic acids isolation had been performed by a modified Boom method [4]. Human and salmon genomic DNA and clinical samples of human blood serum and saliva were used as model biomaterials. The extraction efficiency was estimated by the quantitative RT-PCR [3] to be 83–94 %. No impurities that can inhibit the PCR were detected during operations. It was found that the purity of the extracted DNA was suitable for the PCR analysis in clinical diagnostics.

Thus, the synthesized γ -Fe₂O₃/SiO₂ nanocomposite suspension meets the basic requirements to sorbent for commercial DNA isolation kit.

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Photoelectric characterization of P3HT polymer / PbS nanocrystals composites

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The need of low-cost renewable energy motivates scientific researches on looking for effective and cheap solar cells. One of potential solutions is hybrid solar cells, which can merge advantages of both organic and inorganic semiconductors, such as strong absorbance, mechanical flexibility, low specific weight of conjugated polymers, and high conductance and tunable band gap of inorganic nanocrystals [1].

In this research, we investigated photocurrent kinetics of new type hybrid solar cells created on the base of semiconductor nanocrystals doped polymer. The purpose of this research was to evaluate the mobility of electrons and holes and it dependence on composition and fabrication of samples.

Thin films (roughly 100 nm thick) with different mass ratio of poly(3-hexylthiophene) (P3HT) polymer and PbS nanocrystals were investigated by using “transient photocurrent” and “charge carrier extraction by linearly increasing voltage” (CELIV) methods. By using the first method we registered photocurrent kinetics on several time scales (Fig.), and dependencies of charge carrier extraction times on

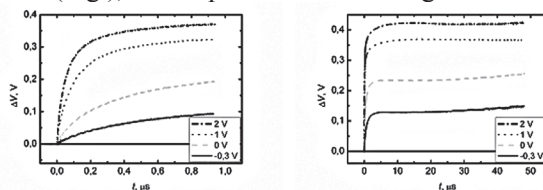


Fig. Photocurrent affected voltage drop ΔV at different time scales on applied electric field.

applied electric field and polymer/nanocrystal composition ratios were evaluated.

The results of research showed that photoconductivity of samples and charge carrier extraction times were strongly dependent on the sample composition ratio and fabrication procedures. Analysis of photocurrent kinetics and their dependencies on composition ratio enabled us to distinguish the electron and hole motion. By increasing concentration of polymer the mobility of holes increases, however, the mobility of electrons decreases. The extraction times were by about 5 times shorter in samples annealed during fabrication. Furthermore, qualitative analysis of the photocurrent kinetics revealed that the charge carriers extraction time can be expressed as $1/E\mu$ in all samples, where $\mu \sim E^{1/2}$.

By using CELIV method only few samples were measured, because others had too high conductance. The results matched with those measured by the “transient photocurrent” method.

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Low-temperature synthesis and the study of nanostructured Co–TiO₂ ferromagnetic compositions

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In recent years nanostructured (1D-, 3D-dimensional) TiO₂-based materials have become a subject of intense research due to unique physicochemical properties and original morphology [1, 2]. A large ion exchanging capacity combined with high surface area make them attractive for direct applications as magnetooptical, ion-conducting, and spintronic devices, photocatalysts, selective sorbents of radioactive ions, materials absorbing a radiofrequency radiation, as well as high activity participants in fabricating delicate composites. The aim of this work was to study the possibility to produce nanostructured TiO₂-based material with high concentration of Co-containing components via alkaline hydrothermal treatment of TiO₂ and CoCl₂ · 6H₂O powders in the presence of hydrazine.

The properties of hydrothermal products have been studied by Raman and IR spectroscopy, scanning electron (SEM) and transmission (TEM) microscopy, powder X-ray diffraction (XRD), an energy dispersive X-ray (EDX) and magnetic analysis. As a result, optimal conditions for synthesis of nanostructured Co–TiO₂ compositions were determined. It has been found that hydrothermal products are formed in shape of one-dimensional elongated structures Co-doped titanium dioxide and the Co-containing globular nanoparticles (Figure). The elongated

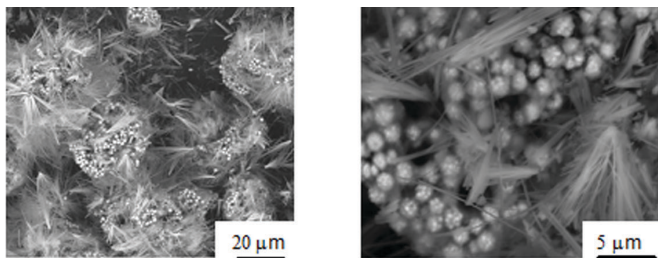


Fig. SEM images of hydrothermal nanostructured Co-TiO₂ product

nanostructures have lengths exceeding several hundred of nanometers. A higher magnification reveals that one-dimensional structures are characterized by a well-ordered multilayered morphology. The globular nanoparticles are composed of smaller rounded formations having very similar dimensions. After low-temperature air treatment at 60 oC, nanostructured products of hydrothermal synthesis demonstrate abnormally high ferromagnetic properties. An effect of hydrazine on the texture, morphology, and phase composition of products is discussed.

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Design of new functional materials based on chalcogenide glasses, polymers via modification and nanocomposite techniques

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The purpose of this work is to analyze the ways for design and synthesis of new nanocomposite materials based on chalcogenide glass semiconductor (ChGs) and organic polymers and dyes and overview their optical and principal solid-state properties and some applications. Our research was concentrated within next directions: study the influence of doping on properties of chalcogenide glasses; chalcogenide glasses nanomultilayer structures of various compositions; polymers, composites “polymers – chalcogenide glasses”; and study of their optical, other physical and chemical properties, their properties as recording media and some applications.

Influence of doping with transitional metals and rare-earth elements on properties of chalcogenide glasses was studied. X-ray diffraction measurements confirmed the amorphous structures of doped by transition metals and rare-earth elements chalcogenide glasses. Radial distribution functions have shown no significant changes in distance for nearest neighbourhood with the change of dopant concentration. In Raman spectra the main effect observed under the introduction of dopants was the change in relative concentration

of main and non-stoichiometric structural units characteristic for chalcogenide glasses.

Thermal properties (T_g values for undoped and doped glasses) were studied using DSC technique. Activation energy of glass transition was estimated with the use of Kissinger's expression. Optical properties of doped chalcogenide glasses were studied in 700–4000 cm^{-1} spectral region. The observed changes of the vibrational absorption bands were considered to be connected with the interaction of the introduced dopants with the non-stoichiometric structural elements present in glass and inherent impurities of the host glass such as hydrogen and oxygen. The main feature of Raman spectra under the introduction of transitional and rare-earth impurities into chalcogenide glass matrix was the change in relative concentration of the main and non-stoichiometric structural elements typical for initial glasses. Luminescence of chalcogenide glasses doped by transitional metals was studied in 800–1600 nm region ($T = 77 \text{ K}$,). Luminescence intensity increased with the metal concentration thus denoting the enlarged level of defects which is in accordance with the modified Tanaka's model. Chalcogenide glasses modified by Yb had two bands of luminescence in near IR region (near 980 and 1060 nm, excitation at 980 nm wavelength, room temperature). In this case transitions were observed characteristic for Yb^{3+} ion. Pure chalcogenide glasses are diamagnetics. Introduction of transitional and rare earth impurities changed the magnetic properties of investigated chalcogenide glasses. In the fields near 5T the $M(T)$ dependence was observed typical for paramagnetics and ferromagnetics in the paramagnetic temperature range.

$\text{As}_2\text{S}_3\text{--Se}$ and $\text{Ge}_5\text{As}_3\text{S}_5\text{S}_8\text{--Se}$ nanomultilayers were studied as recording media. Optical constants of nanomultilayers, thickness and optical band-gap energy were obtained from transmission using Swanepoel method. Optical properties of nanomultilayer structures were analysed within the frames of single-oscillator model.

Diffraction gratings were recorded using DPSS green laser ($\lambda = 532 \text{ nm}$ and power 100 mW) with synchronous diffraction efficiency measurement at $\lambda = 650 \text{ nm}$ in the first diffraction order. Atomic force microscopy (AFM) studies of the surface of holographic gratings with a period $\Lambda = 1 \text{ }\mu\text{m}$ recorded on nanomultilayers $\text{As}_2\text{S}_3\text{--Se}$ and $\text{Ge}_5\text{As}_3\text{S}_5\text{S}_8\text{--Se}$ have shown high optical quality of the obtained relief. Diffraction efficiency η values of the gratings was $\sim 20\text{--}30 \%$ in transmission mode at wavelength $\lambda = 0.65 \text{ }\mu\text{m}$. Due to the changes in transmission, reflection, and in thickness under the influence of laser irradiation, $\text{As}_2\text{S}_3\text{--Se}$ and $\text{Ge}_5\text{As}_3\text{S}_5\text{S}_8\text{--Se}$ multilayers can be used for effective amplitude-phase optical information recording, for the production of surface-relief optical elements.

Two-component nanocomposites based on chalcogenide glass semiconductor (ChGS) and metal phthalocyanine were obtained by simultaneous condensation of the two components on the surface of substrates in vacuum. Surface morphology of the samples was investigated using AFM. In the optical absorption spectra of composites characteristic bands of phthalocyanine were present. Comparison of Raman spectra of nanocomposite films and ChGS or Me–ChGS allowed us to identify the main structural bounds. Metal atom formed additional coordinating bonds with chalcogen atoms in nearby ChGS matrix.

Layers of polyepoxypropylcarbazole (PEPC) were studied as a media for holograph-

ic recording. The polymer was synthesized as the host polymer matrix and iodoform CHI₃ was used as the photosensitizing dye. As the pure polymer material was sensitive only in the UV spectral range its sensitivity had to be shifted to the type of recording laser region. To shift the spectral sensitivity to the blue region of spectrum the sensitizing dye such as iodoform CHI₃ has been introduced into the samples. The dependence of photosensitivity of the deposited films on the content of iodoform CHI₃ was studied earlier, where it was established that the optimal concentration of the iodoform was ~10 wh. %. Thin polymer films with thickness ~ 1.3 μm were prepared from homogeneous polymer solution in toluene by spin coating procedure using programmable spin-coater "SGS Spincoat G3P-8". For the determination of film thickness in this work the modified interferometric PC measurement based on MII-4 interference microscope was applied.

With the purpose of firmly assessing the nature of the synthesized material, a detailed characterization by IR and UV-VIS spectroscopy was applied. 473 nm 100 mW DPSS laser was used for holographic characterization. Diffraction gratings were recorded on these films by keeping the beam ratio as 1 : 1 and spatial frequency 1000 lines/mm. On exposing to the interference pattern, the CHI₃ molecules get excited and electron transfer takes place between carbazole ring and CHI₃. Carbazole radical is produced in the reaction and this radical initiates the polymerization reaction. Polymerization takes place at the region of constructive interference and, as a result of this polymerization (crosslinking), contributes to the structurization of co-polymer. This structurization takes place without significant change in the refractive index and transmittance of film which leads to the hidden grating formation. After recording the wet chemical treatment was applied for the surface relief formation. Etching treatment was controlled by measuring the diffraction efficiency of the gratings in transmission mode at the 633 nm wavelength within the equal time interval. The carbon tetrachloride was chosen as etching agent. Evolution of diffraction efficiency of the gratings in dependence on recording and etching time was studied. After the recording the diffraction efficiency (η) of all samples was less than 0.1 %. After chemical etching due to surface relief formation the diffraction efficiency value was grown up to 18 %. Diffraction efficiency of gratings in dependence on the etching time of polymer films was studied.

Obtained results show that optical, thermal, luminescent and magnetic properties of chalcogenide glasses can be changed by doping of transitional and rare-earth metals. Chalcogenide glasses can be a host for rare-earth metals that provides the possibility of simultaneous change both in luminescent and magnetic properties of glasses.

Nanomultilayer composites based on chalcogenide glasses and inorganic (chalcogenide glass) – organic (polymers, dyes) composites are perspective as holographic recording media. Direct surface recording or recording with consequent selective etching can be realized. New functional materials based on chalcogenide glasses, polymers and produced via modification and nanocomposite techniques are perspective for the applications in optics, optoelectronics and integrated optics.

ELECTROCHEMISTRY

Dependence of the underpotential shift of metals cathodic deposition tellurium on the Gibbs energy of metal telluride formation

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Metal adlayer on a foreign substrate is an important intermediate product in the electrochemical layer-by-layer assembly of nanostructured materials [1–2]. The adlayers are formed by underpotential deposition (UPD) that is a cathodic reduction of the corresponding metal cations above the reversible potential $E(\text{Mez}^+/\text{Me})$. The underpotential shift characterizing the difference between the potential of UPD (EUPD) and $E(\text{Mez}^+/\text{Me})$, has been known to depend linearly on the difference of the work functions of the substrate and the deposited metal in the UPD of metals on foreign metals [3]. The UPD of metals on tellurium shows much similarity with the UPD of metals on a foreign metal electrode in cyclic voltammetry, with few significant differences. The UPD on tellurium is more irreversible and the underpotential shift of the deposition potential shows no correlation with differences in the work functions of the metal that is deposited underpotentially and the substrate material. In the investigation of the UPD peculiarities on tellurium with voltammetric and nonstationary impedance techniques, we have derived a correlation of the UPD shift with the free energies of formation of the corresponding metal tellurides which is helpful for predicting UPD shifts in those adlayer deposition processes on tellurium that do not give clear voltammetric response of UPD for different reasons. Different methods of the UPD shift derivation from voltammetric data and potentiodynamic electrochemical impedance spectroscopy will be also discussed in the report.

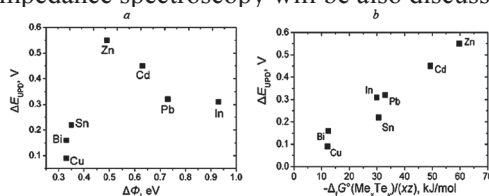


Fig. Underpotential shift versus (a) the work function difference $\Delta\phi$ of tellurium and metal, (b) normalized Gibbs energy of metal telluride formation

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Electrochemical formation of functional materials of new generation: nanostructured coatings with pre-set properties (for electronics and energy)

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Proposed work deals with the fundamental problem of the modern electrochemistry: synthesis of materials with tailor-made structure and properties in a controlled and repeatable way for various practical applications, as well as with materials science as its methodologies will be used for chemical and structural characterization of obtained materials as well as for determination of functionality.

Concept of the study is to develop a theory and practice of controlling the electrodeposition of functional films of alloy with tailor-made nanostructure and properties. Now such a general theory does not exist in the world, there are only scattered data concerned each particular case. The efficiency of transformation of chemical energy in electric one in fuel cells (FC) is determining the constant of rate of electrochemical electrode reaction, reversibility of electrochemical process and electrochemical resistance of the system. A tendency in creation of electrocatalysts is a transition from monometallic constructions to multi-component with a certain structure and functionalization. The idea of the work consists in the use of bifunctional electrocatalysis, which is conditioned by the action of different in nature catalytic centers included in one structure at a certain spatial arrangement of them. These centers have to be of nucleophilic and of electrophilic nature, that creates conditions for the selectivity and electrocatalysts efficiency.

The problem of the catalytic activity of d-metal alloys in the hydrogen evolution reaction (HER) is discussed in the literature. Hydrogen overvoltage reaction significantly affects the number of vacant d-orbitals in the electronic structure of the metal or alloy, the nature of this influence depends on the limiting step of the process of hydrogen evolution. Based on the analysis of the electronic configuration of metals belonging to the binary alloys it was found that the greatest catalytic effect on the HER should be observed in case when one of the metals has d4–d5, and another d6–d8 electron configuration. From this viewpoint, the alloys of tungsten and molybdenum with metals of the iron subgroup are important for practical applications. These properties have to be inherent to the alloys of metals belonging to iron subgroup with tungsten, and molybdenum (CoW, CoMo, NiW, NiMo, FeW, FeMo) that is necessary for their electrocatalytic activity in hydrogen/oxygen reduction processes and ethanol oxidation.

Since the availability of direct correlation between corrosion and electrocatalytic characteristics of the surface layer of nanostructure catalysts FC (as «core-shell»), the study of corrosion and nanocorrosion properties of catalysts is important and sometimes crucial. The advantage of researches of FC based on ethanol with proton-conductive polymeric electrolyte lays in the possibility of application of the catalytic systems which do not contain platinum. The main trends of this study are 1) to develop the electrochemical deposition of alloys containing nucleophilic and electrophilic component; 2) to create electrocatalysts of ethanol oxidization or hydrogen reduction-oxidization. The ideas of spillover and synergistic effects are also used, which can be realized using bifunctional electrocatalysts on the carbon surface and nanostructure compositions.

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Preparation and electrochemical properties of tin(IV) oxide – graphene oxide film electrodes

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Graphene oxide (GO) is an object of great interest for materials science, due to its use for preparation of membranes of exceptional filtering capacity and strength [1], graphene production via GO by various techniques based on Hummers method [2], etc. Graphene oxide has attracted also much attention recently [3, 4], as electrode material which combines recognized advantages of graphene with additional possibilities for electroactive interfaces design that result from oxygen-containing functional groups in GO molecular structure. In electrochemical applications, the use of a binding component could provide additional benefits. In order to bring about the advantages of the two-component electrode materials, we have developed a method of preparation of tin(IV) oxide – graphene oxide film electrodes and tested the electrodes in the reaction of anodic oxidation of chloride anions and also in lithium cathodic intercalation.

Graphene oxide was prepared from graphite via a modified Hummers [2] method, using the preoxidation stage that was based on optimization of Kovtyukhova et al. [5] procedure. Graphite powder was first preoxidized in a mixture of phosphorous(V) oxide, sodium persulfate and sulfuric acid and further oxidized to graphite oxide in a mixture with potassium nitrate, potassium permanganate and sulfuric acid. Thus obtained graphite oxide was exfoliated by sonic treatment, and the graphene oxide sol was finally separated from graphite oxide residue by centrifugation and identified by Raman spectroscopy. Graphene oxide sol was mixed with SnO₂ sol in different proportions to obtain composite tin(IV) oxide – graphene oxide film electrodes of various composition by dip coating the conducting ITO (mixed indium and tin oxide) glass.

The surface area of the composite electrodes monitored by double layer capacitance showed a strong increase with GO content up to 40 % GO. It was diminishing with the further increase in GO content. The composite electrodes were characterized by high electrocatalytic activity in anodic oxidation of Cl⁻ anions in concentrated aqueous solutions of alkali metal chlorides, in contrast with the unmodified SnO₂-electrode. The anodic reaction manifested strong effect of alkali metal cation, which was explained by the effect of different ion pairing in chloride solutions with different cations and the ion pair interaction with adsorbed chloride. We have also found that the cathodic treatment in the potential range of lithium intercalation in LiCl solution in acetonitrile activated the cathodic reduction of graphene oxide in the composite electrodes.

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Synthesis, structure and electrophysical properties of polycrystalline bismuth films

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Thin bismuth films provide a wide range of practical applications. Owing to a high magnetoresistive effect bismuth layers can be used as components of magnetic field sensors [1]. Many of today's conventional thermoelectric materials are bismuth-based compounds, for example Bi₂Te₃ [2]. The present work is focused on establishing correlation between electrophysical properties of polycrystalline bismuth films prepared by different methods and their microstructure. The films were fabricated by melt spinning and electrochemical deposition techniques.

Electrochemical bismuth deposition was performed from aqueous electrolyte containing 0.174 mol/l Bi(ClO₄)₃ and 3 mol/l HClO₄ onto plates made of a one-sided flexible foil-coated laminate. 70 μm thick Bi films were electrodeposited at room temperature and electrolyte stirring under galvanostatic regime with a current density of 2.5 A/dm². In the melt spinning technique, bismuth (99.9999 %) was melted and then spilled on the cold surface of rotating cylinder made of a polished copper.

Grain structure analysis (electron backscatter diffraction technique) showed that relatively fine-crystalline films (grain size l_G is 0.5–1.5 μm) were formed by electrochemical deposition. Annealing of these films at 540 K for 5–6 h led to a significant growth of the grain size (up to 10–50 μm). Melt spinning technique provided immediate formation of the coarse-grained Bi films ($l_G \sim 5$ –15 μm). Electrophysical characteristics such as resistivity, magnetoresistance, Seebeck coefficient and Hall coefficient of the prepared bismuth films were measured in 4–300 K temperature range under magnetic fields up to 8 T. Relative magnetoresistance $\Delta\rho/\rho_0$ at 4 K under magnetic field 8 T reached 4500 for annealed electrodeposited films, whereas $\Delta\rho/\rho_0$ did not exceed 12 for as-prepared electrodeposited films. Temperature dependence of the resistivity was found to be strongly influenced by Bi grain size. Semiconductor-like behavior was observed for the samples with grain linear size l_G comparable to a charge carrier's mean free path l . Metal-like behavior was inherent to the samples with $l \ll l_G$.

Mobilities and concentrations of electrons and holes were calculated using Lax model for electrons and parabolic dispersion law for holes. Electron and hole concentrations were found to be practically independent of the film fabrication method and were around 10^{24} m^{-3} , increasing five to seven times at the temperature growth from 25 to 300 K. Mobilities for the electrochemically deposited samples were close to $1 \text{ m}^2/(\text{V}\cdot\text{s})$ and depended only slightly on the temperature in the studied range. For the other types of Bi films, mobilities were approximately $10 \text{ m}^2/(\text{V}\cdot\text{s})$ at helium temperatures and declined by an order of magnitude at room temperature.

The observed differences in electronic properties of the Bi films under study can be explained by a profound effect of grain boundaries on charge carriers scattering. For fine-crystalline films (as-prepared electrodeposited films) the grain-boundary scattering plays a significant role, which results in a weak temperature dependence of mobility and a decrease of resistivity with increasing the temperature due to a rise of the charge carrier concentration. In case of coarse-crystalline films (electrodeposited films after annealing and films deposited by melt spinning) a contribution of the temperature-dependent scattering by phonons enhances strongly. As a result, the charge carrier mobility decreases, and the resistivity droningly rises with the temperature increase.

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Synthesis and transport properties of phosphorylated polyvinyl alcohol membranes for redox Fe³⁺/H₂ flow cell

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Fuel cells redox flow batteries are used in the electrochemical energy conversion and electrical energy storage technologies [1–3]. A hybrid Fe³⁺/H₂ redox flow system is very promising among those and the polyvinyl alcohol-based membranes are believed to be components of this system.

A novel method for preparation of phosphorylated polyvinyl alcohol (p-PVA) membranes was developed and used to synthesize a series of membranes with different degree of phosphorylation (4–9 w. % of phosphorus). The optimal mass ratio of PVA : H₃PO₂ was found to be 4 : 1, while the optimal curing time was 3 h at a temperature of 120 oC. The membranes possessed good mechanical robustness and chemical stability in acidic media. A method, based on “diatomic approximation” and combined with the Badger’s rule and Brown’s bond valence concept, was developed to estimate the chemical bonds frequencies with an accuracy of 20–25 cm^{–1} and was used to interpret the IR-spectra of the membranes. The possible pathway of PVA phosphorylation leading to formation of P–C bonds and various chemical functionalities was suggested.

The water flux (6.08·10^{–2} g·cm^{–2}·h^{–1}) and permeability of ferric ions (3.5·10^{–5} cm²·min^{–1}) were comparable to those of commercial Nafion 117 membrane. The dependence of the proton conductivity on the concentration of H₂SO₄ at 22 oC was studied and the intrinsic proton conductivity of the p-PVA membrane (5.5·10^{–3} S·cm^{–1}) was determined. The partial charges on oxygen atoms in structural linkages were calculated and the results indicate on the Grotthuss mechanism of proton transport.

The increased density of negative charges on oxygen atoms in structural linkages results in extra hydrogen bonding within the p-PVA matrix and affects not only proton conductivity, but also water flux through the membrane and other transport properties. The doping of p-PVA membrane with 2NH₂SO₄ increases the proton conductivity to the value close to the conductivity of commercial Selemion HSF membrane.

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Electrochemical deposition of Ni-Cr alloys from ethylene- and propylene glycol solutions

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Protective and functional nickel coatings owing to their high wear, heat and corrosion resistance are demanded in different industry's branches such as electronics, instrumentation, production of household appliances and furniture. The growing demands to the production quality cause the necessity to improve coatings properties. It could be done by the substitution of individual metals by their alloys. Nickel–chromium alloys are of great interest because of their hardness, wear resistance, corrosion stability and high heat resistance that is realized at a certain ratio of nickel and chromium in coatings. These alloys are used as finishing or intermediate coatings in steel molds and in different implements.

Aqueous Cr(III) и Ni(II) containing solutions are known to be used for electrochemical deposition of nickel–chromium alloys. However, they are not widespread because of the difficulties in maintenance the demanded alloy composition that is due to the instability of electrolyte in the result of hydrolysis and hydration isomerism of Cr(III) compounds.

The way to prevent the hydrolysis and hydration isomerism is to use nonaqueous polar solvents instead of water solutions for Ni–Cr alloy electroplating. Polyatomic alcohols such as ethylene glycol (EG), propylene glycol (PG), glycerin can be used as the solvents. Their advantages consist in the alteration of electrode potentials and overvoltages of metal ions reduction, in prevention of the hydrolysis. As a result, the processes of passivation of electrodes with hydroxides and hydrogen evolving are excluded and besides, coatings with low porosity are deposited [1, 2]

The purpose of this work was the investigation of nick-

el-chromium alloy electrochemical deposition from nonaqueous electrolytes with the usage of EG and PG as the solvents.

$\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$ и $\text{CrCl}_3 \cdot 6\text{H}_2\text{O}$ were used as chromium and nickel precursors. Ni(II) : Cr(III) ratio was varied in the range of 1 : 1, 2 : 1, 1 : 2. Boric acid and ammonium chloride were used to increase the electroconductivity of the solution and to diminish its viscosity, as it was recommended in the work [3].

It was revealed that Ni–Cr coatings with reproducible composition were deposited from EG and PG electrolytes containing boric acid under Ni(II) : Cr(III) ratio equal to 1 : 1 with the rate of 3.7 or 3.9 $\mu\text{m/h}$. Chromium content in these coatings was varied in the limits 2–8 at.% in case of PG and EG electrolytes accordingly. The dependence of chromium content in the alloy from current density appeared to be nonlinear and maximal chromium quota was achieved at the current density 7.5 mA/cm^2 . A slight dependence of chromium content on Cr(III) concentration and Ni(II) : Cr(III) ratio has been found.

Metals yield at this current density were equal to 21.4 % for nickel and 1.9 % for chromium in case of EG electrolyte and to 48.5 % for nickel and 0.6 % for chromium in case of PG solutions.

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Electrochemical activity of immobilized enzyme preparation of black horseradish on inorganic carries

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The influence of the inorganic carries (kaolin, aerosil, bentonite and its modified form on the electrochemical properties of black horseradish enzyme was studied using electrochemical impedance spectroscopy (Fig).

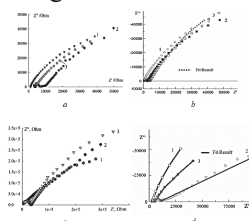


Fig. Impedance images of 0.5 % peroxidase solution, immobilized on horseradish (a), kaolin (b), modified bentonite (c), aerosil – 100 (d). 1 – initial carrier, 2 – native material with the adsorbed peroxidase, 3 – after 3 days in water

It was shown that strong proton-conducting properties of the substrate accelerate the conversion of proton-donor substrate and electron-conducting properties affect the conversion of electron-donor substrate. The results show the possibility to manage peroxidase and oxidase activity of immobilized enzyme.

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An electrochemical study of interaction between contact nonequilibrium plasma and aqueous electrolytes system

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The use of contact nonequilibrium plasma and aqueous electrolytes system (low-temperature glow discharge electrolysis), when the cathode is in a liquid phase and the anode is at some distance from the liquid surface, makes it possible to carry out nonequilibrium oxidation processes in the liquid being treated. In the liquid media the oxidation processes occur which cannot be realized by using conventional electrolysis or by the action of arc-crown-, townsend- or barrier-discharge plasma on the liquid.

The fundamental aspects of low-temperature glow discharge electrolysis action on water and water solutions of different classes of inorganic and organic compounds were revealed. It was shown that the formation of liquid bipolar bifunctional electrode as a conductor of second kind is a basis of faraday processes. This fact presents a peculiarity of low-temperature glow discharge electrolysis and a difference from a classic electrolysis. The mechanism of these electrodes work is considered depending on a direction of polarizing current.

Variation in the pH of water solutions and the formation of hydrogen peroxides during contact electrolysis upon the low-pressure glow-discharge treatment of water were studied. Some physicochemical properties of the products of treatment in these water solutions were presented. The changes of physics-chemical properties of water solutions, features of electrochemical processes during the reduction of metals were investigated.

We have carried out studies on the use of low-temperature glow discharge electrolysis for the purification of industrial wastewater containing inorganic heavy metal salts, radioisotopes, and a wide range of organic compounds, including heavy biodegradable nonionic surfactants and microbiological contaminants.

High efficiency of the effect of low-temperature glow discharge electrolysis is shown for disinfection of bacterial muddied drinks and wastewaters. Possibility of low temperature glow discharge electrolysis application is considered on purpose to remove the artificial radionuclide and transuranium elements compounds.

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Protective ability of electrodeposited and electroless Ni–P alloy coatings on mild steel in saline media

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Nickel phosphorus (Ni–P) alloys are of great interest because of their useful properties such as anticorrosive protection, wear resistance, high hardness, low friction coefficient, paramagnetic characteristics, catalytic activity in hydrogen evolution reaction. Although Ni–P coatings have been intensively studied, their protective properties are still not completely understood [1, 2]. In particular, no comparison of protective ability of Ni–P alloys produced by different methods can be found in literature. Since the commonly used methods for Ni–P coatings production are electrodeposition and electroless deposition, the present work was focused on comparing the protective properties of electroless and electrodeposited Ni–P coatings. The phosphorus content in Ni–P coatings is known to affect strongly their structure and anticorrosion properties. Therefore we prepared the electrodeposited Ni–P coatings with the phosphorus content 5.5, 10.0 and 21.5 at. %, which had microcrystalline, amorphous-crystalline and amorphous structure respectively. Since in the case of electroless deposition the P content in the coatings cannot be varied by changing the parameters of deposition process, we prepared electroless Ni–P coatings containing only 10 at. % of phosphorus which had amorphous-crystalline structure. The thickness of both kinds of the coatings was about 20 μm .

A systematic study of the effect of phosphorus content and the origin of Ni–P coatings on their protective ability on a mild steel substrate in saline media (3.5 % NaCl) was performed. Impedance spectroscopy was used as a powerful method for diagnostics of corrosion processes because of its high sensitivity to surface state in aqueous solutions. Immersion corrosion test of the coatings in saline solution was conducted for 1000 hours (about 40 days). During this period impedance spectra of the samples were periodically recorded under open circuit conditions, and then fitted with Nova software using corresponding equivalent circuits.

The research revealed a great difference in protective ability of the electrodeposited Ni–P coatings with different phosphorus content. Calculated charge transfer resistance (R_{ct}) of the electrodeposited crystalline Ni–P samples strongly fluctuated in the range of 10–40 $\text{k}\Omega\cdot\text{cm}^2$ during the first 10 days and then was stabilized at 10–15 $\text{k}\Omega\cdot\text{cm}^2$. Then after 680 hours of testing the R_{ct} began to rise up to 40 $\text{k}\Omega\cdot\text{cm}^2$. This behavior can be due to the penetration of aggressive chloride ions through pores and microcracks of the coating to steal substrate. Unlike crystalline samples, the R_{ct} of amorphous-crystalline and amorphous coatings increased rapidly in early hours of testing from 15 up to 200 $\text{k}\Omega\cdot\text{cm}^2$, indicating the formation of a thin protective film on the coatings surface. Then the R_{ct} growth rate decelerated, and after 1000 hours of testing the R_{ct} of elec-

trodeposited Ni-P (10 at. % P) was about 300 kOhm•cm². In comparison with the electrodeposited Ni-P coatings, the electroless Ni-P coating containing 10 at. % P demonstrated very low values of the R_{ct} (about 7–8 kOhm•cm²) during the whole period of testing, evidencing active corrosion processes of the samples.

Thus the results obtained show that only amorphous-crystalline and amorphous electrodeposited Ni-P coatings can provide effective protection against corrosion in saline media. Electroless Ni-P coatings with amorphous-crystalline structure do not protect mild steel under these conditions due to their active dissolution.

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Electroless deposition of Pd–Ni–P films from the polyligand pyrophosphate solutions

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Palladium-nickel-phosphorous alloys have high corrosion resistance, good solderability, wear resistance and hardness, low resistance transfer. Due to these properties Pd–Ni–P films are applied as finishing coatings in the production of different electronic devices instead of gold, as a sublayer for the deposition of palladium thin films, as the diffusion barrier at the assembly of electronic circuit boards and optoelectronic devices. As a rule, solutions for electroless Pd–Ni–P deposition contain ammonium, ethylenediamine (En), ethylenediamine tetraacetate or their mixture as the ligands. Sodium hypophosphite and potassium boronhydride are used as the reducing agents. Great difference between the values of Pd²⁺/Pd⁰ and Ni²⁺/Ni⁰ standard electrode potentials and easy reduction of much more electropositive Pd(II) stipulate the predominant content of palladium in Pd–Ni–P alloys and a low stability of solutions. Therefore, to diminish the gap between redox potentials of palladium and nickel and to retard Pd(II) reduction in the solution bulk it is necessary to select ligands or ligands mixtures providing the formation of stable complexes with palladium. That can be achieved in case of $K_s(\text{PdL}_x\text{My}) \gg K_s(\text{NiL}_x\text{My})$, where K_s is the stability constant and L and M are ligands, x and y can be varied from 2 to 4.

The purpose of this work was to develop the composition of stable solution for electroless Pd–Ni–P films deposition containing three types of ligands (pyrophosphate ions, ammonium and En), the investigation of peculiarities of joint Ni(II) and Pd(II) electroless reduction in polyligand solution, the analysis of elemental and phase composition of the coatings obtained and evaluation of their protective properties.

Stable electrolyte with pH 10.2 containing pyrophosphate ions, ammonium and En have been developed. The electrolyte allowed us to depos-

it coatings with the rate 1.5 $\mu\text{m/h}$ with nickel, palladium and phosphorous content equal to 77.0, 12.8 and 10.2 at.%, accordingly. Freshly deposited coatings included Ni₃P, Pd₇P₃ crystalline phases and amorphous palladium. At thermal treatment of Pd–Ni–P coatings crystalline phase of solid solution of palladium in nickel with palladium content equal to 8 at.% appeared.

In the result of voltammetric study of cathodic processes occurred on copper electrodes in polyligand pyrophosphate solutions it was established that the joint reduction of Ni(II) и Pd(II) proceeded with the depolarization effect in comparison with Ni(II) individual reduction but with the effect of overpolarization in comparison with Pd(II) individual reduction in the solutions with the analogous composition. The results of voltammetric experiments conducted with nickel working electrode modeling the later stages of Ni–Pd–P films deposition have shown that the joint Ni(II) and Pd(II) reduction proceeded with the effect of depolarization in comparison with individual Ni(II) and Pd(II) reduction. These results explain high nickel content in the alloy.

Pd–Ni–P, Ni–P, Pd–P coatings 1 μm thick deposited from solutions with the identical composition were tested for corrosion by the weight losses of the samples in the chamber of heat and moisture and in solution containing 3 mass. % NaCl and citrate buffer with pH 6. It was found that these coatings had no sufficient differences in their corrosion stability.

Effect of SnO_2 sol on peculiarities of electrochemical deposition and properties of copper coatings on zink, aluminium and their alloy

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Copper plating on zink, aluminium and their alloys is used for finishing manufactured articles and corrosion stability improvement, but there are principal difficulties in deposition of uniform metal layers with high adhesion and protective ability [1]. This work carries on the previous studies [2, 3] and is devoted to the elucidation of SnO_2 sol effect on the peculiarities of electrochemical deposition, microstructure and properties of copper coatings on zink, aluminium and their alloy.

Copper coatings were plated on zink, aluminium and Zn–Al alloy from slightly alkaline diphosphate copper plating solution containing nanoparticles of hydrated tin dioxide sol 2–4 nm in size which were stable in the electrolyte. It was found that at a small SnO_2 concentration of 0.5–1.0 g/l in copper plating solution there exists a confined range of current densities providing coatings deposition with the rate equal to that in the absence of sol. This optimal range depends on the substrate nature. At the increased sol concentration the rate of copper deposition diminishes and coatings become rough and friable. The intercalation on tin dioxide in coatings

is insignificant and its content in copper matrix does not exceed 1 at. % according to EDX data. Nevertheless, the presence of SnO_2 sol in copper plating electrolyte provides deposition of very fine-grained uniform and dense copper coatings (Fig).

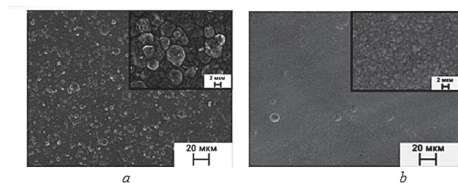


Fig. SEM images of Cu (a) and Cu- SnO_2 (b) coatings on Zn-Al alloy

Average size of copper grains in Cu- SnO_2 coatings deposited on zinc, aluminium and Zn-Al alloy is 2–3 times less as compared with the copper grain size in the absence of tin dioxide. Fine SnO_2 powders consisting of particles 20–100 nm introduced into the electrolyte under investigation did not exert such strong modifying effect on the coatings microstructure. Voltammetric studies of the anodic behavior of zinc, aluminium and Zn-Al alloy in the media of diphosphate copper plating electrolyte showed the diminution of anodic current density and the charge spent on Al, Zn and Al-Zn anodic oxidation in the presence of SnO_2 sol. Corrosion tests of the samples covered with copper doped with SnO_2 showed the heightened ability to retard Zn-Al alloy corrosion in the acid and chloride media compared with corrosion of the samples covered with coatings deposited in the absence of SnO_2 .

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Chemical and electrochemical formation of nanostructured aluminium mesh for display applications

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Nowadays, deposited indium-tin oxides (ITO) are the industrial standard materials for display applications. These materials possess good optical transparency and electrical conductivity. However, the deposition of the ITO films is a costly process demanding complicated equipment. An electrochemical anodization

of thin aluminium layers can manufacture adoptable transparent conductors for display. In this case, the anodization is accompanied by the formation of porous alumina layer on metal surface. At a moment when the bottoms of pores reaches sodium glass the rest of the metal presents an invisible Al mesh [1]. Furthermore, anodization of thin aluminium is one of low cost processes in industry.

In this work nanostructured aluminium mesh was produced by a simple anodization of aluminium, which was carried out in oxalic acid solution at a voltage of 50 V. The duration of anodization was determined by the current drop. Oxide films were removed by chemical etching in a mixture of 5 wt. % H_3PO_4 and 2 wt. % H_2CrO_4 at 30 °C for 0.2 h. The acid resistant paint was dissolved in acetone after anodization [2].

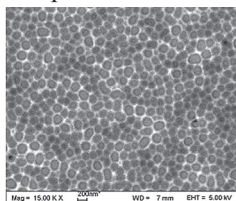


Fig. SEM image of invisible Al meshes after Al anodization in 0.3 M oxalic acid and chemical etching

Typical SEM image of invisible aluminium meshes after anodization and chemical etching is shown in Fig.

Defects in hexagonal arrangement of the mesh were caused by deference in the rate of the self-organized growth of pores. Conductivity of invisible meshes was determined by the thickness of the rest of aluminium nanostructure. These nanostructures can be used for the production of display devices.

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Voltammetric behavior of dinitrophenyl and phenol at their joint presence

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Phenol and its derivatives t refer to pollutants of the second class of hazard, their total content in the water should be less than 0.5 mg/l. The known method of their analysis is voltammetric determination of phenol and dinitroethylbenzene using glassy carbon electrode (GCE) [1, 2].

In our work the electrochemical behavior of the modified GCE in different background electrolytes containing 2,5-dinitrophenol, 2,4-dinitro-

phenol under their individual or joint presence and in the phenol availability have been studied. VAM-curves were recorded in a three-electrode cell with electrochemically modified GCE as a working electrode.

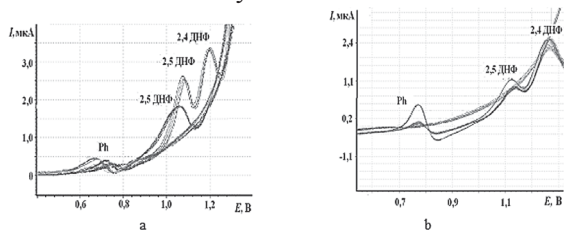


Fig. VAM-curves illustrating the behavior of electrochemically modified GCE electrode in acetate buffer background solution containing phenol, 2,5-dinitrophenol and 2,4-dinitrophenol:
a – phenol is added to 2,5-dinitrophenol and 2,4-dinitrophenol;
b – 2,5-dinitrophenol and 2,4-dinitrophenol are added to phenol

In case of acetate buffer background solution the analytic signals on current-voltage curves were observed as peaks at potentials $E_{2,4\text{-DNP}} = 1,250 \pm 0,150$ B and $E_{2,5\text{-DNP}} = 1,100 \pm 0,110$ V, the value of which increased with the enlargement of concentration. At the addition of a mixture of 2,4- dinitrophenol and 2,5- dinitrophenol in a ratio of 1 : 1 a broad total peak at $E = 1,100$ V appeared. At the increase of 2,4- dinitrophenol concentration to the ratio of 3 : 1 the separation of peaks was observed. The addition of phenol provided the separation of the measured peaks of phenol, 2,4-DNP and 2,5-DNP on the current-voltage curve. At the joint presence of phenol and dinitrophenols in the background solution three separate good measured peaks were observed on the current-voltage curves (Figure). The results show the possibility of the use of electrochemically modified GCE electrodes in voltammetric analysis of phenol and its derivatives at their joint presence in acetate buffer background solution.

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Effect of heat treatment of TiO₂ nanotubular layer on electrocatalytic activity of Au nanoparticles/TiO₂ system in oxygen electroreduction reaction

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Oxygen reduction reaction (ORR) significantly limits widespread applications of fuel cells due to relatively slow kinetics of oxygen formation and decomposition on most electrodes [1]. Platinum and its alloys are mostly used as anode and cathode catalysts in these applications, but this metal is costly and of limited reserve. Therefore, recently extensive research efforts have been devoted to the development of non-platinum electrocatalysts. Gold in alkaline medium can display effectiveness in ORR close to that of platinum. In or-

der to achieve a high specific surface area and particularly minimize the cost, gold is typically dispersed in the form of nanoparticles (NPs) and immobilized on solid surface [2]. However, the catalytic activity of NPs can depend strongly on the nature of the substrate.

In the present report, to study the influence of heat treatment of the substrate on electrocatalytic activity of gold NPs, electrochemically synthesized TiO_2 nanotubular layers on Ti were annealed at 350 °C, 450 °C and 550 °C for 3 h. Colloidal Au NPs were prepared by mixing HAuCl_4 , sodium citrate and sodium borohydride solutions. Aqueous colloidal suspension of Au NPs was coated onto the TiO_2 surface and then dried at room temperature. After Au loading, the samples were briefly post-heated at 200 °C to eliminate water and to assure more intimate contact between the NPs and TiO_2 surface. The electrocatalytic activity of the Au/ TiO_2 electrodes in ORR was then examined by cyclic voltammetry (CV) using an Autolab potentiostat in 0.1 M KOH solution saturated with O_2 .

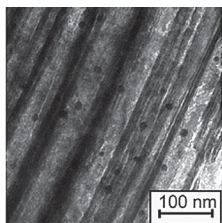


Fig. 1. TEM image of Au nanoparticles within TiO_2 nanotubes

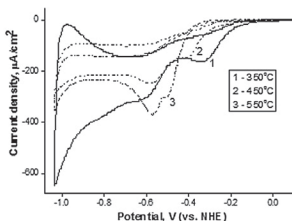


Fig. 2. CV curves of ORR in 0.1 M KOH solution on nanotubular TiO_2 layers heated at different temperatures and then loaded with Au nanoparticles

Fig. 1 shows TEM image of the Au-loaded TiO_2 nanotubular layer, the average size of Au NPs is 7–10 nm. CV curves for TiO_2 samples without Au NPs have one wave of ORR at potentials more negative than -0.5 V (Fig. 2). For Au/ TiO_2 electrodes an additional wave corresponding to O_2 electroreduction on the Au surface appears at less negative potentials. This wave is shifted to the negative direction with increasing the temperature of TiO_2 substrate annealing. This substrate-dependent influence on the Au-catalyzed ORR can be rationalized if we take into account the variation of semiconductor properties of TiO_2 as a result of its annealing.

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CHEMISTRY OF SURFACE AND THIN FILMS

The ways of the obtaining of antibacterial composite films

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The purpose of the investigation was the search and practical realization of the simple and effective ways of different materials protection

from biopollution under exploitation. Especially it concerns silica-alumina ceramics used in manufacturing of filters for liquids sterilization cleaning.

In this work the possibility was found to impart prolonged antibacterial properties to the silica-alumina ceramics by the formation on its surface of silver containing composition films 150–200 nm in thickness by the method of hydrolytic decomposition of the substances included into the impregnating solutions.

The solutions used for deposition of silver containing films represented poorly coagulating sols which were prepared by mixing of isopropil solutions containing silver nitrate and easily hydrolyzing compounds of titanium, titanium and tin, titanium and aluminium, titanium and silicon. Antibacterial films thus obtained included the amorphous products of oxo- and hydroxo compounds of these metals and AgCl nanoparticles 100–150 nm in size which were responsible for biocide action.

Antibacterial properties of the films were analyzed by the conventional diffusion method against Gram-positive and Gram-negative bacteria. The results of the experiments were evaluated by analyzing the width of the inhibition zones of bacteria growth around the ceramic samples coated with antibacterial coating. Diameters of these zones varied from 2 to 15 mm showing the availability of the biocide effect. The largest zones appear in case of the samples containing the products of titanium and tin compounds hydrolysis. The zones were absent in case of the samples containing silver nanoparticles obtained by the treatment in the alkaline formaldehyde solution. Nevertheless, transformation of Ag nanoparticles into AgCl ceeds by treatment in NaCl – H₂O₂ provided the appearance of zones and the rise of biocide activity. The reasons of distinctions in antibacterial properties of silver and silver chloride are discussed in the report.

Changes in structural and chemical composition of carbon-bearing components in porous anodic alumina during heat treatment

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It was shown earlier that composite materials based on ordered porous anodic alumina are widely used in biotechnology [1]. In the present study we aimed to obtain amorphous carbon/anodic alumina composite material with high carbon content by double-sided aluminum anodizing in aqueous solution of tartaric acid at constant current density and investigate the effect of heat treatment on structural and chemical changes in carbon bearing components in the obtained porous anodic alumina. By SEM it was shown that anodic alumina obtained in tartaric acid

electrolyte had well-ordered porous structure with the pore diameter about 90–100 nm and the distance between pores about 400–440 nm. By semi microanalysis it was also established that in as-anodized samples carbon content was about 3.2 % (wt.). Results of FTIR spectroscopy indicated the presence of three-dimensional polymeric structures composed by sp² and sp³ hybridized carbon atoms; and sp² type threefold coordinated bonds were dominating in as-anodized and heat treated in air at 200–700 °C samples (Figure). The ESR signals with $g\ 2.0033$ and $\Delta B =$

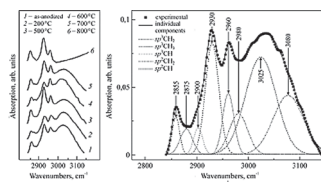


Figure. FTIR spectra of the carbon bearing anodic alumina in the C–H stretching modes heat treated at different temperature (a); the curves are separated to show the details; deconvolution of FTIR spectra on individual components (b); maxima in the individual components spectra are marked with arrows

0.68 mT resulted from electrons localized on the dangling bonds of tetrahedrally and threefold coordinated carbon atoms were observed. After heat treatment at 800 °C the structure of carbon bearing anodic alumina changed significantly. Carbon atoms in sp² hybridization were almost completely oxidized; and the ESR signal was caused by electrons localized on the dangling bonds of tetrahedrally coordinated carbon atoms.

Acknowledgment. This research was partly supported by the grant for joint project no. TAP LB-12/2015 from the Belarusian Republican Foundation and Research Council of Lithuania Foundation.

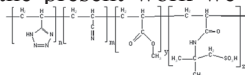
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Copper(II) sorption with tetrazolated Nitron D-5 polyacrylonitrile fibre

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Due to coordination ability polymers containing tetrazole derivatives are attractive as a sorbents for isolation of heavy metals from aqueous solutions [1–4]. In continuation of our investigations in the field of synthesis and chemistry of tetrazole derivatives [5] in the present work we studied the possibility of isola-



tion of Cu²⁺ from aqueous solutions using films of polymers prepared by azida-

tion of the commercial Nitron D-5 polyacrylonitrile fibre. Tetrazolation of the initial fibre was carried out using $\text{NaN}_3/\text{NH}_4\text{Cl}$ as azidation agent in dimethylformamide at 100°C . Obtained polymers present copolymers of 5-vinyltetrazole, acrylonitrile, methyl acrylate and 2-acrylamido-2-methylpropanesulfonic acid.

The content of tetrazolyl moieties varied from ~ 10 to $\sim 90\%$ was adjusted by changing the azidation agent : initial polymer ratio.

Films of polymers investigated was found to sorb Cu^{2+} from dilute solu-

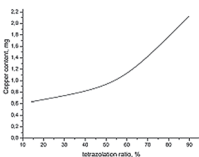


Fig. Dependence of sorbed Cu^{2+} amount vs tetrazolation ratio of sorbent (sorbent – 100 mg, $2.7 \cdot 10^{-4}$ M $\text{Cu}(\text{NO}_3)_2$, 24 h, 20°C).

tions of $\text{Cu}(\text{NO}_3)_2$. The degree of sorption increased with increasing of tetrazolation ratio (Fig), that indicated a key role of tetrazolyl moiety in the interaction of Cu^{2+} with a sorbent. The adsorbed Cu^{2+} ions were shown to be quantitatively removed from polymer formed by treatment with 0.1 M HCl. Sorbent regenerated were suitable for the further extraction of metal ions.

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The advantages of sulfur/graphene oxide materials

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Elemental sulfur is a promising cathode material for lithium rechargeable battery, due to its high theoretical specific capacity of 1.672 mAh g^{-1} [1, 2]. Furthermore, due to the advantages of natural abundance, low cost and environmental friendliness, sulfur shows great potential as the cathode material for the next generation of highenergy rechargeable lithium batteries [3].

However, the lithium/sulfur system confronts some great challenges, prior to its widespread practical realization. Recently, great efforts have been devoted

ed to improve the electrochemical performance of sulfur cathodes. Various carbonaceous and conductive polymer materials have been used to composite with sulfur [4–10]. The oxidized derivative of graphene, graphene oxide (GO), can be regarded as a functionalized graphene, bearing oxygen functional groups on its basal planes and edges, and, as it was found by Zhang et al., the functional groups on the GO surface play the role of immobilizers and can effectively confine any polysulfides from dissolving [7]. In the work we expect the formation of a highly porous structure consisting of sulfur with uniform graphene oxide coating on its surface at heat treatment at 150°C to obtain the S/GO composite (Fig).

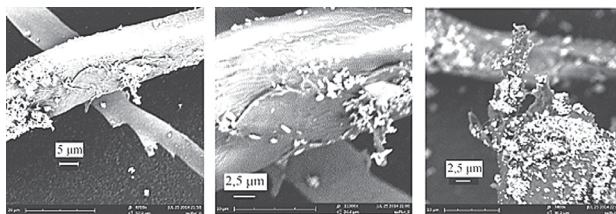


Fig. SEM images of morphology of the obtained S/GO mixture

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Removal of nitrate ions from natural water by nanofiltration

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Pollution of water with nitrates is a global problem. The aim of this work was to study the basic regularities of nanofiltration removal of nitrate ions both from model aqueous solutions and real natural waters.

Experiments were conducted by means of a laboratory nanofiltration membrane cell equipped with OPMN-P and OFAM («Vladypor», Russia) membranes. The membranes area in the cell was 38.5 cm². The operating pressure was created by com-

pressed nitrogen. The experiments were carried out with model solutions of nitrate ion with concentration of 50 mg/l. KNO_3 and $\text{Ca}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$ salts were used to prepare the solutions. A separate set of experiments was performed with natural water. The concentration of nitrate ions in the samples was determined by nitro analyzer pX - 150.1. pH values of the solutions were adjusted by means of NaOH and H_2SO_4 .

It was found that the nitrate retention with OPMN-P membrane appeared to be the highest in alkaline medium. This fact can be explained by the electrochemical mechanism of membrane separation. The nitrate retention decreases with an increase in a degree of the permeate selection. This was caused by the concentrating of a feed solution, which resulted in the enhanced concentration polarization effect [1].

The retention of nitrate ions with OFAM membrane was the highest in a neutral solution. Apparently this happened because the OFAM membrane had a higher ξ -potential comparing with OPMN-P membrane.

The addition of a cationic polyelectrolyte such as polydialildymethylammonium chloride in a nitrate-containing solution did not lead to an increase in nitrate retention.

It was established that while water purification from nitrate ions in neutral medium the OFAM membrane had a maximal nitrate retention of 73.2 %, while the retention for OPMN-P membrane was 42.9 %. In the acidic medium the retention of nitrate ions with the OPMN-P membrane reached 60.1 %, while for OFAM membrane it was 45.7 %. In alkaline medium the maximal retention of nitrate ions with OPMN-P and OFAM membranes was 77.1 % and 71.3 %, respectively.

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Investigation of antibacterial properties of ultrafiltration polymeric membranes

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The aim of this study was to investigate the effect of the chemical nature of the membranes surface on their biofouling. To obtain composite membranes with different chemical nature of the surface, a method of photoinitiated graft polymerization was used. Antibacterial properties of synthesized membranes were evaluated with *Escherichia coli* (*E. coli*) suspension, which was prepared by the method described previously [1].

Microfiltration polyethersulphone and polyvinidene fluoride membranes with an average pore size of 0.22 μm (Millipore Express and Millipore Durapore) have been used in the study. 2-acrylamide-2-methyl-1-propanesulfon-

ic acid (AMPS), 2 hydroxyethylmetacrylate (HEMA) and quaternized 2- (dimethylamino) ethyl methacrylate (kDMAEM) were used as modified agents.

The membrane tendency to biofouling has been evaluated during filtration of *E. coli* suspension in a dead-end membrane cell with an effective membrane area of 24.6 cm². The operating pressure was created by compressed nitrogen. The rotation speed in the membrane cell was set as 300 ± 20 r/min. The membrane flux was determined as:

$$J = V / S \tau,$$

where J is membrane flux (dm³/m²h), V is permeate volume (dm³) passed through the membrane area of S (m²) during filtration time of Δ (h) at operating pressure of ΔP (bar).

The results of microbiological tests reveal that the membranes modified with kDMAEM possess a strong bactericidal effect. AMPS modified membranes showed much weaker antibacterial properties, while HEMA modified membranes practically did not exhibit any bactericidal action.

The performed studies have also shown that the mechanism of antimicrobial action of the obtained composite membrane was probably similar to the same for guanidine substances [2]. It was found that the surface chemistry of the composite membranes essentially affects their susceptibility to biofouling. The membranes with hydrophilic surface were less fouled with *E. coli* cells comparing with hydrophobic membranes while the ability to recover the membrane flux upon washing was higher for the membranes with a chemically neutral surface than for charged membranes.

Thus, targeted chemical modification of the membrane surface can increase the membrane resistance to biofouling, especially when aqueous solutions with low concentrations of foulants are used for filtration.

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Background of nanoscale gradient formation in the structure of steel 9HF at hard plastic deformation

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The notion of multi-level nature of the deformation considers a deformed solid as a hierarchically organized multilevel system. The plastic flow of deformation develops consistently as a gradual evolution of the local shifts causing the crystal stability loss on the interconnected nano-, micro-, meso- and macroscale levels.

The origin of nanoscale gradient structure in thin foils, occurring in the surface layers of the back-up rolls of the rolling mill, made of steel 9HF, characterized by the original lamellar pearlite structure was investigated by electron diffraction microscopy [1].

Nanoscale (100 nm) level of gradient structure formation and phase composition was manifested, and its appearance was associated with the movement of the atoms of alloying elements in the process of thermo-mechanical impact on the steel 9HF samples. Mechanisms of the lamellar pearlite evolution in the process of steel deformation were revealed.

It was shown that the process of destruction of the cementite plates in steel was accompanied by the transfer of carbon atoms from cementite plates in the nuclei of moving dislocations with the subsequent formation of ferrite in the bulk of nano-sized cementite particles, by cutting plates and the movement of individual particles of cementite according to Geguzin-Krivoglaz mechanism in the fields of internal stresses.

Thus, it was found that steel deformation caused the gradient of carbon concentration in the samples of steel 9HF and the gradient of the volume fraction of cementite particles. Both gradients had nanometer scale.

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Multiple hafnium germanate interphase for SiC / SiCf composites

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Fiber-reinforced ceramic composites achieve high toughness through distributed damage mechanisms. These mechanisms are dependent on matrix cracks deflecting into fiber/matrix interfacial debonding cracks. Oxidation resistance of the fiber coatings often used to enable crack deflection is an important limitation for long-term use in many applications. Hafnium germanates have a high potential as interface coating in fiber reinforced ceramic composite materials due to a number of thermomechanical properties and oxidation resistance. Unfortunately, there is not a lot of information about hafnium germanates. Especially, the method of thin films deposition on substrates of complex geometric shape has not been studied.

The aim of this work was to prepare stable sol suitable for forming the nanosized coatings on the SiC fibers and to investigate the surface modification SiC fibers in terms of morphology and the tensile strength.

The special sol-gel approach was developed to obtain stable for a long period of time sols via dissolving the stoichiometric quantities of HfOCl_2 and GeO_2 in de-ionized water. Both solutions were then mixed and stirred. The precipitate was washed and dissolved in water by ultrasonic dispersion. Further, a small

amount of polyethylene glycol (PEG) was added. The fibers were immersed in mixed oxide sol, dried and then calcined at 900 °C. The elemental, phase composition and morphology were studied by modern analytical techniques. The tensile strength of single filaments was measured using Instron machine.

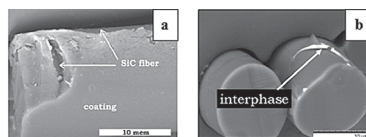


Fig. SEM images of the coated SiC fiber (a), fracture surface of SiC/HfGeO₄/SiC₂ minicomposites (b)

According to SEM images the coating was relatively uniform throughout the length of the fiber (Fig). The thickness of the first layer was equal to 200–250 nm. It was found that the accumulation of defects at the surface increases with the amount of the coating layers and sol concentration. The PEG addition allowed us to improve the surface morphology. It was established that the mechanical tensile strength of the fibers only slightly decreased in comparison with that of the initial fiber treated at the same temperature.

The effective fire protection of nonwoven polyether material

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Permanent fireproof processing of the non-woven polyester materials is a very difficult task, because their fibers are chemically inert and have a very smooth surface with nonporous microstructure (Fig, a). Commonly, two and trivalent metals-ammonium phosphates used as non-toxic inorganic flame retardants are fixed on the polyester materials surface in the insufficient quantity even in case of the use of stannous-containing mediator agents applied for a chemical binding of the burning inhibitors to a polymeric matrix [1, 2]. Thus, deterioration of the exploitation properties of the fire protected polyester materials is observed mostly due to the growth of their hardness. It was assumed that the replacement of inorganic burning inhibitors by nitrogen and phosphorous-containing organic products containing reactive functional groups can provide an increase in the resistance of fireproof effect to washings of the polyester materials and the elimination of their hardening. One of the effective fire protectors for polyolefin polymers could be 5-aminotetrazol phosphate, containing reactive amino groups [3].

In this work the nonwoven polyester fabric previously etched in alkaline solution was treated with 5-aminotetrazol phosphate alcohol solution. The fire protected material had satisfactory physical-mechanical properties such as softness, flexibility,

elasticity. It was revealed that ~25–30 mass. % of the burning inhibitor was preserved on the surface of the protected fiber after washing of polyester fabric that was confirmed by electron microscopic researches (Fig.e b). For comparison, the fiber treated with inorganic burning inhibitors lost them in the result of the material washing.

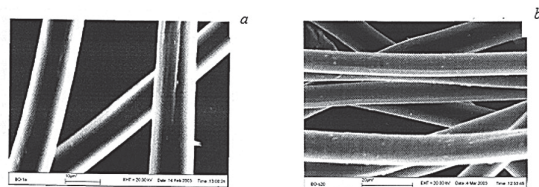


Fig. The surface morphology of initial (a) and fire protected (b) polyester fibers

By fire tests it was shown that the rate of the burning of the washed fire protected polyester material appeared to be 2–3 times under this rate in case of the initial sample. The results make it possible to conclude that the processing of polyester fabric with 5-aminotetrazol phosphate alcohol solution provides permanent fireproof effect.

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Improved alkali resistance of basalt fibers with zirconia and titania coatings

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Construction that is performed in extreme climate such as polar climate gives a rise to develop strength, resistant and sustainable materials for building. Reinforcement of a concrete by a fiber is an important step to increase the fracture toughness, water and frost resistance, bending and tensile strength of concrete. Basalt fiber is one of widespread types of such fiber. Due to some of its characteristics such as operating temperature, elastic modulus, tensile strength, basalt fiber is superior compared to most kinds of glass fiber. A disadvantage of the basalt fiber is its degradation in an alkaline medium such as a hardening concrete mass. The most promising way to solve this problem is the application of barrier coatings to basalt fiber that could slow the degradation process. The advantages of this method are targeting (maximum concentration in the reaction zone), cost (material cost reduction compared with other methods) and high adaptability. Also such technique can be easily scaled and integrated into the technological cycle of basalt fiber production. Properties of ZrO_2

and TiO_2 allow these oxides to be used for the application in alkali-resistant coatings.

The aim of this work was to develop zirconia- and titania-coated basalt fibers and to study their alkaline resistance.

As precursors $\text{ZrOCl}_2 \cdot 8\text{H}_2\text{O}$ and TiCl_4 were used for preparation of hydrated zirconia and titania sols with a concentration of 0.1–1.0 M and 0.2–0.8 M, respectively. Fibers were briefly dipped into a sol followed by drying and heat treatment to remove the solvent and to form the crystalline ZrO_2 and TiO_2 coatings. 2M NaOH solution and saturated solution of Ca(OH)_2 were used as a media for alkaline etching.

It was found that coatings were uniform and smooth with the thickness of 300–400 nm and 400–1000 nm for ZrO_2 and TiO_2 , respectively. One can note the presence of elongated aggregates (traces of the sol) on the surface of some fibers which are due to the retention of the sol between fibers which are close to each other. The morphology, phase and elemental composition, mechanical properties of the etched fibers were investigated. The surface morphology of basalt fibers etched in different alkaline media changed greatly. The formation of a layer of hexagonal Fe(OH)_2 plates was observed both for NaOH and Ca(OH)_2 media. The rate of the formation of this layer is much slower for Ca(OH)_2 media. Another feature was the morphology of calcium carbonate drusen, namely, dense spheres were formed in NaOH solution, whereas needle-like spheres or flower-like drusen were formed in Ca(OH)_2 solution. It was found that the presence of dense protective ZrO_2 and TiO_2 coatings on the surface of basalt fibers can significantly slows down the etching process.

Inhibition of steel corrosion by, Co(II), Zn diphosphates

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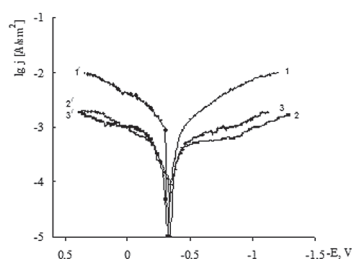


Fig. 1. Polarization dependence obtained on steel 08kp in $5 \cdot 10^{-3}$ mole/l solution of H_2SO_4 without additives (1,1') and with the addition of diphosphates $\text{Mn}_{0.54}\text{Zn}_{1.26}\text{P}_2\text{O}_7 \cdot 5\text{H}_2\text{O}$ (2,2'); $\text{Mn}_{1.17}\text{Co}_{0.83}\text{P}_2\text{O}_7 \cdot 6\text{H}_2\text{O}$ (3,3')

In actual practice of technological processes intensification in chemical, machine-building and metallurgical industry the special attention is devoted to questions of anticorrosive protection of metals and equipment. The aim of this work was to investigate the anticorrosive properties of new Mn(II), Co(II), Zn diphosphates solid solutions. $\text{Mn}_{2-x}\text{Co}_x\text{P}_2\text{O}_7 \cdot 5\text{H}_2\text{O}$ ($0 < x \leq 0.83$) and $\text{Mn}_{2-x}\text{Zn}_x\text{P}_2\text{O}_7 \cdot 5\text{H}_2\text{O}$ ($0 < x < 2.00$) solid solutions obtained as described in [1]. Corrosion researches of steel 08kp samples were conducted by the technique described in [2]. We used $5 \cdot 10^{-3}$ mole/l H_2SO_4 solution (background) as the model corrosion environment. Concentration of diphosphates in solution was $5 \cdot 10^{-3}$ mole/l. The gravimetric corrosion researches have shown that the addition of diphosphates to the background solution provided the reduction of steel cor-

el corrosion environment. Concentration of diphosphates in solution was $5 \cdot 10^{-3}$ mole/l. The gravimetric corrosion researches have shown that the addition of diphosphates to the background solution provided the reduction of steel cor-

rosion rate in 2.5–3.5 times that corresponded to protection degree of 59–70 %.

The results of electrochemical researches showed that the largest corrosion currents were observed in the background H₂SO₄ solution (Figure). The addition of diphosphates into the acid solution significantly altered the shape of polarization curves. Anodic current density in the presence of diphosphates was reduced almost on the order of magnitude, in comparison with a current density in the background solution, throughout the region of potentials under study. Thus, at the potential –0.18 V the value of current density logarithm in case of background solution was –2.64 and it was reduced in the presence of manganese-zinc and manganese-cobalt diphosphates to –3.26 and –3.22, respectively. In case of steel electrode in the background solution cathodic current density logarithm at potential –1.0 V reached –2.15. In the presence of diphosphates it decreased to –3.02 and –2.84, respectively. The magnitude of steel corrosion potential of steel (E) in the background solution was –0.32 V (regarding to NHE). Addition to the background solution of Mn(II), Co(II), Zn diphosphates practically did not shift the E value, that demonstrated an equal inhibition of cathode and anode processes at steel corrosion. The revealed anticorrosive action of diphosphates can be stipulated by the formation of protective coatings on a steel surface. They were found out by visual, gravimetric and X-ray researches. Thus, the experimental results show that for the first time synthesized Mn(II), Co(II), Zn diphosphates solid solutions revealed anticorrosive properties and can be used as inhibitors of steel corrosion in the acidic environment.

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Nano- and ultradisperse powders of superhard materials as modifiers of liquid lubricant

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Resource and mobility of tribocoupling of machine components depend not only on the type and quality of materials, careful manufacturing details from them, operation conditions, but also on the lubricants used in their work. The initial period of running-in of friction pair elements is a particularly crucial moment, and formed favorable conditions for their contacting form in the future.

Structural, technological and operational features of assembly units are very diverse, so it is recommended to use a specific lubricant for each particular case. Such a recommendation is advisable to use depending on the period of operation of the mechanism since interaction condi-

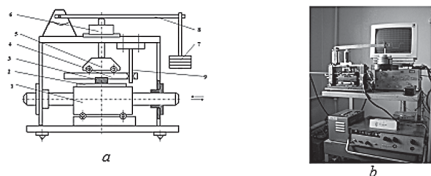


Fig. Plot (a) and appearance (b) of automated tribometer

tions of tribological conditions are continuously changing therein over time.

Properties of lubricants are regulated by the introduction of certain additives to the base oil that can help to reduce friction and wear of the assembly parts. Tribological tests were performed on an automated lubrication tribometer.

The purpose of this work was to investigate in terms of the oil I 40 the effect of the additives of synthetic diamond nanodisperse (7–8 nm) powders and silicon carbide ultradisperse (7–12 μm) powders on the running-in and lubricant ability. Diamond as well as silicon carbide has extremely high hardness (10.0 and 9.8 scores on Mohs scale, respectively).

However as it has been established during AFM analysis due to extremely high dispersion, the abrasive properties of the first one are virtually absent, and in the second one they are expressed to a small extent. Whereas the particle size of the powder modifiers is less or equal the size of the surface irregularities the process of components breaking-in at the presence of oil with these powders additives occurs mainly not by the removal of microroughness on their surface, but by filling roughness of the relief and leveling the surface. This provides an increase in the bearing area of twin contact and more uniform load distribution over the surface. As a result, a specific load in tribocontact decreases. Furthermore this mechanism of breaking-in of tribocouplings, that is implemented by modifying the oil with these dispersions, provides a significant (1.5–2 times in comparison with the oil without additives) reduce of its duration and also affects on the wear resistance of the friction pair and the coefficient of friction.

The most notable reduction of the linear wear and friction coefficient are recorded using diamond nanomodifier.

Estimation of surfactants adsorption in oil dispersive systems

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Investigations initiated to change physicochemical properties of oil dispersed systems (ODS) and to modify them by surfactants are of special urgency nowadays. A number of scientific problems are directly connected with adsorptive interactions between surfactant and ODS, but information about the study of surfactant adsorption from nonaqueous media in such colloid systems is practically absent in literary sources. The aim of this work was to study adsorptive interaction between surfactant and dispersed asphaltene particles in ODS.

Two surfactants that are quaternary ammonium compound ether based on triethanolamine, oleic acid and methosulphate (EQAC) and ethylenediamine tetrakis (EO-PO) block copolymer ((EO-PO)-EDA) have been used as the test subjects. The oil bitumen of gel type performed the role of ODS and contained next chemical elements (wt. %): C – 76,87; H – 10,55; N – 2,35; S – 2,21; O + metals – 8,02. ODS have been modified at 170 ± 5 °C under intensive mixing with surfactant (1 wt %). Methods of thin-layer chromatography with flame-ionization detection and Fourier-transform infrared spectroscopy have been applied for investigations.

Determination of chemical group composition of ODS allowed us to establish that under ODS modification by surfactant the asphaltene percentage in system is reduced and composition of dispersion medium is changed: EQAC increases resins content by 3.6 %, but (EO-PO)-EDA raises the quantity of aromatic hydrocarbons in ODS by 1.5 %. Probably, it is connected with different mechanism of adsorption owing to interaction between the surface and polar groups of surfactants that can be caused by distinctions in the way of self-organization of surfactant molecules in discrete micelles on the surface of asphaltenes.

Results IR-spectroscopy and the data on elements composition of ODS give evidence to the fact that there are active polar centers in bitumen structure on the surface of disperse asphaltene particles being able to interactions with surfactant molecules distributed in dispersion medium of ODS. So, comparative analysis of infrared spectra gives evidence that besides characteristic absorption peaks observed in initial ODS spectrum new peak appear in case of ODS modified with EQAC. It belongs to stretching vibrations of the sulfoxide group $-S=O$ (1031 cm^{-1}), but as compared with EQAC spectrum it is less intensive and shifts for 30 cm^{-1} to the near-wave spectral region. The weak ‘ammonium’ line (2358 cm^{-1}) characterizing stretching vibrations of aminogroup in unsaturated and aromatic amines has been also found out.

In addition to characteristic absorption lines observed in initial ODS spectrum, in case of ODS modified with (EO-PO)-EDA the line at 1290 cm^{-1} appears, which is responsible for stretching vibrations of $-C-N$ group in $Ar-N-R_2$. As compared with surfactant spectrum, it has weaker intensity and is shifted to near-wave spectral region. Moreover, the weak ‘ammonium’ line (2356 cm^{-1}) verifies chemical interactions with formation of aromatic amines. Four lines, typical for (EO-PO)-EDA, that belong to stretching vibrations of $-C-O$ group, were not discovered in modified ODS spectrum. Evidently, it is related with the transformation of alcohol and ether groups $-C-O$ in carbonyl groups $-C=O$, connected with aromatic structures peculiar to aromatic ketones, aldehydes and acids, that is confirmed by the availability of peaks belonging to stretching vibrations at 1697 и 2727 cm^{-1} .

Thus, it had been found that the studied surfactants of cationic and nonionic nature are bound up with the surface of dispersed phase in ODS by means of Vandervaals forces and chemisorptive interaction forces. So, the surfactant adsorption on nucleophilic parts of low-polarity particles of dispersed phase occurs due to the acid-base interaction of functional polar groups and provides screening of dispersible particles in oil dispersion and an increase in its stability.

Study of anodizing mode effects on synthesis of self-ordering TiO₂ nanotubes

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TiO₂ nanotubes were obtained by Ti anodizing in ethylene glycol solution. TiO₂ foil of 99.5% purity, 250 μm thickness, purchased from AlfaAesar was used in the experiments. The electrochemical set-up consisted of an electrolysis power supply consort EV 243 and a classical two electrode cell. A sample was positioned vertically between two stainless steel plates as cathodes at a distance of ~ 13 mm from each other. A one-compartment thermostat bath was applied for Ti anodizing. The anodizing solution was stirred continuously using a magnetic stirrer and its temperature was fixed between 5 and 40 °C by thermostat. The anodizing electrolyte consisted of 0.1, 0.3 and 0.5 wt.% ammonium fluoride (NH₄F) in ethylene glycol + 2.0 vol. % H₂O. The current-time curves for the anodizing were recorded by means of a computer. The morphology, diameter and length of TiO₂ nanotubes were determined by scanning electron microscopy (SEM). The cross-section images were taken from cracked layers after bending of the samples. The outer diameter and length of the nanotubes reported were the average over at least five locations.

The effect of parameters such as applied voltages, anodizing time, electrolyte temperature and pH of electrolyte on the outer diameter of nanotubes and length of TiO₂ nanotubes were investigated. In the experiments the following parameters were used: applied voltage from 30 to 60; electrolyte temperature from 5 to 40 °C; 6, 7 and 8 for pH of electrolyte and 3, 6 and 10 hours for anodizing time. SEM study showed that length and diameter of the synthesized nanotubes were in the range of approximately 9–70 μm and 80–170 nm respectively.

Based on our results, nanotube length increased with increasing voltage, temperature and anodizing time. The outer diameter of nanotube increased also with increasing voltage and temperature, whereas outer diameter of nanotubes decreased significantly with increasing pH and no considerable change was observed with increasing anodizing time.

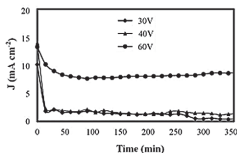


Fig. 3. The current-time curves for Ti anodizing in ethylene glycol solution + NH₄F + 2 vol.% water at constant voltage of 30, 40 and 60 V

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Simulation of the process of crystal surfaces chemical polishing

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Chemical polishing of the surface is used in many fields of science and technology. In particular, the process is applied in the manufacture of miniaturized devices on the basis of single-crystal silicon (e. g. MEMS, NEMS). As devices are scaled down to the nanosize, the formation of more and more high-quality surfaces is required, up to obtain atomically smooth topography [1, 2]. Modern technologies can not provide the formation of a surface with the required quality for advanced silicon devices. One of the most promising ways to study and improve the process of chemical polishing is to simulate it at the atomic level and to identify the ways of developing the theory and technology of monocrystalline surface treatment by comparing the simulation results with the desired structure of the surface [3, 4]. We have outlined the ways of forming a perfect surface Si(001) using an improved atomic dissolution model of diamond-like crystals (Figure). The model takes into account the effect of the second indirect neighbors on the rate of surface atoms removal.

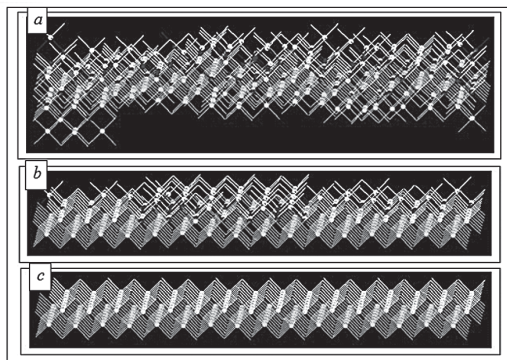


Fig. An operation example of the new model:
a – rough surface (001); *b* – surface *a* after the partial polishing;
c – perfect surface (001) after the finishing polishing of surface *a*

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Stability and rheology of silica suspensions stabilised by surface active substances

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Suspensions based on nanosized silica modified by ionogenic and nonionogenic surfactants have been obtained. The dispersion composition, stability and rheological properties have been investigated. Laser diffraction method, scanning electron microscopy and R/S Brookfield rheometer system have been used for the description of the suspensions under study. The influence of different surfactants on the dispersion composition, stability and rheological properties of 25 wh. % OX-50 suspensions has been investigated. The comparison of rheological properties of aerosol suspension stabilized by ethylenglycol as a low molecular weight stabilizer and by polyethylenglycol as a high molecular weight stabilizer showed that the viscosity of suspension is higher for the last one. The more shear rate the higher suspensions' viscosity is observed in both cases. This phenomenon is known as a dilatancy [1]. Modification of suspension by anionogenic surfactant (sodium do-

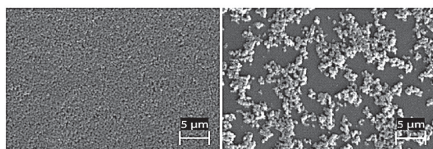


Fig. SEM-image of dried residues of aerosol suspensions:
49.1 ± 0.1 % stabilized by sodium dodecylsulphate (left);

decylsulfate with concentration under critical concentration of micelle formation, CCM) promotes the formation of the stable suspension containing 49 wh. % dispersion phase while modification by nonionogenic surfactant (glycerin monooleate with concentration above CCM) promotes the formation of the stable suspension containing 39 wh. % dispersion phase. As follows from the data of figure the space network of aggregated aerosol particles is formed in the suspension stabilized by glycerin monooleate. In contrast to it the stabilization by sodium dodecylsulphate results in the homogeneous distribution of particles in the volume of suspension. The residue of this suspension has compacted structure after drying. The findings can be applied for developing the technology of synthesis of concentrated stable suspensions used for chemical-mechanical polishing of semiconductor plates [2].

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Au-Sn powders production by cementation from solutions

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Au-Sn eutectic alloy is one of the most used soldering materials for packaging. It is indispensable for integrated circuits, laser diodes and other devices because it provides hermetic sealing owing to good surface wettability of the surfaces under connection, low viscosity at melting point and filling the cracks in a substrate [1]. Nowadays, Au-Sn alloy powders production is of great interest for usage in solder pastes. Traditionally, gold-tin powders are produced by sputtering of metallurgical alloy in vacuum. This technology is energy-consuming and requires expensive equipment that is why the search of new methods of powder production is of great importance. Cementation processes based on the reduction of metal ions by a metal with more positive electrode potential proceed in aqueous solutions on metal surfaces of complex shape. They provide to produce metal coatings and powders by a cheap and simple way without complicated installation [2]. Moreover, it is known that intermetallic compounds are formed sometimes during the cementation process [3], but there is no information about gold(I) reduction with tin.

In this work the process of gold cementation on Sn powders with formation of Au-Sn alloys was studied. Commercial tin powder was used as a substrate. Gold cementation was carried out at 90 ± 2 °C in solutions containing potassium dicyanoaurate(I), citric ions as a ligand, and ammonium chloride as a buffering additive providing an initial pH 7.

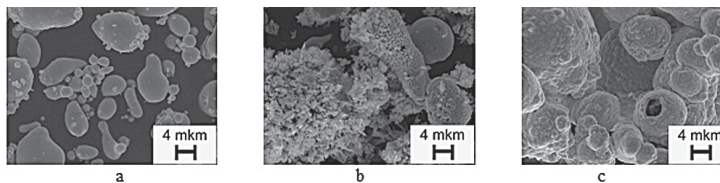


Fig. SEM photos of the surface of Sn (a) and Au-Sn (b, c) powders of different composition:
b – AuSn₂ phase, 25 at. % Au; c – AuSn and Au₅Sn phases, 75 at. % Au

The research revealed that Au(I) was reduced from solution by tin with the formation of Au-Sn alloy. That fact was confirmed by the change of tin powder color, by the results of EDX and X-ray phase analysis. The elemental and phase composition of the alloy powders depended on the duration of the process and molar ratio of Au(I) : Sn. The latter was determined by the weight of tin powder introduced into Au(I) cementation solution and the volume of this solution. Thus, the excess of tin powder resulted in the formation of AuSn₄ intermetallic compound. At molar ratio Au(I) : Sn equal to 1 : 5 and 1 : 2 phases of AuSn₂ and AuSn were obtained respectively. The optimal molar ratio for the formation of the eutectic alloy (Au₅Sn, AuSn; 70

at.% Au and 30 at.% Sn) was 1 : 1. The excess of Au(I) led to the formation of a product with high (83 at.%) content of gold included into phases of AuSn intermetallic compound and amorphous gold. The morphology of Sn grains sufficiently changed during Au(I) reduction. The size and form of the particles in the cementation product appeared to be of great dependence on its elemental and phase composition (Fig).

Thus, the obtained results show the possibility to produce Au–Sn alloy powders by Au(I) cementation from solution and to control the elemental and phase composition of the alloy.

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CHEMISTRY OF METAL COMPLEXES

Molecular structure and paramagnetic properties of lanthanides complexes with bisdiisobutyl dithiophosphinate and 1,10-phenanthroline using NMR

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Magnetic Resonance Imaging (MRI) is routinely used in the clinic to visualize the structure and function of organs. For several applications, including tumor and cardiovascular imaging in clinic and in vivo studies, an enhancement in contrast is an absolute requirement to improve the sensitivity and the diagnostic contents of the images. For this, several contrast agents (CAs) have been developed over the past years, most of which incorporate paramagnetic gadolinium ions (Gd^{3+}). Currently, complexes of different lanthanides (Ln, other than Gd), remain largely unexplored as probes for nuclear magnetic resonance spectroscopy (NMR) and MRI.

The features of the molecular structure and paramagnetic properties of Ln complexes with the dithiophosphinate R_2PS ($R = i-Bu$) and 1,10-phenanthroline ligands $[Ln(1,10-Phen)((i-Bu)_2PS_2)_2(NO_3)]$ {where Ln = Nd^{3+} (I), Eu^{3+} (II), Dy^{3+} (III), Yb^{3+} (IV) and Lu^{3+} (V)} in $CDCl_3$ have been studied by 1H NMR techniques. These complexes are of interest due to the prospect of using some of them as fluorescent sensors for biology and medicine. They are also considered as potential NMR thermometric probes (see our approach in [1, 2]). The structure of complexes was studied in detail by three independent 1H NMR techniques that are analysis of lanthanide-induced shift (LIS) magnitudes, method of the separation

of Fermi-contact and pseudo-contact contributions of LIS [3], and calculation of paramagnetic lanthanide-induced relaxation rate enhancements [2]. The structure results obtained for these paramagnetic complexes by relaxation spectroscopy (RS) of NMR and LIS analysis in solution are mutually consistent with the results found for model complex of yttrium by X-ray analysis in the crystalline phase. Paramagnetic complexes (I–IV) investigated in this work represent a new type of thermometric NMR sensors and lanthanide paramagnetic probes for in situ temperature control in solution. The report also contains: (1) comparison of the results obtained and those found for other Ln complexes; (2) the information about the molecular structure and the dynamics of related Ln coordination compounds with crown-ethers, (EDTA-like) ligands and DOTA-like molecules in solutions.

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Bioactive Cu(II) and Zn(II) complexes with Mannich bases

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Cu(II) and Zn(II) complexes with various organic ligands are known to possess anticonvulsant, antiproliferative, anti-inflammatory, antiviral, antiparasitic, and antimicrobial activity. A higher antimicrobial effect of the complexes as compared with that of the initial ligands is achieved due to their higher lipophilicity resulting from complexation as well as to the influence of the metal ions on the cellular structure and processes. To produce effective antimicrobial agents, it is necessary to carry out further investigations of Cu(II) and Zn(II) with already known and novel ligands and to determine their structural, thermodynamic and pharmacological characteristics.

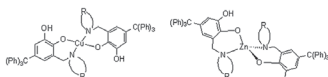


Fig. Structural schemes of the Cu(II) and Zn(II) complexes with the ligands HL¹–HL⁴

The process of complexation of Cu(II) и Zn(II) ions with Mannich bases in water-THF was investigated. It was found potentiometrically that complexes with the ratio M : L = 1 : 2, were formed, their stability constants were determined ($\beta = 11,78 \text{ } 14,26$). The complexes synthesized were shown to be neutral, amorphous and thermally stable. Their coordination polyhedra had the composition [MN₂O₂] and square-planar or tetrahedral geometry (Figure). A high antifungal activity (RI

= 80–100 %) of the metal complexes against moulds *Alternaria alternata*, *Fusarium* spp., *Sclerotinia sclerotiorum* was established.

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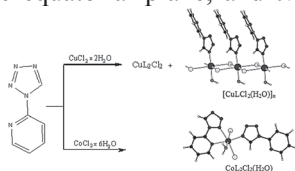
The crystal structure of 2-(tetrazol-1-yl)pyridine complexes with Cu(II) and Co(II) chlorides

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As a part of our investigations concerned with the synthesis of tetrazole derivatives and their complexes with transition metals, 2-(tetrazol-1-yl)pyridine (L) was prepared by heterocyclization of 2-aminopyridine with triethyl orthoformate and sodium azide.

The interaction of L with $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$ (molar ratio 1 : 1) in ethanol at 70°C results in two complexes: 1) CuL_2Cl_2 , deposited as a fine turquoise powder by cooling the reaction mixture to the room temperature; 2) $[\text{CuLCl}_2(\text{H}_2\text{O})]_n$, crystallizing by slow evaporation of mother solution after separation of CuL_2Cl_2 to obtain crystals suitable for X-ray analysis. X-ray data of $[\text{CuLCl}_2(\text{H}_2\text{O})]_n$ showed that it is monoclinic (S.G. P21/n). The compound presents 1D coordination polymer formed due to chlorine atoms (Cl1 and Cl2) acting as two bridges between neighboring copper atoms inside the chains. Both bridges, Cu–Cl1–Cu and Cu–Cl2–Cu, are asymmetrical, in which one bond Cu–Cl is of usual length and another bond is considerably elongated. The copper atoms have essentially elongated octahedral coordination, with the tetrazole ring N4, O atom of the water molecule together with two Cl atoms in the equatorial plane, and two Cl atoms in the axial sites.



$\text{CoL}_2\text{Cl}_2(\text{H}_2\text{O})$ complex was crystallized by slow evaporation at room temperature of ethanol solution containing L и $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ at molar ratio 2:1. According to single crystal X-ray analysis, it presents a molecular complex, crystallizing in the monoclinic space group P21/c. The cobalt atom forms a distorted octahedral coordination with O atom of the water molecule, two Cl and three N

atoms of two ligands L. One ligand is bonded to the metal monodentately via the tetrazole ring N⁴ atom, whereas another one shows bidentate chelating binding through the tetrazole ring N² and the pyridine ring N atoms. It should be noted that the tetrazole N² atom, as a rule, is not coordinated by metal atoms in 1-substituted tetrazoles, and only solitary examples are known with this coordination.

Acknowledgment. This study is supported by Belarusian Republican Foundation for Fundamental Research, project X14P-038.

Synthesis and investigation of transition metal coordination compounds with isomeric tetrazole Schiff bases

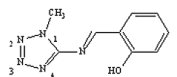
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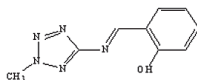
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Recent developments in coordination chemistry of transition metals are determined by application of complexes as novel multifunctional materials. Schiff bases present promising class of simple ligands which can ensure progress in the above area. Among Schiff bases tetrazole derivatives are unexplored



2-(((1-methyltetrazol-5-yl)imino)methyl)phenol – L¹



2-(((2-methyltetrazol-5-yl)imino)methyl)phenol – L²

ligands. The aim of the present study is the development of methods for synthesis of tetrazole based Schiff bases and their transition metal complexes. L1 and L2 were prepared by reaction of salicylic aldehyde with corresponding 5-amino-N-methyltetrazole in ethanol under argon [1]. Hydrated cobalt(II), nickel(II) and copper(II) chlorides were found to react with L1 and L2 in EtOH–MeCN or MeOH–MeCN mixtures with formation of complexes MeXnLm of the following composition:

Me = Co, X = Cl, CH₃COO, n = 2, m = 1 or 2;

Me = Ni, X = Cl, n = m = 2; X = ClO₄, n = m = 4;

Me = Cu, X = Cl, ClO₄, BF₄, n = m = 2.

The yield of these complexes was 70–80 %. Lower yields of target complexes were measured up when using individual solvents (EtOH, MeOH, MeCN).

Powdered cobalt, nickel and copper readily reacted with L1 and L2 in DMSO or DMF in the presence of ammonium salts according to the following scheme:

Composition of perchlorate complex obtained is unusual since weakly coordinated perchlorate-anion facilitates to increase coordination capacity of metal cations.

Complexes obtained were characterized by means of elemental analysis, far

(400–50 cm⁻¹) and middle (4000–400 cm⁻¹) IR spectroscopy, thermal analysis and powder X-ray diffraction. Expected structures of complexes are discussed based on data obtained.

Acknowledgment. The support from BRFFR (grant X13K-018) is gratefully acknowledged.

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Chromotropism of coordination compounds

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One of the most attractive aspects of coordination chemistry consists in a manifold range of colors inherent to metal complexes. Of particular interest both from theoretical and from practical points of view are compounds exhibiting chromotropism, i. e. the ability to change their color under the influence of external conditions or under changing the physical parameters of the environment. Chromotropic compounds are capable of changing color under the influence of temperature, pressure, irradiation with certain wavelength or being affected by electric field. These phenomena could overlap, e. g. a compound could exhibit photo- piezo- and thermochromism or thermo- and solvatochromism simultaneously.

The report considers transition metal complexes with the ligands of different classes exhibiting chromotropism, in particular solvatochromism, photochromism, thermochromism and piezochromism.

The most representative and well-studied class of chromotropic compounds can be presented by metal complexes which exhibit thermochromism. A special attention in the report is devoted to this phenomenon. In most detail there are considered two representative classes of thermochromic compounds such as iron(II) complexes with poly-nitrogen-containing ligands, wherein which the phenomenon of thermochromism is combined with the spin crossover, as well as compounds containing a complex cation and a complex anion, with the composition of [MLn][Cr(SCN)6]. Both classes of the compounds exhibit the transition temperature depending the compound composition, which allows one to obtain thermochromic substances changing the color thereof at different temperature values. The complexes can withstand to many cycles of heating – cooling. The compounds exhibiting thermochromism can be used in different technological processes, in education, in biological research, as well as for the protection of securities and cultural values.

Acknowledgment. The investigations were carried out within the framework of the State contract № 02.740.11.0628, performed within the framework of the Federal Target Program «Scientific and scientific-pedagogical personnel of innovative Russia» for 2009-2013, as well as were supported by the Russian Foundation for Basic Research (grant № 14-03-90006 Bel_a).

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Biologically active complexes of Pt(II), Pd(II), and Cu(II) with nitrogen-containing ligands

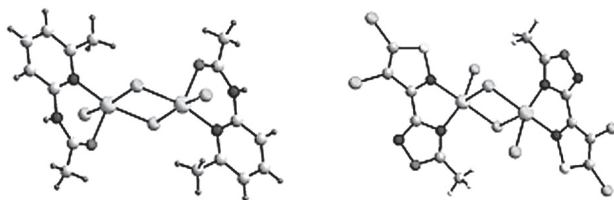
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Complexes of copper(II), platinum(II), and palladium(II) with nitrogen-containing ligands are interesting in view of biological activity of the ligands, which is now under investigation. Some nitrogen-containing compounds, such as isothiazole and pyridine, can intensify pyrethroid insecticide action against the Col-



orado potato beetle (*Leptinotarsa decemlineata*), and they are known to be very effective. We expect to increase this effect if their transition metal complexes will be used. This work is devoted to new coordination compounds of copper(II), platinum(II), and palladium(II) with pyridine and isothiazole derivatives, their X-ray crystal structure and study of their synergistic and cytotoxic activity.

2-(N-acetylamino)-6-methylpyridine (L1), amide of 4,5-dichloroisothiazole-3-carboxylic acid (L2) and 3-(4,5-dihlorizotiazol-3-yl)-5-methyl-1,2,4-oxadiazole (L3) were chosen as biologically active ligands. Various copper salts form complexes of different composition with L1 such as $[\text{Cu}^2(\text{L}^1)_2\text{Cl}_4]$ (1) (left Figure), $[\text{Cu}(\text{L}^1)_2\text{Br}]\text{Br}$ (2), $[\text{Cu}(\text{L}^1)_2(\text{H}_2\text{O})](\text{NO}_3)_2$ (3) and $[\text{Cu}(\text{L}^1)_2(\text{H}_2\text{O})](\text{ClO}_4)_2$ (4). The reaction of different metal salts with L² and L³ yields in complexes

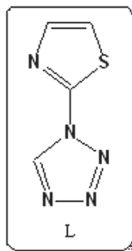
$[\text{Cu}(\text{L}^2)\text{Cl}_2]_n$ (5), $[\text{Cu}(\text{L}2)\text{Br}_2]$ (6), $[\text{Cu}(\text{L}2)(\text{H}_2\text{O})_2](\text{ClO}_4)_2$ (7), $[\text{Cu}(\text{L}^2)_2(\text{H}_2\text{O})_2](\text{BF}_4)_2$ (8), $[\text{Cu}_2(\text{L}^3)_2\text{Cl}_4]$ (9) (right Figure), $[\text{Cu}(\text{L}^3)\text{Br}_2]$ (10), $[\text{Pd}(\text{L}^3)\text{Cl}_2]$ (11), and $[\text{Pt}(\text{L}^3)\text{Cl}_2]$ (12). The compounds have been identified and characterized by a set of methods including elemental analysis, IR-spectroscopy, single-crystal X-ray diffraction analysis, and magnetic susceptibility measurements in the range 5–300 K. Fungicide properties of complexes in case of plant pathogenic fungi *Botrytis cinerea* and *Fusarium* sp. were investigated. It was shown that the complexes have high fungicide activity and completely suppress fungi pathogenic process. Insecticidal properties of the complexes against the Colorado potato beetle larvae as synergist of insecticide “Kerber” were investigated in vitro. It was shown that the complexes were effective against the Colorado potato beetle larvae.

Cytotoxicity of some complexes in comparison with cisplatin in HEK 293 (human embryonic kidney) and U937 (leukemic) cell lines was investigated. Our results showed that cisplatin and complexes inhibit HEK 293 cell line in a dose and time dependent manner, toxicity of complexes was similar to that of cisplatin. The U937 cell line is significantly less sensitive to complexes compared to cisplatin. However, this selective sensitivity can be useful for the selection of drugs with reduced sensitivity to normal cells.

Acknowledgement. The work was financially supported by the Russian Foundation for Basic Research (Grants No. 14-03-31539 mol_a and 14-03-90006 Bel_a).

Synthesis and crystal structure of CoII chloride complex with 2-(1H-tetrazol-1-yl)thiazole

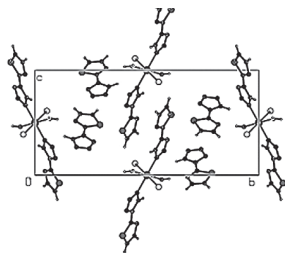
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Complexes of cobalt(II) as well as of iron(II) and iron(III) with organic ligands attract much attention as promising compounds in the field of manufacturing molecular magnets and spin-crossover area. Azole derivatives are suitable ligands to provide magnetic ordering and spin-crossover effects in such complexes. Here we present a novel coordination compound of cobalt(II) with a sulfur-containing tetrazole derivative, namely 2-(1H-tetrazol-1-yl)thiazole (L).

This complex was synthesized in 48 % yield by reaction of equimolar amounts of L and $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ in boiling propanol-2 followed by slow evaporation of reaction mixture at room temperature.

The synthesized compound was investigated by single crystal X-ray analysis at room temperature. As follows from X-ray data, its crystals include complex molecules together with co-crystallized non-coordinated molecules L and correspond to the composition $[\text{CoCl}_2\text{L}_2] \cdot \text{L}_2$. The complex is monoclinic, S.G. P21/c, the unit cell dimensions $a = 5.94922(8)$, $b = 23.3420(3)$, $c = 11.08945(16)$ Å; $\beta = 101.8147(5)^\circ$, $Z = 4$.



The cobalt atom is settled in the inversion centre, imposing C_i symmetry of the complex molecule. The metal atom has an elongated octahedral environment formed by two tetrazole ring N4 atoms of two ligands L, two chlorine and two water oxygen atoms. The chlorine atoms occupy the axial sites of the octahedron.

There is a system of classic and non-classic hydrogen bonds in the crystal structure of $[CoCl_2L_2] \cdot L_2$. Some of them connect neighboring complex molecules, the other act between complex molecules and non-coordinated molecules L. There are also the hydrogen bonds only between non-coordinated molecules L.

Acknowledgement. This study was supported by Belarusian Republican Foundation for Fundamental Research, project X14P-038

Complexation of Cu^{2+} with 1-tert-butyltetrazole in the presence of triethylamine

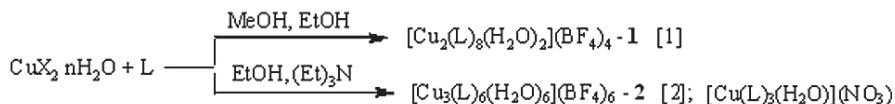
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It is well known that the properties of coordination compounds strongly depend on structural factors which are determined by a nature of ligand as well as genesis of a compound. In this connection investigation of the influence of different reagents on complexation of tetrazole derivatives along with development of traditional synthetic procedures are of current interest. Here we report results of our studies of Cu^{2+} complexation with 1-tert-butyltetrazole in the presence of triethylamine as a strong organic base according to the scheme: Previously, we found that the above tetrazole ligand interacts with copper(II) tetrafluoroborate in ethanol or methanol with formation of complex 1. X-ray analysis showed binuclear structure of 1 with N(4)-monodentate coordination of tetrazolyl moiety [1]. The formation of the binuclear complex was unexpected since 1-monosubstituted tetrazoles usually generate mononuclear complexes with metal(II) tetrafluoroborates under similar conditions. Unusual behavior of the ligand studied is due to the presence of a bulky tert-butyl substituent at the N1 endocyclic atom. Despite the remoteness from the main coordination site N4, this substituent significantly influences on architecture of complexes formed.



$\text{X} = \text{BF}_4$, $n = 6$; $\text{X} = \text{NO}_3$, $n = 3$

We have found that interaction of 1-tert-butyltetrazole with copper(II) tetrafluoroborate in the presence of equimolar amount of triethylamine leads to the formation of complex 2. According to the X-ray single crystal analysis complex 2 presents trinuclear copper complex with rare N(3),N(4)-bridging coordination of 1-monosubstituted tetrazole ring [2]. The role of triethylamine is not clear. Taking into account strong nucleophilic properties of the nitrogen atom of amine one can assume the initial formation of an intermediate complex of triethylamine with copper(II) tetrafluoroborate. Further the above complex slowly reacts with tetrazole ligand generating thermodynamically preferable trinuclear complex 2. In the absence of amine the direct interaction of ligand and copper salt leads to the formation of kinetically preferable binuclear complex 1.

Using amine-assisted procedure we also prepared complex of 1-tert-butyltetrazole with copper(II) nitrate 3. Complex obtained was characterized by IR spectroscopy and elemental analysis.

Evidently, further study of the influence of triethylamine on complexation of tetrazoles is of interest in order to design novel coordination compounds with target structures and desired properties.

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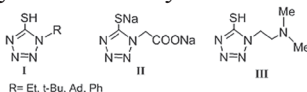
1-(N,N-Dimethyl)aminoethyl-5-mercaptopotetrazole as novel capping ligand for stabilization of palladium nanoparticles in water

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Physical-chemical properties of nanoparticles substantially depend on the metal nature and the type of capping agent. Growing interest to tetrazole derivatives in recent years have been stipulated by their thermally induced decomposition leading to a high



percentage of gaseous products and complexing properties [1–3]. It was found that some commercial tetrazole derivatives (I–II) provide nanoparticles with solubility in organic [2, 4] and aqueous media [5]. Throughout this work we investigated commer-

cial tetrazole derivative (III) in order to obtain water soluble palladium nanoparticles.

The novel stabilizing ligand, 1-(N,N-dimethyl)-aminoethyl-5-mercaptotetrazole (III) has been applied for synthesis of palladium nanoparticles in aqueous media. The morphology of the synthesized particles and some properties were determined by TEM, FT-IR and UV-visible spectroscopy, thermogravimetric analysis, EDX analysis.

It was found that the reduction of PdCl_4^{2-} with NaBH_4 in the presence of III in water yielded nearly spherical nanoparticles (NPs) with diameter 3–7 nm. A freshly prepared aqueous solution of sodium borohydride (1 ml, 0.16 M) was poured under stirring into the solution of PdCl_4^{2-} (0.01 mmol) and III (0.01 mmol). After stirring for 3 h at room temperature, reaction mixture was concentrated under reduced pressure. NPs were precipitated by t-butanol and redissolved in water. The synthesized Pd-NPs show no sign of decomposition or loss of solubility even after 8 months storage at room temperature. The presence of III on the surface of NPs had been provided by comparative analysis of the FT-IR spectra of the synthesized NPs and corresponding free ligand. All samples showed characteristic bands of capped ligand in FT-IR spectra. TG curves of III and Pd-NPs capped with this ligand indicate some differences in thermolysis of the free and capped ligand. Thus, pure ligand decomposes at $\sim 230^\circ\text{C}$, but being deposited on the surface of NPs it decomposes at $\sim 230\text{--}290^\circ\text{C}$. EDX data show no changes in atomic ratio of Pd : S = 6,7 : 1 on NPs surface under thermolysis. Obviously, the products of the ligand decomposition are evacuated from the NPs surface leaving their sulphide anions.

The novel stabilizing ligand, 1-(N,N-dimethyl)-aminoethyl-5-mercaptotetrazole has been applied for simple synthesis of palladium nanoparticles in aqueous medium. The interaction of nanoparticles' surface with ligand has been investigated.

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New tetrazole-containing Schiff's bases and their biological activity

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Since N-heterocyclic pharmaceuticals play a significant role in therapeutic and diagnostic medicine, the discovery and development of new tetrazole containing drugs remain an ever-growing area of research in medicinal chemistry. The new tetrazole containing Schiff's bases (**L**¹–**L**⁵), presented in Fig, and some metal complexes with these bases have been obtained by earlier published methods [1–2].

All compounds were fully characterized by elemental analyses, IR spectroscopy

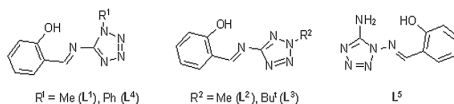


Fig. Schiff's bases containing tetrazole

copy, thermal analysis and powder X-ray diffraction. Since the biological activity of tetrazole derivatives is influenced by substituent R it was of interest to test the above-mentioned activity of the synthesized ligands and complexes with some metals. The obtained compounds were screened for their in vitro antimicrobial activities against the eight standard bacterial strains such as *Staphylococcus aureus*, *Escherichia coli*, *Staphylococcus saprophyticus*, *Sarcina lutea* and the fungi. It was observed that bacterial strains show an absence of sensitivity to tested ligands L1–L5. Nevertheless, effective biological activity of N-heterocyclic tetrazole containing Schiff's bases was found against a series of fungi (Table). The inhibition of mycelia growth was observed under concentration of ligand 250 µg/mL.

Fungi	Fungicidal activity of ligands L ¹ –L ⁵				
	Inhibition level, %				
Ligand	<i>Alternaria alternate</i>	<i>Aspergillus niger</i>	<i>Fusarium oxysporum</i>	<i>Penicillium lividum</i>	<i>Trichoderma viridae</i>
L ¹	100	20	30	0	17
L ²	100	30	50	0	25
L ³	100	100	100	100	100
L ⁴	28	0	40	0	17
L ⁵	100	40	100	0	100

Fungicidal activity of ligands L¹–L⁵

Some metal complexes with Schiff's bases have been investigated on antibacterial and fungicidal activity. The most prominent results were observed for CoCl₂L², NiCl₂(L⁴)₂ and CuCl₂L⁴. These compounds showed both selective antibacterial and fungicidal activity.

Thus, it was found that tetrazole containing Schiff's bases, as well as some complexes with Co(II), Ni(II) and Cu(II), selectively inhibit mycelia growth of a series of fungi and bacteria.

Acknowledgment. The work was supported by grant X13K-018 of the Belarusian Republican Foundation for Fundamental Research.

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d-Metal thiocyanate complexes: effect of the structure on the anion exchange extraction by quaternary ammonium salts

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The interest to detailed and systematic investigation of aqueous solutions of d-metal thiocyanates is due to the fact that the coordination mode of NCS^- largely determines the course of anion exchange extraction of metal thiocyanate complexes by quaternary ammonium salts (QAS) and it can be used for separation and preconcentration. This publication reports a systematic study of aqueous solutions of Co^{2+} , Zn^{2+} , Cd^{2+} , Hg^{2+} , Fe^{2+} , Ni^{2+} , Mn^{2+} thiocyanates by IR spectrometry. As a result, the coordination mode of NCS^- ions to metal ions was elucidated, and an explanation for the relationship between the structure and anion exchange extraction of thiocyanate complexes by QAS complexes was proposed.

The IR spectrum of zinc(II) thiocyanate (0.1 M NCS^-) shows a vaguely split high intensity $\nu(\text{CN})$ band at about 2065 and 2088 cm^{-1} , which provides the conclusion that Zn^{2+} is bound to NCS^- in the isothiocyanate mode. As the NCS^- concentration increases (1.0 M), only one $\nu(\text{CN})$ stretching band at 2053 cm^{-1} remains in the spectrum, indicating clearly that SCN^- is coordinated to Zn^{2+} through nitrogen.

The IR spectrum of a solution of cobalt(II) thiocyanate (0.5 M NCS^-) exhibits a medium intensity $\nu(\text{CN})$ band at about 2104 cm^{-1} and a shoulder at about 2134 cm^{-1} , which testifies to Co^{2+} binding with NCS^- through sulfur. As the NCS^- concentration increases to 1.0 M, a high intensity band $\nu(\text{CN})$ at 2058 cm^{-1} appears in the IR spectrum of cobalt(II) thiocyanate, which attests to Co^{2+} binding with NCS^- through nitrogen. The inflection at 760 cm^{-1} and a weak but sharp band at 730 cm^{-1} can be assigned to the $\nu(\text{CS})$ stretching mode of the NCS^- ions coordinated with Co^{2+} through sulfur. The weak band at 445 cm^{-1} is due to the $\delta(\text{NCS})$ bending mode of the NCS^- ions connected with Co^{2+} through the sulfur atom. When the concentration of the NCS^- ions is up to 1.0 M, both thiocyanate and isothiocyanate forms coexist in the cobalt(II) thiocyanate solution. At further increase in the ligand concentration (>1.0 M), the IR spectrum of cobalt(II) thiocyanate shows only a high intensity $\nu(\text{CN})$ band at 2062 cm^{-1} , which unambiguously points to Co^{2+} binding with NCS^- through nitrogen. Ni^{2+} , Mn^{2+} (at 1.0–2.0 M NCS^-), Cd^{2+} , Hg^{2+} , and Fe^{2+} ions coordinate NCS^- through the sulfur atom.

From the obtained results, it becomes clear why the $\text{Zn}(\text{NCS})_4^{2-}$ ions have the highest anion exchange affinity for the ion exchanger phase. Indeed, high affinity for the hydrophobic phase of QAS is inherent to hydrophobic ions. In the case of thiocyanate complexes, these are compounds in which the thiocyanate group is coordinated to the metal through nitrogen with the sulfur atoms protruding outwards, i. e. $\text{Zn}(\text{NCS})_4^{2-}$. The second most extractable ions are $\text{Co}(\text{NCS})_4^{2-}$ in which

mixed coordination mode of Co^{2+} to NCS^- is observed in cobalt(II) thiocyanate solutions at NCS^- concentration of 0.5 M, while on further increase in the NCS^- concentration, the isothiocyanate coordination mode, like that found in zinc(II) thiocyanate solution, predominates. In the Hg^{2+} , Fe^{2+} , Ni^{2+} , Cd^{2+} , Mn^{2+} thiocyanate complexes, the central ion coordinates NCS^- through sulfur, while the hydrophilic nitrogen atoms protrude outwards; thus, their affinity for the QAS phase is weaker.

It is important that the obtained results have practical applications. The high anion exchange affinity of isothiocyanate complexes $\text{Zn}(\text{NCS})_4^{2-}$ for hydrophobic QAS enables the development of $\text{Zn}(\text{NCS})_4^{2-}$ -selective film electrodes based on them with high analytical characteristics. With appropriate selection of the supporting KNCS concentration (~2.0 M) in which isothiocyanate complexes, $\text{Co}(\text{NCS})_4^{2-}$, predominate in the solution, $\text{Co}(\text{NCS})_4^{2-}$ -selective electrodes can also function successfully [1]. The development of electrodes for determination of Mn^{2+} , Ni^{2+} , Fe^{2+} , Cd^{2+} , and Hg^{2+} ions as thiocyanate complexes is impracticable.

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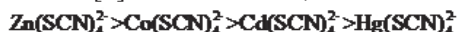
Anion-exchange extraction of Zn(II), Cd(II), Hg(II) and Co(II) complexes from thiocyanate media by high quaternary ammonium salts

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The high quaternary ammonium salts (QAS) as an effective anion-exchange extractant are widely used for extraction, concentration and analytical determination of different types of anions [1]. Certain metals, which are able to form anion com-



plexes, could be extracted by solutions of such QAS by anion-exchange reaction:

The degree of conversion of this anion-exchange reaction depends on the structure of QAS, its anionic form, the solvent applied as well as the nature of extractive metal complex. The thiocyanate anions are the most suitable for cation transfer and formation of rather strong anionic complexes, especially with cations like Zn^{2+} , Cd^{2+} , Hg^{2+} , Co^{2+} .

The present paper is focused on study the anion-exchange extraction of the above mentioned cations from thiocyanate aqueous solutions using high QAS with different structure in various organic solvents. Original experimental techniques for investigation the extraction of metal complexes in the form of double-charged anions have been developed.

The influence of different experimental conditions (the nature of cation and the length of the hydrocarbonic radical of QAS, type of used organic solvent for QAS)

on the ability to extract metal complexes is investigated. Conditional and concentration exchange constants of double-charged metal-complex anions interchange on the anions of the acid dye and standard chloride anion have been calculated.

Based on experimental data and quantum-chemical calculations of the structure of extractable metal complexes a row of extractibility can be presented as follows: :

The practical aspects of selective extraction, separation and analytical determination of Zn^{2+} , Cd^{2+} , Hg^{2+} , Co^{2+} are discussed.

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Synthesis and structural-chemical investigations of coordination compounds of metals with 4-methyl-1,2 cyclohexyldicarboxylic acid

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Metal complexes of aromatic dicarboxylic acids such as phthalic and terephthalic acid have been synthesized and investigated. It is known that these metal complexes have a chain structure and do not dissolve in neutral organic solvents [1, 2]. It was found that composite materials based on metal complexes of aromatic dicarboxylic acids provide the improvement of rheological properties of a variety of heavy oils by reducing their viscosity and preventing paraffin and salt formation due to the ability to form non-valency associations by self-assembling and self-organization.

This work was aimed to synthesis of the coordination compounds of transition metals with 4-methyl-1,2 cyclohexyldicarboxylic acid (4-methyl-1,2-CHDA) which differs by the degree of saturation from phthalic acid as its aromatic analogue. The purpose was to study complexation of this acid with transition metals.

For the first time we synthesized 4-methyl-1,2-CHDA from its anhydride in the form of polycrystalline powder. This acid does not dissolve in neutral organic solvents but easily dissolves in acetone, partly in water and tetrahydrofuran. Its melting temperature is 159–160 °C.

Synthesis of complex compounds of 4-methyl-1,2-CHDA with transition metals was conducted in two stages. At the first stage sodium salt of 4-methyl-1,2-CHDA was synthesized. Synthesis was conducted by mixing of sodium salt and the acid in the ratio $CH_3-C_6H_9(COOH)_2 : NaHCO_3$ equal to 1 : 2. At the second stage the solutions of water-soluble salts of transition metals were added to the water solution of 4-methyl-1,2-CHDA sodium salt. The ratio of components was equal to 1 : 1. The products of the synthesis were analyzed by different methods including elemental analysis, X-ray diffraction, IR spectroscopy and

differential thermogravimetric analysis. In the result of the investigation chemical composition of complex compounds and their structure were determined.

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Polynitrogen azoles as potent ligands in design of metal-based anticancer agents

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Recent years, polynitrogen-containing heterocycles, e. g. tetrazoles and triazoles, have been gaining more attention as promising ligands in design of novel biologically active metal complexes, in particular metal-based antiproliferative agents with broader spectrum of antitumor activity and/or lower in vivo toxicity as compared to established platinum drugs [1–4]. Here we present synthesis, characterization and evaluation of antiproliferative activity of a new triazole-based cisplatin analog, viz. cis-dichloridobis[1-tert-butyl-3-(N-tert-butylamino)-1,2,4-triazole]platinum(II) (1). Compound 1 was obtained by the reaction

Antiproliferative activity of 1 against human cancer cell lines

Cdl line/ tissue	IC ₅₀ , μM 1	IC ₅₀ , μM Cisplatin
HT-29/ colon	1.10 ± 0.17	4.1 ± 0.3 [5]
MDA-MB-231/ breast	1.30 ± 0.20	7.8 ± 0.8 [5]
CH1/ ovarian	0.70 ± 0.13	0.14 ± 0.03 [6]
A549/ lung	1.15 ± 0.05	1.3 ± 0.4 [6]
SW480/ colon	0.57 ± 0.04	3.3 ± 0.4 [6]

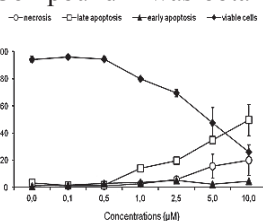


Fig. Proapoptotic activity of 1 in SW480 cells after 24 h exposure

of $K_2[PtCl_4]$ with the corresponding tert-butylated 3-amino-1,2,4-triazole and characterized by elemental analyses, HRESI MS, DCS/TG, IR, and NMR (¹H, ¹³C, and ¹⁹⁵Pt) spectroscopies. According to the results of biological evaluation, the complex demonstrates significant cytotoxic activity in five human cancer cell lines with IC₅₀ values in low micromolar range (Table) as well as pro-

nounced proapoptotic activity in cisplatin resistant SW480 cell line (Figure).
Acknowledgment. T.V.S. acknowledges the financial support of Saint Petersburg State University (postdoctoral grant 12.50.1560.2013).

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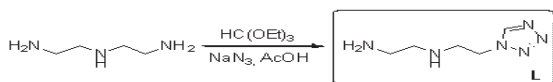
1-(5-Amino-3-azapentyl)tetrazole and its copper(II) complexes

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1-Monosubstituted tetrazoles are of considerable interest as ligands due to intriguing properties of their complexes with transition metals. Specifically, complexes of 1-alkyltetrazoles with copper(II) halides were found to be low-temperature ferromagnetics, while iron(II) coordination compounds show thermal- and light-induced spin transitions. Here we report a novel functionally substituted ligand, namely, 1-(5-amino-3-azapentyl)tetrazole (L), and its copper(II) complexes.



The ligand L was prepared by heterocyclization of diethylenetriamine with triethylorthoformate and sodium azide in acetic acid. ¹H and ¹³C NMR data of the product as well as X-ray analysis of its dihydrochloride showed that only one primary amino group was involved in heterocyclization in spite of an excess of orthoformate used.

Tetrazole L was found to react with copper(II) chloride or tetrafluoroborate in

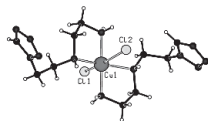


Fig. 1. Molecular structure of $[\text{CuL}_2\text{Cl}_2]$ complex

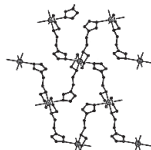


Fig. 2. Fragment of 2D polymeric coordination of cation in the crystal structure of $\{[\text{CuL}_2](\text{BF}_4)_2\}_n$

aqueous solutions forming crystalline complexes. According to single crystal X-ray analysis, the obtained $[\text{CuL}_2\text{Cl}_2]$ chloride compound presents a molecular

complex (Fig. 1) with a distorted octahedron around the Cu atom. The axial sites are occupied by semi-coordinated Cl atoms, whereas four N atoms of 5-amino-3-azapentyl groups of two ligand molecules lie in the equatorial positions, being bonded in chelate manner. The tetrazole ring N atoms do not participate in the coordination.

The obtained tetrafluoroborate complex $\{[\text{CuL}_2](\text{BF}_4)_2\}_n$ consists of polymeric cationic layers $[\text{CuL}_2^{2+}]_n$ (Fig. 2), connected with BF_4^- anions via non-classic hydrogen bonds $\text{C}-\text{H}\cdots\text{F}$. The coordination cationic layers are formed due to bridging ligand molecules, bonded to one Cu atom through the tetrazole ring N3 atom and to another one through both N atoms of 5-amino-3-azapentyl group in chelate mode. The tetrazole N³ atoms, being in axial sites of CuN_6 octahedrons, are semicoordinated.

Quantum-chemical calculations and electrochemical investigation of iron complexes with amide-containing ligands

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Coordination polymers, metal-organic frameworks and other hybrid materials as well as functional coatings based on them are gaining interest as electrochemical sensing materials and non-precious metal catalysts for fuel cell applications. Development of methods for obtaining of such coatings requires the ascertainment of mechanism and main regularities of influence of the ligands geometric and structural parameters, as well as the regime of deposition on their physico-chemical and functional properties. In present study, the influence of 5-benzyl-4,6-dioxo-1,9-diamino-3,7-diazanonan (BDDD) and its transition metal complexes, in particular with Fe ions, on kinetics of the metal ionization processes were electrochemically and computationally investigated and the mechanism of surface modification in such systems was proposed.

Polarization measurements were carried out in sulphuric acid solutions in a three-electrode cell with a carbon steel as working electrode, platinum as the counter-electrode and an $\text{Ag}|\text{AgCl}|\text{KCl}(\text{sat.})$ electrode as the reference one. Quantum-chemical calculations were performed on DFT and MP2 levels of theory with the 6-311G* and cc-pVTZ basis set respectively using the NWChem 6.5 computational chemistry package [1].

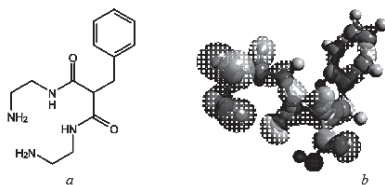


Fig. BDDD structural formula (a) and optimized geometry with HOMO density plot (b)

It was discovered, that the influence of BDDD on the kinetics of metal ionization is comparable to the amino acids, in particular acetylcysteine. At the same time, BDDD showed higher drop in current density on reverse portion of anodic polarization scan, that can be caused by the accelerated formation of the phase metalorganic layers on the metal surface. Computational studies including geometry optimization and calculations of electron structure showed a relaxed geometry and the electron density distribution of the ligand (Figure). According to the simulations performed, this 3D structure facilitates the formation of coordination polymers instead of chelate complexes that explains the observed electrochemical behavior. Thus, the mechanism of phase metal-organic layers formation in the system under study can follow chelate-bridging pattern which was proposed and investigated in detail for amino acids [2] and might be the basis for surface modification methods for obtaining the functional coatings.

Acknowledgment. Authors are grateful to Dr. Lampeka Y.D. for the synthesized BDDD samples.

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The structure and properties of the triple polymer-metal complex of chitosan-Cu(II)-polyhexamethyleneguanidine

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Currently researches in the field of chemistry of polymer-metal complexes are becoming more relevant. Processes of polymeric metal complexes formation are used for the concentration, separation and analysis of metal compounds solutions, creating new polymeric catalysts, new materials and pharmaceuticals [1]. Studies aimed at the synthesis and examination of polymer complexes with biocidal properties are of a particular interest.

The aim of this work was to study the structure and biocidal activity of the synthesized triple polymer-metal complex based on chitosan, Cu²⁺ ions and polyhexamethyleneguanidine hydrochloride (PHMG).

Polymer metal complexes were prepared in an aqueous medium at a temperature of 20 °C by adding an equimolar aqueous solution of the polymer

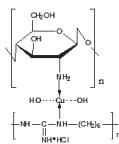


Fig. Schematic structure of the coordination unit of the triple polymer-metal complex: chitosan-Cu(II)-PHMG

mixture and copper chloride(II) and subsequent neutralization with sodium hydroxide.

The structure of the complexes was studied by potentiometric titration, viscometry, IR, EPR, UV spectroscopy. Biological activity was examined for bacterial cultures (*E. coli* B, *B. subtilis* 168) and fungi (*Trichoderma viride*, *Aspergillus niger*).

An internal sphere of complexes of such polymers was found to be formed of two molecules and two hydroxyl groups, with the chitosan hydrochloride PHMG forming coordination bonds by the free electron pair of the nitrogen atoms in amine groups (Figure). The preparation of such complexes is accompanied by a decrease in the characteristic viscosity of the solution, which is explained by the formation of intramolecular structures.

Evaluation of biocidal activity of polymeric complexes showed that the most efficient complexes were synthesized in a pH range between 5 and 7. The minimum inhibitory concentration of the compounds against bacteria *B. subtilis* 168 was 10 µg/ml.

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New rare earth ferrocenoylacetates.

Synthesis, structure, magnetism and thermolysis

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Chelate complexes of polyvalent metals based on β -diketonates have long been known; they find various applications. The derivatives of β -diketonates containing stable organometallic fragments, ferrocenyl in particular, are relatively scantily studied. The data on the derivatives of such substances and rare earth elements (which represent the original type of heterometallic 3d-4f-complexes) are especially poor [1–3].

New rare earth ferrocenoylacetates $[\text{Ln}(\text{FcCOCHCOMe})_3(\text{bpy})] \cdot \text{MeC}_6\text{H}_5$ ($\text{Ln} = \text{Pr}$ (1), Gd (2), Tb (3), Dy (4), Ho (5), (Fc – ferrocenyl; bpy – 2,2'-bipyridyl) and $[\text{Eu}(\text{FcCOCHCOMe})_2(\text{NO}_3)(\text{bpy})] \cdot \text{MeC}_6\text{H}_5$ (6) were prepared. In the crys-

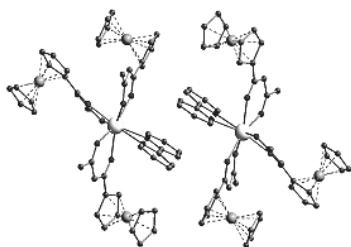


Fig. 1. The structures of 1–5

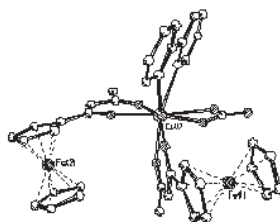


Fig. 2. The structure of 6

tal lattice of the isostructural complexes 1–5 two molecules form quasi-dimeric structure due to stacking interactions between the bpy molecules (Fig. 1). Such stacking is absent in the structure of 6. DC magnetic susceptibilities for 2–5 and AC susceptibilities for 3–5 were studied. Magnetic behavior of 3–5 corresponds to the presence of slow magnetic relaxation which is a significant property of single molecule magnets. It was shown that ferrocenyl moiety quenches the luminescence of Eu^{3+} ion in 6. Thermal decomposition of the compounds was studied by means of DSC and TGA. According to X-ray powder analysis data the final products of thermolysis of 1–5 under air contain perovskites LnFeO_3 and garnets $\text{Ln}_3\text{Fe}_5\text{O}_{12}$, therefore these compounds can serve as potential precursors for the functional complex oxides similarly to rare earth ferrocenecarboxylates [4]. **Acknowledgment.** The work was supported by Russian Science Foundation, project 14-13-00938.

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Polymeric lanthanide cymantrenecarboxylate complexes. Synthesis, magnetism and thermolysis.

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Carboxylate derivatives of stable organometallic molecules are perspective building blocks for polynuclear 3d-4f-heterometallic complexes which are able to combine specific properties of an organometallic moiety and a rare earth ion. Until recently mostly the derivatives of ferrocene were known. Lately we have obtained and studied several series of 3d-4f-carboxylates containing cymantrenyl ($\text{Cym} = (\eta^5\text{-C}_5\text{H}_4)\text{Mn}(\text{CO})_3$) moiety [1-4]; most of those complexes are binuclear.

Crystallisation of the products of exchange reaction between CymCO_2K and LnCl_3 from H_2O -MeOH-THF media afforded polymeric cymantrenecarboxylates $[\text{Ln}(\eta^2\text{-O}_2\text{CCym})_2(\mu\text{-OOCcym})_4\text{Ln}(\text{ROH})_4]_n \cdot m\text{Solv}$ ($\text{Ln} = \text{Nd}$ (1), Gd (2), Dy (3), Ho (4), Er (5); $\text{R} = \text{H}, \text{Me}$; Solv - solvent molecule). Their structure is based on the alternating of specific coordination centers (Fig. 1).

By means of exchange reactions between Ln acetates and CymCO_2H in H_2O -THF-MeOH media the following isostructural complexes having polymeric structure based on tetradentate acetate groups connecting three Ln^{3+} ions (Fig. 2) were obtained: $[\text{Ln}(\text{CymCO}_2)_2(\text{OAc})(\text{MeOH})]_n$ ($\text{Ln} = \text{Nd}$ (6), Gd (7), Dy (8); $\text{Cym} = (\eta^5\text{-C}_5\text{H}_5)\text{Mn}(\text{CO})_3$). In H_2O -THF-*i*-PrOH solvents media the same reaction results

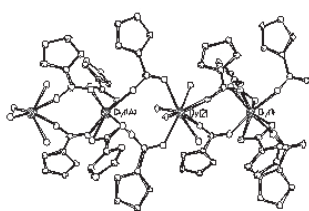


Fig. 1. The structure of 3.

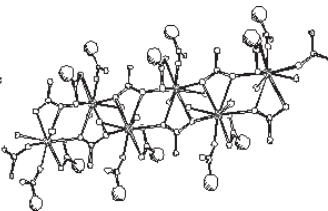


Fig. 2. The structure of 7.

in $[\text{Nd}(\text{CymCO}_2)_2(\text{OAc})(\text{H}_2\text{O})_2]_n$ (9), $[\text{Gd}(\text{CymCO}_2)_2(\text{OAc})(\text{H}_2\text{O})_2]_n$ (10) and $[\text{Dy}(\text{CymCO}_2)_2(\text{OAc})(\text{H}_2\text{O})]_n$ (11) polymers that differ in structures and in the quantity of solvate molecules. In all of the cases CymCO₂ groups are situated in the periphery of the chain and play chelate, monodentate or bridging role. Magnetic susceptibility of complexes 7 and 10 was measured in the 300 – 2K temperature range in a magnetic field of 5 kOe; the weak antiferromagnetic interactions between Gd³⁺ ions for 2 ($J = -0.03738 \text{ cm}^{-1}$) and ferromagnetic ones for 5 ($J = 0.01483 \text{ cm}^{-1}$) were found. Thermolysis of 6-11 was studied by means of TG and DSC in 30 – 900°C temperature range under air and Ar atmosphere; in the first case it affords LnMn_2O_5 phases, some of which exhibit the properties of multiferroics [4].

Acknowledgment. The work was supported by Russian Science Foundation, project 14-13-00938.

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CHEMISTRY OF MOLECULAR SYSTEMS

Chemical aspects of vitamin- and antioxidant-based therapy of oncological diseases

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The activities aimed at finding out new anti-tumor agents being performed in the world's most advanced research centres are mainly based on recent progress in molecular biology and genetics, the areas of knowledge which established the key factors determining genesis, development and proliferation of tumors.

Along with the genetic causes leading to the development of cancer, there are also other mechanisms of cancerogenesis. The aerobic glycolysis mechanism, discovered by O. Wartburg, has been found to be the main feature of metabolism disturbance in cancer patients, while the metabolic reprogramming of the energy exchange is a fundamental characteristic of a cancer cell and constitutes a mandatory item in the list of cancer signs. The most of the reactions taking place in cells and resulting in a release of energy involve oxygen molecules and occur according to free-radical mechanisms. Therefore, free-radical processes play an important role in the normal functioning of an organism; however, their activation could be the cause of various pathologies. While assessing the role of such processes in proliferation of malignant cells, one should take into account the fact that their proliferation occurs under conditions of hypoxia. In this connection, the availability and analysis of information about free-radical processes taking place in biologically relevant substances in the presence of various oxygen concentrations appears to be of importance.

Our studies have shown that a characteristic feature of free-radical transformations taking place in carbohydrates, amino acids, glycerophospholipids and sphingolipids under hypoxia conditions is a fragmentation reaction occurring in their respective radicals, involving simultaneous rupture of two bonds located in β -position with respect to the radical centre and leading to formation of the signaling molecules [1].

A particular attention deserves the fact established for the first time in our studies, namely the phenomenon of phosphatidic acid (PA) formation under the action of γ -radiation [2] or various redox systems [3] on glycerophospholipids. In healthy cells, PA is known to play an important role in regulation of cell proliferation and apoptosis processes. It has been established in recent studies that PA is a lipid messenger in the processes promoting the apoptosis switch-off and enhancing thereby the cancer cell survival [4]. Consequently, the PA accumulation would affect negatively the efficacy of chemo- and radiotherapy. Therefore, a rational strategy for anti-cancer therapy should be aimed at regulation of PA levels. We have found [5] that the best blockers of non-enzymatic pathways of PA formation under hypoxia conditions are quinones, as well as substances containing a conjugated carbonyl group in their respective structure, such as curcumin, phenylpropanoids, vitamins B, C and K [6, 7]. The possibility and outlooks of using the substances of such type in various combinations with other redox-active compounds in the treatment of oncological diseases will be discussed in the oral report.

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Radiation induced reactions of carbon-centered radicals with pyrimidine nucleobases and their derivatives

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Interactions of reactive products of water radiolysis with biomolecules play an important role in radiation-induced damage of biosystems. In the presence of oxygen processes of oxidation and oxidative destruction take place. They proceed mainly with participation of cell membrane lipids, proteins and nucleic acids. Oxidative modification and destruction of the latter could trigger biochemical replication of mutant biomolecules.

Under hypoxic conditions radical products of water radiolysis can induce free-radical fragmentation of hydroxyl-containing organic molecules, which occurs via formation of corresponding carbon-centered radicals.

In contrast to the normal cellule, cancer cells are duplicated under hypoxic conditions and the process of their oxidation during exposure to radiation is realized with lower probability [1]. It is widely known that DNA in nuclei is packed with protein and this total structure is called histone. ROS can lead to formation of carbon-centered radicals of protective protein histone and other molecules, which accompany DNA. It is reported [2], that these radicals are able to make cross-links between DNA and proteins. Taking this into account, it is relevant to study a mechanism of radiation induced carbon-centered radicals interaction with the components of nucleic acids under hypoxic conditions.

In order to find evidence for the cross-linking hypothesis on molecular level and to find possible sites of interaction, there were investigated the reactions of nucleic bases with the model carbon-centered α -hydroxyl containing radicals, which were generated via steady state radiolysis in pure ethanol. To establish the described mechanism of interaction uracil and thymine were used. It was found that the addition of uracil and thymine to pure ethanol decreased the yield of the butanediol-2,3 in contrast to 5,6-dihydrothymine and 6-methyluracil. This fact indicated that uracil and thymine can form adducts with α -hydroxyethyl radicals. In order to prove it we used hydroxyl group specific derivatizing agent (TMSI) and GS-MS-EI or LC-MS-ESI as methods of identification. The capability of uracil and thymine to be oxidized and to form adducts with α -hydroxyethyl radicals was observed unlike 5,6-dihydrothymine and 6-methyluracil. Their α -hydroxyl containing isomeric adducts were identified via GS-MS, their concentrations increased linearly with the raise of irradiation dose. This fact showed the crucial role of the presence of 5,6-double bond and the position of methyl group in the compound for ability of interacting with α -hydroxyethyl radicals.

Summarizing, we have revealed the ability of α -hydroxyethyl radicals as a model of carbon-centered radicals of biomolecules to interact with nat-

ural pyrimidine nucleobases and to modify their structure and properties.

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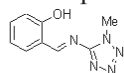
New tetrazole-containing Schiff bases

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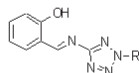
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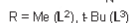
Schiff bases are well known for their biological applications as antibacterial, antifungal, anticancer and antiviral agents. On the other hand, tetrazole derivatives also possess important pharmacological properties (antibacterial, antifungal,



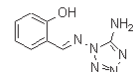
$L^1 = 2-(((1\text{-methyltetrazol-5-yl})\text{imino})\text{methyl})\text{phenol}$



$L^2 = 2-(((2\text{-methyltetrazol-5-yl})\text{imino})\text{methyl})\text{phenol}$



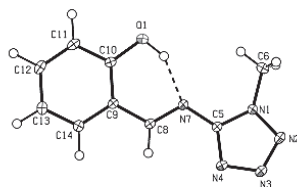
$L^3 = 2-(((\textit{tert}\text{-butyltetrazol-5-yl})\text{imino})\text{methyl})\text{phenol}$



$L^4 = 2-(((5\text{-aminotetrazol-1-yl})\text{imino})\text{methyl})\text{phenol}$

analgesic, anti-inflammatory, antitubercular etc.). Hence tetrazole-containing Schiff bases are considered as the compounds which can provide better therapeutic results, this circumstance causes the interest to them. Here we present four new tetrazole-containing Schiff bases, L1–L4, synthesized by the interaction of 5-aminotetrazole derivatives with salicylic acid under heating in ethanol.

The obtained compounds L1–L4 were identified by single crystal X-ray analysis, carried out with a SMART APEX II diffractometer at 100 K. The crystal structures were solved by direct methods and refined on F2 by full matrix least squares technique. All compounds show trans-configuration with respect to the C=N double bond and rather flattened skeletons of the molecules, which favor the conjugation of the azomethine group $-\text{C}=\text{N}-$ with the π -systems of the



Molecular structure of compound L^1 .

benzene and tetrazole rings. In all molecules there are rather strong intramolecular hydrogen bonds $O-H\cdots N$ between the hydroxy H and azomethine N atoms.

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Investigation of the chitosan based microstructured materials using CARS microscopy technique

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This work describes Coherent anti-Stokes Raman Scattering (CARS) microscopy [1] technique as an analytical method for the investigation of the spatial structure and chemical composition of microstructured materials based on chitosan. We used nitrogen-hydrogen vibrations in the high wavenumber region of Raman spectrum as a spectral marker of chitosan. High resolution images revealing size, geometrical shape, porosity and localization of chitosan in the microstructures such as powder, microfibers and aerosol nanoparticles are presented. We demonstrate chemically selective imaging of chitosan particles in the sample with the addition of polystyrene microspheres, which confirms our proposal to use nitrogen-hydrogen vibrations to identify chitosan.

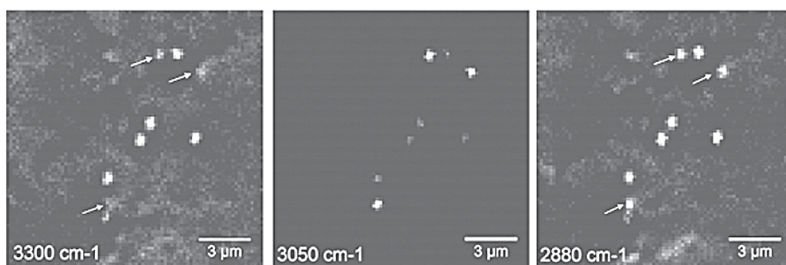


Fig. CARS images of chitosan and polystyrene particles on a surface of coverglass. Arrows show polystyrene particles. The images reveal the particles of: chitosan at 3300 cm^{-1} , polystyrene at 3050 cm^{-1} , both chitosan and polystyrene at 2880 cm^{-1}

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Molecular modelling of human oxysterol-7 α -hydroxylase complexes with ligands

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Human oxysterol-7 α -hydroxylase (cytochrome P450, CYP7B1) is a microsomal enzyme which catalyzes 7 α -hydroxylation of oxysterols and steroids [1]. CYP7B1 is associated with several physiological functions, such as bile acids biosynthesis [2], metabolism of steroid hormones (including neurosteroids) [3], regulation of immunoglobulin production [4] and metabolism of estrogen receptor ligands [5, 6]. Dysfunction of oxysterol-7 α -hydroxylase leads to a number of genetic disorders such as liver failure in newborns due to accumulation of toxic oxysterols and different neuropathies in adults [1]. There are 8 sense mutations which are associated with uprising of such disorders, but molecular mechanisms of this process are still unknown.

Recombinant CYP7B1 and its mutant forms were obtained earlier and it was shown that oxysterol-7 α -hydroxylase with amino acid substitution Arg486Cys (R486C) possesses modified activity toward neurosteroids [7].

To cast light on mechanisms of such specific alteration of protein–ligand recognition, a full-atomic model of human CYP7B1 and its mutant form was developed, and docking of natural substrates and their derivatives to the active site of the enzyme was performed. The results obtained reveal that Arg486Cys mutation has dramatic effects on protein structure and can lead to decrease in enzyme conformational stability. It was also shown that α -helix B' changes its position in CYP7B1 active site due to investigated amino acid alteration. This can be a reason of modified affinity of R486C toward several steroids.

Molecular docking of known ligands allowed us to determine amino acids which are important for substrate stabilization in the active site of CYP7B1. It was shown that conservative Ser115, Leu118, Leu119, Phe282, Ala 292, Ile369 were crucial for ligand binding that is in agreement with the results of multiple alignment of steroid-7 α -hydroxylases from different species. Using the alanine scanning for determination of the contribution of amino acids, forming the CYP7B1 substrate-binding region, to the free energy of ligand binding also confirmed this hypothesis.

The parameters of the binding enthalpy of substrates are in agreement with the data obtained in vitro by using of spectrophotometric titration method [7].

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New NBD-labeled fluorescent steroids as molecular probes for mammalian steroid-converting enzymes: in silico evaluation

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Previously we have shown that known 7-nitrobenz-2-oxa-1,3-diazol-4-yl (NBD)-labeled fluorescent 3 β -hydroxy-5-en-steroids, trivially mentioned as 22-NBD-cholesterol and 25-NBD-cholesterol, can be converted into their 3-oxo-4-en-derivatives (22-NBD-one and 25-NBD-one, respectively) by bacterial cholesterol oxidase and cholesterol dehydrogenase [1–3]. Recently further metabolism of these compounds by bacteria, expressing 3-ketosteroid-1-dehydrogenase (KSD), has been predicted using molecular docking [4]. All of the compounds bear NBD fluorophore in their side chain. Thus, structure and synthesis of an alternative fluorescent cholesterol analogue, based on cholestan scaffold, has been designed. The synthetic scheme included two steps, namely reductive amination with ammonium acetate and NaBH₄ followed by electrophilic substitution of chlorine in 4-chloro-7-nitro-2,1,3-benzoxadiazole with steroidal amines. Two isomers of 3-((NBD)-amino)-cholestane, probably 5 β -H-3 α -(NBD)amino- (3NC1) and 5 α -H-3 β -(NBD)amino (3NC2) [5], have been obtained and their physical properties have been confirmed using fluorimetry, spectrophotometry and mass-spectrometry.

Using the same synthetic scheme 20 α - (more hydrophobic) and 20 β -isomers of 20-((NBD)-amino-pregn-5-en-3 β -ol (20NBDP) as well as 17 β -(NBD)-amino-estr-1,3,5(10)-trien-3-ol (17NE) have been synthesized. The yield was relatively low (10 %) and the main side product of 17NE synthesis was found to be estradiol. The fluorescent product ([M–H][–] with *m/z* 433) has been quantitatively purified from reaction mixture using Al₂O₃-based column chromatography followed by reversed-phase HPLC.

In this study using Autodock 4.2 software we have focused on a prediction of binding affinity/features of 3NC1, 3NC2, 20 α - & 20 β -isomers of 20NBDP and 17NE in active sites of some steroid-converting mammalian enzymes with known 3D-structures, namely cytochrome P450 vitamin D 24-hydroxylase (CYP24; pdb code: 3K9V), P450 17 α -hydroxylase/17,20-lyase (CYP17; pdb code: 3RUK), P450 aromatase (CYP19; pdb code: 3S7S) and steroid sulfatase (SULT; pdb code: 1p49). Our docking simulation results indicate affine and, in some case, substrate-like binding of the fluorescent steroids in the active sites of CYP24 (3NC1, 3NC2, 20NBDP), CYP17 (20NBDP), CYP19 (17NE) and SULT (20NBDP, 17NE). The calculations pointing out on the potential of the low-molecular compounds as fluorescent probes for screening of new inhibitors of the enzymes, playing important roles in steroid homeostasis as well as in pathogenesis of prostate cancer (CYP24, CYP17) and breast cancer (CYP19, SULT) [6, 7].

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Preparation of metal complexes of sulfonated polyacrylamide with Cr(III) using frontal polymerization method

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Frontal polymerization is a nonisothermal process propagating by an autowave mechanism. This process can be performed in continuous reactors in laminar and, particularly, turbulent flows [1]. Thermal frontal polymerization can be applied to the widest range of materials. The major advantage of thermal frontal polymerization is the high rate of conversion. Hydrogels have been prepared frontally, which have superior properties to those prepared by conventional methods [2]. It was shown earlier that complexation of Cr^{3+} with carboxylate groups is a driving force of polyacrylamide cross-linking in the presence of chromium acetate [3].

The aim of this work was to study the possibility to prepare the complexes of sulfonated polyacrylamide with Cr(III) through polymerization in the frontal regime. Test tubes with inner diameter of 5 mm and length of 150 mm were filled with dilute aqueous solutions of 1 : 1 molar mixture of acrylamide and 2-acrylamido-2-methyl propane sulfonic acid (AMPS), containing 1 mol % of ammonium persulfate as initiator and different amounts of chromium acetate as a cross-linker. Frontal polymerization process was initiated through heating the upper part of test tubes with a soldering iron. Front rate was measured visually. Maximum front temperature was measured with digital thermometer. Gel fraction and equilibrium water absorption were measured gravimetrically. Water absorption firstly decreased with an increase in chromium acetate concentration and then it was diminished due to oxidation of some of Cr^{3+} ions to Cr^{6+} ones in the presence of AMPS and persulfate. The decrease in maximum front temperature and front rate with an increase in the cross-

Table. Characteristics of frontal polymerization in the presence of different ratios of cross-linker

Cross-linker / monomers, wt/wt	Maximum front temperature, °C	Front rate, cm/min	Water absorption, g H ₂ O/g hydrogel	Gel fraction, %
1 / 400	118	1.20	1425 ± 190	20.3
1 / 350	114	1.00	1140 ± 150	43.7
1 / 300	110	1.00	1875 ± 250	73.0

linker concentration confirms the idea of Cr^{3+} oxidation at higher chromium acetate concentrations. It seems that the extent of polymeric metal complex formation is adequate to an increase in the gel fraction with the raise of the chromium acetate concentration. IR study of prepared hydrogels detected their low residual monomer content.

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Spectroscopic properties of benzotiadiazole based compounds

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Due to unique physical properties organic multifunctional compounds containing benzotiadiazole, fluorene and carbazole moieties are of great concern for applications in optoelectronic devices. Therefore, current state of the art molecular compounds are often composed of several building blocks responsible for one or another material functionality. Carbazole or fluorene presenting strong electron-donating chromophores are most common building blocks in design of molecular compounds in which intramolecular or intermolecular charge transfer is desirable. Benzotiadiazole moiety is a strong electron acceptor and is also quite common in materials for molecular electronics.

New benzotiadiazole compounds with carbazole or fluorene chromophoric units were synthesized in this work, and their optical properties as well as excited state dynamics were investigated in solutions and in solid films. Steady-state absorption and fluorescence properties of solutions and thin films of the studied compounds revealed formation of long-wavelength absorption and fluorescence bands related to low energy charge transfer states. These benzotiadiazole molecules in solutions have large fluorescence quantum yields exceeding 50 %, which drop slightly in solid films. In comparison with solutions the fluorescence spectra of both compounds in solids moves to the blue spectral region.

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Antiviral properties of the natural and synthetic cinnamic acid derivatives

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Anti-inflammatory, antiviral, antimicrobial, anticancer, cyto- and hepatoprotective activities of a lot of herbal medicines are associated with cinnamic acid (1) and its ester derivatives which they contain [1]. Taking it into account we have synthesized a number of O-methylated caffeic and ferulic acids derivatives (5, 7–9) to study their antiviral activity. Antiviral properties of the natural and synthetic cinnamic

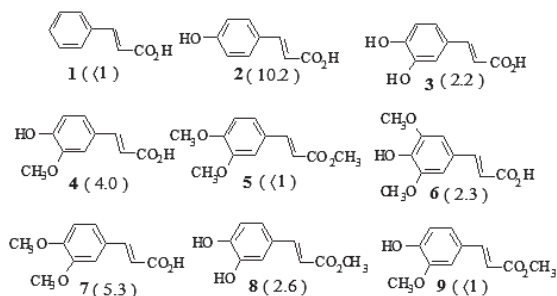


Fig. Natural and synthetic cinnamic acid derivatives tested (MTC/EC₅₀)

acid derivatives were studied in cell culture against herpes simplex type I virus (HSV-I). The investigations were performed in the human rhabdomyosarcoma cell culture with HSV-1 using the cytopathic effect evaluation method, as described earlier [2]. Concentrations of the tested compounds providing suppression of the virus replication by 50 % (the average effective concentration, EC₅₀) were also calculated, as well as the ratios of maximum tolerated concentration (MTC) to EC₅₀. The ability of 4-hydroxycinnamic (2), ferulic (4) and 3-(3,4-dimethoxyphenyl)-2-propenoic (7) acids, as well as methyl-3-(3,4-dihydroxyphenyl)-2-propenoate (8) to suppress replication of herpes virus has been established (Figure).

The tested compounds demonstrated the following structure-activity relationship. In the set of caffeic (3) – ferulic (4) – 3-(3,4-dimethoxyphenyl)-2-propenoic (7) acids the consecutive methylation of hydroxyl groups provided an increase in antiviral activity. In the range of substituted methyl esters of cinnamic acid derivatives we observed the opposite tendency, namely, compounds 5, 9 did not inhibit virus reproduction. Only sample 8 had a weak activity.

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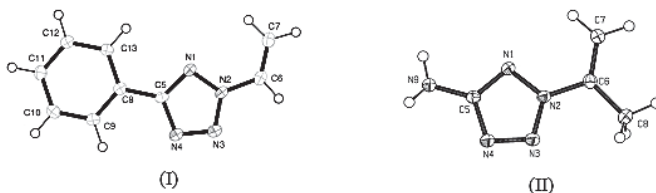
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Molecular and crystal structure of 5-phenyl-2-vinyl-2H-tetrazole and 2-(prop-1-en-2-yl)-2H-tetrazol-5-amine

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N-Vinyltetrazoles present valuable intermediates in organic synthesis and starting monomers for preparing polymeric materials. To date, a range of 1-vinyltetrazoles have been synthesized and some of them structurally characterized. However, structural data of 2-vinyltetrazole derivatives have not been reported, except for 1-tert-butyl-3-(prop-1-en-2-yl)tetrazolium perchlorate, prepared by quaternization of 2-(prop-1-en-2-yl)tetrazole [1]. In the present work, we fill to some extent the

deficiency by reporting molecular and crystal structures of two 2-vinyltetrazoles, namely 5-phenyl-2-vinyl-2H-tetrazole (I) and 2-(prop-1-en-2-yl)-2H-tetrazol-5-amine (II). Hitherto unknown monomer (II) was synthesized by dehydrobromination of 2-(1-bromopropan-2-yl)tetrazol-5-amine obtained by alkylation of tetrazol-5-amine with allyl bromide in sulfuric acid using an adapted procedure [2]. Single crystal X-ray data of compounds (I) and (II) were obtained at 100 K. Both compounds were found to be S-cis-(N1) conformers. The planes of the vinyl groups are close to those of the tetrazole rings. In compound (I), the vinyl atoms C6 and C7 lie out of the tetrazole ring plane on 0.0053 (19) and 0.058 (2) Å, respectively, and corresponding values for compound (II) are still lower, namely of –0.0028 (9) and 0.0010 (3) Å. These data agree with a conclusion derived by quantum-chemical investigation of 2-vinyltetrazoles [3] that consists in the following. In case of the absence of steric hindrances in vinyltetrazoles the vinyl groups have a tendency to be placed in the tetrazole ring plane to favor the conjugation between the π -systems of the ring and the vinyl group.



In compound (II), the amino group shows somewhat flattened configuration, nevertheless it is pyramidal, with a sum of the valence angles around the amino N atom equal to 347.4°. Two amino H atoms are located on the same side of the tetrazole ring plane.

There are hydrogen bonds in the crystal structures of the compounds. In (I), intermolecular non-classic hydrogen bonds $C_6-H_6 \cdots N_3$ between the vinyl H and the tetrazole N3 atoms form dimeric units comprising hydrogen-bonded rings $R_2^2(8)$. In (II), intermolecular classic hydrogen bonds $N_9-H_9A \cdots N_3$ and $N_9-H_9B \cdots N_4$ between the amino H and the tetrazole ring N atoms are responsible for the formation of polymeric ribbons.

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Destruction of blood sphingolipids under the action of reactive chlorine species

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Sphingolipids have emerged as key signaling molecules involved in the regulation of a variety of cellular functions including cell growth and differentiation, proliferation and apoptotic cell death. Sphingolipids have been implicated in several diseases such as cancer, obesity, atherosclerosis and sphingolipidoses; however, the efforts addressing blood sphingolipidomics are still limited. Interest in blood sphingolipids has been broadened by the development and clinical application of the immunosuppressive drug FTY720, which targets sphingosine-1-phosphate receptors resulting in lymphocyte sequestration [1]. It has since become increasingly essential to determine the mechanisms by which sphingolipid biosynthesis and turnover regulate cell function and pathology.

The mechanisms by which the sphingolipids act on cells have a complex nature. Not much is known about the metabolism of sphingolipid breakdown products. For example, sphingosine-1-phosphate lyase catalyses the final step of sphingolipid degradation, namely the irreversible cleavage of the carbon chain, thereby yielding 2-hexadecenal and phosphoethanolamine. 2-Hexadecenal possesses a wide spectrum of biological activity; in particular, it provokes reorganization of the cell cytoskeleton, induces apoptosis and forms adducts with DNA which can induce mutagenic consequences [2–3]. Furthermore, it has been established that the action of hypochloric acid on aqueous sphingolipid dispersions produces 2-hexadecenal [4]. These processes occur in polar moieties of the lipids and include formation of nitrogen-centered radicals, which undergo decomposition via rupture of two β -bonds.

In this study, new data have been obtained on the formation of 2-hexadecenal in human blood cells which contain sphingolipids under the exposure to reactive chlorine species. Analysis of the effect of hypochloric acid on extract of blood erythrocytes indicates 2-hexadecenal to be formed. Blood of healthy volunteer was collected to heparin tubes and centrifuged to obtain erythrocytes and plasma. The reaction of erythrocytes with a freshly prepared NaOCl solution was performed at room temperature, in short time while stirring. To separate the aldehyde from the biological samples, we used a modified “Bligh & Dyer” extraction procedure. We developed method based on high performance liquid chromatography using fluorescence detection to quantify the sphingolipid destruction product 2-hexadecenal.

The obtained results suggest the described mechanism of free radical fragmentation of sphingolipids that can be implemented on a cell culture under stress of reactive chlorinating species.

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An investigation of thermal destruction of caprolactam solid oligomers generated at polyamide-6 production

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Low molecular weight liquid or solid products of oligomerization are formed in the process of caprolactam polymerization occurring at the polyamide-6 production. Polymers and oligomers with free end groups, in particular, all types of polyamides (PA-6, PA-66) contain small quantities of cyclic oligomers, which largely effect the physical and mechanical properties of polymers. Similar to the ϵ -caprolactam all cyclic oligomers polymerize readily at heating in the presence of water or acids. However, the most interesting property of cyclic oligomers is their ability to transform into ϵ -caprolactam.

Thermogravimetric studies of caprolactam samples and solid wastes of polyamide-6 production were carried out to determine the optimal conditions for ϵ -caprolactam synthesis by thermolysis of cyclic oligomers.

Thermal analysis was carried out using NETZSCH STA 449 C thermal analyzer provided with a thermogravimetry (TG) module and a differential scanning calorimetry (DSC) cell. Standard measurements were performed at a heating rate of 5° min^{-1} in the air atmosphere and in nitrogen flow at the temperature range 30–500°C.

By means of DTG and DSC it has been revealed that solid wastes represent a mixture of cyclic dimers, trimers, tetramers and linear oligomers of caprolactam, which can be converted into ϵ -caprolactam under certain conditions. It has been found that maximal temperature of linear oligomers decomposition is 156.3°C, while trimer or their mixture with tetramer decompose at 240.1°C. The maximal decomposition temperature of the most thermally stable dimer lies in the region 338–340°C. Therefore heating of the reaction vessel during the synthesis of caprolactam should not be below this temperature.

The processes of solid caprolactam oligomers thermal destruction in vacuum have been investigated in the presence of various catalysts (SiO_2 , TiO_2 , H_3PO_4 , NaOH , KOH). Thermolysis was carried out at 250–340°C in vacuum at a pressure of 1.3–2 Pa. It has been found that about 5 % of caprolactam is released under these conditions in the absence of any catalyst. However, according to the DSC data the samples of solid oligomers initially contain caprolactam and its release during thermolysis is not associated with the destruction of cyclic oligomers. It has been established that the yield of caprolactam in the process of thermolysis significantly depends on the nature of the catalyst. Thus at the thermolysis in the presence of SiO_2 the yield of caprolactam does not exceed 24 %, while maximal regeneration of caprolactam (90–92%) from cyclic oligomers occurs at their thermolysis in the presence of alkali metal hydroxide (KOH , NaOH).

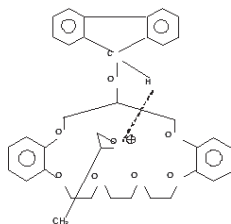
The dependence of caprolactam yield on the catalyst concentration has been investigated on the example of sodium hydroxide. It has been shown that an increase of

the catalyst concentration to a certain limits provides a rise of the caprolactam yield. Thus, during the thermolysis in the presence of 2 wt. % NaOH the yield of the caprolactam reaches 90 % and does not increase with increasing catalyst concentration to 10 %.

Thermogravimetric study and the results of thermolysis of cyclic and linear oligomers of polyamide-6 were a prerequisite for creating recycling technology of solid wastes, generated in the production of polyamide-6.

Usage of the fluoreneoxy substituted crown compounds in the allotment of optical isomers

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It is known that the introduction of alkyl radicals in the macrocyclic ring of crown esters changes the conformation of the macrocyclic ring [1]. To prevent conformational transition by the rotation around carbon-carbon bonds fluoreneoxy substituted crown esters were synthesized by the introduction of the large bulky substituent which was fluorenyl group into the macrocyclic ring [2]. Propylene oxide can be allotted with the help of the chromatographic column into the enantiomers with the usage of fluoreneoxy crown ester as the adsorbent. Phenyl groups which are in the fragment and hydrogen in the group bounded with oxygen are very active. Hydrogen takes part in the formation of hydrogen bond with the ring of oxirane and in the result oxonium cation is formed. Oxonium cation is formed with crown ester in molecular supramolecular clathrate with the type of «guest–host». S- and R- isomers of propylene oxide are captured with the ring of crown ester and active hydrogen of fluorene by different forces and the effectiveness of such interaction is different. That is why the duration of their exit from the chromatography column is different.

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Development of novel biologically active food supplements based on flaxseed oil

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Flaxseed oil is a rich vegetal source of ϵ -linolenic acid (ALA), which belongs to the family of omega-3 polyunsaturated acids (PUFA). 49–66 % of the total fatty acid content of flaxseed oil falls to the share of this acid, and for this reason it is widely used as a basis for development of biologically active food supplements (BAFS) effective for prevention and treatment of many diseases. The high ALA content entails high susceptibility of flaxseed oil towards oxidation because of the presence of three reactive double bonds in the fatty acid structure. A common drawback of flaxseed oil-based BAFS, including those in capsule forms, is their low resistance to oxidation, and hence a short storage period and insufficient efficacy, which limit their presence on the market of biologically active food supplements.

The Laboratory of Chemistry of Free-Radical Processes at the Scientific Research Institute for Physical Chemical Problems of the Belarusian State University performs the research work aimed at the development of novel flaxseed oil-based BAFS characterized not only by unique preventive and therapeutic properties due to a combined action of the flaxseed oil components and the biologically active substances (BAS) added, but also by high resistance to oxidation.

The effect of BAS including Q10 coenzyme, carotinoids (β -carotene, lutein, zeaxanthin), vitamin E in its various forms, fat-soluble ascorbic acid derivatives and organic selenium compounds on the oxidative resistance of flaxseed oil was studied as a function of concentration and composition of the additives. The effect of BAS on the storage conditions was also revealed. Concentrations of the BAS used for the flaxseed oil enrichment were selected taking into account their recommended safe daily doses for the proposed dosages. Kinetic data on accumulation of peroxide compounds, as well as other oxidation products including carbonyl compounds (α - and β -unsaturated aldehydes) and free fatty acids, have been obtained under various storage conditions of the oil with BAS added and without additives. Some BAS being added to flaxseed oil were found to provoke enhancement of the oxidation processes taking place in the oil. The effectiveness of inhibition of such processes by the synthetic and natural antioxidants, as well as compositions thereof, was assessed under storage at room temperature and under accelerated oxidation conditions using an 892 Professional Rancimat instrument. The BAS depletion rate was studied for the BAFS being stored in the presence and in the absence of various stabilizers.

It has been shown that fat-soluble ascorbic acid derivatives and their combinations with stabilizing legume-seed-based compositions, which we had developed earlier for edible flaxseed oil, can be used for ensuring anti-oxidative protection of a range of nutrient products. These additives enable significant inhibition of the free-radical oxidation and oxidative destruction processes taking place in PUFA, tocopherols, carotinoids and other unsaturated

components of flaxseed oil (and the BAFS on its basis), substantially improving thereby the resistance to oxidation and prolonging self-life of the products.

Formulations and production technologies for 4 oxidation-resistant flaxseed oil-based BAFS have been developed from the results obtained in this research work that were «Coenzyme Q10 – flaxseed oil plus», «Beta-carotene – flaxseed oil plus», «Selenium –vitamin E – flaxseed oil plus», and «Milk thistle seed oil – flaxseed oil plus», the former one having storage period of 9 months, and the latter 3–12 months. These BAFS possess antioxidant, radioprotector, anti-cancerogenic, immuno-stimulating, adaptogenic and geroprotecting properties. The respective official registration certificates have been obtained and manufacture of these BAFS has been started at an enterprise of the ClubPharmEco Company in 2014.

Anomalous temperature dependences of luminescence of alkoxy-substituted stilbenes

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Common luminescent materials typically demonstrate monotonic decrease of emission with the temperature rise [1, 2]. We have found anomalous temperature dependence of luminescence (ATDL) of alkoxy-substituted stilbenes (Figure a). The emission maximum shifted towards the shorter wavelength (blue shift) with the temperature increase. Effects of alkyl chain length and polymer matrix on thermal dependence of luminescence were studied. As shown in Figure b the doping of polymer matrix with a stilbene dye provides a linear decrease in luminescence with an increase in temperature, thus ATDL is not observed. Polymer matrix reduces interaction between stilbene dyes molecules and a shift of emission maximum to the blue region of wavelengths occurs. ATDL can be attributed to structural changes in thin films at temperature increase. It should be pointed that ATDL effect is observed at temperatures above the transition of crystalline phase into isotropic phase.

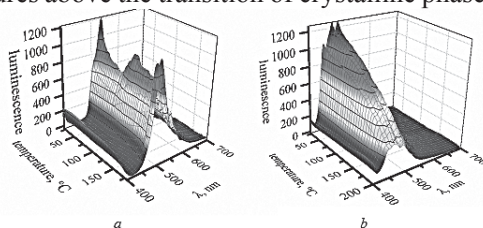


Fig. Temperature dependence of stilbene dye luminescence in thin film (a) and in polymer matrix (b)

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Multi-elemental analysis by ICP-AES in authentication of geographical origin of wines

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It is known that macro and trace element composition of plants and living organisms depends on the elemental composition of the environment [1]. European researchers have found that even 10 years after bottling, the wine continues to bear the «chemical signature» of the vineyard and the wood of the barrel, in which the wine was matured. Naturally, this fact can be used to confirm the origin of wines with geographical appellation, as well as to detect wine falsification [2]. The authentication of the product at the place of origin means that it has some special features related to this area because of the unique natural and climatic conditions and existing traditions. Also, the geographical appellation bears the information that there is some control over this production. In 2011 the OIV (International Organization of Wine) issued the book of recommended methods for multi-elemental analysis of wine, must and grape juice [3]. The analysis has to be carried out by atomic emission spectrometry with inductively bound argon plasma (ICP-AES or ICP-AES) and mass spectrometry with inductively coupled argon plasma (ICP-MS or ICP-MS).

In this work there are presented the results of tests carried out in order to validate trace elements analysis of wines by ICP-AES. Studies were carried out by atomic emission spectrometry with inductively bound argon plasma at ICPE-9000 instrument (ICP-AES, Shimadzu Co., Japan). We used standard for ICP, Fluka Trace CERT-ISO/IEC 17027, ISO Guide 34 (Sigma-Aldrich GmbH). For preparation of calibration solutions, water and nitric acid class Trace SELECT Ultra were used. For the multi-elemental analysis of wine two sets of standards were used that were series (1), including trace elements (zinc, copper, arsenic, lead, cadmium, iron, aluminum, etc.) and series (2), including macro-elements (sodium, potassium, calcium, magnesium, lithium). For the first series, the multi-elemental standard was prepared with 5 % solution of ethanol, and for the second series the influence of alcohol was not taken into account, since a significant dilution of the samples (25–100 times) negates its effect.

It was determined that the content of trace elements depended not only on the composition of the probe, but also on the applied technological operations. The content of micro and macro-elements also depended on the crop year. In particular, relatively low levels of elements such as copper and iron indicated the absence of exogenous metals, of agronomic or technological origin. Relatively low levels of potassium suggested that technological operations such as treatment with potassium metabisulfite, potassium ferrocyanide, clarification with potassium alginate or caseinate, etc. were not used.

The multi-elemental analysis performed by ICP-AES method is of a considerable interest to confirm the geographical origin of the product, as well as it is a source of information on the applied technological methods. In fact, this analysis has to be primary for wines of designated origin. Besides, this method can be used to identify the counterfeit products.

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Frontal copolymerization of sodium acrylate and sodium 2-acrylamido-2-methylpropanesulphonate

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Acrylic acid salts and acrylamide copolymers solutions gelled by transition metal complexes are widely used in oil recovery to shut off fractures and zones of high permeability in oil-bearing rock formations [1]. A common gel used in field treatments is usually obtained by cross-linking of partially hydrolyzed polyacrylamide (sodium acrylate and acrylamide copolymer) with chromium acetate. The initial stage of the crosslinking is the interaction of chromium acetate with carboxyl group of copolymer.

In previous studies [2], the possibility of gel formation of sodium acrylate and sodium 2-acrylamido-2-methylpropanesulphonate copolymers, synthesized in aqueous solution, in the presence of chromium acetate as crosslinker was ascertained. But the molecular weight of such copolymers was low. The frontal copolymerization of solid monomers can eliminate an ability of dissociation and mutual repulsion of ionic monomers, and thus it is able to promote an increase in the length of polymer chain and a decrease in polymer concentration in gelling compositions.

The purposes of the present work are to synthesize homo- and copolymers of sodium acrylate and sodium 2-acrylamido-2-methyl-propanesulphonate by frontal polymerization of solid monomers and to determine minimal concentration providing gel formation in aqueous solutions of copolymers containing chromium acetate as cross-linking agent at oil reservoir temperature 95 oC.

Copolymers were prepared by solvent-free frontal free-radical polymerization with the descending mode of thermal waves propagation in the presence of benzoyl peroxide initiator (1 % from the weight of monomers mixture) and molar ratio of monomers 1 : 1. The length of macromolecular chain was evaluated by measurement of intrinsic viscosity of pure copolymer in 5M aqueous NaCl solution. The gelation process was determined based on the Sydansk's gel strength code [3] by observing the appearance of the gel structure on the wall of the bottle when the bottle was inverted.

Copolymers of sodium acrylate and sodium 2-acrylamido-2-methyl-propanesulphonate were for the first time obtained by frontal polymerization of solid monomers. Synthesis of sodium polyacrylate via frontal polymerization resulted in a cross-linked, insoluble product. Frontally polymerized sodium poly-2-acrylamido-2-methyl-propanesulphonate had linear structure, could be dissolved in water, but its solutions were not able to crosslinking by chromium acetate. Frontally polymerized copolymers of sodium acrylate and sodium 2-acrylamido-2-methyl-propanesulphonate also had linear structure and could be dissolved in water, but they were able to form gels in aqueous solutions containing chromium acetate. It was established that the value of the intrinsic viscosity of copolymer prepared by frontal polymerization of solid monomers was 1.7 times higher than the value of viscosity of copolymer synthesized in aqueous solution. Due to the increase in the length of polymeric chain it was possible to decrease the concentration of copolymer

in gelling compositions from 10 to 2 wt.%. The concentration of chromium ions was constant and equal to 800 mg/l. Under the equal conditions gel formation of frontally polymerized copolymer compositions had higher rate than gel formation of the compositions of copolymer synthesized in concentrated aqueous solutions.

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Lubricating additives for low sulphur fuels

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The term “lubricity” refers to the ability of a liquid to form a hydrodynamic and/or boundary grease films and reduce friction between sliding surfaces. The significance of lubricity issues in fuel formulations has been decisively proved in recent years, when the advent of low-sulfur fuels, as forced by environmental regulations [1], led to numerous failures of vehicle engines. Being a key driver in the push for cleaner fuels, desulfurization resulted in a loss of fuel's inherent lubricity responsible for anti-wear protection of injectors and pumps, which are lubricated by the fuel itself.

Fatty acids methyl esters (FAME), obtained via trans-esterification of canola oil,

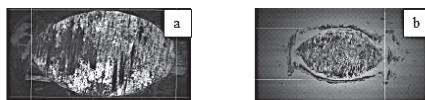


Fig. Microscopic pictures of wear scars of pure K5 diesel (a) and diesel with 3 wt% of FAME (b)

and their mixtures with free fatty acids (FFA) were examined as lubricating additives for K5 diesel fuel in the current work. The samples were tested for friction and wear with the High-Frequency Reciprocating Rig (HFRR) testing method [2] with the use of measuring-calculating complex system “Smazka DT” developed by Belarusian intercollegiate center BMC. The lubricity of the pure fuel, organic additives and their mixtures were evaluated by the diameter of wear scar formed under friction of steel ball sliding against stationary metal plate immersed in a studied liquid.

It was found that 1–7 wt. % FAME additives did not cause a sufficient increase in diesel fuel viscosity or density (< 2 % difference) and did not change the fuel energy characteristics. The lubricity tests testified that the addition of FAME to the oil diesel fuel improved its lubricity by 1.5–2 times. The optimal concentration of FAME was estimated to be 3 wt. % which corresponded to the wear scar diameter decrease from 696 to 427 μm . Further increase in the concentration of FAME did not provide sufficient improvement of the fuel lubricity.

FAME and FFA blends were found to be even better lubricating additives as they caused a decrease of wear scar diameter at their much lower concentrations (0.02–0.03 wt%). Particularly, a sufficient change in wear scars diameter from 696 to 380 and 343 μm was observed under the addition of 0.02 and 0.03 wt% of FAME and FFA blend to K5 diesel fuel respectively. The same trend was observed in case of the addition of FAME and FFA mixtures to kerosene.

The obtained results clearly proved the advisability of the use of FAME and FFA as lubricating and anti-wear additives for low sulphur oil diesel fuels.

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Extraction of aromatic hydrocarbons by methanol solutions of various organic salts

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Nowadays extraction systems consisting of an aliphatic hydrocarbon and an organic salt solution in polar solvent or ionic liquids have not been investigated well. Ionic liquids are known to show specific affinity to aromatic hydrocarbons [1]. But they are expensive and not available on a large scale. An organic salt solutions in polar solvent can be used as alternative.

Distribution of aromatic hydrocarbons containing from 2 to 9 aromatic rings in extraction systems consisting of n-heptane and an organic salt (1-butyl-3-methylimidazolium chloride or 1-methylquinolinium benzenesulfonate) methanol solution, has been studied for the first time. Distribution constants (P) in systems n-heptane – polar phase for aromatic hydrocarbons and the increments of methylene group (ICH₂) have been calculated. UV-spectrophotometry was used to determine the concentration of aromatic hydrocarbons in phases of the system.

It has been found that increasing the salt concentration strengthens the

Substance \ Concentration of salt, M	0,0 [2, 3]	0,5	1,0	1,5	2,0	2,5	DMSO [2, 3]	DMF [2, 3]
I_{α_2}	0.08	0.12	0.14	0.17	0.19	0.21	0.20	0.12
Naphthalene	1.2	1.3	0.88	0.76	0.72	0.76	0.50	0.29
Anthracene	2.1	0.53	0.46	0.32	0.26	0.27	0.40	0.18
Tetracene	2.3	0.56	0.22	0.10	0.07	0.04	0.33	0.13
Diphenyl	1.3	1.1	1.0	0.83	0.88	1.1	0.59	0.32
p-terphenyl	1.9	1.2	0.88	1.0	0.65	0.64	0.47	0.14
$\alpha\alpha'$ -dinaphthyl	3.1	1.6	1.4	1.1	0.74	0.97	0.40	0.10
Perylene	1.4	0.28	0.25	0.13	0.08	0.03	0.11	0.050
Chrysene	1.1	0.45	0.28	0.21	0.16	0.13	0.11	0.061

structure of polar phase and at the same time decreases distribution constants of aromatic hydrocarbons. In addition, the most significant drop of distribution constants occurs for condensed polyaromatic hydrocarbons.

It has been established that the extraction system consisting of n-heptane and 2,5 M 1-methylquinolinium benzenesulfonate methanol solution was much more efficient for condensed aromatic hydrocarbons' extraction than the best known extractants such as DMSO and DMF

[2, 3]. This system demonstrates the best differentiation of P-values for monocyclic and condensed aromatic hydrocarbons (Table). It is very important that the above-mentioned system have remarkable ability to differentiate P-values of aromatic hydrocarbons having isolated and condensed benzene rings in molecules. This phenomenon gives an opportunity to develop new sample preparation methods for objects consisting of mixed aromatic hydrocarbons. It may be promising to use these salts and their solutions as stationary phases in chromatography.

Values of increments of methylene group (ICH₂) and distribution constants of aromatic hydrocarbons in systems n-heptane – 1-methylquinolinium benzenesulfonate methanol solution, n-heptane – DMSO, n-heptane – DMF

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Synthesis and study of antiradical and antioxidant properties of agidol derivatives

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Due to the ability to inhibit free-radical processes of oxidation of organic substances phenolic compounds have found broad application in various spheres as

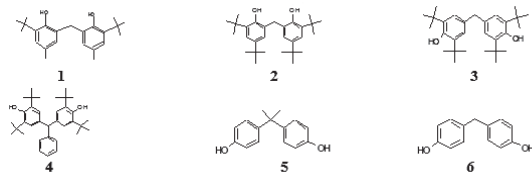


Fig. Agidol derivatives under study

stabilizers of food and industrial fats, polymers and petroleum [1]. Some of them have found application as therapeutic agents [2]. Natural and synthetic phenolic antioxidants play an important role in the regulation of lipid peroxidation [2]. Antioxidant properties of commercial stabilizers such as ionol and agidol (1) are among the most well-studied substances [1]. The importance of homolytic processes involving carbon-centered radicals during free radical-induced damage of biomolecules under hypoxic conditions have been shown in the recent publications. Agidol antiradical activity has been demonstrated earlier [3]. It appears important to study agidol derivatives reactivity to various radical intermediates.

For this purpose agidol derivatives (2–6) (Fig.) have been synthesized. Systematic comparative studies of agidol and its derivatives reactivity to oxygen- and carbon-centered radicals have been performed. We have studied the influence of such compounds on the formation of hexane and ethanol radiation-induced transformations products in the presence and in absence of oxygen that allowed us to evaluate the reactivity of the studied substances to various types of radicals. In accordance with the experimental data industrial antioxidants, such as agidol (1) and its derivatives (2–6) have shown to be effective inhibitors of hexane oxidation processes. Unlike hexane, the tested compounds did not inhibit ethanol oxidation. Addition of agidol and its derivatives caused only minor changes in the yields of hexane major radiolysis products in the absence of oxygen. However, compounds (1, 2, 3, 6) significantly decreased 2,3-butanediol yields during deaerated ethanol radiolysis. This indicates their high reactivity to α -hydroxyethyl radicals.

Thus, radical-regulatory properties of the studied substances depend not only on their structure but also on the nature of the target compound. Therefore, these results should be taken into account when choosing appropriate antioxidants intended for the protection of multicomponent systems such as bioobjects from the damages resulting from free-radical processes.

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Radiation-induced carbon skeleton destruction of 2-aminoethanol derivatives in aqueous solutions

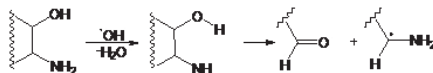
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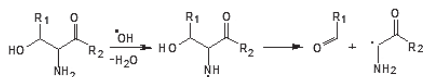
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Amino alcohols and their derivatives such as hydroxyl-containing amino acids, phospholipids and amino sugars have a great biological significance. It is well known that reactive oxygen species (ROS) such as hydroxyl radicals ($\bullet\text{OH}$) can cause dam-

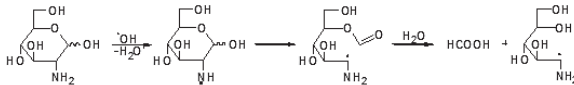


age to biomolecules [1, 2]. In our work we have used γ -irradiation model for OH -radicals generation. We have performed the radiolysis of aqueous solutions of 1-amino-2-propanole, serine, threonine, glucosamine and related compounds. The irradiation conditions (pH value of solutions, the presence of oxygen and additives) were varied. The chromatographic techniques coupled with UV-visible, flame ionization and mass spectrometry detectors were used for qualification of the investigated compounds destruction products. It was confirmed that molecules with 2-aminoethanol moiety, such as 1-amino-2-propanole, serine, threonine and containing these amino acids residues on the N-terminal parts of the molecules dipeptides, as well as glucosamine undergo radiation-induced carbon skeleton destruction in aqueous solutions. The proposed free radical mechanism of the destruction included N-centered radicals formation and their further fragmentation according to the general scheme (1):



$R_1 = \text{H, CH}_3$
 $R_2 = \text{H, Val-residue, Ala-residue, Leu-residue}$

(2)



(3)

For the realization of this type of fragmentation the presence of unsubstituted and non-protonated amine-groups in the biomolecules is necessary. On the contrary, the presence of protonated amine-groups (in the case of investigated compound acidic solutions), substituted amine-groups (in the case of N-acetylglucosamine) or the 3-aminopropanol moieties (in the case of homoserine) in compounds inhibited the process (1). We have proposed that serine, threonine, dipeptides, containing these amino acids residues in the N-terminal parts of the molecules, and glucosamine under radiolysis of their solutions transform per schemes (2) and (3) respectively:

It was found that reducing compounds such as cysteine can inhibit carbon skeleton destruction process (1) of studied vicinal amino alcohols and their derivatives in the irradiated aqueous solutions.

The results discussed above supposed to be taken into account during investigation of ROS-induced pathophysiological processes involving biomolecules with 2-aminoethanol moiety and finding the ways of these processes suppressing.

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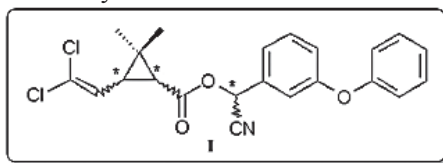
Insecticidal composition with improved characteristics on the basis of alpha-cypermethrin

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When grazing or staying on the farms the livestock undergoes to attacks of a large number of different parasites like mites, insects and others, which drastically reduce the productivity of animals and causes enormous scathe to the national economy. Various insecticidal preparations including the derivatives of alpha-cypermethrin (I) are used in order to combat with parasites [1–3]. Along with high efficiency, they have several disadvantages, in particular, they are insufficiently resistant to the effect of atmospheric condensation.



We have developed and investigated a novel alpha-cypermethrin based composition, which is resistant to atmospheric condensation. The composition is appropriated for the prophylaxis of animal parasites in agriculture and veterinary.

The effectiveness of the composition against insects and mites was confirmed by trials performed in the laboratory, pets and farm animals. For example, 500-fold dilution of the composition had 100 % efficiency against common scab, *Bovicola bovis* infestation and siphunculosis on cattle. Along with high target efficiency, the composition also shows wound-healing effect and resistance to atmospheric condensation.

Aprerequisite for widespread application of insecticides is the absence of their residues in food. For this reason we have developed a method for quantitative determination of residual alpha-cypermethrin in animal products. The method was based on gas

chromatography and mass spectrometry and provided the detection of alpha-cypermethrin in meat and milk in concentrations above 0.02 mg/kg with an accuracy of $\pm 5\%$.

Analysis of samples of meat, liver and kidneys of animals after single and double treatment with insecticidal composition developed have shown that alpha-cypermethrin was completely eliminated from the animal body after 10 days. Moreover, alpha-cypermethrin was not detected in the milk of treated cows.

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Tetrazolization of commercial Nitron D-5 polyacrylonitrile fibre

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The original properties of tetrazole derivatives caused by sufficiently high thermal stability of the heterocycle along with its considerable energetics, high nitrogen content, acid-base properties, biological activity and coordination ability predetermine a great interest to tetrazole-containing polymers as promising multi-purpose materials [1].

In the present study we have investigated commercial Nitron D-5 polyacrylonitrile fibre, copolymer of acrylonitrile, methyl acrylate and 2-acrylamido-2-methylpropane-sulfonic acid (produced by the Polymir plant, JSC Naftan) as a precursor in the tetrazolization process. Transformation of nitrile groups into tetrazol-5-yl moieties was found to proceed smoothly in dimethylformamide using $\text{NaN}_3 \cdot \text{NH}_4\text{Cl}$ as azidation system.

Reaction kinetics has been studied at 100 °C. The obtained kinetic curve presented in Figure indicated that the reaction proceeded relatively slowly. Conversion degree increased gradually and reached 80–85 % after 11–12 h. It could be adjusted by changing the amount of azidation agent used that allowed us to obtain polymers with the desired content of tetrazolyl groups.

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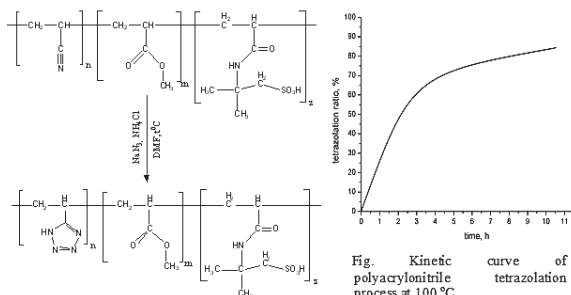


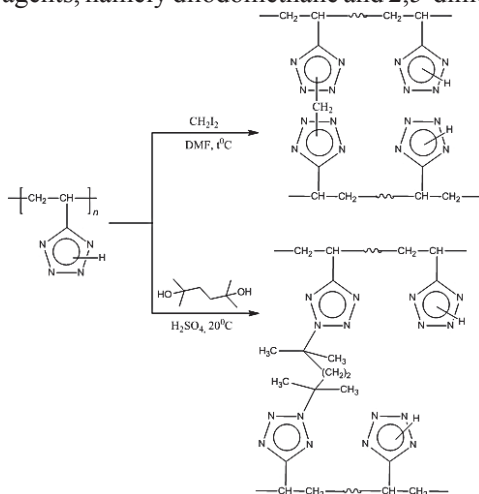
Fig. Kinetic curve of tetrazolization process at 100 °C

Preparation of cross-linked polymers by alkylation of poly-5-vinyltetrazole with bis-alkylating agents

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Cross-linked tetrazole containing polymers are studied poorly. Information about the methods for their preparation and properties are too limited [1, 2]. In order to prepare novel polymers from this series we have studied alkylation of poly-5-vinyltetrazole with bis-alkylating agents, namely diiodomethane and 2,5-dimethylhexane-2,5-diol.



It was found that use of the above alkylation agents allow to prepare cross-linked polymers. The degree of crosslinking can be regulated by changing of poly-5-vinyltetrazole – alkylating agent ratio. Increasing of the crosslinking degree leads to decreasing of solubility of polymers formed in organic solvents as well as in basic aqueous solutions. However, these products are capable of swelling under action of solvents. Cross-linked tetrazole containing polymers obtained are attractive as promising ion exchange materials and templates for the synthesis and stabilization of metal nanoparticles.

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CHEMISTRY TRAINING AND TEACHING IN HIGH SCHOOL

Means of organizing the system for independent work on chemistry at high school

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Independent work as basis of education at high school was and still remains the keystone of this problem. It is necessarily included into the students activity, but the degree of independence can be varied.

The student's coursework including scientific research elements is the most effective type of independent work. Pedagogic experiment on investigation of the worked-out didactic means [1; 2] effect on a general level of students' independent work has been carried out. Problems of content and sequence of the course work at studies "General and Inorganic Chemistry" by the students of engineering-ecologic specialization are considered in the work [1], as well as the required means of writing and criteria of its assessment.

Computer program "Assessment of Student's Coursework" for the assessment of the course work [2] is worked out. It realizes a unique algorithm for assessment, which takes into account the main items and peculiarities of writing a course-paper by the students of chemical-ecologic specialization. The main task of the worked out program is to unify the criteria for estimating the students' works, as well as to make teachers' work more effective and rational. Special function of the program makes it possible to perform a report on all the parameters for each coursework. So the student is able to analyze his work personally as if by teachers eyes and to make it more effective taking into consideration all the remarks.

The didactic means worked out for organizing the system of students' independent work provide an increase in the level of action and give not only algorithms for such activity but possibilities for more objective self-assessment and self-control. As a result of carried out investigation it was shown that independent work in this approach becomes more effective, and the function of control is transferred from the teacher to the student.

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The tasks of entrance examinations in chemistry (adaptation to new conditions)

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Today, in accordance with the Education Law of Russian Federation, the selection of entrants in Russian universities is conducted on the basis of the sum of Unified State Exam points. Thus, the MSU Chemistry Department applicants have to submit their points in mathematics, chemistry, physics, and Russian language. Only Moscow and St. Petersburg State Universities have the right to conduct one additional written entrance exam. For applicants of the Chemistry Department this is an exam in chemistry, so the additional test in mathematics is not provided. The quality of pretenders and first-year students of the University is reported to decrease every year, and direct correlation between their progresses in mathematical and in chemical disciplines is revealed. Thus, under condition of the absence of entrance examination in mathematics, the need to evaluate the real level of mathematical knowledge of applicants arose.

One of the ways to solve the above problem is to control mathematical component of chemical tasks offered at the Olympiads and the entrance exams. We have analyzed about 2000 published tasks of written entrance examination and Olympiad tasks in chemistry (since 1990 until now) in order to reveal the dynamics of saturation of the tasks with mathematical content. All tasks were divided into two groups: purely chemical problems without mathematical elements (represented mainly with so-called chains of chemical transformations and theoretical questions) and the tasks, which include mathematical component. The second group was classified according to the type of mathematical operations needed to solve the tasks. Analysis revealed that during the last 25 years the mathematical level of chemical tasks was significantly increased and the diversity of mathematical operations needed for solution had grown also. So, in the early 1990s, an examination card consisting of seven tasks usually included two tasks with mathematical content. But now, the number of such problems within the examination card increased to six out of ten.

We have found that except control function, mathematical content of the tasks of chemical Olympiads and entrance examinations performs another function. It prepares the school students to the fact that serious employment of chemical science often implies good mathematics knowledge; mathematics is useful and often necessary for solution of many chemical problems. Moreover, rapidly developing computer chemistry applies mathematical methods to modeling molecular structures or to simulation of the reactions, enabling us to investigate complex biochemical processes.

The revealed changes in chemistry exam tasks are a kind of adaptation of the applicant selection system to the modern educational reforms in our country. A constant monitoring of the level of mathematical train-

ing of our entrants is needed to create an adequate set of examination cards.

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Case technology in chemistry active learning by future teachers

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In recent years the case method takes a special place in vocational education among the modern technology and teaching methods.

According to the literature [1], the case method allows you to create professional skills, relevant expertise in the integration of elements of real professional activities in the learning process. In addition, the case method allows you to organize the transfer of educational knowledge in the field of professional activity.

The main purpose of case-method is organization of independent individual or group activities of students to develop their thinking skills in the course of solving the educational and professional tasks and exercises. For example, at studying general professional disciplines the case method provides the effective cooperation of students, promotes understanding of the problem situation and its resolution.

In general, in the case method the tasks are presented in a form of description of a specific practical situation. The situation has to be described sufficiently for understanding and explicit or implicit problems have to be quite clear.

Thus, the essence of this method is that the training material should be supplied to the students in the form of problems (cases), and the knowledge should be acquired as a result of an active creative work. In other words, the case method is a method of active learning.

The cases are presented in various forms such as several proposals for a single page or a large number of pages. However, case technology often presents difficulties in analysis of a problem situation. A certain standard of case studies presentation is absent in the current literature.

We have prepared and tested in the learning process the cases in analytical chemistry [2] and physical chemistry including the topics «Thermochemistry», «Thermodynamics of chemical equilibrium», «Phase Equilibria», «adsorption equilibrium» for students enrolled in the direction of Teacher Education (chemistry profile). A series of tests includes historical material.

For example, in one of the cases on thermodynamics a historical fact is presented with the description of the explosion while trying to break up a compacted mixture

of nitrate and ammonium sulphate [3]. It is offered to assess on the basis of thermodynamic calculations the extent of danger of decomposition of ammonium nitrate.

In another case the question on thermodynamics is raised about the possibility of potassium chlorate spontaneous decomposition. The effect of this salt purity on its sensitivity to friction and the combustion in the presence of sulfur and phosphorus is described, and a historical fact on application of this phenomenon into production of the matches is presented.

The case technology in chemistry studies can be considered as a complex integrated system of active learning.

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Computer technology energy education in the study of natural sciences

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The Russian Federal Law «On energy saving and energy efficiency improvements and on Amendments to Certain Legislative Acts of the Russian Federation» adopted by the State Duma on November 11, 2009 and approved by the Federation Council 18 November 2009 actualizes the need for advocacy for energy conservation in higher educational institutions, secondary and general education in the study of natural sciences [1].

Since the modern economy is based on the use of fossil energy reserves which are not renewed, energy plays a key role in the conservation of natural resources and the prevention of environmental disaster. In addition, the implementation of the project on energy efficiency in educational institutions will contribute to the formation of ecological culture among the younger generation.

Learning the basis of energy conservation in educational institutions is aimed at attracting students to conscious efforts to conserve biodiversity and conservation, environmental safety in the process of learning and in life. The goal requires solving the following tasks: analysis of modern energy-saving measures and identification of the most effective ones; development of the appropriate recommendations; carrying out the measures of effective energy saving in educational institutions and at home, analysis of their effectiveness.

The solving of the problems is seen by the inclusion of elective courses (elective courses for high school) in the curriculum. Moreover, according to the literature recommendations [2] it is necessary to include computer animation and virtual models of human events in science education. Sys-

tems and objects become a part of digital educational resources. Learning the basis of energy savings is possible in the process of studying the chemical disciplines on examples of computer models of the natural processes.

For example, in the course of physical chemistry at studying the topic «Thermodynamics of chemical processes» based on the first law of thermodynamics, you can demonstrate the importance of energy saving in terms of energy utilization using computer multimedia presentations. The animation helps to show how not to waste the energy in vain and to use the energy more efficiently. The examples are connected with the application of cost-effective energy-saving lamps, usage of industrial waste heat for home heating. It can be concluded that, transforming the energy into the desired form it is possible to solve the problem of its shortage in the future. Then, on the base of the thermodynamics second law it can be shown that this process is quite complicated due to energy losses. Otherwise, in the process of energy transformations the useful energy decreases due to its dispersion in the environment (energy quality is lost). The conclusion follows that the energy saving in accordance with the second law involves the use of bioenergy, chemical and thermal energy instead of electricity. Then it is advisable to introduce computer models to compare the quality of energies such as the use of electrical (lighting, heating and mechanical work) and thermal energy (for heating, and losses). In this case the computer models have to meet certain requirements: to reflect the familiar and popular natural science processes in the life-saving measures, ways of assessing the impact of their implementation.

In conclusion, we note that the energy education involving computer technology will improve the quality of learning and motivation, enhance interdisciplinary communication and build modern eco-directed scientific outlook on the basis of scientific knowledge.

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Interdisciplinary collaborations as a condition of the holistic natural scientific worldview formation while chemical education at the Technical University

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Chemistry plays a central role in formation of the natural scientific worldview. Unfortunately, at the Engineering and Technical Universities the General Chemistry is mere one of disciplines which the students begin to study and end their education in this subject for a very short time. Day by day all students are meeting with different materials consisting from chemical substances with concrete structures and with many types of chemical processes including different types of chemical reactions. So, for example, we can look at the process of the storage battery charging as the reaction where electrons are moved between two components of physical and chemical system. Though, this process is interesting not only from the viewpoint of experimental and theoretical chemistry, but from the viewpoint of other areas of knowledge. Integrity of the process of learning about

the world and the human knowledge about it, as well as the increasing amount of information on chemicals, materials and chemical processes necessitate the inclusion of an interdisciplinary approach to teaching Chemistry at Engineering and Technical Universities. This approach within the learning process can be achieved through the use of the intersubject communications involving Chemistry on one hand and other natural and/or engineering discipline on the other hand [1]. In our view, interdisciplinary collaborations should cover both the content of academic disciplines as well as the students' learning skills which are acquired by them during the course of their study at the University.

The interdisciplinary collaborations involving disciplines such as Chemistry and Material Science is discussed in this presentation. Different chemical substances and chemical reactions are the objects of studies in Chemistry. The objects of studies by Material Science include different materials and the chemical processes for their obtaining. The material is the chemical substance which has a specific structure and properties. At the same time the chemical processes for obtaining materials are the chemical reaction which occurs under specific conditions. So both these disciplines have a common object of the studies. Therefore interdisciplinary collaboration between them have to be revealed. The similarities between the objects of the study enables to obtain interdisciplinary thesaurus for training purposes, using generalized categories of sensory and rational levels of studying the objects of educational subjects. The interdisciplinary thesaurus for training can be used as a sort of «interdisciplinary data field» and it is the basis for integrating the content level of such disciplines as Chemistry and Materials Science.

The didactic principles of continuity, consistency and regularity were used for integrating the content of these disciplines. We isolated the list of particular algorithms of the students learning activities during the laboratory work on Chemistry and Material Science and the list of common training algorithms and used them for interdisciplinary collaboration at the procedural level.

So, this presentation illustrates a model of interdisciplinary collaborations involving disciplines of Chemistry and Materials Science at the content and procedural levels. The possibility of involving some of other academic disciplines into interdisciplinary collaboration is discussed. We believe that the implementation of an interdisciplinary approach in chemical education induces further knowledge of Chemistry, promotes an acquiring of higher aggregate skills, advantages the development of individual systematic thinking and creativity and develops students' abilities to quick adaptation in the modern world.

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Structuring of the content of future engineers chemical education based on content lines

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Structuring the syllabus of chemical courses for would-be engineers is an actual problem in methodology of high school education. There are some approaches for

design of chemical education content. One of them is using the “content lines”. For the first time these approaches they have been applied in the late 1970s in didactics of mathematics. Since the middle of 1980s the content lines began to be used in didactics of informatics (computer science). Now they are accepted as an element of standards in the secondary education in Belarus and Russia for various subjects. Last years content lines became more common in university education for different curricular units: from theory of architecture to machine-building. The definition of content lines is diffuse and is not conventional. At the beginning the content lines were presented as titles of syllabus clusters. Semakin (2002) defined a list of content lines as a first level of hierarchy of syllabus [1]. He alleged that the titles of content lines have to correspond with general concepts of a science. Content lines should pass through all syllabus. Mychko et al. (2002) in explanatory note to the Educational Standard for chemistry explained that content lines should set scientific level of material presentation [2]. They should form intellectual framework and syllabus matrix of chemistry in secondary school. According Mychko et al. every unit of syllabus has its own set of unique content lines.

In Brest State Technical University content lines were used by the author as an instrument of structuring the content of chemical education for would-be engineers. Content lines form the basis of syllabus. The following lines have been used:

- substance: composition, structure and properties,
- chemical process: energetic, rate and equilibrium,
- chemical methods of identification and quantification of substances.

These three lines form invariant part of syllabus for students of different specialties. They correspond to classical course of general chemistry. Next three additional lines were also proposed:

- chemistry and engineering as an area of future professional activity,
- chemistry and environment protection,
- chemistry and every-day life.

These three content lines form variable part of syllabus. They help to adjust the content of chemical education to needs of future profession of students. A fight against prejudice with the regard to chemical science is another important function of these lines. Clearly they help students to realize the significant role of chemistry in sustainable development and environment protection.

On our deep opinion content lines make education area more transparent for the students. They make general chemistry syllabus more holistic and understandable for all participants of the education process.

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Teaching of chemistry in high school using e-learning course

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The peculiarities of the development and usage of an electronic training course “inorganic chemistry” based on a distance learning platform Moodle are described. We have created an electronic course to study a discipline «Chemistry» for the first-year students of technological specialties. The educational material of this course is structured as follows: general information about the course; contents; final examination.

General information about the course includes the work program calendar plan, glossary and a list of printed and Internet resources. All material through the retention rate is divided by modules. The content of modules includes the following materials.

1. Theoretical training material.
2. Laboratory (practical seminars) work.
3. Tasks for independent work.
4. The modular control.

Theoretical training material includes the structured lectures, presentations and the test questions for the lectures.

The guidelines and a list of individual tasks are provided both for each laboratory work (a practical work, seminars) and self-study activity. The different options for submission of the results such as graphs, charts, comparative tables, presentations, etc. are provided for students' self-study work.

The students send the completed tasks to a teacher via online. The gained points are fixed in an electronic journal.

For module control the different types of the tests have been created, for example to determine compliance, to set a correct sequence with a single or multiple choice of a correct answer, open tasks, the case studies with a numerical answer, etc. Each module contains a self-control test, control questions and quizzes.

The final examination contains test questions and tasks to prepare the students for exams and a final test. The results of a final test are issued as certification statement.

The distinctive feature of e-learning course as compared with electron textbooks is a clearly structured educational and methodological material. The teachers and the students actively interact throughout all the study. There is also a possibility for a teacher to take control over all learning activities of the students.

This course in chemistry has to be tested during one semester module. Thereafter such a course needs to be certified and passed through three expertises: structural and functional, content-scientific and methodical.

Syllabus as the means of educational technologies in training agricultural engineers

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In teaching the fundamental sciences to agricultural engineers chemistry plays a particular important role in formation of the professional competency.

In order to be prepared for effective solving the changing professional tasks of different complexity an agricultural engineer should possess a set of special knowledge. At the Belarussian State Agrarian Technical University (BSATU) the necessary attention is paid to the timely development of syllabus for new courses that provides a high level of professional education. The course “Physical and Chemical Properties of Substances” was introduced in the syllabus of the future agricultural engineers as the logical extension of the basic chemical knowledge obtained by the students. The important means of exercising contemporary educational technologies is the course syllabus.

The structure of the developed “Physicochemical and Toxic Properties of Substances” syllabus complies with the concept of the course “Chemistry”, developed and introduced in the educational process by the Chair of Chemistry of BSATU [1]. The syllabus includes:

- training program [2];
- educational means (educational publications and academic manuals of different purposes);
- assessment means (tests of various difficulty for current, midterm and final assessment).

The course “Physicochemical and Toxic Properties of Substances” comprises the learning of basic properties of various organic and inorganic substances used in the agriculture. According to the study plan, the course “Physicochemical and Toxic Properties of Substances” is accounted for 72 academic hours: 36 class hours, 18 hours of lectures and 18 hours of laboratory operations comprised. The established program is divided into two teaching modules: “Physicochemical and toxic properties of the I–VII periodical group elements compounds” and “Physicochemical and toxic properties of organic compounds”. The necessary theoretical material, laboratory operations and individual assessment tasks were developed for each module. The tasks are designed with the provision of the knowledge and skills acquired during the course “Chemistry” and include the elements of the work with certain chemical compounds in account of their toxic properties. The skills acquired during the execution of laboratory operations allow the future agricultural engineers to expand their professional competencies. The education with the use of the developed syllabus will promote the effectiveness of the educational process. At the same time it meets the requirements of the innovative teaching technologies.

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The elective course “Nanotechnology”

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One of the significant trends in the modern natural science education is the increased interest to nanoproblematics. This tendency demands the development of corresponding learning programs and courses which deal with the rules and regularities, working in the low-dimensional systems. The elective course “Nanotechnology” elaborated by the specialists of the Inorganic Chemistry Chair at the BSU Chemical Department is an example of this tendency realization at the classic university. The peculiarities of this course are discussed in the report. This course program includes firstly the theoretical block, in which the problem field of nanotechnology is determined and nanoobjects and their special properties are discussed as well as the methods of the nanoparticles and nanostructures formation and investigation.

The large practical block introduces the students to such important methods of nanostructures study as electron microscopy, electronography and X-ray analysis. The material of the course has been selected on the base of the succession and teaching-and-research principles.

Case-method in the study of the course “General Chemistry”

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The problem of the introduction of case-study in the practice of higher education at the present time is very urgent, due to the next two trends:
—oriented education in the formation of professional competence, capacity to learn, shift of thinking paradigm and the ability to process massive amounts of information;
—requirements to the quality of specialist, which should also have the ability to optimal behavior in different situations including systematic and effective action in a crisis.

At the implementation of case method in the study of “General chemistry” by the first-year students at the Voronezh State University Chemistry Department we carried out a preliminary survey, which revealed the degree of readiness of the students to work. The results showed that students were not trained in the format of case-study. Only certain students possessed the ability to create presentations and use them as a method of presenting information and writing reports in the learning process.

The work with the cases “Atomic structure. Periodic Law” and “Chemical bond”, analysis and discussion of the results in small groups, their representation in the form of presentations in front of the whole team allowed us to conclude about the effectiveness of case-study for teaching of junior students. Using

a case-study in the learning process contributed to the formation of the ability to search for information and analyze it, developed the skills of oral communication and reasoning of the students' position, the work in a team, the ability to construct models of problem solving. Application of case-study technologies motivated students to study chemistry, enhanced cognitive and creative activity.

Studying chemistry at the museums in the content of lifelong learning

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One of the main functions of the museums is the educational function. The basic principles of studying chemistry at the museums are: continuity of chemical education at all its steps, namely kindergarten, high school, higher education institution, self-education for adults and succession upon transition from one step to another. Among other important principles of teaching of chemistry in the context of lifelong learning at the museums it should be noted the following: integration of natural science and humanities in the content of classes; developing teaching, including the upbringing of early subject interest in chemistry; activity approach.

The analysis of the Moscow Polytechnic Museum activities in the sphere of its educational function as one of the main museum functions is presented in the report. Materialization of the principles of lifelong chemical education in museums is shown on the examples of its continuity at all stages, integration of chemistry with other natural sciences and humanities in the content of the classes, developmental teaching, the development of early subject interest, activity approach. The work of the chemical laboratory of the Polytechnic Museum on supporting all stages in continual chemical education that are familiarizing preschool children with natural sciences, school students and professionals training, promoting science for adults is demonstrated.

The audience studying chemistry at the museums is divided into the following age groups: pre-school children (3–6 years), younger school students (7–10 years), younger (11–13 years) and senior (14–17 years) teenagers, students and adults (who are a part of family groups). Studying chemistry at the museums for different age group has its specific features, namely the purposes and the content of education adequate to them and education, the corresponding forms of the organization of these processes, their results and methods of assessment. All these first of all depend on physiological and psychological characteristics of each age.

At pre-school age specially organized teaching in natural sciences helps to order the impressions obtained by the child from the world around. Teaching is also of great importance in training children for school, in formation of bases for educational activity.

The purposes of informal chemical education of younger school children are to provide supplementary materials and activities for the course «World around us», first of all, through carrying out corresponding chemical experiment; to de-

velop this course through pupils' practical activities with small impregnations of theory, as a rule, at the beginning of classes as an introduction to a subject.

At younger teenage natural science classes help to fill a gap between the courses «World around us» at elementary school and the systematic course of chemistry which begins only in the 8th class of high school. The purposes of museum chemical education for senior teenagers are the same as for younger school children, but they concern a course of chemistry of the 8-11th classes.

Students have a wide range of purposes to attend museum classes in chemistry, from satisfaction of their own curiosity to professional interests. For family audience the main goal of such classes is the possibility of the joint education for different generations with differentiation of the program material according to interests and age resources of the participants.

In accordance with the age there is a reduction of game activities, an increase in duration of classes (from 30 minutes for pre-school children to 1 h 30 min for the senior teenagers and all older), mainly due to the expansion of a theoretical component of classes.

In the long-term study of the problem it is necessary to build a system of the origins and the development of chemical knowledge for the chosen age groups.

**Formation of chemical education succession in the vertical
“stage I – stage II – higher education institute”
through the scientific research activities of the learners**

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One of possible stages in formation of the succession in the system of chemical education appears to be organization of practical scientific research activity of the learners at school. This activity can be conventionally divided into two following steps:

- training activity in the field of the techniques and methods that correspond to the research activity carried out in primary and secondary school;
- direct experimental researches that can be proceeded on the base of universities and research institutes (carried out in high school).

All this permits the learners of the senior school to develop their intellectual abilities, helps them to choose the institute of higher education in the 8–10 form already and to do this choice consciously.

The joint work of the school and the institute of higher education resolves the problem of psychological adaptation to new conditions and to peculiarities of education, to unaccustomed teaching methodology. Organization of practical scientific research work in chemistry at school can help to form the continuity in the system of chemical education.

The choice of the topic of the investigation and the problem statement appears to be the most difficult issues in the realization of the scientific research work.

On this stage the leading role belongs to the teacher or to the scientific adviser. Moreover in case of the research work in the field of chemistry it is important to choose where and how the experiment would be carried out, because the laboratory equipment at school is not always quite enough to conduct necessary experiments. The outgo of this situation consists in the collaboration with the institutes of higher education and scientific research institutes of our republic.

Gymnasium is always ready to communicate, and, from the other hand, each institution of higher education is interested in the involvement into the education not only of capable students, but also of talented pupils on purpose to engage and to prepare the best matriculants. In order to help the learners to sort out their propensities and abilities, to decrease the quantity of the mistakes that learners and their parents commit while choosing their future profession eliminating the individuality, we enable the children to realize their scientific abilities and inclinations. In this case learners can get into the real chemical laboratories not only as the excursionist or the participant of the Open Information Weekend, but to try themselves in science by their own actions and reasoning, and, therefore, to correlate themselves with the chosen profession.

The problem of forming multipurpose training activity in context of methodical training of future chemistry teachers

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The evolution of pupils' personalities is considered to be one of the most important aims of the modern educational system. Observing the results of pupils' teaching one can distinguish types like: personal, subjective and universal ones. Universal results are connected with producing cognitive, directive and communicative multipurpose training activity (MTA). Thus each subject contributes to organization of MTA. Nevertheless regarding the formation of MTA only in pantopedagogical case is uncorrectable, because the forms, methods and ways of organizing educational activity are determined by the specificity of each school subject and particularly of Chemistry. Thereby, present-day chemistry teacher should organize educational process in a specific way in order to form holistic notion of the most important terms, principles, theories and methods of Chemical science, at the same time including the organization of MTA into the educational process. For this aim implementation it is necessary to improve the system of specialized training of future chemistry teacher. This system should satisfy all the demands of modern school and should be even outrunning. It is important to teach future chemistry teachers to be able to form MTA knowledge while teaching their pupils. It is necessary to point out the importance of using chemical situational exercises [1]. Our research brought out clearly the necessity to create conditions for using situational exercises during the Chemistry lessons, elective courses, because it promotes the MTA formation.

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Educational mobile service Socrative in the knowledge control of the chemistry department students

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The results of the application of the mobile testing software Socrative for the students of chemical specialties on the example of «Organization of production and management in pharmacy» course are presented. Socrative service is one of the most convenient objectification of the trend of modern mobile technologies application in the higher education system. Service looks like a website and mobile application implemented for iOS and Android platforms. Socrative is an effective tool for the work with the learning content in a personal account on all devices (computer, tablet, mobile phone), does not require special equipment. It is free of charge and available to students and teachers. It has been shown that the service provides not only an express control of students' knowledge, but helps the students to learn the material better, to develop arguing and exchange of opinions skills, thereby improving their current performance. The use of the program helps to achieve several objectives such as the students' knowledge assessment in a real time, the motivation of students and the ensuring of interactive learning.

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Using the case method for forming information competence of students in teaching chemistry at school

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With the introduction in 2008 of the new Federal State Educational standards based on competence approach, the requirements for the educational process have been changed. The article discusses several classifications of competences, information competence and features of its formation in studying Chemistry in particular. The ability of students to independent acquisition of knowledge, to continuing education and self-education, readiness for handling information on paper and electronic-based is interpreted as an information competence. We believe that this competence is one of the most important as it provides the student's ability to deal with information contained in any school subject and also in the surrounding world as well. For the creation and development of information competence, we suggest using the case method. A case is a set of described situation and additional information submitted in the form of text, graphs, videos, etc.

Active learning methods are widely used for teaching Chemistry at school in Russia. In recent years, the case method has been introduced along with other innovations. The method promotes the developing information competence of students, particularly the ability to perceive and evaluate information that comes in verbal and nonverbal forms both in paper and electronic media. The importance of the case method is in mastering various social roles of students in a group, forming skills to formulate and express their positions, to communicate, to discuss a problem. The advantage of cases compared with the typical problems deals with the existence of multiple solutions and alternative routes leading to them. Our research involves developing a series of Chemistry cases that foster and develop students' information competence. Relying on the experience of Russian scientists, we have developed an algorithm permitting teachers to create a case on the basis of a real problem or situation related to the Chemistry subject. Several examples of using the algorithm for compiling the case «Heavy metals and their influence on humans» for studying the topic «Metals» in high school are presented in the report.

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Relevancy analysis in the search for chemical information as a part of the competency-based learning in teaching chemistry students

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In the beginning of the XXI century, the need for moving away from a «knowledge» paradigm became actual in education. The awareness of the need per se does not mean the solution of the problem. The possible option exists to implement the competency-based learning, that is actively advocated and developed in our country and abroad.

One of the principles of organization of the educational process in this case [1] is to create conditions in gaining the experience in self-regulation of solving cognitive, communicative, organizational, moral and other problems that constitute the content of education.

In fact, it means the shift to self-regulation of learning and learning to learn. In the «Recommendation on Key Competences for Lifelong Learning», which was adopted by the European Parliament and the Council of Europe in 2006, self-regulation and learning to learn is indicated as one of the eight key competences.

The latest issue (№ 5, 2014) of the European Educational Research Journal is devoted entirely to the research on self-education and self-study and their perspective in the European education. In this case, one of the most important elements in the practical implementation of this approach is applying information and communication technologies (ICTs).

In literature, there is an obvious excess of publications concerning basic research on this subject and a distinct lack of applied studies that are so necessary for the real work. It should be noted that particular implementations of the competence approach contain more peculiarities than common features.

In 2011, we embedded the ideas of the competence approach in the Information Retrieval round of intellectual competitions for chemistry students at the Belarusian State University [2–4]. The tasks of the round require flexible planning of the strategy of the online search and subsequent thorough analysis of the relevancy and reliability of the retrieved documents.

In this report we examine the practice of combining educational and research goals of students activities in the course of the Olympiads. Examples of tasks and analysis of students solutions are presented. The feasibility of a wider implementation of the competency-based approach within the educational process is discussed.

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Dialog learning chemistry on the basis of the gender approach

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Gender approach presents an objective generic feature of political culture, characterized by active representative democracy, the essence of which is taking into account the interests of both socio-sex groups in society. The main point of this approach is to find special measures to achieve gender equality. Phenomena that occur in the society, have different effects on the male and female population, causing different reactions. Awareness of this is the aim of gender approach.

Gender access is intensively implemented in education. This happens in two ways. One of them is realized in a higher educational institution, and the second one is carried out in secondary schools, lyceums, gymnasiums, institutions of primary and secondary professional education. Dialog training is often used in intensive learning. In order to learn and be able to apply such

methods into practice, it is necessary to know various methods of group interaction on the basis of gender conception. These methods cannot replace conventional lectures, but they help to understand better the new material, the gender approach helps to build a relationship in a team, ability to compromise.

At the lesson the teacher does not provide ready-made knowledge, but offers the trainees the algorithms of action for each group. As compared with the traditional form and method of performing exercises, at the dialog-based learning gender approach the teacher is interchanging roles with the trainees. The activity passes to the learner and the task of the teacher becomes to create conditions for its implementation.

The experience of gender approach gives evidence that by organizing educational interaction regardless of the sex differences of students, teachers condemn their pupils to a one-sided development that happens on the reason of the lack of knowledge about the physiological capabilities of children. The absence of gender consideration in education can infringe the legal values of personalities equality and lead to gender discrimination. On the contrary, gender approach promotes better realization of personal inclinations and abilities.

When organizing the group work, it is necessary to pay attention to the following aspects of gender approach. It is useful to ensure that students have the knowledge and skills to perform the group task. The lack of knowledge very soon will cause the absence of the students' efforts to do the job. It is important to make all instructions as clear as possible. It is forbidden to accept more than two tasks simultaneously. That is why the instructions have to be written on the board and (or) cards. It is necessary to provide the team with enough time to complete the task.

Problems of fundamental chemical education

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The mission of university is preparation of experts who, on the one hand, are able to see the basic directions of a science development and independently choose the most prospective areas of realization of knowledge and feel aspiration for research work, and on the other hand, are capable of qualitative and creative implementation of concrete everyday scientific work. The paper represents the results of the analysis of current state of university chemical education in Russia on the example of MSU Chemistry Department.

Today one of the main problems is the permanent decrease in the quality of knowledge of school-leavers which leads to a decrease in the quality of the university applicants. Also it should be noted that the decrease in interest in science and technical professions causes the significant reduction of competition on the corresponding specialties in university. As a result, we observe the lack

of preparedness of students enrolled for the first year. However, educational process at the university takes place so rapidly that the student does not have time for elimination of gaps in school knowledge. We have no time for complementary “adaptive” courses in core subjects of high school, namely in mathematics, chemistry and physics. Similar problems with school background are characteristic for junior-course students of other MSU natural-science departments [1].

Every year we analyze the “geography” of pretenders and first-year students. Here are the two trends. For a quarter of century, despite changes in the forms and methods of attracting students to higher education, geography of students from Russia enrolled in the first year is not varied and remains quite wide. But the share of foreign students decreased from above 10 % at the turn of the century to 2 % in 2014. The main trajectory of admission of foreign applicants to Chemistry Department was and remains the International Mendeleev Chemistry Olympiad. At the beginning of the century annually about 15 Mendeleev Olympiad winners were enrolled to the Chemistry Department without exams, and these students were the leaders [2]. We can conclude that MSU is becoming less attractive for foreign students.

For a quarter of century the entrance examinations on chemistry at the MSU are conducted in written form, and all the problems and their solutions together with MSU Olympiad tasks are systematically published. Annually we analyze the quality and complexity of tasks on entrance examinations in chemistry. This helps to specify the sections of the program, most difficult for applicants.

The ways to solve the problems in the university chemistry education are indicated. First of all, it is the development of close interaction between high school institutions and university, organization of various chemistry Olympiads for high school pupils and pretenders, helping to attract young people to chemistry and to university. After that, it is the preparation of qualitative textbooks for school pupils and pretenders. We underline the necessity to publish and maximum wide spread the tasks of exams and Olympiads in order to illustrate the level of knowledge required at the university.

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Using the case-based technology as means of implementing problem-based teaching chemistry

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The need for changes in education is dictated by the life realities today connected with the fact that our civilization is becoming more and more informa-

tional. The role of high school teachers lays in changing modern pedagogical paradigm. Pedagogical culture of the modern teacher assumes a high level of development of all components of pedagogical activity that are axiological, technological, personal and creative. When using explanatory and illustrative techniques the possibility of active perception of educational material is negligible.

Therefore, the methods of active interaction of the teacher and the learners in the process of formation of the required level of activity acquire more and more importance in the training of students and SDF students. These methods involve the acquisition of experience of independent activity on the basis of universal knowledge and are characterized by the formation of skills, which are a holistic unity of the most important knowledge, and the ways of activities in the field of chemistry, which become updated and enriched during the participation of students in the real, vital situations.

To form the competences it is necessary to create the tools and procedures of organization, conducting and evaluation of activities of students. An example of the formation of subject competences technology could be the case-technology, which takes its name from the Latin 'casus' ('confused') or English «case» – 'situation'.

Let us consider the following scenario, which can be used to study the topic «The chemical properties of sulfuric acid.» The background information raises the question or riddle and describes the real situation. «At a railway station a master told two workers to clean up an empty rail tank, which transported concentrated sulfuric acid, in order to use it for another traffic. The workers washed the walls of the tank with water from hoses and sat on the edge of the neck, sparked off a cigarettes. There was an explosion, the workers were injured.»

In the analysis of the offered test, students should go the way of the formation of competencies. The stages of the work and their content are the following.

- Search for sources of information. Information «support»: chemical properties of concentrated and dilute sulfuric acid, solutions, substances to dissolve in water, thermal conditions at dissolution, the chemical properties of hydrogen.
- Extraction and primary processing of information: reading the text, finding the characteristics of the substances.
- Processing the next information and making a decision on its base: opposed properties of concentrated sulfuric acid from that of dilute, dilute acid ability to interact with metals, etc.
- Presentation: developing information and logic scheme and explanation of the situation.

Making a report on the implementation of tasks in order to help in the formation of values and meanings, educational and informative, general cultural competence. The report can be presented in the form of a story, composition, report, essay, etc. If the work on the topic is organized in groups, it will contribute to a greater degree of communicative competence formation.

Methodology of additional education in the natural science disciplines for the freshmen at the Peoples' Friendship University of Russia

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Chemistry and physics are among the most difficult basic disciplines which are studied by the first-year students of different learning fields at the Peoples' Friendship University. This is evidenced by the large number of unsatisfactory graded final examinations and lowest average scores (compared to other disciplines). In our opinion, the most important reasons are the low level of training in chemistry and physics in most secondary schools and not enough hours in the school curriculum needed to follow such complex disciplines. It should be noted that graduates of schools show very low level of awareness of the disciplines that underlie the basic training of engineers, doctors or ecologists. That is why the "Chemistry" discipline in the curriculum at the university is a surprise for the students of engineering courses and "Physics" is unexpected for the students of medical profile. Most of them do not have enough basic knowledge on these subjects.

In order to solve this problem and improve the ranking of students at the faculty of physical, mathematical and natural sciences at the Peoples' Friendship University, where basic courses in chemistry and physics for secondary specialties are taught, a special two-stage additional education process is organized. At the initial stage of the first-year students teaching the so-called «adaptation» course within 16–20 hours (depending on the basic speciality and level) is offered. Groups are formed on a voluntary basis of first grade full-time students who pass the required initial testing to identify their level. The program offered in this course is a transition one from school to university and it includes the basic laws and concepts of chosen disciplines. In addition, it contributes to the formation of skills of application of physical and chemical concepts, laws, and formulas to address simple examples and problems. The control of the acquired knowledge is made through regular testing with increasing complexity. According to the results of two years of work, we can conclude that the majority of freshmen, that studied the «adaptation» course, successfully mastered the material of the basic course.

One additional course was offered for re-learning the particular discipline to the students who have not mastered adequately the base of the discipline and failed on the final examination. It was larger than "adaptation" course (28–36 h), as the students were generally less motivated to learn and objectively more poorly prepared. These courses were fully consistent with the main basic program of the University, but by teaching in small groups of 7–9 students we became able to focus attention on the most important and difficult in understanding parts of chemistry and physics, as well as to pay more attention to the lagging students.

Although such a two-stage system of additional courses in chemistry and phys-

ics to some extent is a compulsory measure, however, it helps to fill in the gaps of school education and allows the majority of freshmen to pursue their education goals.

Physical quantities, terminology and symbols in chemistry

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As D. I. Mendeleev rightly observed, science begins when one starts to measure, and exact science is inconceivable without measures. Scientific terms and physical quantities are the precise instruments by which the scientific community shares the results of researches. The consequence is the importance of a coherent applying of physical quantities within research and educational groups and in the scientific community as a whole. A particular issue is the problem of continuity in the familiarization with the terminology and physical quantities at different levels of education (school, university).

The approaches to the interpretation of physical quantities in the section «Stoichiometry» of school and university textbooks according to the latest recommendations of the International Union of Pure and Applied Chemistry (IUPAC) [1] are discussed in the report. The main issue is the concept of the chemical amount of substance. For a correct understanding of the concept at the initial stages of studying chemistry it is recommended to use the formula: $n_B = \frac{m_B}{M_B}$, where the symbol B denotes a structural unit of the substance, n_B – chemical amount of the substance in its predetermined portion, m_B – mass of the substance, M_B – molar mass of the substance, N_B – number of atoms, molecules, formula units in this portion, N_A – Avogadro constant. According to the IUPAC recommendations it is essential to specify the entity (atom, molecule, formula unit) of the given substance while using the physical quantity «chemical amount».

Methods of specifying the quantitative composition of the solution (mass, number, amount, surface concentrations; mass, volume, amount fractions) are discussed.

The report examines the most common misconceptions regarding the applicability of concepts and physical quantities in chemistry. For example, «molality of a substance» in a solution is not a concentration, although one can find such statement in textbooks. According to the latest recommendations, the term «concentration» by default may replace the previous term «molar concentration». It is not recommended to use the term «molar concentration of the equivalent of the substance». Moreover, since 1989, a number of leading scientific journals (Journal of Analytical Chemistry, Analytical Chemistry) do not accept papers with the last mentioned term.

The report provides the structure of the course «Physical quantities in chemistry, chemical terminology and symbols» for students of the pedagogical branch of the Faculty of Chemistry of the Belarusian State University. The experience of seminars and workshops is discussed/

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Prospects for creating integrated system of continuous entrants training for centralized testing in chemistry

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At present, the understanding of the value of continuing education trend reorientation in the educational process demands an application of knowledge aided by technological innovation processes and pedagogical character. The aim of the study was to ensure continuity of chemical education through the creation of an integrated system of continuous three-stage training; comparison of the results of students learning activities in training as a part of the experiment, with the results of other groups of students. Over fifteen years of work in the pre-university education, we have seen insufficient subject and psychological training at school and came to a natural conclusion about the necessity of its development through changes in both organizational and substantial plan. The researches in the field of higher education problem on the theme "Studies of the effect of innovative educational technologies on the quality of the educational process at the Medical University» carried out at the Department of Chemistry, Faculty of pre-university training and vocational guidance are directed to create an integrated system of continuous three-stage training of the faculty students to the centralized testing in chemistry and learning in higher education. A study of the possibility to organize an integrated three-stage training system for students of the evening chemistry preparatory courses (grades 9–11) is carried out in close cooperation with other departments of the university such as the Department of toxicological and analytical chemistry, information technology course digital library, as well as departments of distance learning and educational work. In the experiment on training complex development, the most satisfying students, which entered the university and learned in it, obtain the task to evaluate the performance of the created system. The experimental results have led us to the feasibility of combining classical forms of classroom work and modern information, communication and educational technologies in the following forms:

- preparation of the reports on the studied subjects with multimedia support;
- lectures and practical classes with multimedia support;
- computer testing system of distance learning platform Moodle and organizations of independent work based on it;
- search activity of students and remote consulting services through the Internet;
- laboratory studies at the Department of Toxicology and Analytical Chemistry.

The effectiveness of such an organization of continuous training of schoolchildren for centralized testing in chemistry within the three-stage integrated system is confirmed by a comparative analysis of the results of tests carried out at the beginning of the school year and its duration. We fulfilled a complex of tasks that were aimed to correct the students' knowledge, to teach them to perform model calculations provided by the program, to lay the foundation for further training for centralized testing by forming training abilities and skills, to create a welcoming atmosphere of open educational process. Thus, a solid foundation was created for effective functioning of the entire integrated system of three-stage training, orienting students to increase the level of demands to themselves, to form a conscious motivation and to lay a solid foundation upcoming academic success in high school. It is focused on further practical training of specialists with a holistic natural-science outlook, systematic thinking formed by a set of universal, subject and professional competencies.

Innovative training manual with electronic application for theoretical foundations of organic chemistry

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The modern period of development of information technology offers great opportunities for a radical revision of the basic principles and methods of historical patterns of classical secondary and higher education. At present, the continuous memorization of extremely large amount of knowledge in continuously expanding flow of new scientific and technical facts becomes almost impossible. Formation of specialists who are ready to learn new scientific developments and technological processes requires the use of new educational technologies, combining traditional forms of learning and different methods of computerization of educational process.

The aim of this work was to create innovative training manual "Theoretical Foundations of Organic Chemistry. Training Manual with Electronic Application for Independent Work and Knowledge Control".

In accordance with this task the general concept has been formulated and the structure of three thematic modules corresponding by their content to the material of Organic Chemistry theoretical sections has been worked out. These modules were "Classification, Nomenclature and Structural Isomerism of Acyclic Organic Compounds"; "Chemical Bond. Stereoisomerism"; "Chemical Reaction. Theory of Acids and Bases".

The extensive electronic database of jobs (575 options) was offered. Three modes of academic work organization were used including training, teaching, and monitoring. To enable the independent individual work of students the blocks of tests for each module were supplemented with thematic text comments on the theory and practice of tasks solving. In accordance with the standard and working

training programs banks of test items covered all teaching material in this section and were used as a tool for monitoring students' knowledge. All tasks were adapted to both final ten-point system of assessing students and rating system of knowledge assessment adopted by the Department of Organic Chemistry of BSTU. Original in its structure and conceptual filling, this textbook is the first in our country.

On the bases of this manual new educational technology "New format of organizing practical training on "Theoretical Foundations of Organic Chemistry" for students of chemical and technological specialties of BSTU has been introduced into the educational process.

This new structural form of practical classes helps to combine traditional (classroom) and innovative forms of discipline studying modes "student-teacher" and "student-to-computer" successfully, allowing it to personalize the learning process and to organize systematic control of the current assessment of students learning with a client-server software.

Using of electronic learning resource in the education process at the chair of High Molecular Compounds of the Belarusian State University

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Further introduction of electronic learning resources is one of the foreground directions of the development of educational process at the chair of High Molecular Compounds at the BSU Chemical Faculty.

After the publication of schoolbook «High Molecular Compounds» by M. V. Shishonok in 2012 year [1], electronic version of this book was placed in electronic library systems and now it is of wide use in learning of the same named discipline. Standard, basic and working educational programs of disciplines and elective courses of the chair, which had been worked out by the lecturers of the department, were placed on the BSU Web site.

Multimedia presentations, including animations and videos are predominantly used at the lectures. Electronic format of illustrations gains time and helps to increase a volume of studying material. As result of visualization students perceive a material better. Computer testing for intermediate monitoring of knowledge is also realized. Control of student's individual work is carried out in a form of the reports of abstracts made with the help of electronic presentations also. Students find information themselves in Internet network and systematize it. This form of the work promotes them to obtain the original knowledge and motivates to research work.

Attraction of computer technologies makes it possible to carry out virtual laboratory works, which cannot be practically realized by the reason of toxicity and explosiveness of initial compounds. Opera-

tion of the equipment for molding polymers is shown in dynamic mode.

The application of electronic learning resources has some disadvantages. The accessibility of information obtaining does not motivate students for its memorization. More intensive control of knowledge is realized, when tasks are given in the open mode, but not in the form of computer testing. Virtual laboratory work is not able to substitute a value of practical experience, which is acquired as a result of real laboratory work realization. On the base of self-experience it was realized, that electronic learning resources should be used in combination with traditional educational technologies.

The retrieval of available resources in the Internet network has shown [2] that principally chemical educational software products are available for secondary schools. Software products for higher school can be found for inorganic, organic, analytical and physical chemistry. There is a little amount of Internet resources for macromolecular chemistry and their level is low. Therefore, the formation of multimedia data base for using in educational process is one of the foreground directions of the research work for lecturers, working in the field of macromolecular compounds.

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The effectiveness of the development process focused on future specialist secure professional activity

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The main component of a professional orientation is the motive that represents a set of external and internal conditions causing the activity of the individual and determining its orientation. The researchers note that motives can be variously organized, be in different relations of subordination, strengthen or weaken each other, engage in mutual contradiction and conflict with existing capabilities towards achieving the objectives [1]. So the purpose of professional activities can be the achievement of high professional results, professional efficiency. This goal attainment can be accompanied by professional risks, the admissibility of which is not always adequately assessed by a specialist. Moreover, in the course of professional activity the contractor often does not reflect, analyze and simulate situations that could be dangerous [2].

At the stage of high school training, in particular in the framework of disciplines such as «Life Safety», «Ecology», «Chemistry», «Physical Chemistry» it is necessary to focus the students on a clear understanding the needs and motives of secure professional activity, values corresponding to the beliefs and attitudes.

At studies these disciplines the emphasis has to be done on the knowledge of the rules, standards and regulations on health and safety together with the safety measures when performing laboratory works. In connection with this, a problem of orientation of students, in particular of chemical and metallurgical specialties, to secure professional activity becomes especially actual for the modern theory and practice of higher education. It requires pedagogical organization of the search for efficient measures of professional orientation of students throughout the entire period of training and practice in high school and in the future professional activity.

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Forms of submission of help data and their use in educational process

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Considerable amount of literature has been dedicated to upsetting of equations of oxidation-reduction reactions (redox reactions), as it is one of the bases in the academic courses of many university disciplines.

This work discusses the possibility of completing a number of subtasks that are necessary in figuring redox reaction equations which are the following: a) to choose an oxidizing agent and a reducing agent; b) to characterize them as strong, weak, etc.; c) to prove the possibility of the reaction between them; d) to single out the products of the reaction with the help of physical quantities represented in various forms of data: Pourbaix diagram, Tables of oxidation-reduction potential, Latimer's diagrams and Frost's diagrams.

We completed the comparative analysis of all the ad-hoc forms, and showed the options and the confinements of every form of data presentation.

The tables of standard electrode potentials contain partial reactions and values of the standard electrode potential in the media with pH 0. However, the electrode potential of a partial reaction depends on the acidity of the media. That is why we cannot use values of potential from the table in completing the equations of reactions proceeding in the acid or basic media. Latimer's diagrams present electrode potential figures for the definite media; that allows it to complete the equation of a redox reaction and substantiate its possibility in the given media. Diagrams of oxidation state (Frost's diagrams) represent the graphic picture of the dependency of the electrode potential and the number of the transposed electrons, which is also known as V- equivalent, on the oxidation state of the atoms of an element.

For completing redox equations, the use of Frost's diagrams enables to

solve one of the crucial tasks, which consists in selection of the most stable compound for the given media. This answer cannot be obtained from the data on electrode potentials. As every form has certain drawbacks, the first group of tasks is the development of the needed forms on the basis of other forms.

The second group of tasks is aimed at the use of reference books for completing equations of redox processes with different feed data from the tasks with a complete set of agents to the tasks with arbitrary choice of both agents and media.

Modern methods of teaching chemistry and its development prospects

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Modern methods of teaching chemistry present themselves the independent pedagogical science which has its own specific objects, the methodology of their studying, results and methods of their measurement. The subject of methods of teaching chemistry is the theory and practice of teaching chemistry, as well as pupils education and development while learning chemistry.

Having its own research subject and specific methods of a research the status of methods of teaching chemistry can be accentuated as an independent pedagogical science. Like any pedagogical science the methods of teaching chemistry belong to humanitarian and applied science.

Methods of teaching chemistry belong to an integrative science formed as a result of the synthesis of four systems that are didactics, theory of education, psychology (the objects of their study are, respectively, educational, educative and developmental functions of the learning) and chemistry. On the one hand these four systems are independent ones, on the other hand they are a part of the methods of teaching chemistry as structural elements of its contents.

The most important problems of modern methods of teaching chemistry relate with computerization, profilization and practical orientation of the chemical education at secondary and high school. As a result, the branches of methods of teaching chemistry widely developed today are associated with the development of:

- theory of continuous chemical education on the basis of continuity of teaching chemistry at secondary and high school;
- programs and schoolbooks in chemistry for all levels of the educational process at secondary and high school;
- scientific and methodological support of profiling chemistry teaching at the institutions of secondary education;
- use of information and communication technologies in teaching chemistry and teacher training for this work;
- electronic educational resources in chemistry and methods for their use;
- test measuring materials in chemistry.

Chemical applications for mobile devices using Android platform and prospects for their use in teaching chemistry

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Today there is a sharp decline in interest to learn chemistry among pupils and students. It should be noted that visiting libraries, reading popular science magazines, encyclopedia and reference books have been also reduced unfortunately. It rarely happens to see a book in the hands of the modern youth. At the same time, all pupils and students are actively using their mobile devices. The Internet has become accessible to everyone.

The majority of modern smartphones and tablets work on the basis of the operating system Android. However, a relatively small number of Russian-language applications using this platform have been developed yet for the chemical industry. Among them we can mention only the program «Chemistry» (author Denis Chaschin), which can be useful to search for products of chemical reactions and interactive periodic Table «Periodic Table» (JQ Soft), which can be used as a reference.

Another problem that has its impact on reducing the level of chemical education is the expansion of «reshebnik» and websites for homework. The solution to this problem should be the use of «cloud technologies» in the organization of knowledge control, including the preparation of homework. For example, it could be the computer testing system Moodle, or individual tasks using file sharing or cloud data stores, such as Dropbox.

A large number of educational content is available on the social network «Vkontakte», which is particularly popular today among young people. In this social network, they can find groups specialized in chemistry. For example, the group «Chemistry» (<http://vk.com/onlychemistry>) contains more than 37,000 subscribers and about 1,500 participants visit this page every day. In this community, we are also the editors. In the group a large number of publications on all chemical disciplines of different levels are permanently published beginning from the entertaining chemistry for pupils to special questions of fundamental chemistry. It is possible to search quickly for topics of interest. When searching for a key in front of the tag you should put a symbol #. Also there are some useful groups of «Vkontakte» that present «Impossible chemistry» (http://vk.com/impossible_chemistry), «The great science of chemistry» (http://vk.com/velikaya_nauka_himiya) and others. A lot of chemical literature and educational videos can be downloaded. They could be recommended for use in independent students' work.

Thus, the use of chemical applications for mobile devices opens a wide problematic field for teachers, professors and chemistry trainers.

Realization of succession and professional orientation of chemistry course in the system of continuing education school – college – university

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The rapid increase in the rate of development of human society, science and technology, globalization of economic and increasing international cooperation in various fields, increase in mobility of capital and human resources are accompanied by modernization of industry and introduction of new technologies. These trends are reflected in the economic development strategy «Europe 2020: a strategy for intelligent, sustainable and inclusive growth». One of the activities of this strategy is to enhance the performance of education systems and to promote the involvement of young people into the labor market. At the same time considerable attention is paid to professional education. The training of specialist with certain skills and personal qualities, such as the ability to competently develop technological innovations; adapt quickly to the constant renewal of production, possession of information technology, teamwork, is very significant. In this situation, the role of natural and technical sciences, including chemistry is important. Chemical education in many countries is considered as a factor that greatly affects the economic development of the state. This entails not only the need for highly qualified chemists, but also the necessity to improve chemical literacy in society as a whole.

The principle of professional orientation of chemical education can be realized by incorporating elements of professional knowledge, facts, examples in the theoretical material; they are used when performing chemical experiments, solving chemical problems. Professionalization of education can be carried out by incorporating relevant information in basic educational disciplines, and the creation of chemical courses integrated with subspecialties.

It is necessary to incorporate elements of professional knowledge in the basic chemistry course in primary and secondary schools. At the same time the role and place of chemistry in engineering and technology of concrete production, the prospects of its development based on the latest achievements of science must be shown to students. In universities, professional information should be considered in the basic chemical courses and subspecialties. Questions providing a better understanding of the processes occurring in industry have to be considered in detail.

Realization of succession in the system of continuing professional education can be achieved by integrating existing educational structures into multi-level educational institutions that work in close relationship and implement a wide range of programs of general and vocational education. Educational programs in this multi-level institutions can be realized at different levels: from general secondary and vocational education to higher education, including adult education.

In this connection it is interesting to examine the functioning of Universities of applied sciences in the European Union, representing a wide range of practice-oriented training programs. For example, Vilnius College of Higher Education / University of Applied Sciences offers more than 40 undergraduate programs of professional education at 7 faculties.

Adaptive model of principles of nanotechnology in educational process

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The study of the gradient properties of metallic systems based on studies of the formation and evolution of structural and phase states at the active deformation of metals and alloys is an important scientific problem. The theory of deformation process considers a deformed solid as a hierarchically organized system. The plastic flow at deformation process develops self-consistently through a consistent evolution of the local shear stability loss of the crystal on the interconnected nano-, micro-, meso- and macroscale levels.

This scientific problem can be the basis for the organization of the creative approach to the modeling of scientific thinking of students as a part of training courses related to nanotechnology.

One of the main problems of this approach in the first place is to identify the range of talented, not a standard-minded students as well as their involvement into scientific research, education in this process of scientific thinking and organization methods of scientific analysis of unsolved scientific problems.

After a basic introduction to the basic concepts and problems of selected research area students are encouraged to work individually to analyze, for example, the problem of studying the structure of nanodimensional level occurring in the surface layers of back-up rolls of the rolling mill [1].

As a result of scientific research, students produce a decomposition of the problem into independent subtasks, determine the direction, appoint the specialists in these areas and consult with them. The students find the available information on the problem, as well as the purpose of the issue and its importance in the system of the main problems. They identify the research methods and the necessary laboratory equipment.

The results of the research work are discussed, the strengths and weaknesses of the proposed projects are identified. These results can become the basis for the course work.

References

1. V. V. Kovalenko, V. V. Kozlov, Y. F. Ivanov, V. E. Gromov. Physical nature of formation of gradient structural-phase modes in steel and alloys. Novokuznetsk: Co Ltd "Polygraphist" (2009): 557.

PROGRAMM
7-TH INTERNATIONAL CONFERENCE ON
CHEMISTRY AND CHEMICAL
EDUCATION
SVIRIDOV READINGS 2015

ПРОГРАММА
7-ОЙ МЕЖДУНАРОДНОЙ
КОНФЕРЕНЦИИ ПО
ХИМИИ И ХИМИЧЕСКОМУ
ОБРАЗОВАНИЮ
СВИРИДОВСКИЕ ЧТЕНИЯ-2015
7-10 апреля 2015 года

Минск 2015

Программный комитет
конференции «Свиридовские чтения -2015»

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Стронский А.В. – Институт физики полупроводников им. Лашкарева (Украина);

Швиркст Я. – Латвийский университет (Латвия)

ВТОРНИК, 7 апреля

9.00 – 10.00 Регистрация участников, ул. Бобруйская 5, холл первого этажа

10.00 –14.00 Открытие конференции, ул. Бобруйская 5, зал заседаний

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Секретарь – д.х.н., проф. Т. Н. Воробьева

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6. Д.Л. Янович
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7. к.х.н., доцент Т.А. Савицкая

Современные формы в системе вузовского обучения: лекционный подкастинг
Белорусский государственный университет, Минск, Беларусь

8. к.х.н., доцент О.Н. Рыжова

Проблемы фундаментальности химического образования.

Химический факультет Московского государственного университета имени
М.В. Ломоносова, Москва, Россия

СРЕДА 8 апреля

Секция «Синтез, структура и свойства неорганических веществ. Химия наноструктурных систем. Катализ, фотокатализ»

Председатели – д.х.н., проф. Т. Н. Воробьева, д.х.н., проф. Браницкий Г. А.

Секретарь – к.х.н. Н. Е. Боборико, к.х.н. М. Н. Ничик

10.00 – 15.45 устные доклады,

ул. Ленинградская 14, ауд. 717

15.45–17.00 стендовая секция,

ул. Ленинградская 14, холл 3-го этажа

Секция «Организация учебного процесса и преподавание химии в высшей школе»

Председатели – к. х. н., доц. Е. И. Василевская; к. х. н., доц. Д. И. Мычко

Секретарь – к. х. н., доц. О. В. Сергеева

9.00 – 17.00 устные доклады,

ул. Ленинградская 14, ауд. 401

ЧЕТВЕРГ 9 апреля

Секция «Электрохимия. Химия поверхности и тонких пленок»

Председатель – д.х.н., проф. Е. А. Стрельцов

Секретари – к.х.н., доц. Рабчинский С. М., м.н.с. А. М. Мальтанова

9.30– 13.15 устные доклады

ул. Ленинградская 14, ауд. 401

14.00–15.00 стендовая секция,

ул. Ленинградская 14, холл 4-го этажа

Секция «Металлокомплексы. Химия молекулярных систем»,

Председатель – д.х.н., проф. Н. И. Логинова, к.х.н., доц. Т. В. Ковальчук
Секретари – к.х.н. А. Г. Лисовская, к.х.н. С. Н. Самович

10.00–13.15 устные доклады

ул. Ленинградская, 14, ауд. 714

14.00–15.00 стендовая секция,

ул. Ленинградская, 14, холл 3-го этажа

Подведение итогов конференции, 15.00 ауд. 401

СРЕДА 8 апреля,

Секция «Синтез, структура и свойства неорганических веществ.

Химия наноструктурных систем. Катализ, фотокатализ»

Председатели – д.х.н., проф. Т. Н. Воробьева, д.х.н., проф. Браницкий Г. А.

Секретарь – к.х.н. Н.Е. Боборико, к.х.н. М. Н. Ничик

10.00 – 15.45 Устные доклады,

ул. Ленинградская 14, ауд. 717

1 Композиционные материалы в системах $\text{SiO}_2\text{--TiO}_2$, $\text{TiO}_2\text{--Al}_2\text{O}_3$, модифицированные макроциклическими эндорецепторами

А.Н. Мурашкевич, О.В. Федорова, И.М. Жарский, О.А. Алисиенок
Белорусский государственный технологический университет, Минск, Беларусь

10.00–10.15

2 Устойчивость сульфидных силикатов на основе SBA-15 в водных средах

С.А. Козлова, Ю.Н. Зайцева, С.Д. Кирик

Институт химии и химической технологии СО РАН, Красноярск, Россия

10.15–10.30

3 Соединения аммония как нежелательная примесь в конструкционных строительных материалах на основе бетона

К.В. Халецкая, Н.П. Яловая

Брестский государственный технический университет, Брест, Беларусь

10.30–10.45

4 Приборы и химические сенсоры для контроля за утечками газов на предприятиях концерна «Белнефтехим»

Г.Ф. Каркоцкий, Д.И. Мычко, Ж.А. Цобкало

Белорусский государственный университет, Минск, Беларусь 10.45–11.00

5 Синтез и термическая устойчивость низших гидратов хлорида и сульфата лантана

О.Г. Поляченко, Т.Г. Огородникова, С.И. Войтенко,

- Е.И. Ашмянская, Е.Н. Дудкина, Л.Д. Поляченко
Могилевский государственный университет продовольствия, Могилев, Беларусь 11.00–11.15
- ПЕРЕРЫВ 11.15–11.30
- 6 Эффект УФ воздействия на свойства TiO_2 с добавками золота
Н.С. Трофимов, Д.В. Троян, Т.К. Чехлова, И.И. Михайленко
Российский Университет Дружбы Народов, Москва, Россия 11.30–11.45
- 7 Синтез и структура твердого раствора $\text{Bi}_{0,95}\text{La}_{0,05}\text{FeO}_3$ с использованием прекурсора $\text{Bi}_{1,8}\text{La}_{0,2}\text{Fe}_4\text{O}_9$
А.А. Затюпо, Л.А. Башкиров, Г.П. Дудчик, Г.С. Петров
Белорусский государственный технологический университет, Минск, Беларусь 11.45–12.00
- 8 Химический транспорт некоторых бинарных сульфидов
А.Ю. Завражнов, С.С. Березин, А.В. Косяков, К.К. Черненко
Воронежский государственный университет, Воронеж, Россия 12.00–12.15
- 9 Низкотемпературный синтез и исследование наноструктурированных Co-TiO_2 ферромагнитных композиций
Зима Т.М.
Институт химии твердого тела и механохимии СО РАН, Новосибирск, Россия 12.15–12.30
- 10 Магнитные и фотолюминесцентные свойства твердых растворов со структурой перовскита $\text{La}_{1-x}\text{Nd}_x\text{InO}_3$ ($0,007 \leq x \leq 0,05$)
Л.А. Башкиров, Е.К. Юхно, Н.А. Миронова-Улмане, А.Г. Шараковский, П.П. Першукевич, Л.С. Лобановский, С.В. Труханов, Э.И. Богданов
Белорусский государственный технологический университет, Минск, Беларусь 12.30–13.00
- ПЕРЕРЫВ 13.00–14.00
- 11 Коллоидный синтез и оптические свойства двумерных полупроводниковых гетеронаноструктур типа AlPbV
А.В. Антанович, А.В. Прудников, М.В. Артемьев
Учреждение Белорусского государственного университета «Научно-исследовательский институт физико-химических проблем», Минск, Беларусь 14.00–14.15
- 12 Поведение различных моделей графена при растяжении. Квантово-химическое исследование и расчеты в рамках метода конечных элементов
Вадим Э. Матулис, Виталий Э. Матулис, Ю.Е. Нагорный, В.И. Репченков, О.А. Ивашкевич
Белорусский государственный университет, Минск, Беларусь 14.15–14.30
- 13 Новейшие микроскопические и спектроскопические решения для получения изображений наночастиц и поверхности различных материалов

В.С. Неудачина

Московское представительство Intertech Corporation, Москва, Россия

14.30–14.45

14 Надмолекулярные системы с необратимым резонансным переносом энергии на основе тороидального нанокластера Mo138 и Родамина-Б

К.В. Гржегоржевский, А.А. Остроушко, О.В. Корякова, И.Г. Овчинникова, Г.А. Ким

Уральский федеральный университет им. первого Президента России Б.Н. Ельцина, Екатеринбург, Россия 14.45–15.00

15 Особенности каталитических свойств перовскитоподобных ферритов в углекислотной конверсии метана

Т.А. Крючкова¹, И.А. Хайруллина¹, Т.Ф. Шешко¹, Ю.М. Серов¹ М. И.В.Числова², И.А. Зверева²

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Санкт-Петербургский государственный университет, Санкт-2Петербург, Россия

15.00–

15.15

16 Перовскитоподобные ферриты как катализаторы гидрирования монооксида углерода

Т.Ф. Шешко¹, Ю.М. Серов¹, М.В. Дементьева¹, А. Шульга¹, И.В.Числова², И.А. Зверева²

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15.15–

15.30

17 Суперпарамагнитные композитные частицы для выделения и очистки геномной ДНК

В. Натаров¹, Д. Котиков¹, В. Сурвило², А. Попова², А. Перчик², В. Паньков¹.

¹Белорусский государственный университет, Минск, Беларусь

²ООО «Вега», «АлкорБио», Санкт-Петербург, Россия 15.30–

15.45

15.45–17.00 Стендовая секция,

ул. Ленинградская 14, холл 3-го этажа

1 Ленгмюровские пленки золя золота в обращенных мицеллах аэрозоля ОТ

А.В. Абакшонов¹, Н.В. Каратай¹, И.В. Парибок¹, А.Н. Еремин¹, В.Е. Агабеков¹, М.К. Муханна²

Институт химии новых материалов НАН Беларуси, Минск, Беларусь¹,

King Abdulaziz City for Science and Technology, Саудовская Аравия²

2 Квантовый порядок протонов в кристаллической решетке водорода
М.А. Ионцев

Физический институт им. П.Н.Лебедева РАН, Москва, Россия

3 Синтез металлических наночастиц и их влияние на оптические свойства органических красителей

С. Стрекайте, Д. Пеккус, Р. Аугулис, Т. Тамулевичус, С. Тамулевичус, В. Гулбинас

Институт физики, Центр физических наук и технологий, Вильнюс, Литва

4 Морфология серебряных наночастиц, синтезированных в присутствии нитрилтриуксусной кислоты

Г.П. Шевченко, В.А. Журавков

Учреждение Белорусского государственного университета «Научно-исследовательский институт физико-химических проблем», Минск, Беларусь

5 Термодинамическое подобие многослойных конических нанотрубок и графита

Г.Я. Кабо, А.В. Блохин, Е.В. Павлечко, О.В. Войткевич, Т.Н.Левицкая

Белорусский государственный университет, Минск, Беларусь

6 Сенсорные свойства твердых растворов на основе кобальтитов редкоземельных элементов и феррита висмута

Н.Н. Лубинский, Г.С. Петров, А.А. Затюпо, С.В. Шевченко, Л.А. Башкиров, Т.А. Шичкова

Белорусский государственный технологический университет, Минск, Беларусь

7 Термическое поведение системы $\text{H}_3\text{BO}_3\text{--NH}_4\text{PO}_3$

Е.А. Абрамович, А.Ф. Селевич

Учреждение Белорусского государственного университета «Научно-исследовательский институт физико-химических проблем», Минск, Беларусь

8 Сонохимическая модификация поверхности гальванического никеля в присутствии ванадиевой кислоты

А.С. Логвинович, Т.В. Свиридова, Д.В. Свиридов

Белорусский государственный университет, Минск, Беларусь

9 Новые гидрофосфаты $\text{MH}_3(\text{PO}_4)_2 \cdot 0.5\text{H}_2\text{O}$ ($\text{M} = \text{Er}, \text{Y}$)

Л.С. Ивашкевич, А.С. Ляхов, А.Ф. Селевич

Учреждение Белорусского государственного университета «Научно-исследовательский институт физико-химических проблем», Минск, Беларусь

10 Изменения структуры и химического состава углеродсодержащих наполнителей пористого анодного алюминия при термообработке

К.В. Чернякова¹, Р. Карпич², С.М. Завадский¹, Д. Ковгер², О. Н. Поклонская³

¹Белорусский государственный университет информатики и радиоэлектроники, Минск, Беларусь;

²Государственный научно-исследовательский центр физический науки техно-

логий, Вильнюс, Литва;

3Белорусский государственный университет, , Минск, Беларусь

11 Кристаллизация конденсированных фосфатов хрома в системе CrO_3 – NH_4PO_3

Е.А. Абрамович, А.Ф. Селевич

Учреждение Белорусского государственного университета «Научно-исследовательский институт физико-химических проблем», Минск, Беларусь

12 Твердофазный синтез твердого раствора $(\text{Mg}_{1-x}\text{Co}_x)_2\text{P}_4\text{O}_{12}$

Н.М.Антрапцева1, Г.Н.Била2, И.С.Новак1

Национальный университет пищевых технологий, Киев, Украина

13 Изменение парамагнитных центров в MoO_3 и композитах TiO_2 : MoO_3 после прогрева в восстановительной атмосфере

Н.Е. Боборико, Д.И. Мычко

Белорусский государственный университет, Минск, Беларусь

14 Микроволновой синтез YFeO_3

Е.В. Томина, Ю.Н. Гудкова, Ю.А. Белашкова, Н.И. Бойков

Воронежский государственный университет, Воронеж, Россия

15 Об участии кристаллогидратной воды в твердофазном гидролизе $\text{Mn}_2\text{P}_2\text{O}_7 \cdot 5\text{H}_2\text{O}$

Л.Б. Коваль, Н.М. Антрапцева, Н.В. Солод

Институт общей и неорганической химии им. В.И. Вернадского НАН Украины, Киев, Украина;

Национальный университет биоресурсов и природопользования Украины, Киев, Украина

16 Состав продуктов термообработки Co(II)-Zn дигидрогенфосфатов в изотермических условиях

Л.Б. Коваль, Н.М. Антрапцева, О.В.Турко

Институт общей и неорганической химии им. В.И. Вернадского НАН Украины, Киев, Украина

Национальный университет биоресурсов и природопользования Украины, Киев, Украина

17 Синтез и электрохимическое осаждение фосфатов кальция в поливиниловом спирте

О.Н. Мусская, В.К. Крутько, А.И. Кулак,

Институт общей и неорганической химии НАН Беларуси, Минск, Беларусь

18 Свойства пленок сульфида свинца, осажденных из комплекса $[\text{Pb}(\text{CH}_3\text{COO})_2(\text{N}_2\text{H}_4\text{CS})_2]$

Н.М. Овечкина, А.Н. Лукин, В.Н. Семенов, Л.Н. Никитин

Воронежская Государственная медицинская академия им. Н.Н. Бурденко Воронеж, Россия

19 Получение наночастиц AgInS_2 в системах AgNO_3 – In_2S_3 – $\text{C}_2\text{H}_4(\text{NH}_2)_2$

Г.М. Гусейнов

Нахчыванское отделение Национальной Академии Наук Азербайджана «Институт природных ресурсов», Нахчыван, Азербайджан

20 Огнезадерживающие и атмосферостойкие свойства азот-фосфор-содержащих суспензий на основе доломита и трепела

В.В. Богданова, О.И. Кобец

Учреждение Белорусского государственного университета «Научно-исследовательский институт физико-химических проблем», Минск, Беларусь

21 АСМ-исследования морфологии поверхности гетероструктур V_2O_5/InP

Е.В. Томина, Л.С. Зеленина, Б.В. Сладкопевцев, Е.И. Вагайцев

Воронежский государственный университет, Воронеж, Россия

22 Особенности термолитиза тетрагидрата дигидрофосфата марганца(II)

Н.М. Антрапцева, Н.В. Солод, Л.Б. Коваль

Институт общей и неорганической химии им. В.И. Вернадского НАН Украины, Киев, Украина

23 Синтез и свойства индатов $TbxLa_{1-x}InO_3$ ($x \leq 0,15$)

И.Н. Кандидатова, Л.А. Башкиров, П.П. Першукевич, С.В. Труханов,

Л.С. Лобановский

Белорусский государственный технологический университет, Минск, Беларусь

24 Особенности кристаллизации и химическая природа дифосфатов в системе $MnSO_4 - CoSO_4 - K_4P_2O_7 - H_2O$

Н.В. Солод, Н.М. Антрапцева

Институт общей и неорганической химии им. В.И. Вернадского НАН Украины, Киев, Украина

25 Синтез, свойства и структура твердых-растворов на основе $Bi_2Fe_4O_9$.

А. А. Затюпа, Л.А. Башкиро, И.А. Великанова, Г.С. Петров

Белорусский государственный технологический университет, Минск, Беларусь

26 Фотоэлектронная характеристика композита P_3NT /нанокристаллы PbS

В. Бертасиус¹, В. Гулбинас², С. Гиансанте³

¹ Университет Вильнюса, Вильнюс, Литва;

² Институт физики, Центр физических наук и технологий, Вильнюс;

³ NNL-CNR Istituto di Nanoscienze via per Arnesano, Lecce, Italy

СРЕДА 8 апреля,

Секция «Организация учебного процесса

и преподавание химии в высшей школе»

Председатели – к. х. н., доц. Е. И. Василевская; к. х. н., доц. Д. И. Мычко

Секретарь – к. х. н., доц. О. В. Сергеева

9.00 – 17.00 Устные доклады,
ул. Ленинградская 14, ауд. 401

- 1 Современная методика обучения химии и перспективы ее развития
Е.Я. Аршанский
Витебский государственный университет им. П. М. Машерова, Витебск, Беларусь 9.00–9.15
- 2 Анализ релевантности в процессе поиска химической информации как элемент компетентностного подхода в обучении студентов-химиков
В.Н. Хвалюк, А.А. Рагойша
Белорусский государственный университет, Минск, Беларусь 9.15–9.30
- 3 Междисциплинарное сотрудничество как условие формирования целостного естественнонаучного мировоззрения в процессе обучения химии в техническом университете
Л.Г. Горбунова
Котласский филиал ФБГОУ ВПО «Государственный университет морского и речного флота имени адмирала С.О. Макарова», Котлас, Россия 9.30–9.45
- 4 Структурирование содержания химического образования для инженерных специальностей вузов с помощью содержательных линий
В.А. Халецкий
Брестский государственный технический университет, Брест, Беларусь 9.45–10.00
- 5 Методология дополнительного образования по естественно-научным дисциплинам для первокурсников РУДН
С.Б. Страшнова, Т.С. Тамурова, С.П. Карнилович
Российский университет дружбы народов, Москва, Россия 10.00–10.15
- 6 Система интегративно-дифференцированного обучения химии в вузе на основе самостоятельной работы студентов
А.М. Стихова
Государственный морской университет имени адмирала Ф. Ф. Ушакова, Новороссийск, Россия 10.15–10.30
- 7 Изучение химии в духе учения в течение всей жизни в музеях
Н.С. Шакирова
Политехнический музей, Москва, Россия 10.30–10.45
- ПЕРЕРЫВ 10.45–11.00
- 8 Использование образовательного мобильного сервиса SOCRATIVE в контроле успеваемости студентов химического факультета
А.Н. Трифонова
Белорусский государственный университет, Минск, Беларусь 11.00–11.15
- 9 Конкурсные задачи по химии – адаптация к новым условиям
Е.А. Белевцова
Московский государственный университет имени

- М. В. Ломоносова, Москва, Россия 11.15–11.30
- 10 Перспективы создания непрерывной интегрированной системы подготовки абитуриентов к централизованному тестированию по химии
Л.Е. Тригорлова, Э.Е Якушева
Витебский государственный медицинский университет, Витебск, Беларусь
11.30–11.45–
- 11 Применение кейс-технологии для развития информационной компетенции учащихся на уроке химии
И.Б. Мишина, Т. А. Боровских
ГБОУ ЦО № 1464, Москва, Россия 11.45–12.00
- 12 Проблема формирования универсальных учебных действий учащихся в контексте методической подготовки будущего учителя химии
Н.В. Жулькова
МБОУ СОШ №53, Ульяновск, Россия 12.00–12.15–
- 13 Учебно-методический комплекс как средство образовательных технологий в подготовке инженеров-аграриев
И.Б. Бутылина, Д.Т. Кожич, С.В. Слонская
Белорусский государственный аграрный технический университет, Минск, Беларусь 12.15–12.30
- 14 Кейс-технология в системе активного обучения химии будущих учителей
С.И. Гильманшина, В.С. Бурлакова, Г.Ф. Валитова
Казанский федеральный университет, Казань, Россия 12.30–12.45
- 15 Элективный курс «Нанохимия»
Т.Н. Воробьева, Л. С. Ивашкевич, О.В. Сергеева
Белорусский государственный университет, Минск, Беларусь 12.45–13.00
- ПЕРЕРЫВ 13.00–14.00
- 16 Инновационное учебное пособие с электронным приложением по теоретическим основам органической химии
А.Э. Щербина, М.А. Кушнер, Т.С. Селиверстова, О.Я. Толкач.
Белорусский государственный технологический университет, Минск, Беларусь 14.00–14.15
- 17 Химические приложения для мобильных устройств на платформе Android и перспективы их использования в обучении химии
А.А. Белохвостов
Витебский государственный университет им. П.М. Машерова, Витебск, Беларусь 14.15–14.30
- 18 Физические величины, терминология и символы в химии
А.С. Тихонов
Белорусский государственный университет, Минск, Беларусь 14.30–14.45
- 19 Формы представления справочных данных и их использование в учебном процессе

Б.В. Румянцев

Московский государственный педагогический университет, Институт биологии и химии, Москва, Россия 14.45–15.00

20 Практика использования электронных средств обучения в образовательном процессе кафедры высокомолекулярных соединений БГУ

Л.Б. Якимцова, Л.П. Круль

Белорусский государственный университет, Минск, Беларусь 15.00–15.15

21 Диалоговое обучение химии на основе гендерного подхода

Н.Г. Щавелева

Казанский (Поволжский) Федеральный Университет, Казань, Россия

15.15–15.30–

22 Обучение химии высшей школе с использованием курсов электронного обучения

О.Д. Кочкодан

Национальный университет биоресурсов и природопользования Украины, Киев, Украина 15.30–15.45

23 Компьютерные технологии обучения энергосбережению в процессе изучения естественнонаучных дисциплин

С.И. Гильманшина, Р.К. Ямалдинов, И.Р. Гильманшин,

Р. И. Рахимова

Казанский (Поволжский) федеральный университет, Казань, Россия

15.45–16.00

24 Метод кейсов при изучении курса «Общая химия»

Е.В. Томина, Б.В. Сладкопцев, Е.В. Кривотулова

Воронежский государственный университет, Воронеж, Россия 16.00–16.15

25 Формирование преемственности химического образования в вертикали «I Ступень образования – II Ступень образования – ВУЗ через научно-исследовательскую деятельность обучающихся

Л. Е. Ермачек

ГУО «Гимназия № 32», Минск, Беларусь 16.15–16.30–

26 Использование кейс-технологии как средства реализации проблемного обучения химии

О. И. Сечко

Белорусский государственный университет, Минск, Беларусь 16.30–16.45

27 Реализация преемственности и профессиональной направленности курса химии в системе непрерывного образования школа-колледж-университет

Е. И. Василевская¹, С. И. Швядене², Н. П. Лепене²

¹Белорусский государственный университет, Минск, Беларусь

²Вильнюсская коллегия, Вильнюс Литва 16.45–17.00

ЧЕТВЕРГ 9 апреля,
Секция «Электрохимия. Химия поверхности и тонких пленок»

Председатель – д. х. н., проф. Е. А. Стрельцов
Секретари – к. х. н., доц. С. М. Рабчинский, м. н. с. А. М. Мальтанова

9.30–13.15 Устные доклады
ул. Ленинградская 14, ауд 401

1 Электрохимическое исследование взаимодействия контактной неравновесной плазмы с водными электролитами
В.С. Кублановский, А.В. Кравченко, А.А. Пивоваров,
О.Л. Берсирова
Институт общей и неорганической химии им. В.И.Вернадского НАН Украины
Киев, Украина 9.30–9.45

2 Химическое и электрохимическое формирование наноструктурированных алюминиевых сеток для дисплейного производства
В.В. Жилинский, Н.В. Богомазова, О.С. Волюнец, А.А. Черник, В.С. Безбо-
родов
Белорусский государственный технологический университет, Минск, Бела-
русь 9.45–10.00

3 Зависимость потенциалов катодного осаждения металлов на поли-
кристаллический теллур от энергии Гиббса образования теллуридов
Е.Н. Анискевич, П.В. Чулкин, Г.А. Рагойша, Е.А. Стрельцов
Белорусский государственный университет, Минск, Беларусь 10.00–10.15

4 Электрохимическое формирование функциональных материалов но-
вого поколения: наноструктурированных покрытий с заданными свойствами
(для электроники и энергетики)
О.Л. Берсирова, В.С. Кублановский
Институт общей и неорганической химии им. В.И. Вернадского НАН Украи-
ны, Киев, Украина 10.15–10.30

5 Синтез и исследование электрохимических свойств тонкопленочных
электродов диоксид олова / графен – оксид
Е.А. Бондаренко, П.В. Чулкин, Т.А. Авчинникова, Е.А. Стрельцов, Г.А. Рагой-
ша
Белорусский государственный университет, Минск, Беларусь 10.30–10.45

6 Эффективная огнезащита нетканого полиэфирного материала
О.В. Рева¹, В.В. Богданова², Т.Н. Андреева¹, А.Н. Назарович¹, А.С. Лукьянов

ГУО «Командно-инженерный институт» МЧС РБ, Минск, Беларусь
2Учреждение Белорусского государственного университета «Научно-исследовательский институт физико-химических проблем», Минск, Беларусь
10.45–

11.00

ПЕРЕРЫВ

11.00–11.15

7 Защитная способность безэлектролизно и электрохимически осаж-
денных Ni-P сплавов на сталь в солевых средах

С.С. Перевозников, С.К. Позняк, Л.С. Цыбульская

Учреждение Белорусского государственного университета «Научно-исследо-
вательский институт физико-химических проблем», Минск, Беларусь

11.15–11.30

8 Улучшение щелочной стойкости базальтовых волокон путем нанесе-
ния покрытий из диоксида циркония и диоксида титана

В.А. Рыбин, Н.И. Бакланова, А.В. Уткин

Институт химии твердого тела и механохимии СО РАН, Новосибирск, Рос-
сия 11.30–11.45

9 Многослойная интерфаза на основе германата гафния для SiC/SiCf
композитов

В.Э. Прокип, А.В. Уткин, Н.И. Бакланова

Институт химии твердого тела и механохимии СО РАН, Новосибирск, Рос-
сия 11.45–12.00

10 Синтез, структура и электрофизические свойства поликристалличе-
ских висмутовых пленок

А.С. Федотов¹, С.К. Позняк², Л.С. Цыбульская², И.В. Свито¹, В.Г. Шепеле-
вич¹, А.В. Мазаник¹, А.К. Федотов¹, Т.В. Гаевская²

¹Белорусский государственный университет, Минск, Беларусь

²Учреждение Белорусского государственного университета «Научно-ис-
следовательский институт физико-химических проблем», Минск, Беларусь

12.00–12.15

11 Влияние золя SnO₂ на закономерности электрохимического осажде-
ния и свойства медных покрытий на цинк, алюминий и их сплавы.

Т.Н. Воробьева^{1,2}, О.Н. Врублевская¹, Д.И. Насонова²,

А.О. Конаков²

Учреждение Белорусского государственного университета «Научно-исследо-
вательский институт физико-химических проблем», Минск, Беларусь;

Белорусский государственный университет, Минск, Беларусь 12.15–12.30

12 Моделирование процесса полировки кристаллической поверхности

А.В. Юхневич, И.А. Майер, А.Е. Усенко

Белорусский государственный университет, Минск, Беларусь 12.30–

12.45

- 13 Стабильность и реология суспензий оксида кремния(IV) стабилизированных поверхностно-активными веществами and
Т.А. Савицкая¹, И.М. Кимленко¹, Е.А. Шахно¹, В.Е. Гайшун²,
Я.А. Косенок²
¹Белорусский государственный университет, Минск, Беларусь
²Гомельский государственный университет, Гомель, Беларусь 12.45–
13.00
- 14 Получение порошков Au-Sn в растворах методом цементации
М.П. Пяткевич¹, А.М. Мальтанова², Т.Н. Воробьева^{1,2}
¹Белорусский государственный университет, Минск, Беларусь;
Учреждение Белорусского государственного университета «Научно-исследовательский институт физико-химических проблем», Минск, Беларусь
13.00–
13.15
- 14.00–15.00 Стендовая секция,
ул. Ленинградская 14, холл 4-го этажа
- 1 Вольтамперометрическое поведение динитрофенов и фенола при совместном присутствии
И.К. Ускова, П.Д. Халфина, Е.А. Левкович
Кемеровский государственный университет, Кемерово, Россия
- 2 Ингибирование коррозии стали дифосфатами Mn(II), Co(II), Zn
Н.В. Солод, Н.М. Антрапцева, Г.Н.Била
Национальный университет биоресурсов и природопользования Украины,
Киев, Украина
- 4 Исследование влияния режимов анодирования на формирование упорядоченных нанотрубок TiO₂
Д. Ковгер¹, К.В. Чернякова², Р. Карпич¹, А. Ягминас¹
¹Государственный научно-исследовательский институтский центр физический наук и технологии, Вильнюс, Литва;
²Белорусский государственный университет информатики и радиоэлектроники, Минск, Беларусь
- 5 Структурно-химические превращения углеродсодержащих компонентов в пористом анодном оксиде алюминия при термическом отжиге
К.В. Чернякова², Р. Карпич¹, С.М. Завадский², Е. Ковгер¹, О.Н. Поклонская²
¹Государственный научно-исследовательский институтский центр физический наук и технологии, Вильнюс, Литва;
²Белорусский государственный университет информатики и радиоэлектроники, Минск, Беларусь
- 6 Способы получения антибактериальных композиционных пленок
Г.А. Браницкий, Н.А. Беясова, Л.И. Антоновская, В.Г. Соколов

Учреждение Белорусского государственного университета «Научно-исследовательский институт физико-химических проблем», Минск, Беларусь

7 Синтез и транспортные свойства фосфорилированных мембран на основе винилового спирта для окислительно-восстановительных $\text{Fe}^{3+}/\text{H}_2$ проточных ячеек

В.П. Глыбин, В.Р. Пупкевич

Западный Университет, Лондон, Канада

8 Нано- и ультрадисперсные порошки сверхтвердых материалов в качестве модификаторов жидкой смазки

Л.И. Южик, Е.В. Карпинчик, В.И. Жорник, С.А. Ковалева

Институт химии новых материалов НАН Беларуси, Минск, Беларусь

9 Электрохимическое осаждение сплава Ni-Cr из этилен- и пропиленгликолевых растворов

А.С. Какарека¹, В.А. Прокошина², О.Н. Врублевская²

¹Белорусский государственный педагогический университет им. Максима Танка, Минск, Беларусь;

²Учреждение Белорусского государственного университета «Научно-исследовательский институт физико-химических проблем», Минск, Беларусь

10 Электрохимическая активность энзимного препарата *Raphanus Sativus* L. Var. *Niger* (корнеплода редьки черной), иммобилизованного на неорганических носителях

М.О. Ходыкина, Е.Д. Першина, К.А. Каздобин

Институт общей и неорганической химии им. В.И. Вернадского НАН Украины, Киев, Украина

11 Безэлектролизное осаждение пленок Pd-Ni-P из полилигандных пирофосфатных электролитов.

И.В. Сакович, О.Н. Врублевская

Учреждение Белорусского государственного университета «Научно-исследовательский институт физико-химических проблем», Минск, Беларусь

12 Влияние температуры прогрева слоёв нанотрубок TiO_2 на электрокаталитическую активность системы «наночастицы Au/TiO_2 » в реакции восстановления кислорода

А.М. Мальтанова, С.К. Позняк, Т.Н. Воробьева, М.И. Ивановская

Учреждение Белорусского государственного университета «Научно-исследовательский институт физико-химических проблем», Минск, Беларусь

13 Тетразолирование коммерческого полиакрилонитрильного волокна Нитрон Д-5

Ю.В. Григорьев, И.М. Григорьева, О.А. Ивашкевич

Учреждение Белорусского государственного университета «Научно-исследо-

вательский институт физико-химических проблем», Минск, Беларусь

14 Удаление нитрат-ионов из природных вод наночистоточным методом

О.Д. Кочкодан, В.М. Кочкодан, Г.М. Бойко

Национальный университет биоресурсов и природопользования Украины, Киев

15 Адсорбция Cu(II) продуктом тетразолирования полиакрилонитрильного волокна Нитрон Д-5

Ю.В. Григорьев, И.М. Григорьева, С.В. Войтехович, О.А. Ивашкевич

Учреждение Белорусского государственного университета «Научно-исследовательский институт физико-химических проблем», Минск, Беларусь

16 Исследование антибактериальных свойств ультрафильтрационных полимерных мембран

В.М. Кочкодан, О.Д. Кочкодан, Т.И. Левадная, В.С. Ковтун

Национальный университет биоресурсов и природопользования Украины, Киев

17 Оценка адсорбции ПАВ в нефтяных дисперсных системах

Н.В. Яковец, О.Н. Опанасенко, Н.П. Крутько

Институт общей и неорганической химии НАН Беларуси, Минск, Беларусь

ЧЕТВЕРГ, 9 апреля

Секция «Металлокомплексы. Химия молекулярных систем»,

химический факультет БГУ, Ленинградская, 14, ауд. 714

Председатель – д. х. н., проф. Н. И. Логинова, к. х. н., доц. Т. В. Ковальчук

Секретари – к.х.н. А.Г. Лисовская, к.х.н. С.Н. Самович

10.00–13.15 Устные доклады

1 Структура и свойства тройного полимер-металлического комплекса хитозан-Cu(II)-полигексаметиленгуанидин

В.А. Добыш, В.А. Тарасевич, В.В. Корней, Л.И. Антоновская

Институт химии новых материалов НАН Беларуси, Минск, Беларусь

10.00–10.15

2 Аномальная температурная зависимость люминесценции алкокси-замещенных стильбенов

А.В. Станкевич, Ал.А. Муравский, Ан.А. Муравский, В.Е. Агабеков

Институт химии новых материалов НАН Беларуси, Минск, Беларусь

10.15–10.30

3 Биоактивные комплексы Cu(II) и Zn(II) с основаниями Манниха

Г.И. Горбачевич, Т.В. Петрашевская, Т.В. Ковальчук, Н.В. Логинова, И.И.

Азарко, Н.П. Осипович, Г.И. Полозов

Белорусский государственный университет, Минск, Беларусь 10.30–10.45
4 Биологически активные комплексы Pt(II), Pd(II) и Cu(II) с азотсодержащими лигандами

Е.В. Лидер^{1,2}, А.И. Смоленцев¹, В.И. Поткин³, Л.Г. Лавренова^{1,2}

¹Институт неорганической химии им. А.В. Николаева СО РАН, Новосибирск, Россия;

²Новосибирский государственный университет, , Новосибирск, Россия;

³Институт физико-органической химии НАН Беларуси, Минск, Беларусь
10.45–11.00

5 Полиазотсодержащие азолы как перспективные лиганды в дизайне металлокомплексов с противоопухолевой активностью

Т.В. Серебрянская, А.А. Легин, С.В. Войтехович, Б.К. Кеплер, В.Ю. Кукушкин.

¹Санкт-Петербургский университет, Институт химии, Санкт-Петербург, Россия;

²Институт неорганической химии, Университет Вены, Вена, Австрия;

³Учреждение Белорусского государственного университета «Научно-исследовательский институт физико-химических проблем», Минск, Беларусь
11.00–11.15

6 Синтез и структурно- химические исследования координационных соединений металлов с 4-метил-1,2-циклогексендикар-боновой кислотой
М.М. Сеидов, Б.Т. Усубалиев, М.М. Гасанова

Научно-исследовательский институт «Геотехнологические проблемы нефти, газа и химия», Баку, Азербайджан
11.15–

11.30

7 ПЕРЕРЫВ 11.30–11.45

8 Молекулярная структура и парамагнитные свойства бис-диизобутилдитиофосфинатных комплексов лантанидов с 1,10-фенантролином по данным ЯМР

С.П. Бабайлов, Е.Н. Заполоцкий, Ю.А. Брылева

Институт неорганической химии им. академика А.В. Николаева СО РАН, Новосибирск, Россия 11.45–12.00

9 Радиационно-индуцированные реакции углерод-центрированных радикалов с пиримидиновыми азотистыми основаниями и их производными
В.А. Бараев¹, Р.Л. Свердлов^{1,2}, И.П. Едимичева², О.И. Шадыро^{1,2}

¹Белорусского государственного университета, Минск, Беларусь

²Учреждение Белорусского государственного университета «Научно-исследовательский институт физико-химических проблем», Минск, Беларусь
12.00–12.15

10 Получение металлокомплексов сульфонированного полиакриламида

с Cr(III) с использованием метода фронтальной полимеризации

М.Б. Газинежад, Е.В. Гринюк, Л.П. Круль

Белорусский Государственный Университет, Минск, Беларусь 12.15–12.30

11 Экстракция ароматических углеводов метанольными растворами хлорида 1-бутил-3-метилимидазолия и бензолсульфоната 1-метилхинолина.

С.М. Лещев, А.В. Онищук, Е.Б. Окаев

Белорусский Государственный Университет, Минск, Беларусь 12.30–

12.45

12 Новые катализаторы для реакций кросс-сочетания на основе комплексов Pd(II) с замещенными изоксазолами и изотиазолами

Н.А. Бумагин, А.В. Клецков, С.К. Петкевич, Е.А. Дикусар, В.И. Поткин

Институт физико-органической химии НАН Беларуси, Минск, Беларусь

12.45–

13.00

13 Влияние расположения катионов кобальта в структуре NZP на каталитические превращения пропанола-2

Е.И. Поварова, А.И. Пылинина и И.И. Михаленко

Российский университет дружбы народов, Москва, Россия 13.00–

13.15

14.00–15.00 Стендовая секция

ул. Ленинградская, 14, холл 3-го этажа

1 1-(5-амино-3-азапентил)тетразол и его комплексы с медью(II)

С.В. Войтехович, Ю.В. Григорьев, А.С. Ляхов, Л.С. Ивашкевич,

О.А. Ивашкевич

Учреждение Белорусского государственного университета «Научно-исследовательский институт физико-химических проблем», Минск, Беларусь

2 Кристаллическая структура комплексов 2-(тетразол-1-ил)пиридина с хлоридами Cu(II) и Co(II)

Ю.В. Григорьев, А.С. Ляхов, Л.С. Ивашкевич, С.В. Войтехович,

А.И. Лесникович

Учреждение Белорусского государственного университета «Научно-исследовательский институт физико-химических проблем», Минск, Беларусь

3 Комплексообразование Cu^{2+} с 1-трет-бутилтетразолом в присутствии триэтиламина

К.А. Набебина¹, М.М. Дегтярик², С.В. Войтехович², О.А. Ивашкевич¹

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4 1-(N,N-диметил)аминоэтил-5-меркаптотетразол как новый лиганд для стабилизации наночастиц палладия в воде

М.Н. Ничик¹, С.В. Войтехович², А.И. Лесникович¹

¹Белорусский государственный университет, Минск, Беларусь;

²Учреждение Белорусского государственного университета «Научно-исследовательский институт физико-химических проблем», Минск, Беларусь

5 Новые тетразолсодержащие основания Шиффа и их биологическая активность

М.Н. Ничик¹, Р.А. Желдакова, М.М. Дегтярик², А.И. Лесникович¹

¹Белорусский государственный университет, Минск, Беларусь;

²Учреждение Белорусского государственного университета «Научно-исследовательский институт физико-химических проблем», Минск, Беларусь

6 Анионообменная экстракция комплексов Zn(II), Cd(II), Hg(II) и Co(II) высшими четвертичными аммониевыми солями из тиоцианатных сред

Е.Е. Трофименко, А.Л. Гулевич, Е.М. Рахманько

Белорусский государственный университет, Минск, Беларусь

7 Синтез и исследование координационных соединений переходных металлов с изомерными тетразолсодержащими основаниями Шиффа

Е.В. Кежун, М.М. Дегтярик, А.И. Лесникович

Учреждение Белорусского государственного университета «Научно-исследовательский институт физико-химических проблем», Минск, Беларусь

8 Полимерные цимантренкарбоксилатные комплексы лантанидов. Синтез, магнетизм, термолиз

П.С. Коротеев, Н.Н. Ефимов, А.В. Ильяхин, Ж.В. Доброхотова, В.М. Новотворцев

Институт общей и неорганической химии им. Н.С. Курнакова РАН, Москва, Россия

9 Синтез и кристаллическая структура хлоридного комплекса CoII с 2-(1Н-тетразол-1-ил)тиазолом

А.С. Ляхов, Л.С. Ивашкевич, Ю.В. Григорьев, А.И. Лесникович

Учреждение Белорусского государственного университета «Научно-исследовательский институт физико-химических проблем», Минск, Беларусь

10 Молекулярная и кристаллическая структура 5-фенил-2-винил-2Н-тетразола и 2-(проп-1-енил-2)-2Н-тетразол-5-иламина

А.С. Ляхов, Т.Н. Андреева, С.В. Войтехович, Л.С. Ивашкевич

Учреждение Белорусского государственного университета «Научно-исследовательский институт физико-химических проблем», Минск, Беларусь

11 Тиоцианатные комплексы d- металлов: влияние структуры на обменную экстракцию анионов четвертичными аммониевыми солями

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