SVIRIDOV READINGS – 2021

BOOK OF ABSTRACTS
OF 9TH INTERNATIONAL CONFERENCE
ON CHEMISTRY AND CHEMICAL EDUCATION

Minsk, Belarus, April 13–14, 2021

BELARUSIAN STATE UNIVERSITY
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КАФЕДРА НЕОРГАНИЧЕСКОЙ ХИМИИ

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СВИРИДОВСКИЕ ЧТЕНИЯ – 2021

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Abstracts are devoted to modern problems in chemistry and teaching of chemistry in universities.

Тезисы докладов представляют современные научные проблемы химии и преподавания химии в вузах.

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Synthesis and characterization of ammonium-vanadium(III) double cyclophosphates $(NH_4)_2V_2P_8O_{24}$ and $(NH_4)_3V_3P_{12}O_{36}$

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This work continues our systematic research on ammonium-metal(III) double condensed phosphates, which are potential fire retardants for polymeric materials [1]. The aim of this work was to synthesize and characterize ammonium-vanadium(III) double cyclophosphates $(NH_4)_2V_2P_8O_{24}$ and $(NH_4)_3V_3P_{12}O_{36}$. Double cyclooctaphosphate $(NH_4)_2V_2P_8O_{24}$ has been synthesized in the system V–NH_4PO_3 at the temperature of 300 ºC and at the molar ratio V : P = 1 : 12. X-ray studies have been performed for powder sample of compound: monoclinic system, S.G. $I2/m$, a = 16,6604(12), b = 12,4435(15), c = 5,2205(8) Å; β = 95,518(8), V = 1077,28 Å^3, Z = 2.

Double cyclododecaphosphate $(NH_4)_3V_3P_{12}O_{36}$ has been synthesized in the system $V(H_2PO_4)_3$–NH_4PO_3 at 350 ºC and at the molar ratio V : P = 1 : 15.

Main crystallographic data for $(NH_4)_3V_3P_{12}O_{36}$ have been calculated: cubic system, S.G. Pa-3, a = 14,38841(77) Å; V = 2978,78 Å^3, Z = 4.

A comparison of main crystallographic data of $(NH_4)_2V_2P_8O_{24}$ and $(NH_4)_3V_3P_{12}O_{36}$ with those of $(M^I)_2(M^{III})_2P_8O_{24}$ and $(M^I)_3(M^{III})_3P_{12}O_{36}$ (M^I – monovalent cation, M^{III} – trivalent cation) indicates that they are isotypical, respectively [2–4]. Thermal behavior of the compound has been investigated within the temperature range of 30–1000°C. It was found that both $(NH_4)_2V_2P_8O_{24}$ and $(NH_4)_3V_3P_{12}O_{36}$ demonstrated high thermal stability. They start to decompose at the temperature of about 500 °C. Final crystal products of thermal decomposition of the compounds are $V_4(P_4O_{12})_3$ and/or $V(PO_3)_3$–C.

The data obtained allow to conclude that cyclooctaphosphate $(NH_4)_2V_2P_8O_{24}$ as well as cyclododecaphosphate $(NH_4)_3V_3P_{12}O_{36}$ having high chemical and thermal stability may used as fire retardant additives to thermoplastics [5].

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Investigating the influence of the trivalent and monovalent metals ionic radius on the structure of the synthesized double condensed phosphates

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The purpose of the work was to produce new condensed phosphates with a structure of double inorganic oligomers, cyclic compounds and long chain polymeric composites via condensation of polyphosphoric acids and to reveal the effect of the trivalent and monovalent metal ionic radius on the structure of the product. High temperature synthesis (100-600 °C) was used to produce multi-component phosphates of the general formula $M^I_2O{-}M^{III}_2O_3{-}P_2O_5{-}H_2O$ (where M^I − Ag and alkali metals, M^{III} – Al, Ga, In and Sc).

Over the last few years, numerous researchers have been paying serious attention to the careful synthesis and investigation of condensed phosphates – so called inorganic polymers. This was possible afterward remarkable development of different fields of new technologies, as well as expanding the research area of nanotechnology and fundamental general researches. By analyzing the crystallization conditions and properties of polymers, the synthesis of new inorganic polymers with targeted properties will be possible, as well as identification of the optimal regimes for formation of mono-crystals and in some cases of nano-composites [1].

Phase composition and the structure of the phosphates obtained were defined. It was found that the stability of highly condensed phosphates of the type $M^IM^{III}(PO_3)_4$ and $M^{III}P_5O_{14}$, and the stability of oligophosphates decreases with an increase in the radius of the M^{III} cation. Concerning alkali metals, it was revealed that generally, Li forms long-chain double polyphosphates, Na forms tetraphosphates, K and Rb generate cyclooctaphosphates. Most characteristic feature of cesium is the formation of highly condensed forms such as cyclododecaphosphates [2, 3]. We determined that some inorganic oligomers and polymers can be used in practice as new technological materials, such as binders and cementing compounds, fertilizers, ion exchangers and substances with catalytic activity.

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Electrochemical route to Bi-Bi_2Te_3 superlattice

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Synthesis of Bi-Bi_2Te_3 superlattice is a promising way to break the trade-off between thermal and electrical conductivities, which limits the thermoelectric efficiency of individual bismuth telluride [1,2]. We present the electrochemical route for fabrication of such superlattice, which is based on concurrent electrochemical deposition of bismuth telluride and bismuth adlayers [1,3]. The process was controlled by periodical switching of the electrode potential between the regions of a predominant electrodeposition of bismuth telluride below $E_{\mathrm{Bi}^{3+}/\mathrm{Bi}}$ equilibrium potential and a predominant Bi adlayer electrodeposition above $E_{\mathrm{Bi}^{3+}/\mathrm{Bi}}$. The superlattice is formed via the stacking of the elementary building blocks of the layered Bi_2Te_3 crystal structure: Te-Bi-Te-Bi-Te quintuples with Bi adlayers on the both sides of the quintuples, so that each pair of Bi adlayers gives a biatomic interlayer in the resulting $(\mathrm{Bi}_2)_\mathrm{m}(\mathrm{Bi}_2\mathrm{Te}_3)_\mathrm{n}$ superlattice structure. The obtained films were examined by SEM in order to optimize electrodeposition conditions for the preparation of compact uniform $(\mathrm{Bi}_2)_\mathrm{m}(\mathrm{Bi}_2\mathrm{Te}_3)_\mathrm{n}$ films. Cyclic voltammetry coupled with quartz crystal microbalance techniques allowed to monitor Bi adlayer and bilayer transformations during the electrodeposition and anodic decomposition of the superlattice. Bismuth bilayers in a superlattice are electrochemically labile and can be removed via selective anodic oxidation, preserving the expanded superlattice structure that was proved by refinement of XRD data.

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Kinetics sorption of Co(II) and Cr(III) ions on ion exchange resin from acidic solutions

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Currently, many factories dispose waste water containing various toxic and non-ferrous metal ions [1]. In particular, an increase in concentrations of Co(II), Cr(III), Cu(II) and Zn(II) in waters adversely affects the environment [2]. This study demonstrate the possibility of remove Co(II) and Cr(III) from aqueous solutions by the formation of the polyampholyte based on polyvinylchloride. The calculated parameters of the pseudo-first and second order of sorption of Co(II) and Cr(III) on PVC- (SO_3H) (NH) are presented in Table. According to the results of the investigation the kinetics of the adsorption of Co(II) and Cr(III) with polyampholyte on the base of PVC is close to the data integrity of the pseudo-first-order model compared to the pseudo-first-order model.

Table. Kinetic parameters for Co(II) and Cr(III) adsorption with polyampholyte on the base of PVC

Initial conc (mol/L)	Calculated equilib. uptake q_e (mg·g^{-1})	k_2 (g mg^{-1} min^{-1})	h (g mg^{-1} min^{-1})	R^2
0,010	37,04	0,000497	0,682	0,989
0,0125	50,00	0,000163	0,407	0,937
0,025	58,82	0,000092	0,321	0,848
0,050	90,91	0,000076	0,635	0,871
Average k_2	0,000112			
0,010	45,45	0,000374	0,773	0,987
0,0125	76,92	0,000219	1,311	0,993
0,025	100,0	0,000145	1,451	0,990
0,050	125,0	0,000066	1,033	0,967
Average k_2	0,000113			

Pseudo-second order adsorption coefficient the coefficient of correlation in the (R^2) relative to the combined Co(II) (R^2=0,989) and Cr(III) (R^2=0,987). This means that the sorption process is influenced not only by the nature of the ions, but also by the sulpho- and amine- groups in the ion exchanger.

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Low remperature heat capacity and phase transition parameters of strontium and barium ferromolybdates

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The results of low temperature heat capacity and phase transition study of strontium and barium ferromolybdates $Sr_{2-x}Ba_xFeMoO_{6-\delta}$ with $x = 2.0$ (I), $x = 1.6$ (II), $x = 1.0$ (III) and $x = 0.8$ (IV) are represented. Barium addition to the $Sr_2FeMoO_{6-\delta}$ leads to decrease of Curie temperature, and, hence, to higher values of negative magnetoresistance, saturation magnetization and to significant magnetocaloric effect at room temperature [1].

The temperature dependences of heat capacities of solid solutions were measured in the range (5 – 370) K using the vacuum adiabatic calorimeter TAU-1 0 («Termis», Moscow, Russia) [2]. The relative expanded uncertainty of the measurements was determined to be 0.4 % in the range (20 – 370) K, 1% in the range (10 – 20) K and 2% in the range (5 – 10) K. There were reproduc ible anomalies on the heat capacity curves of samples I, II and III at temperature higher than 240 K. It was explained by transition from ferromagnetic to paramagnetic state of compounds. There were no anomalies on the heat capacity curve of sample IV below 370 K. Curie temperatures corresponded to excessive heat capacity maximum in the phase transition region and obtained from the temperature dependences of magnetization were agreed within (1 – 2) K. It was found that Curie temperatures nonlinearly decrease, and excessive enthalpies and entropies of phase transitions nonlinearly increases with an increase in the barium content in the samples (with the increase in x). It was found that the Debye cube law does not hold for the heat capacities of solid solutions at temperatures below 15 K. These anomalies were most likely caused by non-cooperative magnetic transformations and indicated the realization of the superparamagnetic state in double perovskites. Standard thermodynamic functions of the samples were calculated in the range (0 – 370) K from the data obtained.

Acknowledgment

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Synthesis of nanosized Cu, Co and Ni stabilized by poly-5-vinyltetrazole

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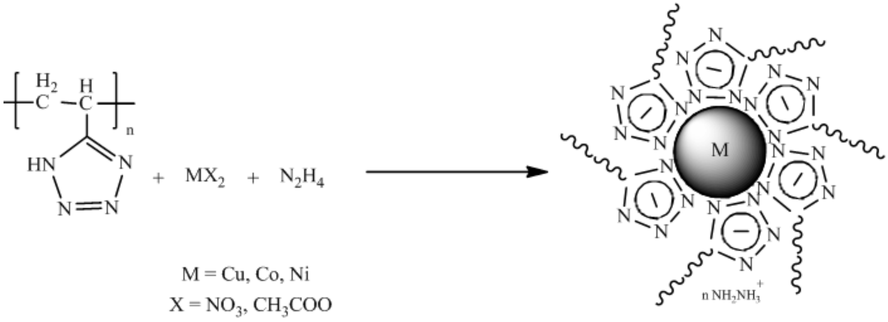
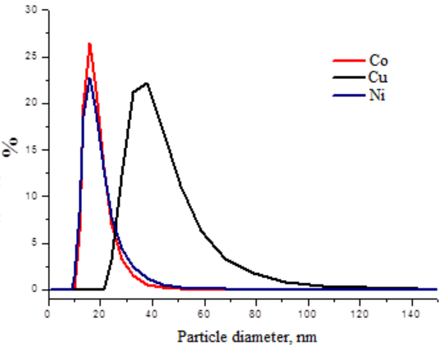
Within the framework of this research, we studied the possibility of using poly-5-vinyltetrazole (PVT) to obtain stable solutions of nanodispersed Cu, Co, and Ni. As a result, it was found that the reduction of the salts of the above metals ($Cu(CH_3COO)_2$, $Cd(NO_3)_2$, $Ni(NO_3)_2$) in an aqueous solutions of hydrazine in the presence of PVT leads to the formation of aqueous solutions of nanodispersed Cu, Co and Ni. Confirmation of the participation of precisely PVT molecules in the stabilization processes of the obtained nanodispersed metals are the results of blank experiments carried out under similar conditions, but in the absence of PVT, and leading to the production of finely dispersed precipitates of these metals. Most likely, the stabilization of the obtained metal nanoparticles occurs due to the interaction of their surface with the tetrazolyl fragments of PVT.



M = Cu, Co, Ni
X = NO_3, CH_3COO

According to the measurements, the diameter of the synthesized nanoparticles is predominantly laying in the range of 20 - 100 nm for Cu and of 10 - 40 nm for Co and Ni.



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Thermal behavior and dielectric properties of $Bi_2CaNb_{2-x}Fe_xO_{9-\delta}$

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Solid solutions of $Bi_2CaNb_{2-x}Fe_xO_{9-\delta}$ were obtained by the method of solid phase synthesis. The thermal analysis of the samples revealed diffuse low- and high-temperature exo-effects in the DSC curves in the temperature ranges of 493–673 K and 1123–1223 K. According to the high-temperature X-ray diffraction results, the exothermic effect in the range of 1123–1223 K is related to ferroelectric phase transition from polar (A21am) to nonpolar phase (I4/mmm). The high-temperature X-ray diffraction detected no reconstructive phase transitions in calcium bismuth niobate or its solid solution in the low temperature range of 493–673 K. The study of the electrical properties of $Bi_2CaNb_{2-x}Fe_xO_{9-\delta}$ samples ($x = 0.06$ and 0.10) showed that the substitution of niobium with iron led to the increase in the direct current electrical conductivity of the sample. In this case, the dielectric loss decreased and the dielectric permittivity increased. The studied solid solutions were characterized by the low-frequency ion-migration polarization. The radical change in the electrical characteristics including the almost double activation energy growth, the maxima of the LF and HF relaxation times and the maximum of polarization inhomogeneity were observed at the temperatures of 573–598 K. That was probably caused by the phase transition accompanied by activation of oxygen ions. Thus, the impedance spectroscopy and thermal analysis data correlate well pointing the reproducibility of the low-temperature effect recorded by the thermal analysis methods.

Mn doped $BiNbO_4$ ceramics: phase transitions, magnetic properties, NEXAFS and EPR spectra

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Magnetic susceptibility, NEXAFS and ESR of solid solutions $BiNb_{1-x}Mn_xO_{4-\delta}$ in triclinic and orthorhombic modifications have been studied. The reversibility of the phase transition from the high-temperature triclinic modification to the orthorhombic one has been revealed by means of magnetic dilution and X-ray phase analysis on the example of polycrystalline samples of the solid solutions $BiNb_{1-x}Mn_xO_{4-\delta}$ [1]. The manganese-containing $BiNbO_4$ solid solutions were obtained at $x \leq 0.06$. The ESR spectra of solid solutions in triclinic modification revealed sextet structure of Mn(II) ions with 8.4 mT splitting and some features at $g = 3.80$ and 1.47, and a broad diffuse band with $g \sim 2.2$ having a sextet with 8–9 mT splitting and $g = 2.0$ against its background. The parameters of exchange interactions in dimers and the distribution of manganese atoms (II), (III) and (IV) of $BiNb_{1-x}Mn_xO_{4-\delta}$ in triclinic and orthorhombic modifications have been calculated depending on the concentrations of the solid solutions. The solid solutions $BiNb_{1-x}Mn_xO_{4-\delta}$ as well as iron oxides MnO, Mn_2O_3 and MnO_2 were studied by the NEXAFS spectroscopy in order to determine the degrees of oxidation of iron atoms. The analysis of the NEXAFS Mn2p-spectra of manganese-containing solid solutions and oxides revealed that the studied Mn atoms were mainly in the (II), (IV) oxidation state.

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Conductive composites based on copper- and nickel-containing powders deposited from solutions instead of silver pastes

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Conductive silver pastes and adhesives are used to produce electrical contacts and conductive elements in printed circuit boards, display panels, electrodes of capacitors, etc. [1]. Silver particles are the main conductive component in them providing high electrical conductivity and corrosion resistance. Due to high cost of silver, it is important to replace Ag with cheaper metals. The substitution of Ag with Cu is impossible because of the rapid copper oxidation in the air and a loss of electrical conductivity. Ni is significantly more resistant to corrosion, but has four times less electrical conductivity than Cu. The electrical conductivity of Zn and Ni has close values, but zinc loses its conductibility being covered with an oxide layer in the air. The purpose of this work was to obtain a conductive composite, which is a polymer matrix filled with copper or nickel-containing bimetallic ultrafine particles with a core–shell structure instead of silver powder.

Cu–Ni powder was synthesized by chemical deposition of nickel shell on copper particles for their corrosion protection. Zn–Cu and Zn–Ni powders were obtained by copper or nickel cementation with zinc powder [2]. Zn core performed the function of Cu or Ni cathodic protection against corrosion. In addition to the metal powder, thermally splitted graphite (TSG) was added to the polymer during the paste preparation. TSG plates arranged metal particles in a conductive frame. The resulting paste was applied to a glass surface in the form of strips 60−90 μm thick, simulating electrically conductive elements. The results of measuring their bulk resistivity are presented in the Table. The data show that polymers filled with only copper are non-conductive. The presence of Cu–Ni, Zn–Cu or Zn–Ni powders together with TSG in the polymer matrix provides a decrease of coatings' resistivity to about 3.6−5.1 kΩ·mm^2/m. Their resistance does not change during storage for six months or more.

Bulk resistivity (ρ_V) of metal−polymer composites

Filler	ρ_V, kΩ·mm^2/m
TSG	106
Cu	10^6
Cu + TSG	17.4
Cu–Ni (5 wt.% Ni) + TSG	3.7
Zn–Cu (98 wt.% Cu) + TSG	5.1
Zn–Ni (80 wt.% Ni) + TSG	3.6

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Metal hexacyanoferrates as cathode materials for Zn-ion batteries

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Transition metal hexacyanoferrates (MeHCF) of general formula $A_xMe_y[Fe(CN)_6]_z{\cdot}nH_2O$ (A – alkali metal cation, and Me^{2+} = Mn, Fe, Co, Ni, Cu, Zn, etc.) have an open type channel crystal structure with the size of the channel sufficient for reversible intercalation of Zn^{2+} cations. This makes MeHCF promising cathode materials for zinc-ion batteries (ZIBs) [1, 2, 3].

In this work we synthesized potassium-vanadyl hexacyanoferrate (VHCF), copper(II) hexacyanoferrate, potassium-manganese (II) hexacyanoferrate, cobalt (II) hexacyanoferrate, and manganese (II) hexacyanoferrate and compared their electrochemical behavior in 1M aqueous solutions of $ZnSO_4$.

The cyclic voltammetry of all the MeHCFs in zinc sulfate solutions showed at least two cathodic and (or) anodic peaks. The variation of the transition metal (V, Cu, Ni, Co) in the hexacyanoferrate enables the battery voltage adjustment by the redox potential of the corresponding half-reaction that involves different valence states of the d-element.

VHCF is not well described in the literature, though the variety of available vanadium oxidation states may result in considerably high material specific capacity. Thus we studied its electrochemistry in greater detail, using both aqueous and non-aqueous zinc salt electrolytes. The specific capacity of VHCF cathodes reaches 43 mAh/g in 1M aqueous solutions of $Zn(CF_3SO_3)_2$, while the capacity in 1M $Zn(CF_3SO_3)_2$ solution in acetonitrile was found to be only 20 mAh/g which indicates a significant role of protons in the process of charge storage in aqueous VHCF-based ZIB. The cyclability of VHCF in acetonitrile-based electrolyte was found to be better than that in aforementioned aqueous 1M $Zn(CF_3SO_3)_2$ electrolyte. The usage of concentrated zinc salt solution helps to improve cyclability of aqueous VHCF-based ZIB.

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Synthesis, structure and magnetic properties of $Mn_xFe_{3-x}O_4$ (x = 0,1 – 0,6) for magnetorheological liquids

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Ferrimagnetic micro- and nanoparticles are used as a functional component of magnetorheological fluids (MRF) for magnetically controlled devices. When searching for such materials, high values of the specific magnetization of powders, low values of the coercive force, as well as a high value of shear stress in suspensions based on magnetic particles upon application of a magnetic field are important [1]. A series of powders of Mn-substituted magnetite $Mn_xFe_{3-x}O_4$ (x = 0.1 – 0.6) was synthesized by the method of coprecipitation from aqueous solutions of salts. Powder of composition $Mn_{0.3}Fe_{2.7}O_4$ showed high values of shear stress in magnetorheological suspensions. The particle size of the powder did not exceed 200 nm. It has been established that it is possible to change the magnetization and coercive force of powders by changing the degree of substitution, with the maximum magnetization corresponding to a powder of composition $Mn_{0.3}Fe_{2.7}O_4$. The high value of the shear stress (2 kPa) at a relatively low magnetic induction (~ 650 mT) allows the obtained material to be considered a promising functional filler for magnetorheological fluids (Fig.).

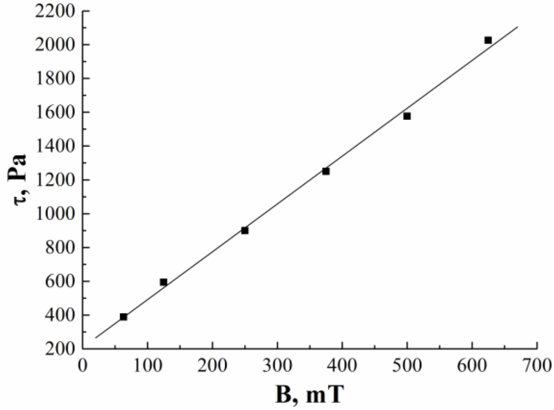

Fig. Dependence of the shear stress of the MRF containing 20 wt.% $Mn_{0.3}Fe_{2.7}O_4$ magnetic particles in Mobil 22 oil on the shear rate in a magnetic field at a shear rate of g = 200 s^{-1}, T = 20 ˚C

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Nuclear magnetic resonance relaxation efficiency of $Mn_{0.3}Fe_{2.7}O_4$ magnetic nanoparticles

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From a series of magnetic nanoparticles of Mn-substituted magnetite $Mn_xFe_{3-x}O_4$ (x = 0.1 – 1.8) that previously were described in [1] the powder of composition $Mn_{0.3}Fe_{2.7}O_4$ showed the highest value of saturation magnetization of relatively unsubstituted magnetite. MNPs $Mn_{0.3}Fe_{2.7}O_4$ were stabilized in the form of colloidal solutions using a number of polyelectrolytes, such as poly(diallyldimethylammonium chloride) (PDDA), chitosan 60 kDa (CH60), copolymer of chitosan 60 kDa and polyethylene glycol 5 kDa ($\chi = 0.15$) (CH60-PEG), copolymer of chitosan 60 kDa and dextran 6 kDa ($\chi = 0.15$) (CH60-DEX) and silica (SiO_2). Nuclear magnetic resonance relaxation of protons in aqueous solutions of $Mn_{0.3}Fe_{2.7}O_4$ stabilized nanoparticles has been investigated (Table).

Table. Physicochemical characteristics of $Mn_{0.3}Fe_{2.7}O_4$ magnetic nanoparticles stabilized by different reagents

MNP composition	Z_{av}, nm	PdI	d_{HD}, nm	Relaxation efficiency, $l\cdot mmol^{-1}\cdot s^{-1}$		r_2/r_1
				r_1	r_2	
$Mn_{0.3}Fe_{2.7}O_4$/PDDA	86,4 ± 0,8	0,153 ± 0,021	68,1	11,7	89,9	7,68
$Mn_{0.3}Fe_{2.7}O_4$/CH60	195,5 ± 1,3	0,294 ± 0,032	78,8	—	61,5	—
$Mn_{0.3}Fe_{2.7}O_4$/CH60-PEG	220,6 ± 3,4	0,241 ± 0,021	68,1 141,8 w	12,3	129,0	10,5
$Mn_{0.3}Fe_{2.7}O_4$/CH60-DEX	214,3 ± 1,3	0,178 ± 0,033	190,1	12,5	135,5	10,8
$Mn_{0.3}Fe_{2.7}O_4$/SiO_2	48.13 1000 (0,1%)	0,247 ± 0,024	—	13,8	105,2	7,62

w – weak intensity

Measurements of spin-relaxation properties have shown that nature of the dispersion stabilizer in most cases has little effect on the relaxation parameters (r_1 and r_2). Typical contrast agents with a r_2/r_1 ratio of 2 to 40 are treated as T_2-contrast agents, while for T_1-contrast agents this ratio is less. The resulting dispersion has a sufficiently high contrasting ability for magnetic resonance studies.

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Theoretical limits of basicity in condensed state and in gas phase

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Brønsted superbases have wide applications in organic chemistry because of their capability to activate C—H bonds [1]. The strongest known neutral Brønsted bases are substituted aminophosphazenes developed in late 1980's by Reinhard Schwesinger [2], their gas-phase basicity surpasses 1200 kJ/mol. Since that time many researchers have been designing even stronger bases, but none of them have been produced experimentally.

In this work, the reasons of instability of very basic compounds are investigated by means of high-level quantum-chemical calculations. Hexamethylphosphoramide is proposed as a reliable ionizing solvent for superbases covering 60 units of pH, while cyclopentane is proposed as a non-ionizing solvent with extremely low acidity. Three novel stable neutral superbases are designed and studied along with metastable and anionic structures possessing record-breaking basicities.

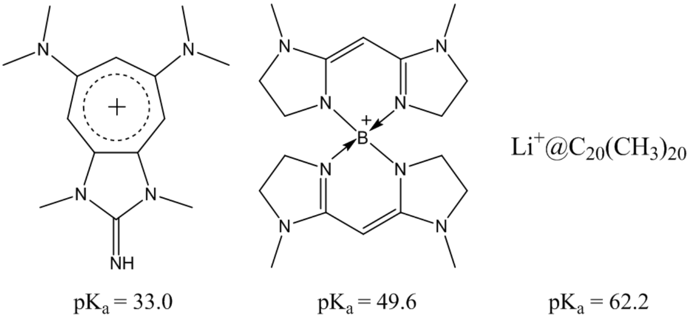

Fig. Protonated forms of proposed bases and their predicted pK_a values in HMPA

It is found that the base $Li@C_{20}(CH_3)_{19}CH_2$ appears to be close to basicity limit in the solution. Gas phase basicity limit for neutral molecules is probably reached by K_3N (1400 kJ/mol) in terms of Brønsted equilibrium; neutral structures that are metastable against self-deprotonation easily surpass gas-phase basicity of 1700 kJ/mol. Anionic species like $K_2F_5^{3-}$ could reach values beyond 2000 kJ/mol, while structures that decompose upon protonation could have no basicity limit at all.

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Thermostable heat-insulating materials based on solid phosphate binders and hollow microspheres

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Liquid phosphate binders are widely used for the manufacture of inorganic heat-resistant composites [1]. However, the liquid binders have several drawbacks and one has to face with some difficulties: over time, crystallization and polycondensation processes occur in solution. This leads to a significant complication of the subsequent technological operations.

The use of solid phosphate binders makes it possible to apply in practice a more advanced technology of dry building mixtures, which ensures the production of high quality target products based on them. The literature and investigations in which solid binders have been employed are very few and such works are related to a narrow range of compositions [2, 3].

Inorganic hollow microspheres (HMS) are one of the promising fillers for thermostable heat-insulating materials (THIM) [4]. During the traditional process of composition preparation by the mixing of lliquid phosphate binders with solid abrasive fillers (corundum, chamotte, etc.) the destruction of HMS occurs. This fact leads to a decrease of HMS efficiency utilization for obtaining. Therefore, in this work we used the technique of the mixing solid binder and fillers in an air-suspended state, which practically does not lead to the destruction of hollow microspheres. In present research, $Mg(H_2PO_4)_2\cdot4H_2O$ was used as a solid phosphate binder, the main filler was a mixture of Al_2O_3(M5) and AlN. Ash HMS and glass HMS were used as a functional fillers.

As a result, the optimal formulations of heat-insulating composites have been developed. It has been found that the content (wt. %) of the main filler is 10–15, and the content of $Mg(H_2PO4)_2{\bullet}4H_2O$ varies in the range from (15–20) for THIM based on ash HMS to (60–70) for THIM based onaglass HMS. The values of the compressive strength and density for the developed composites based on ash microspheres reach 2.5–5.5 MPa and 0.5–0.8 g/cm^3, respectively; for the composites based on glass microspheres these values are 1.0–2.5 MPa and 0.4–0.6 g/cm^3.

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Adaptive lubricants based on metastable molybdenum oxide intercalated with benzotriazole

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The metastable transition metal oxides of lamellar structure (*h*-MoO_3, *h*-WO_3, layered V_2O_5) represent promising lubricant materials capable to diminish radically the coefficient of friction both under dry sliding condition [1] and as the additive to the oil used to reduce the adverse impact of the mechanical load on the friction parts of machines. Thus, the coefficient of friction measured at the pressure in the friction zone of 2.5 MPa decreases two-fold (from 0.08 to 0.04) when 0.01 wt.% *h*-MoO_3 is added to the oil. It is seen from Fig. 1 that the coefficient of friction increases with pressure peaking at *ca*. 5 MPa and then exhibits gradual decrease that can be attributed to the dispergation (stratification) of oxide particles under high pressures. The oxide lubricants added to the oil thus behave as the adaptive antifriction material sensitive to the mechanical load. The layered structure of MoO_3 facilitates the loading of oxide particles with bezotriazole (BTA) known to be an effective corrosion inhibitor. The BTA molecules intercalated into the MoO_3 host during the course of polycondensation synthesis of matrix oxide create only weak links between the lamellae and MoO_3:BTA particles thus retaining antifriction properties. On the other hand, being a source of corrosion inhibitor, the MoO_3:BTA particles effectively suppress the tribocorrosion which is known to be an important cause of wearing.

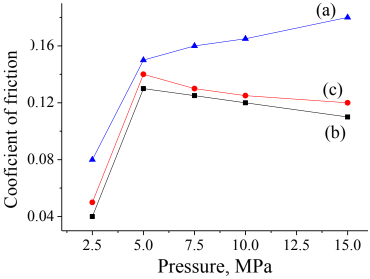

Fig. Dependence of a coefficient of friction on the pressure in the friction zone for oil lubricant: (a) bare; containing (b) MoO_3; (c) MoO_3:BTA. Oxide loading: 0.01 wt.%.

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Hydrothermal crystallization in the natural mineral of Nakhchivan – LiOH + LiCl system

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Hydrothermal synthesis was carried out in the natural mineral of Nakhchivan – LiOH + LiCl system. Hydrothermal synthesis was carried out in Mory type autoclaves with a volume of 18 cm^3, autoclave filling factor F = 0.8. The hydrothermal crystallization experiments were carried out without creating a temperature gradient and without mixing the reaction mass. The ratio of solid to liquid is 1:10. A natural sample was taken from a zeolite-containing horizon in the northwest of the Kyukyuchay River, where its content varies between 75–80%. The samples were Nakhchivan zeolite tuffs, 78.5% of which is the main mineral - mordenite ($Ca_2Na_2K_{2.8}Al_{8.8}Si_{39.2}O_{96} \cdot 34H_2O$), 19.5% quartz ($SiO_2$) and 2.00% anorthite ($Ca_{0.86}Na_{0.14}Al_{1.94}Si_{2.06}O_{8.01}$). The sample was thoroughly washed with distilled water and dried at 100°C for 3 days. The zeolite phase was identified by X-ray diffraction (2D PHASER «Bruker» (CuK_α radiation, $2\theta=20–80^0$)) and elemental (Launch of Trition XL dition refrigerator – Oxford instrument) analysis methods. Hydrothermal crystallization was studied under the following conditions: temperature - 100-300°C, LiOH concentration − 5-30%, LiCl concentration − 5-15%, processing time − 1-100 hours. X-ray diffraction patterns of crystallization products are shown in Fig.

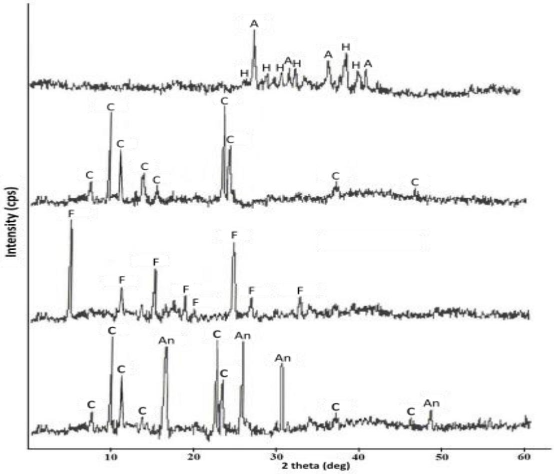

Fig. X-ray diffraction patterns of crystallization products in the natural Nakhchivan zeolite – LiOH + LiCl system (An-analcime, C-clinoptilolite, F-faujasite, H-hydrosodalite, A-albite)

Features of the process of propane dehydrogenation on $LnVO_3$ systems synthesized by solid-phase synthesis

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A number of studies [1] have shown that compounds containing vanadium can catalyze the dehydrogenation of light hydrocarbons and extend their service life. Therefore, the creation of catalytic systems containing both vanadium and rare earth elements is very promising.

The object of our study is the vanadites of rare earth elements of the composition $LnVO_3$ (Ln = La Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb Lu). Orthovanadates are formed by solid-phase high-temperature interaction of stoichiometric amounts of V_2O_5 and REE (III) oxide according to the reaction:

$$V_2O_5 + Ln_2O_3 = 2\ LnVO_4$$

$$LnVO_4 + H_2 = LnVO_3 + H_2O$$

In the thermal cracking of propane, the formation of products began above 773K, and at 873K the conversion was only 2%. In addition to shifting the degree of half conversion to lower temperatures, the selectivity for olefins in comparison with thermal cracking also changes (Figure1). In the case of catalytic cracking in the temperature range 623–1123 K, the yield of olefins increased.

The yield of target products of ethylene and propylene increases from lanthanum to gadolinium, and then declines.

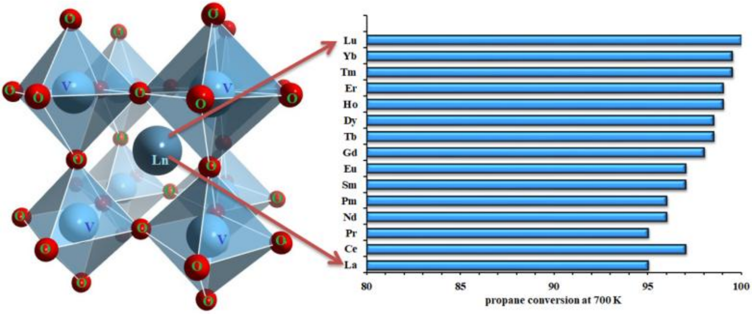

Fig. propane dehydrogenation on $LnVO_3$ systems

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Electrospark purification of waste waters from heavy metals

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Studies on the purification of multicomponent galvanic effluent by the electro-spark method using metal loading (Fe, Al) and low-voltage (up to 1000 V) equipment have been carried out. It is shown that the degree of purification depends on the specific energy of processing, the height of metal loading in the reactor, and practically does not depend on the energy of the pulse and the rate of its input into the liquid being processed (Fig.). The concentrations of heavy metals such as Ni(II), Zn(II), Cr(VI), Cr(III), Cu(II), Fe(II, III) in the treated water are significantly lower than their MPC values regulated in developed countries.

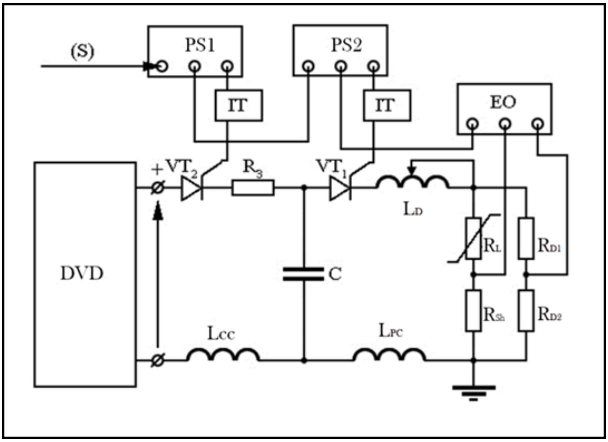

Fig. The electrical circuit of the experimental low-voltage source of discharge currents

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Theoretical insights into the low-lying states of the RaF molecule promising for laser cooling

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Ultracold polar molecules offer prospects for the creation of the molecular Bose-Einstein condensate with possible applications for quantum information and precision measurements [1].

Recently [2, 3], it was shown that radium fluoride RaF is a promising candidate for the direct laser cooling in order to use it for measuring molecular parity violation. According to the *ab initio* FS-CCSD calculations [3], the equilibrium internuclear distances for the ground and first excited states of the RaF molecule almost coincide, which provides high values of the diagonal FCFs.

In this study, *ab initio* state-of-art calculations at the FS-CCSD level of theory of the low-lying potential energy curves (PECs) of the RaF molecule were performed for the first time (Fig. 1). The PECs and spectroscopic parameters were calculated for the following low-lying RaF terms: ground state $X^2\Sigma^+$, and excited states $A^2\Pi_{1/2}$ (T_e= 13298 cm^{-1}), $B^2\Delta_{3/2}$ (T_e= 14988 cm^{-1}), $A^2\Pi_{3/2}$ (T_e= 15332 cm^{-1}), $B^2\Delta_{5/2}$ (T_e= 15745 cm^{-1}), and $C^2\Sigma^+$ (T_e= 16628 cm^{-1}). The results of our calculations are in excellent agreement with experimental values [2].

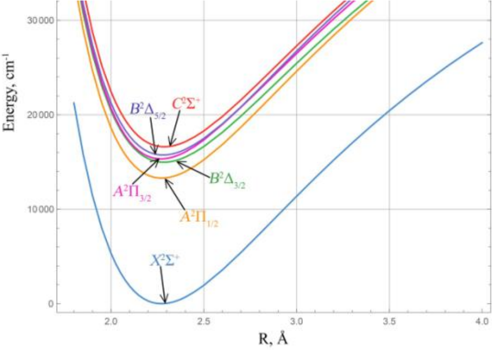

Fig. The PECs of the low-lying doublet states of the RaF molecule.

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Direct synthesis and isolation of complex compounds of Cu(II) nitrate and thiocyanate with 1-ethyltetrazole

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This work presents the results of the direct synthesis of complex compounds (CC) based on the interaction of 1-ethyltetrazole (L) with copper metal powder (Cu^0) in the presence of ammonium salts: NH_4X, where X = NO_3^-, NCS^-. The synthesis of CC was carried out in the medium of lower alcohols (methyl or ethyl) or acetonitrile. It was found that the best solvent for the synthesis of CC with a maximum yield (up to 70 %), in the case of NH_4NO_3, is a mixture of alcohols with triethyl formate in a volume ratio of 5:1, and for ammonium rhodanide – acetonitrile. The synthesis of CC was carried out by heating the reaction mixture to 60 °C with active mixing in the presence of oxygen in air. It should be noted that with the active bubbling of air through the reaction mixture, the dissolution time of copper metal powder (Cu^0) is reduced by about two times. As a result of the slow concentration of solutions in air at room temperature, fine-crystalline complexes are formed, which are separated by filtration, washed and dried in air. Six previously undescribed CC of the composition: CuL_nX_m, where X = NO_3^-, n 1; 3; 4; 6; m=2 and where X = NCS^-, n = 2; 6; m = 2 were synthesized and characterized. The isolated complex compounds were characterized by the methods of elemental analysis. $Cu(NO_3)_2L_n$ with n = 1 and 3 are linear polymers, while with n = 2 and 6 they are complexes of the molecular (island) type. Similarly, in the case of complex compounds of copper rhodanide: $Cu(NCS)_2L_2$ is chain-type compound, and $Cu(NCS)_2L_6$ is island-type complex.

Composite materials on the base of zeolite, clay minerals and highly dispersed silica

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Natural alumosilicates are perspective materials for using in different fields. Structure of these materials as well as variety of active sites makes the special properties connected with adsorptivity and possibilities of forming complex composite systems. That is why using them as adsorbents, “conteiners” for culture media and recurparation of soils needs researches in structure formation of multicomponent systems. Here afterwards the obtained results will contribute to determination of optimal mass transfer of components in dependence on functional purpose of composite material.

The aim of the research was directed to creation of highly function material being the support of BAS (bioactive substance) on the base of natural silicates of alumina and highly dispersed silica, A300, formulation of secondary porosity of composites in dependence on the nature of introduce clay and relation between zeolite and clay, study of BAS delivery from obtained samples.

The kinetics of BAS release is controlled by the chemical nature of the surface and by the porosity of the carrier. Changing porosity and the surface area by using of aluminosilicate matrixes of different structures as carriers allows controlling the release of BAS, prolonging the term of their effective using. In addition to that fact these carriers allow to transport BAS. They have biocompatibility and bioavailability without causing allergic reaction.

Thus, the composite materials of clay / clinoptiolite / silica / vegetable raw materials, where the nature of the inorganic component and the presence / absence of solvent are varied, have been obtained. The dependence of BAS allocation on the structure and composition of the synthesized composite has been established.

Formation and thermal stability of neodymium hydroxychloride

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It is well known [1,2] that rare earth (RE) chlorides $LnCl_3$ form various hydrates with water which give on heating oxychlorides LnOCl and hydroxychlorides $Ln(OH)_2Cl$. All these compounds are very important for chemistry and technology of RE metals, because they are intermediate products in the metallurgy of these metals using a relatively low-temperature chloride technology. Thus on heating of $LnCl_3$ hydrates in order to obtain the necessary anhydrous chlorides, a complex system is formed that includes several solid phases, as well as a gas phase containing water vapour and hydrogen chloride in various ratios. In order to understand the chemical processes in such a complex system, the method of chemical thermodynamics can be effectively used, but this requires sufficiently reliable thermodynamic information about all the components of this system. Work [1] presents the results of a detailed study of formation and decomposition of the chloride hydrates and hydroxychloride of neodymium – one of the most widely used rare earth metal (strong magnets). The hydroxychloride decomposition temperature according to the reaction

$$Nd(OH)_2Cl(s) \leftrightarrow NdOCl\ s + H_2O(g)$$

was determined by the DTA method in the atmosphere of Ar, it is equal to 376 ° C.

However, the water vapour pressure was unknown in this case, apparently, it was very low. Its heat of decomposition, equal to 98.2 kJ /mol, was obtained by the DSC method. However, the latter value differs significantly from the value, corresponding to its enthalpy of formation, found in the dissertation work [2] by the method of dissolution calorimetry. In addition, the analysis of chemical equilibria carried out in [1] did not give an answer to the most important question – by which reaction and at what temperatures the intermediate compound $Nd(OH)_2Cl$ is formed. Therefore we recalculated the equilibria of $Nd(OH)_2Cl$ formation and decomposition reactions. These calculations are based on 2 experimental values: $\Delta H°_{649}$ of reaction (1), equal to 98.2 kJ /mol [1], and the decomposition temperature (669 K) of $Nd(OH)_2Cl$ at the water vapour pressure equal to 1 atm [3]; the approximate value of reaction (1) $\Delta Cp°$ (– 7.3 J/mol•K) was also used. These calculations may be useful for planning and explaining the results of subsequent scientific and technological investigations of such RE systems.

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Stability and activating ability of non-aqueous $SnCl_2$ sols

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We have shown [1] that with regard to chemisorption the ammonium-phosphate flame retardants on the surface of polyester fibers, alcohol solutions of $SnCl_2$ are more effective than aqueous solutions. It was found [1], that the Sn (II) oxidation in ethanol and isopropanol $SnCl_2$ solutions proceeds much more slowly, than in aqueous and aqueous-alcoholic solutions, and colloidal particles in their volume retain their optimal size and concentration much longer. In this regard, it has the considerable interest to study the regularities of Sn(II) oxidation and colloid formation in organic media with different chemical nature, especially acetone and glycol media. These media not only meet a number of conditions good solubility of Sn(II) salts, reduced oxygen solubility, assumed stability with respect to oxidation and hydrolysis of Sn(II) compounds but also able to partially disrupt the surface structure of polyester fibers [2].

As a result of the comparative studies the stability of tin-containing colloidal systems in various organic media, the factors, defining their ability to activate the surface of the polyester matrix in relation to the fixation of an inorganic nitrogen-phosphorus-containing combustion retardant, have been established. It has been proved that a necessary condition for fixing the flame retardant on the polyester surface is the formation of numerous homogeneous colloidal particles with sizes not exceeding 20-25 nm in the volume of the $SnCl_2$ activating solutions.

This condition observed for acetone, water-acetone and ethanol SnCl2 solutions. It should that colloidal particles in the volume of acetone solutions of SnCl2 retain their optimal sizes (5-25 nm) much longer (~1.5-2 times) than in ethanol media, and acetone solutions retain their activating ability in relation to the flame retardant treatment much longer: up to 70 days. In the volume of ethylene glycol and water-glycol solutions, large particles with sizes from 30 nm with an insignificant concentration are formed, which do not show activity in relation to the flame retardant treatment of PET.

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IR absorption spectra of (2–*X*)MgO·*X*(MnO, FeO)·$2Al_2O_3$·$5SiO_2$ (*X*=0–2) ceramic materials

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An magnesium aluminosilicate $Mg_2Al_4Si_5O_{18}$ is a high thermal stability and electrical insulating ceramic material (cordierite). $Mg_2Al_4Si_5O_{18}$ is commonly synthesized at temperatures from 1350 to 1450°C. We examined the effect of MnO and FeO modifiers on the processes of phase formation in the $2MgO\cdot 2Al_2O_3\cdot 5SiO_2$ system [1]. (2–*X*)MgO·*X*(MnO, FeO)·$2Al_2O_3$·$5SiO_2$ (*X*=0–2) ceramic materials were prepared through partial (*X*<2) or complete (equimolecular *X*=2) substitution of MnO or FeO for MgO in a magnesium aluminosilicate system. Samples were synthesized using standard ceramic technology at temperatures of 1050–1250°C [2]. The study is aimed at analyzing the phase structure in the studied system by IR spectroscopy method (Nexus Fourier transform IR spectrometer Thermo, USA). The IR spectra of the materials studied show many absorption bands in the range 400–1300 cm^{-1}. The strongest band, situated at 920–1198cm^{-1}, is mainly due to the asymmetric and symmetric modes of the tetrahedral bond Si–O–Si, common to all silicates. At a sintering temperature as low as 1100°C for the manganesecontaining samples and 1150°C for the ironcontaining samples, the spectra show well defined absorption bands characteristic of rings of [SiO_4]-tetrahedra in the structure of silicates: a strong doublet in the range 912–1180 cm^{-1}, due to the asymmetric stretching mode of the Si–O–Si bond of the [SiO_4]-tetrahedral group. The “ring” band at 766–770 cm^{-1} and the band at 572–578 cm^{-1} are attributable to the formation of six tetrahedras, [Si_6O_{18}] or [Si_5AlO_{18}], characteristic of the $Mg_2Al_4[Si_5AlO_{18}]$, $Mn_2Al_4[Si_5AlO_{18}]$, and $Fe_2Al_4[Si_5AlO_{18}]$ silicates, which have a ring structure of the silicon–oxygen radical, and of their solid solutions. Mn^{2+} and Fe^{2+} substitution for Mg^{2+} influences the distortion of the tetrahedra, their spatial arrangement, and the shift of the bands characteristic of $Mg_{2-y}Mn_yAl_3[Si_5AlO_{18}]$ and $Mg_{2-y}Fe_yAl_3[Si_5AlO_{18}]$ to lower frequencies (1167, 1147, 950, 912, 766, 614, 575 and 1162, 1145, 950, 900, 726, 611, 558 cm^{-1}) relative to the absorption bands of $Mg_2Al_4[Si_5AlO_{18}]$ (1180, 1147, 955, 914, 770, 616, and 577 cm^{-1}). The bands at 1164, 1126, 1084, 950, 738, and 557 cm^{-1} in the spectrum of material were prepared through complete (*X*=2) substitution and synthesized at 1100°C are attributable to the formation of rings of four tetrahedras, [Si_4O_{12}] or [Si_3AlO_{12}], in the structure of $Mn_3Al[Si_3AlO_{12}]$. The IR spectroscopy results are consistent with the XRD data and indicates that MnO and FeO accelerate the phase formation of $Mg_{2-y}(Mn, Fe)_yAl_4Si_5O_{18}$, which is similar in XRD pattern to $Mg_2Al_4Si_5O_{18}$ [2].

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Crystal structure priority controlling topochemical reactions

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Having a topochemical transformation reproduced is the evidence of regularity in the succession of crystal structures of the reagent and the reaction product. The symmetry of the crystal structure can lower not only as a result of topochemical recrystallization but also due to the crystal deformation. Hence, the deformational dissymmetrization can promote the topochemical process or suppress it.

If the reagent crystal has perfect cleavage, then its surface reactivity depends on its topochemical affinity with the reaction product. If the reagent cleavage is imperfect, then the surface reaction outcome is determined by crystallochemical barriers, i.e. the restrictions of positions for structural units that are imposed on those units by the lattice symmetry. In their turn, these restrictions determine "the structural preferences" of the crystallizing phase. The preferences of that kind can be characterized quantitatively by crystallochemical priorities of Fedorov groups, i.e. by relative frequencies of Fedorov groups in crystal structures. Correspondingly, there are primary and rare Fedorov groups of crystal structures. Paradoxal kinetic stability of thermodynamically unstable crystal phases is provided by their structure being of primary (i.e. most probable) type. On the other hand, forming a crystal structure of a rare (i.e. highly unlikely) type is possible only on condition of themodynamical stability of the structure because the rarity of a Fedorov group indicates a low "crystallochemical feasibility" of the corresponding structure.

If the structures of the reagent and the reaction product are meroedrically related then an external mechanical effect can facilitate the reaction or suppress it. The result is determined by the balance of crystalline phase specific volumes before the reaction and after it. The relative frequency of the space group of a structure can be used as an auxiliary criterion for evaluating the credibility of that space group. Fedorov space groups with relative frequencies fewer than 0,5% should be considered as extremely rare ones. The rarity of the Fedorov space group of a insufficiently studied structure should be considered as an incentive for more meticulous analysis of the structure. This recommendation is especially insistent for compounds being advanced as single known representatives of a Fedorov space group.

Dispersing a crystal phase induces forming a structure with a higher crystallochemical priority. Likewise, baric effect promotes forming a structure with a more probable crystallochemical type.

Synthesis of phosphors based on strontium aluminates codoped with Ce^{3+} and Mn^{2+} ions

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In the present work, a comprehensive study of the preparative features of the synthesis (solid-phase and colloid-chemical) of luminescent strontium aluminates codoped with Ce^{3+} and Mn^{2+} ions was carried out. The influence of matrix composition ($SrO:Al_2O_3$ = 1:1 and 3:5), heat treatment temperature (900°C, 1300°C and 1500°C), and heating atmosphere (air and H_2+Ar) on the phase composition, morphology, and spectral-luminescent properties of the samples was studied by the XRD, SEM and photoluminescent analysis (emission and excitation).

It was found that the heating temperature has a significant effect on the luminescence intensity of the samples. At a temperature of 900°C, samples do not exhibit luminescence, and with an increase in the heating temperature to 1500°C, the luminescence intensity increases by a factor of 1.5–2, regardless of the matrix composition. Heat treatment in a reducing environment also has a positive effect on the luminescence intensity. It was discovered that during solid-phase synthesis for the samples obtained using $SrCO_3$, blue luminescence is observed, and when using $Sr(NO_3)_2$ – green luminescence, regardless of the matrix composition. Only for the samples obtained by the colloidal – chemical synthesis, heated at 1500 °C, phosphorescence is observed (Fig.).

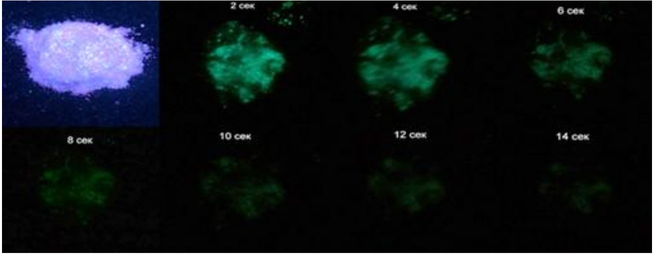

Fig. Photo of $SrAl_2O_4$: 1% Ce^{3+}, 0.1% Mn^{2+}sample after cessation of irradiation with an ultraviolet lamp (λ_{ex} = 312 nm, 10 min) depending on time of irradiation

The reasons for the influence of the studied preparative techniques and synthesis methods on the luminescent properties of the obtained samples will be discussed

Luminescent Films for Silicon Solar Cells

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Today, silicon solar cells (SSC) are still dominant, and improving their efficiency is an urgent task. Therefore, the search for systems that could effectively transform the sun ultraviolet (UV) radiation into SSC maximum spectral sensitivity region is important.

Earlier, we found [1, 2] that CuI-containing oxide films under UV radiation (λ_{max}=720nm) exhibit luminescence in the visible spectral range from 600 to 1000 nm; in the area of maximum photosensitivity of the SC. This work is devoted to the study of SSC efficiency amplification by applying on it an additional layer of luminescent oxide films containing CuI doped with rare earth ions, as well as films of phosphor $Sr_4Al_{19}O_{25}$:Bi, Mn.

It was found that the deposition of luminescent films does not have a negative effect on the dark electrical parameters of the SSC used; but an increase in the parallel resistance of the solar cell is observed, leading to an increase in the current supplied to the load. The largest increase in the external quantum efficiency of photoelectric conversion of solar cells in the near UV range is observed for single-layer films of the composition $50Al_2O_3 - 50CuI$, heat-treated at 280°C for 30 min, which corresponds to a relative increase in the photocurrent upon exposure to radiation with a spectral composition of AM 1.5 (1000 W/m^2) by more than 35%.

The obtained results confirm the efficiency of using luminescent oxide – CuI films to the SSC efficiency amplification.

Acknowledgment

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Influence of liquid-phase oxidation treatments on the purity and hydrophilicity of single-walled carbon nanotubes

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The practical use of single-walled carbon nanotubes (SWCNTs) is hindered by the fact that it is impossible to synthesize them pure (without amorphous carbon and impurities of the catalytic synthesis phase), not subjected to aggregation into bundles during the synthesis process and capable of being dispersed into individual molecules in polar solvents. In this work, we investigated the effect of liquid-phase oxidative treatments on the purification of SWCNTs from organic and inorganic impurities, their structural modifications with oxygen-containing groups for the formation of stable suspensions in polar solvents [1]. The following oxidizing reagents were used: hydrogen peroxide with following treatment of SWCNTs with hydrochloric acid or a mixture of concentrated acids (HNO_3/H_2SO_4) [2]. Treatments were carried out at 105-115 ^{0}C for 1 h using preliminary ultrasonic loosening of SWCNT bundles in surfactant solutions [3]. Finishing substances were studied for their ability to disperse in water, isopropyl alcohol and their mixtures. The structural features of SWCNTs, initial and subjected to oxidative treatment, were studied by transmission electron microscopy, Raman spectroscopy and infrared absorption. Their elemental compositions was studied by X-ray energy dispersive method. Studies have shown that bundles of SWCNTs, due to the adsorption layers of surfactants, are separated without destructive effects on the SWCNT structure when using treatment with an HNO_3/H_2SO_4 mixture (2: 1, vol.). This contributes to the formation of an array of SWCNTs, purified from amorphous carbon and inorganic impurities (the content does not exceed 1.0 wt.%), dispersible in water and an aqueous-alcoholic solution (9 : 1, vol.) with the formation of concentrated and stable suspensions. TEM images of SWCNTs are shown in the Fig.

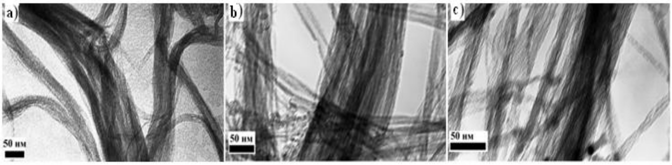

Fig. TEM images of SWCNTs: a – initial, b, c – after treatments respectively in solutions of H_2O_2 and HNO_3/H_2SO_4.

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Metal-organic framework/magnetite composites for electronic devices

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This study is devoted to the development of new composite materials, consisting of framework organometallic compound with magnetite nanoparticles, with potential application for cooling electronic devices using the approach described in [1].

Basolite A520 (aluminum fumarate) was synthesized according to [2]. It has a high specific surface area (1040 m^2/g), good water absorption (about 426 mg/g), a hydrodynamic particle diameter of about 340 nm and a ζ-potential of +20 mV. Two types of Basolite A520-based composites with a mass fraction of magnetite of about 7 % were obtained. The microparticles of the metal-organic framework coated with a $(polymer/magnetite)_6$ shell were obtained by layer-by-layer assembly [3]. The Fe_3O_4/BasoliteA520 composite in which magnetite nanoparticles are surrounded by a matrix of porous material was obtained by admixing them to one of reagents at the early stages of the synthesis. Microphotography of Basolite A520/PSS/$(PEI/Fe_3O_4)_6$ composite shows that the particles have an irregular shape and size from 0.5 to 2.5 microns. Small particles of magnetite are clearly visible on their surface. The FTIR_spectra of the samples have bands characteristic of Basolite A520 and magnetite. Both composites have pronounced magnetic properties.

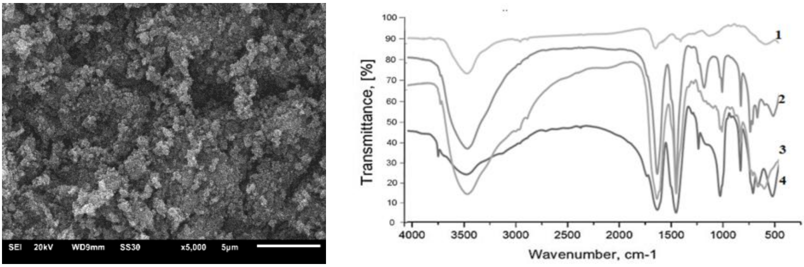

Fig. SEM microphotography of particles Basolite A520/PSS/$(PEI/Fe_3O_4)_6$ (a); FTIR spectra: 1 - Fe_3O_4,, 2 - Basolite A520, 3 – Basolite A520/PSS/$(PEI/Fe_3O_4)_6$, 4 – Fe_3O_4/Basolite A520 (b) .

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Luminescent properties of $SrAl_2O_4$:Bi_2O_4 phosphor

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Scientific interest in the luminescence of bismuth based materials has maintained a steady increase especially pronounced in the last four years [1]. Bismuth has an electronic configuration of $[Xe]4f^{14}5d^{10}6s^{2}6p^{3}$ yielding 5 valence electrons. The outer orbitals responsible for luminescence are unshielded and strongly influenced by the surrounding environment, so that their energies are host dependent, similarly to the case of the f-d transitions of Ce^{3+} and Eu^{2+} ions, which vary according to the host. This makes it possible for bismuth based materials to emit over a wide range of wavelengths. In previous studies [2, 3] for bismuth-dopant phosphors was noted luminescence from the ultraviolet to the infrared with a single rather narrow emission peak. We carried out a series of solid-phase syntheses of phosphors based on bismuth-doped strontium aluminate. Unlike the previously described methods, we used as a source of bismuth not Bi^{3+}, as usual, but the compound Bi_2O_4. Synthesized phosphor has full spectral multi-peak luminescence, which is highly promising for solid state luminescence, especially for single-source white light-emitting diodes [4].

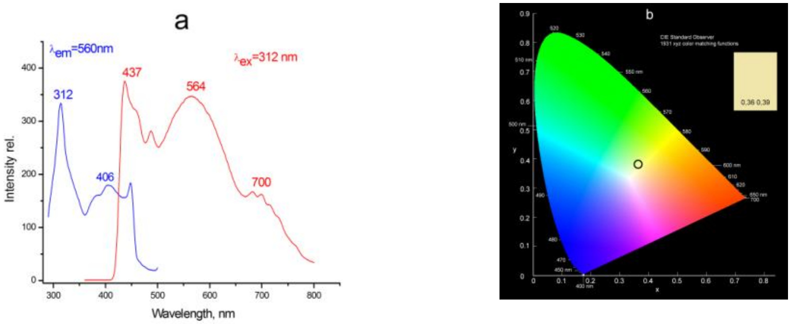

Fig. Excitation and emission spectra of phosphor $SrAl_2O_4$:Bi_2O_4 (a);
CIE chromaticity coordinates diagram of $SrAl_2O_4$:Bi_2O_4 luminescence (b)

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CHEMISTRY OF SURFACE AND THIN FILMS

Wear protection of silicon surfaces by Langmuir-Blodgett monolayers of saturated fatty acids

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The silicon substrate is the most common design element of micro-electro-mechanical devices (MEMS), used in production of micromotors, gyroscopes and accelerometers [1]. Its low wear resistance is a reason of incorrect operation and reduction of lifetime of devices [1, 2]. Therefore, increasing of the wear resistance of silicon surfaces is a considerate worldwide problem, which can be solved by usage of monolayer Langmuir-Blodgett (LB) films of saturated fatty acids, such as docosanoic (DA, $C_{21}H_{43}COOH$) and hexacosanoic (HA, $C_{25}H_{51}COOH$) acids, formed by horizontal precipitation [2] at a surface pressure of 30 and 18 mN/m, respectively, (phase state «solid film»). Linear microtribometer was used for the tribotechnical testing [2]. Testing conditions were: normal load of 1,0 N, 3 mm diameter steel ball as indenter, 3 mm stroke, linear speed of 4 mm/s [2]. It was found that the abrasive wear of the uncoated silicon surface occurs during 1 sliding cycle and after its modification with the DA and HA monolayer the silicon is failed within 356 and 567 sliding cycles, respectively (Fig.). The increase in the wear resistance of the modified silicon surface is due to the transfer of the DA and HA molecules between the rubbing surfaces [1, 2].

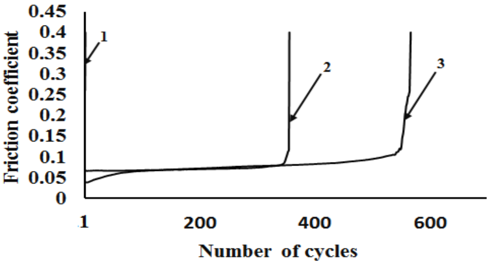

Fig. The friction coefficient as a function of number of sliding cycles:
1 - unmodified silicon surface; 2 – DA; 3 – HA

Thus, LB monomolecular films of DA and HA can be used as protective coatings in MEMS.

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The role of the crystallographic orientation of the oxide materialsin their gas sensing activity

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One of the tools to evaluate gas sensing properties of the oxide materials with a minimal empirical experimental search is molecular dynamics simulation [1]. It allows analyzing the interaction of the detecting molecule with the surface of gas sensing material and revealing the most energy-efficient contacts. The ability of the oxide surface to interact with the molecules of the detecting gas is essential in the forming of gas sensing properties.

It is obvious that the process of adsorption of the gas molecules at thermodynamically unstable oxide surfaces is more efficient in comparison with the adsorption at thermodynamically stable ones. The same statement comes from the analysis of the results of the molecular dynamics simulation of the interaction of CH_4, H_2, C_2H_5OH, and H_2O molecules with TiO_2 and MoO_3 atomic planes of {100} set [1]. The problem is that the existence of thermodynamically unstable planes in a large quantity in a real oxide material is unprofitable and highly improbable. This opens a problematic area of the aimed synthesis of the crystallographically oriented oxide materials.

In the work MoO_3 with the pronounced (010) orientation was synthesized by a simple and fast route by the heat treatment of the mixture of $(NH_4)_6Mo_7O_{24}\cdot 4H_2O$, oxalic acid, and Pluronic F-127 at 450 °C for 4 hours.

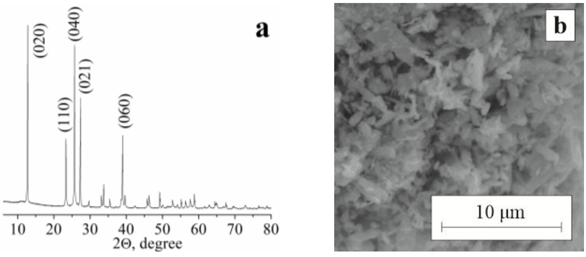

Fig. XRD pattern (a) and SEM image (b) of the oriented MoO_3

Molecular dynamics simulation showed that MoO_3 (010) atomic planes are perspective for the interaction with C_2H_5OH molecules. It was established that the output value towards ethanol of the semiconducting chemical gas sensors on the basis of "TiO_2 - oriented MoO_3" material is about 20 % higher than of the sensors based on "TiO_2 - spherical MoO_3", obtained by the calcination of $(NH_4)_6Mo_7O_{24}\cdot 4H_2O$ at 450 °C.

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Influence of the composition of gas-coke-forming systems on the fire-thermo-insulating properties of expandable composites

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The need for fire-thermo-insulating means that prevent the spread of fire through inter-storey polymer communications in the building sector is an incentive for the development of polymer thermo-foaming composite materials for fire-fighting preventive devices [1].

In order to obtain efficient economical thermally expandable composites (TECs) based on ethylene-vinyl acetate copolymer, a comparative study of the effect of the qualitative and quantitative composition of combustion retarders and inert mineral fillers on the thermal, physical-mechanical properties and fire-thermo-insulating ability of TECs was carried out.

It has been established that thermally split graphite (TSG) and / or a mixture "TSG–gas–coke–forming fire retardant system" provide the effect on increasing the efficiency of the fire-thermally insulating action of the silicate mineral filler. In the absence of a gas–coke–forming system (amine, metal- and / or phosphorus-containing compound), a comparable result in terms of fire resistance was obtained only in the case of a high filling of the composition with a silicate mineral. At the same time, a high content of heat-resistant mineral fillers (40–50%) in the absence of a fire-retardant system in the composition formulation leads to a decrease in the elasticity of the starting material and the strength of the thermally foamed coke residue. It has been shown that a set of satisfactory characteristics of TECs in terms of the required parameters (elasticity, foaming coefficient, mechanical strength of coke residue, total exothermic effect of DSC, flammability group, fire resistance limit) can be achieved by regulating the composition of the gas-coke-forming system and the ratio between the filler components.

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Colloidal silica slurries preparation by ion exchange method for microelectronics application

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Nowadays it is more often required processing of semiconductor wafers with a microrelief which does not exceed atomic scales. That is the reason of the intensive research for the development of new methods for their processing and materials for this purpose. The suspensions should be homogeneous by phase and elemental composition, high stable, easy in obtaining and application, cheap and environmentally friendly. The lack of systematic reviews and little amount of publications on this problem is explained by commercial interests [1-2]. Among the silicic dispersions silica sols attract more attention than aerosol ones.

We have synthesized silica sols by ion exchange technology. The formation of nuclei of sol silica particles with the following growth of colloidal size particles occurred by adding an acid to a dilute solution of waterglass. Waterglass was diluted to a SiO_2 concentration of 3÷5 mass. % and passed through a column filled with ion-exchange resin: cation, anion exchanger and the mixture of them. The possibility of concentrating silica sols by evaporation and ultrafiltration were studied. Since silica sol is a dynamic system, this especially applies to freshly prepared silica sol, its particles undergo changes during their existence (Figure). The polymerization of silica in solution and the sols st

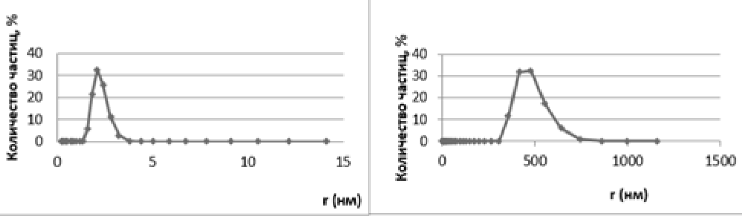

Fig. The particles size distribution of silica sol in 20 and 60 minutes after the preparation

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Gas sensitive materials based on tungsten oxide and graphenometallic composite

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Semiconductor metal oxides are widely used as sensitive elements of resistive-type gas sensors. The gas sensitivity of WO_3 with the addition of a graphene-metal composite was studied [1]. Using the methods of X-ray phase analysis, scanning and transmission microscopy, electron spin resonance, the structure and morphology of the composition of tungsten oxide with graphene were studied. Tungsten oxide was obtained by the sol-gel method, graphene – by solution combustion synthesis. A graphene-metal composite with a content of metal nanoparticles (Cu, Ni) no more than 25 wt.%) was injected into a tungstic acid gel (1.0; 2.0; 3.0; 4.0; 6.0 wt% in terms of WO_3) at the stage of drying the gel in air at $T < 100\ ^0C$. A large (5 or more times) increase in the sensitivity to gases of oxidizing (NO_2) and reducing (acetone, isopropanol) nature of the obtained composites was observed in comparison with the initial WO_3. The ESR study confirms the conclusions about structural disordering and the formation of a complex defect structure in the obtained material. The signals corresponding to a narrow line in the value of the g-factor are characteristic of electrone hole and their associates, radical anion forms of oxygen, and also for *F*-centers. A large increase in the concentration of paramagnetic defects in tungsten oxide is one of the direct reasons for an increase in their gas adsorption activity.

Other reasons for the increase in gas sensitivity are a decrease in the size of crystallites (and, as a consequence, an increase in the specific surface area) compared to WO_3, which does not contain an additive, as well as the presence of residual surface OH groups after annealing.

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Sorption of Zn^{2+} by poly-5-vinyltetrazole from aqueous solutions

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In continuation of our studies of the sorption properties of tetrazole-containing polymers [1], we explored the possibility of using poly-5-vinyltetrazole (PVT) to extract Zn^{2+} ions from dilute (0.0005–0.005 M) aqueous solutions of $ZnSO_4$. PVT samples with various content of tetrazolyl group were obtained by azidation of polyacrylonitrile. The sorption was carried out at room temperature under dynamic conditions using PVT powders with dispersion of 450–600 µm. After sorption, the quantitative content of Zn^{2+} cations in the final solution and the sorbent was determined. The obtained analytical data have good convergence, which confirms their correctness.

It was found that the sorption capacity of PVT towards Zn^{2+} cations increases with an increase in tetrazolyl group content in the sorbent. This shows that tetrazolyl moieties, included in PVT, participate in the ion-exchange sorption. The dependence of the sorption capacity of PVT on the concentration of Zn^{2+} cations in the solution indicates the equilibrium nature of the sorption (Fig.). "Sorption-desorption" equilibrium is achieved within 20 h under studied conditions. Taking into account the fact that the experimentally determined exchange capacity of PVT towards Zn^{2+} cations is about 20% of the theoretically possible one, it can be assumed that ion-exchange processes occur mainly on the surface of PVT particles. Regeneration of the sorbent can be achieved by treating it with dilute hydrochloric acid.

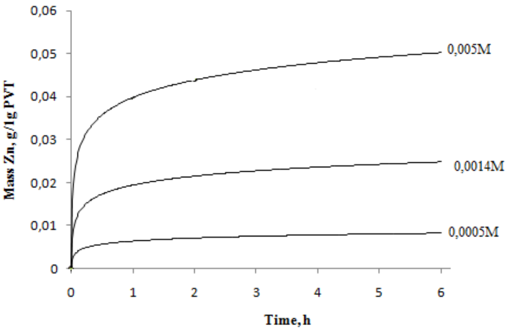

Fig. Sorption curves at various concentrations of Zn^{2+}.

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Preparation of silver nanoparticles in the presence of α-cyclodextrin

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Interest in silver nanoparticles (NPs) is unabated due to their unique physicochemical and antibacterial properties. However, there is an acute issue of directed growth of silver NPs or their targeted delivery. Therefore, the ability of α-cyclodextrin (α-CD) to influence on particles' shape or to penetrate into the cell and transport silver nanoparticles is currently in demand [1].

Silver nanoparticles (NPs) have been obtained by a modified Turkevich method [2]. Ag_2SO_4 of analytical grade was used as a precursor for NPs. Addition of Na_3Cit solution and α-CD was followed by pouring a freshly prepared solution of $NaBH_4$. The synthesized sol has been purified from byproducts by dialysis. The study of the obtained sol was carried out by UV-Vis spectroscopy, TEM, Zeta potential has been studied also.

As a result of the synthesis, along with spherical particles with a size of 7–14 nm, a great number of silver particles with clear cylindrical shape with a cross section of 10–12 nm and a longitudinal section of 5 nm were obtained. It can be seen on TEM images that cylindrical particles are separated from each other. The absorption spectrum of the colloidal solution shows a single peak at 400 nm. The observed flux value of zeta potential of the purified sol (from –21.9 mV to +23.6 mV) means that sol has high stability and resistance to aggregation.

It can be consumed that the reason for the inhomogeneous morphology of particles, lies in the high sensitivity of α-CD to the pH of the medium. Dissolution of $NaBH_4$ is accompanied by hydrolysis, that leads to a partial destruction of α-CD. It can be suggested that undestructed part of α-CD promoted the directed growth and stabilization of silver nanoparticles with cylindrical shape.

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Physical sorption between the molecule [4-(1,2,4-triazol-1-yl)-1-(2',3',5'-tri-O-acetyl-β-D-ribofuranyl)]uracil and CNT (12,12-8)

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Quantum chemistry seeks to accurately predict the chemical and physical properties of molecules and materials, useful in many fields and technology. Predicting chemical properties using an atomic scale approach is a theoretical and computational challenge. Quantum-chemical modeling of the spatial and electronic structure, physicochemical and chemical properties of known and atomic-molecular structures and their combinations is an effective method of chemical research. To carry out quantum-chemical calculations, computer facilities and quantum-chemical programs are needed, which are becoming more accessible and cheaper. The complexity of calculations is determined only by the atomic composition and the studied states of molecular systems. The calculations were performed using the ChemOffice 2016, Nanotube modeller, HyperChem 08, and Gaussian 09W software packages. During the work, we managed to find an energetically favourable complex between [4-(1,2,4-triazol-1-yl)-1-(2',3',5'-tri-O-acetyl-β-D-ribofuranosyl)] uracil and nanotube CNT (12,12-8).

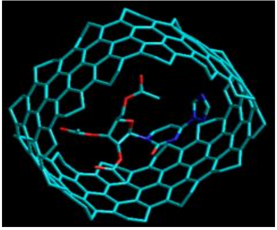

Fig. Complex between [4-(1,2,4-triazol-1-yl)-1-(2',3',5'-tri-O-acetyl-β-D-ribofuranosyl)] uracil and nanotube CNT (12.12-8)

The energies of the CNT (12,12-8) nanotube and the structural analogue of the pyrimidine nucleoside are 129.8 kcal/mol and 126.5 kcal/mol, respectively, that shows the stability of the system. Based on the data obtained, it can be assumed that the nanotube can theoretically act as a transfer agent, thereby having a high chance of penetration of a drug compound into diseased cells.

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Structure and properties of poly(9-vinylcarbazole) thin compositional nanofilms

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The morphology of thin compositional films and careful control of the ratio of the composite components play a crucial role in regulation the processes of charge transfer and optimizing theirs optoelectronic properties.

Compositional poly(9-vinylcarbazole) (PVC, M_w ~ 1 100 000) films with silicon dioxide nanoparticles were obtained from a mixture of PVC and a powder of nanoparticles (NP) SiO_2 (d=10− 20 nm) as NP suspension in chloroform with different volume ratio (1 mol PVK : $0.67 \cdot 10^4$ and $167 \cdot 10^4$ mol SiO_2 respectively.

It was found, that the optimal concentration is of 0.5 mg/ml and surface pressure for forming PVC-films by Langmuir – Blodgett method is varied from 4 to 12 mN/m (Fig. a, b). After incorporation of NPs in a chlorophorm suspension and as powder surface pressure of phase state of the solid film is shift to the value pf 30 mN/m, while the NPs are embedded in the structure of the PVC film. In the case of SiO_2 powder NPs directionally structured layer (Fig. c, d).

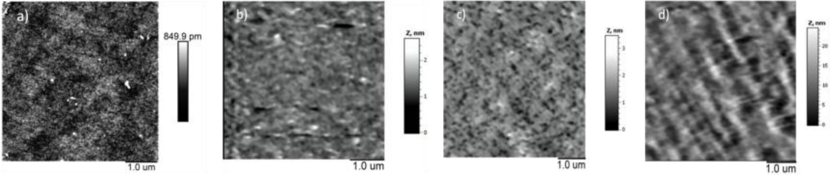

Fig. AFM-structure of PVC films on silicon substrate:
a) PVC, $\pi = 4{,}7$ mN/m; b) PVC, $\pi = 8{,}3$ mN/m; c) PVC + SiO_2, $\pi = 30$ mN/m;
d) PVC + NPSiO_2, $\pi = 33$ mN/m

Contact angle doesn’t depend on structure and composition of film and its value is only 59^0 on silicon substrate. On the glass substrate structure of films is denser and CA increases to the value of 70^0 and in the case of composition films PVC+NP SiO_2 is up to 92^0. For films formed by spin-coating method the surfaces are characterized by conglomerates with sizes from 200 to 400 nm and CA is of $70-85^0$ on the two types of substrates. These films don’t reduce the light transmission of glass and increase scattering in some cases.

The hydrophilic properties of polymeric nanofilms on pretreated substrates by the atmospheric discharge plasma

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The treatment by low temperature dielectric barrier discharge plasma is one of the perspective method of substrates surfaces purification from the adsorbed gasses, water and others substances.

Composition PMMA films with silicon dioxide nanoparticles (NP) were obtained from a mixture of PMMA and SiO_2 in chlorophorm with the ratio of 1 mol PMMA : $1.7\cdot10^2$ mol SiO_2 by Langmuir – Blodgett (LB) and spin-coating (sc) methods. Preliminary, the substrates were treated by low temperature dielectric barrier discharge plasma. The surface of the PMMA film on the glass substrate after plasma treatment is characterized with contact angle 1.5 times less as compared to untreated substrates (Fig.).

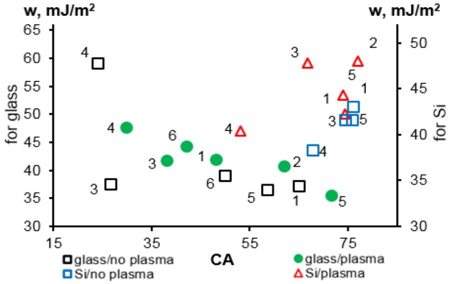

Fig. The value of contact angle and surface free energy of PMMA films with NP of SiO_2 (1 – PMMA, s-c; 2 – PMMA, LB; 3 – PMMA+SiO_2, s-c; 4 – PMMA/SiO_2, s-c; 5 – SiO_2/PMMA, s-c; 6–water treatment) on the glass and silicon substrates

It was shown by AFM method, that SiO_2 NP are structured on the surface of glass substrate after plasma treatment, while on the surface of silicon substrates such effect was not observed. The near-surface layer of glass substrates is both purified, and activated after plasma treatment. The silicon surface is only purified. This difference is due to the content of impurities in the glass; whereupon fragile bonds are breaking and the charge of the surface is changing that provides the formation of structured layers and dense and uniform films on this type of substrates.

Epoxy composites filled with carbon nanotubes and graphene

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Carbon based additives improve thermal, mechanical, electrical properties, electromagnetic interference shielding effectiveness (EMI SE) of the composites [1]. The present work is focused on the preparation of epoxy based polymer composites filled with carbon nanotubes, graphene and characterization of their conductivity, EMI SE, and mechanical properties. Epoxy resin Biresin CR122 and hardener CH122-5 were provided by SIKA. Elicarb® graphene (GNPs) epoxy dispersion and Multiwall carbon nanotubes (MCNTs) NC7000™ were used for composites preparation. MCNTs effectively create a conductive network in the epoxy composites providing their electrical and thermal conductivity. It was found that the percolation threshold for the MCNTs/epoxy composites was 0.013 wt. %. The value of EMI SE grows up to 13 dB when 2 wt.% of MCNTs was loaded in the composite. An addition of GNPs to the MCNTs-loaded composites almost did not influence the conductivity of the composites, but improved their EMI SE in X-band frequency range. The MCNTs loading was found to result in the degradation of the mechanical properties of the composites, while the addition of GNPs only slightly weakens the tensile strength. The mechanical properties of MCNTs + GNPs composites were similar to that of the MCNTs-loaded composites without GNPs.

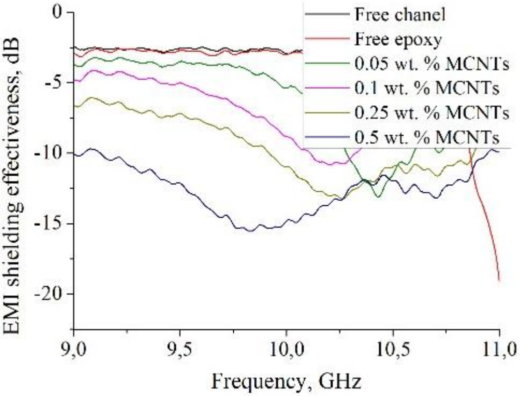

Fig. EMI shielding effectiveness of the composites loaded with different amount of MCNTs

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Effect of brightening additives on phosphorus content in Ni–P coatings

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Electrodeposited Ni–P coatings are well known by its improved properties. It's also known that phosphorus content in these coatings have great effect on their structure and properties. Commonly composition of Ni–P coatings can be regulated by varying phosphorus source concentration (NaH_2PO_2 or H_3PO_3) or parameters of process. Recently saccharin presence in electrolyte was shown to reduce phosphorus content in Ni–P coatings greatly [1]. But an explanation of this phenomenon hasn't given yet. Two ways of saccharin effect can be proposed. Saccharine is a brightener of the first class as it increases polarization of nickel ions reduction slightly. Adsorption of saccharin molecules on the surface of Ni–P electrode can reduce the number of active sites on which phosphorus species reduction can occur. On the other hand, the reduction of saccharin leads to the sulfur atoms incorporation into a deposit. Such sulfur containing coatings have lower catalytic ability in hydrogenation reactions as compared with pure nickel that should decrease intensity of phosphorus species reduction. There were three different additives tested to examine these assumptions. Parasulfamidobenzoic acid (PSBA) also acts as brightener of the first class but doesn't lead to sulfur incorporation to deposit. 2-Butin-1,4-diol is the brightener of the second class and increases polarization of nickel deposition greatly because of strong adsorption to nickel surface. Thiourea also acts as a brightener of the second class but additionally provides an incorporation of large amount of sulfur to coating. As can be seen from Table PSBA doesn't have any effect on phosphorus content in Ni–P coating. 2-Butin-1,4-diol can't be used in 0.005M concentration because it almost stops deposition process and only hydrogen evaluation reaction occurs. When 0.0005 M concentration used, deposition process can occur and P content in coating slightly is decreased. The presence of 0.005M of thiourea in electrolyte inhibit phosphorus incorporation process and leads only to deposition of Ni–S coating (5 at. % of S).

Table. Effect of brightening additives on the phosphorus content in Ni–P coatings

Additive	–	Saccharin	PSBA	2-Butin-1,4-diol	Thiourea
c(additive), mol/dm^3	–	0.005	0.005	0.0005	0.005
χ(P), at. %	21.3	6.1	21.0	16.7	0.1

Thus, it becomes clear that only sulfur presence in the coating has strong effect on phosphorus incorporation to the nickel coating.

Acknowledgment. The work was funded by BRFFR, grant №X19PM-060.

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Effective approach to theoretical investigations of heterogeneous catalytic processes on metal oxides

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Heterogeneous catalysis is widely used in various important industrial processes. Nevertheless, mechanisms of these processes are poorly understood due to lack of effective investigation approaches. Any experimental technique by itself is insufficient for unquestionable determination of mechanism, it has to be combined with thorough theoretical study. In its turn, simulation of crystal surfaces is one of the most challenging problems in computational chemistry. Use of periodic models for these purposes gives rather accurate results but still remains extremely expensive (regarding CPU time); in addition it is difficult to treat charged systems in terms of this approach. Another way is to use cluster models which are cheaper but less accurate. Moreover, there is a problem of reasonable calculation of vibrational frequencies (for locating transition states).

To solve these problems we have developed a new approach for surface calculations based on three-layers embedded cluster models. To obtain such a model one should choose appropriate number of metal atoms that are able to represent the adsorption center and to include them together with all oxygen atoms of their coordination spheres into the first layer. This layer is treated explicitly using large basis set. All metal atoms that are connected with oxygen atoms from the first layer form the second layer of “soft” charges which are described only with effective core potential. The third layer is an array of point charges that are located at the positions of corresponding atoms in the crystal structure of the oxide. This layer can be enlarged without loss of calculations efficiency, because only the resulting background charge distribution is included into the Hamiltonian. Obtained cluster model as a whole should be neutral. The array of point charges takes into account differences in electron density distribution between bulk crystal and cluster. The layer of “soft” charges plays role of a buffer which prevents excessive polarization of the model and its folding. Coordinates of the second and third layers are kept frozen during the optimization. While calculating vibrational frequencies, removing of normal modes that involve contribution of the “soft” charges allows using automatic procedure of transition states optimizations implemented in such programs as Gaussian.

The proposed approach has been tested by calculating methane activation barrier on γ-Al_2O_3[1] and by studying NO reduction process on Ag/γ-Al_2O_3 [2]. Thus, accuracy of our approach is not inferior to that of periodic calculations.

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Electroreduction of Ag(I) in non-aqueous ternary choline chloride containing solvent with the usage of AgCl

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Silver and its alloys such as Ag-Cu, Sn-Ag are widely used in printed circuit boards production [1]. Non–aqueous solution for silver electrodeposition with three-component solvent containing choline chloride (ChCl), ethylene glycol (EG), urea (U) and AgCl as silver source was investigated. It was needed for the development of stable, easily corrected for multiple electrolyte using. AgCl was used owing to its rather high solubility in non-aqueous ChCl containing solution [1]. AgCl concentration was varied in the limits 0.025–0.100 mol dm^{-3}.

Solution is stable for a year and more and can be corrected many times. Current efficiency of Ag(I) reduction depends on silver salt concentration and can be varied in the limits 5.4–43.4%. The maximum rate of silver coatings growth is close to 1.8 µm h^{-1}. It is achieved under the conditions: $C(Ag(I)) = 0.100$ mol dm^{-3}, $T = 20 \pm 2°C$, $i = 1$ mA cm^{-2}. It was found that the usage of the proposed electrolyte allows to deposit crystalline silver coating with highly developed and porous surface in case of C(AgCl) 0.025–0.050 mol dm^{-3} and more tightly packed in case of the $C(AgCl) = 0.100$ mol dm^{-3} (Fig).

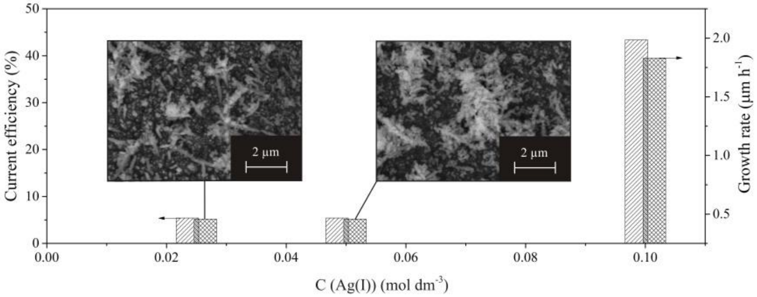

Fig. The dependence of current efficiency (left), coating growth rate (right) and surface morphology (SEM photos) of silver coatings on Ag(I) concentration in electrolyte

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Energy storage photocatalytic systems of Fenton type with the enhanced biocide activity

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Energy storage photacatalytic systems comprising the mosaic films made of TiO_2/ MoO_3 nanoheterojunctions exhibit a long-term biocide activity upon UV expose retaining at least for 8 h. Contrastingly to the conventional TiO_2-based photobiocide coatings exhibiting self-sterilization through generation of hydroxyl radicals under UV irradiation, the pathophysiological activity of TiO_2/MoO_3 photocatalyst is due to hydrogen peroxide production accompanying oxidation of Mo^{5+} centers (produced during the course of photoaccumulation of negative charge) and thus retains in the dark [1]. Our studies have shown that modification of the surface of TiO_2/MoO_3 nanoheterojunctions with $NiMo_6O_{24}H_6^{4-}$ capable of rapid conversion of hydrogen peroxide yielding OH radicals, results in *ca.* 2-fold increase in the probing dye oxidation efficiency (Fig. 1) and leads to the corresponding enchantment of biocide activity against *E. coli* bacteria. Moreover, hydroxyl radicals known to be the most efficient oxidant among other reactive oxygen species behave as the non-selective killing factor, being thus effective against both gram-negative bacteria and gram-positive ones which differ as to the oxidation resistance of lipids forming the envelop. The poyoxometallate molecules immobilized at the TiO_2/MoO_3 surface are also involved in the photoinduced charge storage resulting in the enhanced efficiency of photoaccumulation.

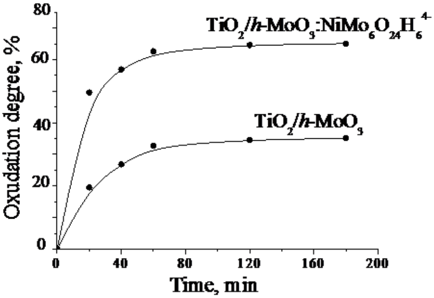

Fig. Degradation kinetics of Rhodamine 6G under dark conditions at photocatalysts pre-exposed to UV light for 10 min. $NiMo_6O_{24}H_6^{4-}$ deposited onto the surface of MoO_3 particles behaves as the catalyst of Fenton reaction.

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Adsorption of surfactant binary mixtures at the oil-water interface

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To increase the efficiency of oil displacement from the surface of rock-forming minerals, surfactants should exhibit high surface activity at the oil-water interface and limited adsorption on the surface of rock-forming minerals [1, 2]. The aim of this work was to study the adsorption capacity of aqueous solutions of binary mixtures of anionic (alkylbenzenesulfonic acid and its sodium salt (ABSNa)) and nonionic surfactant (oxyethylated ester of anhydrosorbitol and fatty acids (OEFA)) on the oil-water interface before and after contact with a finely dispersed quartz surface. It was found that the ABSNa/OEFA mixture has a low adsorption capacity for quartz ($0.5 \cdot 10^{-7}$ mol/g), surfactant components after contact with it remain in solution and, therefore, are adsorbed at the oil-water interface, which is confirmed by a decrease in values of interfacial tension from 25 mN/m to 2.2 mN/m. After the establishment of adsorption equilibrium in the ABSA/OEFA/quartz system, the excess adsorption value is 6.8 times higher than this indicator for ABSNa/OEFA/quartz. The surface tension of the ABSA/OEFA solution after interaction with quartz reaches 65 68 mN/m, practically approaching the value of the surface tension of water (72 mN/m). This fact determines the low adsorption capacity of ABSA/OEFA at the oil-water interface in the presence of mineral material. The interfacial tension value decreases slightly – from 25 mN/m to 16.2 mN/m. The results obtained are confirmed by studies of the kinetics of oil displacement from the surface of quartz with AS/NS solutions and the calculated values of the activation energy of oil displacement.

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Photoselective nickel deposition on SnO_2-coated glass

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Conductive metal patterns on the surface of dielectrics and semiconductors are compulsory elements of printed circuit boards, chips, waveguides, heating devices, etc. Traditionally, to obtain them, a continuous metal layer is first deposited, and then it is selectively removed using photolithography processes. More economical processes are known that consist in metal ions catalytic reduction only on the specified areas of the surface containing palladium nanoparticles as a catalyst. Processes using photosensitive titanium dioxide films have found practical application. Selective metal deposition on titanium dioxide films is due to its semiconducting properties. UV irradiation of TiO_2 film generates photoelectrons which are captured by palladium ions and reduce them either during irradiation or when treated with $PdCl_2$ solution after the UV exposure. TiO_2 films 0.1−0.2 μm thick are obtained by the sol-gel technology using a solution of polybutoxytitanium in isopropyl alcohol, followed by drying and annealing to convert titanium hydroxide into TiO_2 and increase the photosensitivity and adhesion of films [1].

The purpose of this work was to develop a similar method to obtain metal patterns using an aqueous tin dioxide sol for photoinduced reduction of palladium. This sol was obtained by hydrolysis of $SnCl_4 \cdot H_2O$ according to the method proposed in the work [2]. Then it was mixed with a solution of polyvinyl alcohol and applied to a glass by pouring, followed with drying at a temperature of 20 °C. After UV exposure through a stencil for several minutes, the samples were treated in a palladium chloride solution and then in a hypophosphite solution of chemical nickel plating. A shiny conductive nickel films were deposited on the exposed areas. In contrast to the process of obtaining patterns on TiO_2 films, multiple layer-by-layer deposition of SnO_2 films and their heating were not required.

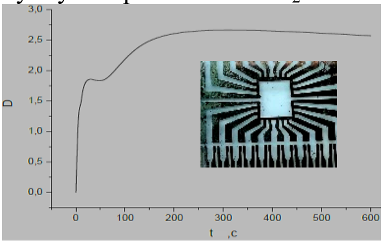

Fig. Dependence of nickel film optical density on the time of UV-exposition and the sample of conductive pattern

The ability of tin dioxide films to reduce palladium ions on their irradiated areas can be preserved for 24 hours and more instead of several seconds.

The Fig. shows the dependence of the optical density of nickel films on the duration of UV irradiation of the SnO_2 film with a mercury-quartz lamp, and a sample of a conductive nickel pattern obtained on the glass.

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Ni-Cu electrodes for hydrogen evolution reaction

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Alkaline electrolysis of water is an excellent method of obtaining an environmenttally friendly energy carrier as hydrogen. It is possible to use not noble metals such as Ni and its alloys with Cd, Bi, Cu as the catalysts for electrolysis [1]. Nickel alloys are obtained electrochemically with the formation of powders or loosely packed coatings at current densities close to the diffusion limit [1, 2]. The purpose of this work was to obtain powders of Ni and Ni-Cu alloys by Ni(II) and Cu(II) reduction with hydrazine hydrate in aqueous media and to analyze the possibility of their using as the catalysts in the process of alkaline electrolysis of water. Powder Ni-Cu alloys with Ni content of 93.0 and 55.0 at.% (solid Cu solution in Ni) have been synthesized. The morphology study of the Ni-Cu powders showed that regardless of composition they consist of small spherical grains 0.2–0.3 µm in sizes and loose aggregates (2–10 µm), Fig. a. The catalytic activity of the powders was assessed by cyclic voltammetry (CV) in 0.1 M KOH in three-electrode cell including working electrodes prepared from powders pressed into tablets with surface area of 1 cm^2, Pt pseudocomparative and indicator electrodes. It was revealed that the catalytic ability of the powders in the alkaline medium decreases in the order of Ni > Ni 93.0 – Cu > Ni 55.0 – Cu, Fig. b. Catalysts stability during cyclic using decreases in the row of Ni 55.0 – Cu > Ni 93.0 – Cu > Ni, Fig. c.

Based on the results of the work performed, it can be concluded that the Ni 95.0 – Cu alloy is the most applicable in alkaline catalysis, since its catalytic activity is close to that for nickel, but it is more resistant to oxidation during cyclic operation.

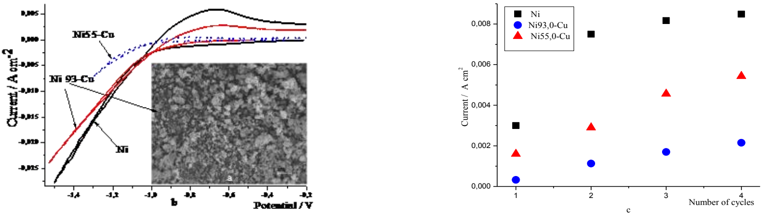

Fig. CV curves for working electrodes from nickel and its alloy powders in 0,1 M KOH (a), SEM photo of Ni 93.0 – Cu powder (b); the dependence of the current in the maximum of the anodic peak characterizing nickel oxidation from the number of cycles (c)

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Nickel–tin alloy as the catalyst in the electrochemical process of alkaline hydrogen evolution

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Hydrogen (H_2) is the most promising alternative energy source for the future. The alkaline water electrolysis is widely used for the production of H_2 and nickel is one of the most suitable metals for its electrocatalytic evolution. It is known [1, 2] that the electrocatalytic ability of nickel increases in case of usage instead of nickel its alloys with Se, P, Mn, Ti.

The purpose of this work was to analyze the possibility to use Ni–Sn alloy as the catalyst in the process of hydrogen evolution in 0.1 M KOH solution. Ni–Sn powder alloy with 72,2±5,8 at.% of nickel was synthesized electrochemically, its phase composition includes crystalline phases of Ni, β-Sn and NiSn, Ni_3Sn, Ni_3Sn_2, Ni_3Sn_4, powder surface area is $1{,}00 \pm 0{,}01\ m^2 \cdot g^{-1}$ (determined by the BET method). CV investigations were conducted in three-electrode cell with Pt counter and reference electrodes. Working electrode was prepared by applying Ni-Sn suspension (mixture of 4 vol.% nafion, 20 vol.% isopropanol, 76 vol.% deionized water, 46 mg of Ni–Sn powder). To compare the catalytic activity, Sn and Ni-P powders were used and CV curves were recorded (Fig.). It was found that synthesized Ni–Sn alloy, in comparison with Ni–P and Sn powders provides the highest value of the current density and the lowest value of hydrogen evolution potential. The electrochemically active surface area of nickel, calculated according to [2], for Ni–Sn powder is two times higher than that for Ni–P powder and equals to 66 $cm^2\ mg^{-1}$. Thus it is shown that Ni–Sn powder is more catalytically active than Ni–P and Sn in the electrochemical hydrogen evolution.

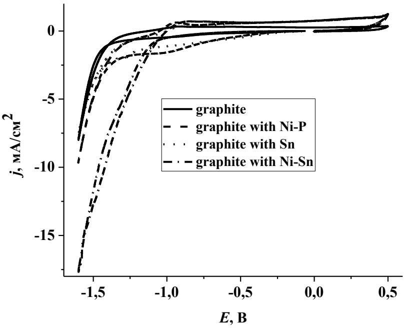

Fig. CV curves in 0,1 M KOH with a scan rate 10 $mV \cdot s^{-1}$

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METAL COMPLEXES

Complexation of N-(1,3-di-*tert*-butyltetrazolium-5-yl)benzimidate with copper(II) chloride

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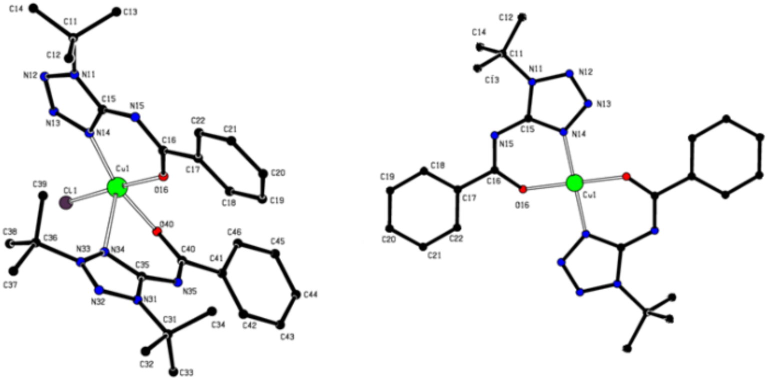
Coordination compounds, based on mesoionic tetrazole-containing ligands, attract today a great attention because of their unique properties such as high energy density, catalytical and magnetic properties [1–3]. However, the complexation of such ligands has not been enough studied.

In the present work, the interaction of N-(1,3-di-*tert*-butyltetrazolium-5-yl)benzimidate (L^1) with anhydrous copper(II) chloride was investigated. It was found that complexation proceeded with de-*tert*-butilation of ligand L^1 to form N-(1-(*tert*-butyl)tetrazol-5-yl)benzamide (L^2). It was shown that ligand-mixed complex $[CuClL^1L^2]$ (**1**) was formed at room temperature, while complex $[Cu(L^2)_2]$ (**2**) was obtained upon heating. Synthesized compounds were identified by single crystal X-ray analysis and IR-spectroscopy. Both compounds present mononuclear molecular complexes (Fig.).



1 **2**

Fig. The structures of complexes **1** and **2**. Hydrogen atoms are omitted for clarity.

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Chromium(III) and REE heterometallic complexes with N, O-donor ligands

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Modern high-tech industries require the creation of new generations of functional materials produced on the basis of synthesized chemical compounds and their compositions. Promising precursors for their production are double complex compounds (DCS) They are used as molecular and ionic precursors, catalysts, analytical reagents, and thermo-indicator colors. For carrying out such studies, information is needed on physicochemical characteristics and structure of DCS precursors, as well as the development of methods for their directed synthesis. Using inert bulk hex (isothiocyanato)chromate(III) - anion, hexathiocyanato chromates(III) of complexes of "hard" rare earth metals and chromium with neutral organic ligands were obtained by direct synthesis from aqueous solutions. All DCSs were studied by the methods of chemical, IR-spectroscopic, X-ray phase, X-ray structural, thermogravimetric analyzes; density, electrical conductivity of solutions, and magnetic characteristics of substances were determined.

Complexes with caprolactam crystallize in three related structural types, the mutual packing in the structures of which corresponds to the topological type of NaCl. Complexes with nicotinic acid have the same structure and differ only in the number of crystallization water models. In the study of the thermal behavior of substances, it was found that they have reversible thermochromic properties with a color change from pale lilac to dark green and vice versa upon heating↔cooling, during their decomposition already at a temperature of about 600 ° C, fine powders are formed, consisting, according to XRF data, from a mixture oxides of rare earth metals(III) and chromium(III). The discovered properties of the substance characterize promising precursors for the production of polyfunctional, including nanomaterials, as well as chemical sensors in thermo-indicator devices.

Synthesis and comparative study of the antibacterial activity of tetrazole-containing Schiff base and its organometallic complex with $CoCl_2$

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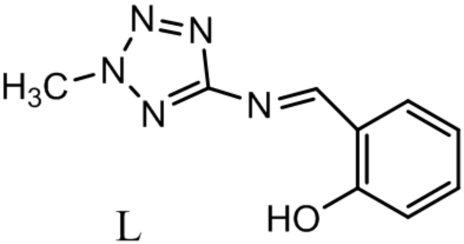
Schiff bases are known as polydentate ligands to obtain coordination compounds of various compositions and properties. The obtained by direct synthesis tetrazole-containing Schiff base is an interesting material that can be used as starting compound for the creation of biologically active substances and other functional materials [1]. Here we report synthesis and some properties of biologically active metal-containing structure of tetrazole-containing Schiff base with $CoCl_2$. It was found that the reaction of $CoCl_2$ and 2-(((2-methyl-1H-tetrazol-5-yl)imino)methyl)phenol (L) in a mixture of ethyl alcohol and acetonitrile (1:1) under heat (65-70 °C) gave rise to a novel organometallic tetrazole derivative $CoCl_2L$ of light b



L

The precipitated in 10 days microcrystalline complex compound (CC) was separated and was washed with a mixture of diethyl ether and ethyl alcohol (5:1). The composition and structure of the synthesized complex compound was investigated by elemental analysis, X-ray phase analysis, X-ray diffraction analysis and IR spectroscopy in the range of 40 – 4000 cm^{-1}. Biological activity of the obtained organometallic tetrazole derivative $CoCl_2L$, as well as pure ligand L was determined against ten bacteria and four fungi strains. It was found that in majority antibacterial and fungicidal activity of the complex compound is much higher (almost two times) in comparison with pure tetrazole-containing Schiff base L. However, organometallic derivative showed no inhibition growth of *fungi Aspergillus niger*. The obtained results allow us to conclude that the $CoCl_2L$ complex, as well as CC Co(II) with other Schiff bases, are promising objects for further study of their biological activity.

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Synthesis of new tetrazole-containing multipodal ligands based on 2-aminobenzonitrile

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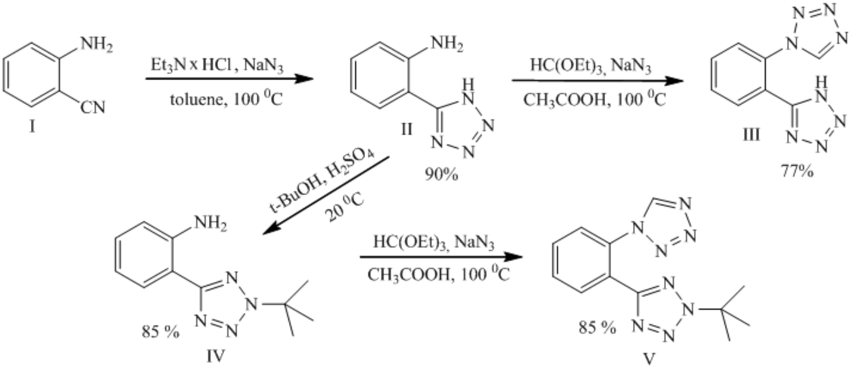
Due to the presence in the hetero ring of four nitrogen atoms capable of forming coordination bonds, tetrazole derivatives are promising objects of research in coordination chemistry [1]. It is known that a convenient method for the preparation of C-substituted tetrazoles is the reaction of 3 + 2-cycloaddition of an azide ion to alkyl or aryl cyanides [2]. 1-Substituted tetrazoles can be obtained in good yield by the heterocyclization reaction of primary amines with triethylorthoformate and sodium azide [3,4]. We have shown the possibility of realizing these approaches to obtain new tetrazole-containing multipodal ligands combining in their structure two tetrazole rings, one of which is N-substituted and the other C-substituted. 2-aminobenzonitrile was used as the initial substrate.



The synthesized multipodal ligands II-V interact with transition metal salts to form coordination compounds.

Acknowledgment

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Magnetically active complexes of 3d metals with nitrogen-containing ligands

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Nitrogen-containing compounds are promising ligands for the synthesis of new coordination compounds with nontrivial physical properties and biological activity. Complexes containing 3d transition metals with the d^4-d^7 electron configuration in octahedral or pseudo-octahedral coordination, for instance, can exhibit spin crossover phenomena, i.e. change spin multiplicity under certain conditions [1-4]. Cooperative interactions in the solid phase of transition metal complexes can turn the spin crossover into an abrupt transition as well as promote various kinds of magnetic ordering associated with exchange interactions between paramagnetic centers [5].

In continuation of our work on the study of iron(II) complexes with 1,2,4-triazoles and tris(pyrazol-1-yl) methanes, which have a spin crossover, we synthesized new Fe(II) complexes with 2,6-bis(imidazol-2-yl)pyridines and various outer-sphere anions of the composition $[Fe(L)_2]A_i{\cdot}nH_2O$ ($i = 1, 2$; $n = 1–2$). The study of the $\mu_{eff}(T)$ dependence in the temperature range 80-520 K showed that they exhibit a spin-crossover $^1A_1 \Leftrightarrow {}^5T_2$. Study of a number of complexes of Co(II), Ni(II) and Cu(II) with derivatives of pyrazole; 1,3,4-thiadiazole and tetrazole showed that they exhibit antiferro- or ferromagnetic exchange interactions between paramagnetic centers.

Acknowledgment

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New polymeric ligands based on polyvinylchloride

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Ion exchange polymers are widely used as ligands for complex compounds. They are used in many market segments and applications globally [1-2]. Purpose of research work is synthesizing cationites containing sulfuric groups by modifying polyvinylchloride and studying the physical and chemical properties of obtained products [3-5]. As a result of the conducted studies optimal conditions for synthesis of cation exchange resin using granular polyvinylchloride as a substrate have been determined for the first time. It has been found that synthesized ionites have high sorption efficiency, thermal and mechanical resistance and are similar to those of commercial cationit KU-2 in terms of abovementioned characteristics. High sorption factors of synthesized cationites for copper, calcium and magnesium ions have been found. The study of a sulfonic cation exchanger based on polyvinyl chloride under dynamic conditions for softening wastewater showed that its sorption properties after several sorption-desorption processes remained unchanged, therefore it can be recommended for repeated use in softening and purifying natural water at industrial enterprises.

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In situ generated 5-(2-mercaptoethyl)tetrazole as a novel capping ligand for silver nanoparticles

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Tetrazole derivatives have received much attention in the recent years in the field of nanostructured materials [1,2]. In particular, they were studied as suitable capping ligands for semiconductor and metal nanoparticles (NPs). So, 5-(2-mercaptoethyl)tetrazole (**1**) was successfully applied to the aqueous synthesis of CdTe and Au NPs [2]. A notable feature of obtained NPs is their ability to build 3D structures in a metal ion assisted gelation process in aqueous solution.

Here we report synthesis and characterization of Ag NPs capped by ligand **1**. It was found that stable aqueous Ag sols can be obtained by reduction of Ag_2SO_4 with $NaBH_4$ in the presence of disulfide **2** (Fig.). In this case, ligand **1** is generated *in situ* by splitting of the S–S bond of **2** upon the addition of reducing agent.

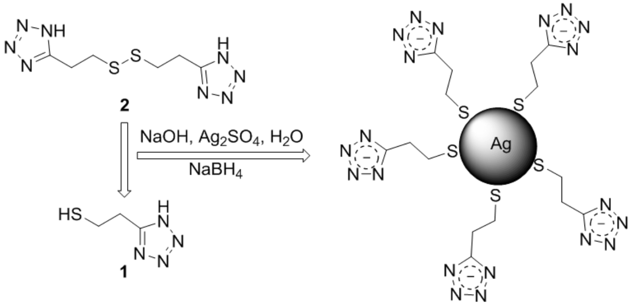

Fig. Scheme for the synthesis of Ag NPs capped by ligand **1**

Synthesized NPs were characterized by transmission electron microscopy (TEM), FTIR and UV-visible spectroscopy, thermogravimetric analysis (TGA). According to the TEM obtained NPs are nearly spherical with a diameter of ~3-5 nm. Yellowish-brown aqueous Ag sols show a single peak at 420 nm in UV-Vis spectra. Comparative analysis of the IR spectra of the powdered NPs and free ligand **1** indicates that the surface of the NPs is covered by thiolate anions. In particular, S–H bands at 2500-2600 cm^{-1} observed for ligand, are disappeared in the NPs spectra. TG curves of **1** and Ag NPs show that thermolysis of the ligand bound to the NPs proceeds at higher temperatures in comparison with the free ligand, which is due to the presence of tetrazolate form of ligand on the surface of NPs.

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Synthesis and characterization of late transition metal complexes with 2-(tetrazol-1-yl)pyridine

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Late transition metal complexes of tetrazolyl-substituted pyridines are of great importance as potential antiproliferative and theranostic agents [1,2]. Majority of the up to date reported species are derived from 5-tetrazolyl pyridines. In the present study, we report on synthesis, structure and properties of Pt(II), Pd(II) and Ru(II)-based complexes with a representative N-tetrazolyl substituted pyridine, namely 2-(tetrazol-1-yl)pyridine [1-pytz]. Complexes M(1-pytz)Cl_2 (M = Pt, Pd) were synthesized *via* direct interaction of the corresponding metal chlorides (K_2PtCl_4 or $PdCl_2$) with 1-pytz under ambient conditions. Ru(II) complex Ru(1-pytz)$_2Cl_2$ was prepared from $RuCl_3$ and 1-pytz in the presence of 2-(tetrazol-5-yl)pyridine in methanol under reflux conditions and argon atmosphere. The resulting complexes were characterized by elemental analyses, ESI(+)-mass-spectrometry, IR-spectroscopy, ^{1}H and ^{13}C NMR spectroscopy, and simultaneous thermal analysis. Molecular and crystal structure of Pd(1-pytz)Cl_2 was established by single-crystal X-ray diffraction analysis (Figure 1). In the structure, 2-(tetrazol-1-yl)pyridine coordinates as a N,N-chelating ligand *via* N atom of pyridine and N^2 atom of the tetrazole ring.

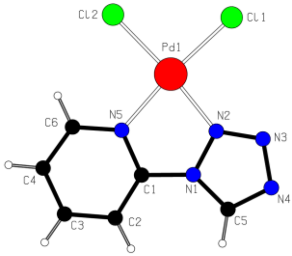

Fig. Molecular structure of Pd(1-pytz)Cl_2

Acknowledgment

The work was supported by BRFFR, grant № X20P-066.

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Antifungal activity of iron group complexes with 4,6-di-*tert*- butyl-2,3-dihydroxybenzaldehyde

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The elaboration of new types of antifungal agents is presently a very actual task because of the fast development of microorganisms' resistance to the antifungals, currently used to treat different plant pathogenic fungal diseases [1]. Iron group metal(II) complexes with hydrazone and thiosemicarbazone derivatives of 4,6-di-*tert*-butyl-2,3-dihydroxybenzaldehyde (L I and L II respectively) have been synthesized and characterized by means of elemental analysis, TG/DTA, IR spectroscopy, XRD and conductivity measurements [2]. Antifungal activities of these ligands and their Fe(II), Co(II), Ni(II) complexes have been determined against *Alternaria alternata, Sclerotinia sclerotiorum, Aspergillus niger*, *Fusarium sp.*, *Penicillium lividum, Mucor sp.*, *Botrytis cinerea* (Figure) using *in vitro* test method described elsewhere [3]. Among the test microorganisms there were plant pathogenic fungi (*Fusarium sp.*, *Botrytis cinerea, Alternaria alternata, Sclerotinia clerotiorum*). Most of the compounds (both the free ligands and the complexes) exert a pronounced antifungal activity (*RI* ≥70 %, *RI* – the degree of inhibition of radial fungal growth), but virtually all of them have the highest inhibitory properties (*RI* = 100 %) against *Alternaria alternata, Sclerotinia sclerotiorum and Botrytis cinerea.* These facts may be of interest in the design of new effective agents against plant pathogenic fungi.

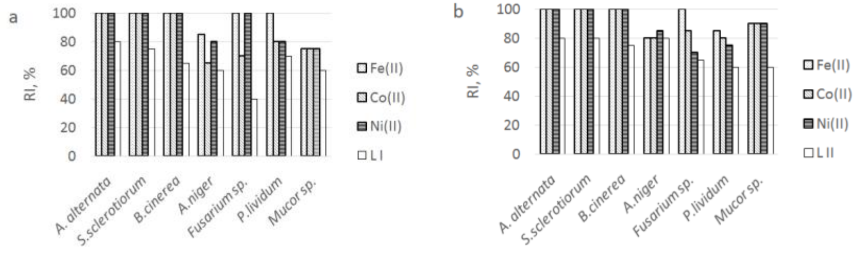

Fig. Antifungal activities of these ligands and their Fe(II), Co(II), Ni(II) complexes with: a – hydrazone derivative of 4,6-di-*tert*-butyl-2,3-dihydroxybenzaldehyde; b – thiosemicarbazone derivative of 4,6-di-*tert*-butyl-2,3-dihydroxybenzaldehyde

Acknowledgement

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Polymeric chain complexes of copper(II) chloride with *N*-substituted tetrazoles: Structure and magnetic properties

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Low-dimensional magnetic compounds are of interest as models for high-temperature superconductors. In this connection, a number of 1D copper(II) coordination polymers were synthesized and their magnetic properties were studied. Chloride ions are suitable bridging ligands for the design of such polymers, since these ions can provide superexchange pathway between the metal cations. Elucidation of correlations between the structure and magnetic properties of complexes is an urgent task of magnetochemical studies.

N-Substituted tetrazoles demonstrate wide variety of structural types of cupric chloride complexes. So, ligands $\mathbf{L^1}$-$\mathbf{L^5}$ were found to generate polymeric chain complexes **I-VI** (Fig.). In all complexes tetrazole rings are monocoordinated *via* N^4 atom, except **III** (N^3,N^4-bridging mode) and **IV** (N^3-monodentate mode). In **V** ligand L^4 shows chelating N^4,N^{amine}-coordination. Complexes **I** and **II** exhibit very weak ferromagnetic intrachain interactions [1], whereas **III–V** [2] and **VI** reveal antiferromagnetic ones. The strongest interactions with J = –17.6 cm^{-1} were observed for complex **III** in which metal cations are also linked by N^3–N^4 bridge. Complexes **IV**, **V** and **VI** have J value of –5.4, –14.2, and –1 cm^{-1}, respectively.

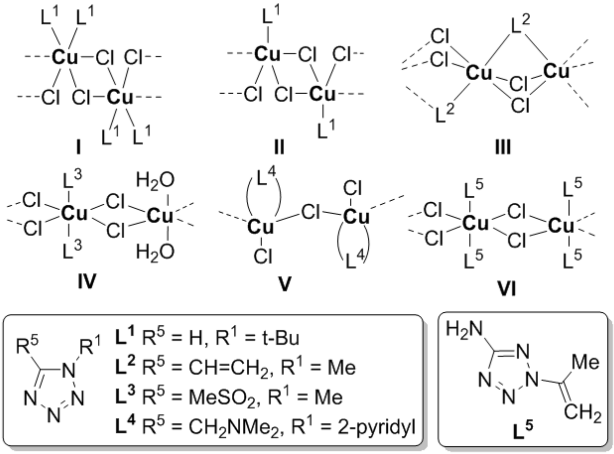

Fig. Structures of copper(II) chloride complexes with N-substituted tetrazoles

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CHEMISTRY OF MOLECULAR SYSTEMS

Thermodynamic properties of some furan derivatives in different aggregate states

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Furan derivatives are promising heterocyclic compounds, which can exhibit unique cytotoxic, antitumor, antispamidic or anti-feeding activities [1]. Ethyl-2-cyano-3-(furan-2-yl)-prop-2-enoate (ECFP) and its phenyl derivative (PhECFP) are prepared via the Knoevenagel condensation reaction. The standard thermodynamic functions of ECFP and PhECFP in the ideal gas state were calculated using statistical thermodynamics approach in the temperature range (0 – 1500) K. The optimized geometry, harmonic vibrational frequencies, potential energy surface scans have been investigated by density functional theory (DFT) on B3LYP method with 6-311++G(d, p) level of theory. An excellent agreement between the optimized geometry in gaseous state and the molecular structure in solid state obtained through X-ray study of ECFP [2] was noticed. The molar heat capacities at 298.15 K were $(201.4 \pm 0.8)\ \mathrm{J \cdot mol^{-1} \cdot K^{-1}}$ and $(279.2 \pm 1.1)\ \mathrm{J \cdot mol^{-1} \cdot K^{-1}}$ for ECFP and PhECFP respectively. These values were compared with the results of Joback's additive scheme. The standard thermodynamic functions of ECFP and PhECFP in the crystalline state were obtained using the temperature dependence of the heat capacity in the range of (80 – 340) K for ECFP and (80 – 370) K for PhECFP.

The standard enthalpies of formation in gaseous state for ECFP and PhECFP were determined using isodesmic reaction scheme and the composite quantum chemical method Gaussian-4. The obtained results were $-(232.2 \pm 1.3)\ \mathrm{kJ\ mol^{-1}}$ for ECFP and $-(111.2 \pm 12.6)\ \mathrm{kJ\ mol^{-1}}$ for PhECFP. The calculated enthalpies of formation in gaseous state are in good accordance with the experimental values [3]: $-(230.0 \pm 8.5)\ \mathrm{kJ\ mol^{-1}}$ for ECFP and $-(113.4 \pm 7.5)\ \mathrm{kJ\ mol^{-1}}$ for PhECFP. Applying of Joback's additive scheme for prediction standard enthalpies of formation in gaseous state for furan derivatives was considered. The way of modifying this scheme was offered.

The additive scheme for prediction standard enthalpy of sublimation based on isodesmic reactions was proposed. The results obtained were (106.5 ± 1.2), (104.3 ± 0.5) and $(111.2 \pm 0.2)\ \mathrm{kJ\ mol^{-1}}$, for 2-furanacrylic acid, 3-furanacrylic acid and ECFP, respectively.

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Synthesis of cellulose carbamate and its properties

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In nature, cellulose is based on plants, which means that cellulose is mainly extracted from plants. However, due to the high demand for cellulose and its derivatives, it does not fully meet the demand for them [1]. The use of local raw materials to meet such requirements can be one of the most important solutions to the problems that arise [2].

One of the most important properties of carbamate cellulose is that it can be used as a filler in disposable polyethylene films used for the cultivation of seasonal crops in open fields. The resulting polyethylene films do not break down under the influence of external factors, leaving no waste, and as a result of this decomposition, carbamate cellulose acts as a fertilizer for plants.

The experiment was performed in a three-nozzle flask equipped with a thermometer, a refrigerant and an automatic mixer. Initially, urea was dissolved in distilled water to prepare solutions at different temperatures as well as urea solutions of different concentrations. This process was performed based on the solubility coefficient of urea. The prepared urea solutions were then slowly added to the cellulose chips and mixed with a mixing mechanism. This process was carried out in the temperature range of 20-30 °C for 3 hours. The resulting product was filtered and placed in an oven at 35-45 °C for drying. The product, dried for about 2 hours, was placed in a Petri dish and placed in a 700 W microwave oven. The product was heated at maximum temperature for 10-15 minutes. The product was then removed from the microwave and thoroughly washed in distilled water. The washed product was stored in an oven at 60 ° C and dried. The result is a light yellow carbamate-cellulose polymer. The resulting product was weighed, compared with the mass of the original raw material, and the reaction yield was calculated. The IR spectrum of the resulting substance was obtained and analyzed. In the next part of our experiment, we studied the effect of solvents on synthesized carbamate cellulose. To do this, we tried 10 g of well-dried fruit. The sample was immersed in several solvents and observed to dissolve over a period of time.

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Thermodynamic Parameters of Poly-5-Vinyltetrazole and its Cu(II)- and Ag(I)-containing Derivatives

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The increasing interest in tetrazole-containing polymers and some of their metal-containing derivatives is explained by the possibility of their use as binders of solid propellants and precursors of a wide variety of products with unusual properties [1]. The results of the thermal behavior study of the poly-5-vinyltetrazole (PVT) and its Cu(II)- and Ag(I)-containing derivatives (CuPVT and AgPVT respectively) are represented. PVT was obtained through polymer-analogous transformation of polyacrylonitrile. CuPVT and AgPVT were synthesized via reaction between aqueous solutions of sodium salt of poly-5-vinyltetrazole and Cu(II)- or Ag(I) nitrates [2]. Metal content in CuPVT and AgPVT was 33 mas. % Cu and 35 mas. % Ag respectively. Thermal decomposition temperatures of the polymers (T_d = 510 K for CuPVT and T_d = 630 K for AgPVT) were determined using TG and DSC methods. The heat capacities of the polymers in condenced state (Fig) were measured in an automatic vacuum adiabatic calorimeter TAU-10 (Termis, Moscow, Russia) [3] between (80 and 370) K. The relative expanded uncertainty of the measurements was determined to be 0.4 %. A solid-phase low-enthalpy reproducible anomaly was observed between (287 and 327) K for PVT. There were no anomalies on the heat capacity curves for CuPVT and AgPVT. The specific heat capacities at 298.15 K were equal to (1.143 ± 0.005), (1.084 ± 0.004) and (0.6451 ± 0.0026) $J \cdot g^{-1} \cdot K^{-1}$ for PVT, CuPVT and AgPVT respectively. The standard thermodynamic functions of the polymers in the condensed state in the temperature range of (80 to 370) K were calculated from the data obtained.

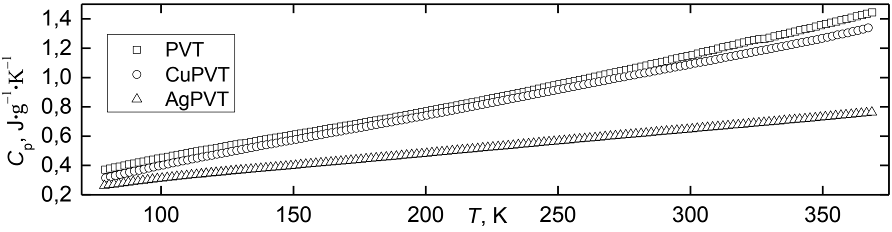

Fig. The heat capacity temperature dependences of the PVT, CuPVT and AgPVT

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Functionalization of mesoionic (1,3-di-*tert*-butyl-tetrazolium-5-yl)amide with benzyl chloride

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Today mesoionic tetrazole containing compounds attract growing interest as a source for obtaining of energetic compounds, catalysts, components of accumulator batteries [1, 2]. Recently it was shown that mesoionic tetrazoles can be selectively functionalized to exocyclic imino-group with acid anhydrates and chloro-anhydrates, phenylisothiocyanates and some other alkylation reagents [3, 4].

A convenient method was proposed for the functionalization of (1,3-di-*tert*-butyl-tetrazolium-5-yl)amide (1) using benzyl chloride in acetonitrile. The reaction proceeds at reflux for 3 h with the formation of tetrazolium salt 2. Then acetonitrile is removed under reduced pressure, the dry residue is washed with several portions of cold diethyl ether and treated in the $NaOH_{water}/CHCl_3$ system. The organic phase is separated, dried with Na_2SO_4, and evaporated to dryness. The resulting solid is passed through chromatographic column with SiO_2 sorbent using ethyl acetate-triethylamine (9:1) system to obtain compound 3 (yield 42%).

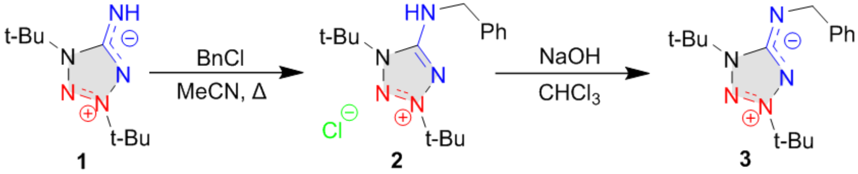

Fig. Scheme of the synthesis of benzyl(1,3-di-*tert*-butyl-tetrazolium-5-yl)amide

Synthesized compounds were identified based on data of IR-, ^{1}H and ^{13}C NMR spectroscopies and elemental analysis.

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Ion-exchange polymer complexing materials based on polyacrylonitrile

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The level of usage of polymer ion-exchange fibrous materials has been increasing at an alarming rate in many developed countries around the globe. In contrast to granulated ion-exchangers, ion-exchange fibrous materials possess a larger specific surface area that promotes the high rate of sorption. In this work we intend to report the latest research results on obtaining anion-exchange materials by chemical modification of "Nitron", an industrial polyacrylonitrile fiber. The modification of the fiber was realized by interaction of the nitrile groups of the polymer with nitrogen-containing bases such as a hydroxylamine (HA), hydrazine (HD), N,N-dimethylhydrazine (DMH), hexamethylenediamine (HMD) and ethylenediamine (EDA).

Stable sorption fibers were obtained during the investigation of reaction of "Nitron" fiber with HA in presence of the cross-linking agent-HD. The chemical modification of polyacrylonitrile fibers with HD and particularly with N, N-dimethylhydrazine in water solution occurs difficultly. Therefore, “nitron” was activated by 1 % solution of NaOH at 90 ^{0}C during 1-3 minutes before the modification by these reagents. Acidic moieties formed in this process accelerated the reaction of -CN groups with HD and DMH. Under the same hydrazidation conditions, the SEC values of activated fibers are much higher than those of fibers obtained without activation.

Furthermore, the catalytic action of HA on hydrazidation reaction of nitron was identified. In the presence of HA in the substrate mixture, the reactions of polymer’s nitrile groups with HD and DMH occurred easier. Besides, a higher degree of conversion was achieved. By treating nitron with HMD and EDA, ion-exchange fibers containing both weakly basic and strongly basic functional groups were obtained. In these cases, the diamines execute the function of crosslinking agent and modifier of nitrile groups at the same time. The reaction of nitron fiber with HMD, without a solvent or in an organic solvent, was carried out at the temperature 130-160^{0}C. Sorption materials (SMA-1) obtained under these conditions mainly contain strong alkaline amidine groups.

Thus, the obtained ion-exchange fiber sorbents are perspective for using in hydrometallurgy, in the purification of industrial wastewater from toxic metals, disinfection of drinking water from natural resources, as well as for production of bactericidal materials for medicine.

Selective synthesis of 1-R-5-phenyltetrazoles

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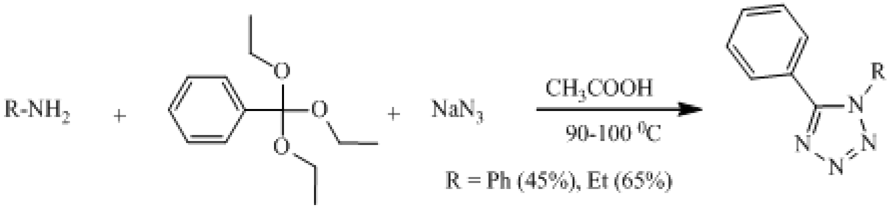
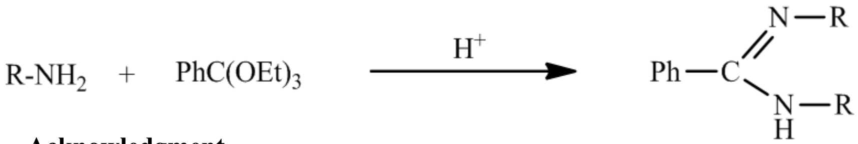
Despite the vast potential for the practical use of tetrazole derivatives, the specific use of many of them is hampered by the lack of convenient preparative methods of synthesis. We have previously shown that a convenient and effective method for the preparation of a wide range of 1-substituted tetrazoles is the heterocyclization reaction of primary amines with triethylorthoformate and sodium azide [1, 2]. In continuation of these studies within the framework of this work, using aniline and ethylamine as examples, we showed that 1-substituted 5-phenyltetrazoles, which are difficult to obtain by other methods, can be synthesized in good yields by heterocyclization of the corresponding primary amines with triethylorthobenzoate and sodium azide.



The maximum yields of the target 1-R-5-phenyltetrazoles, as in the case of using triethylorthoformate, are achieved when the process is carried out in a temperature range of 90–100 ^{0}C at a molar ratio of RNH_2 : $PhC(OEt)_3$: NaN_3 : CH_3COOH = 1 : 3: 1,1: 8. The use of excess triethylorthobenzoate during the process is due to the need to suppress the side reaction of the formation of benzimidamides.



Acknowledgment

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Methylation of 5-phenyltetrazole with dimethyl carbonate

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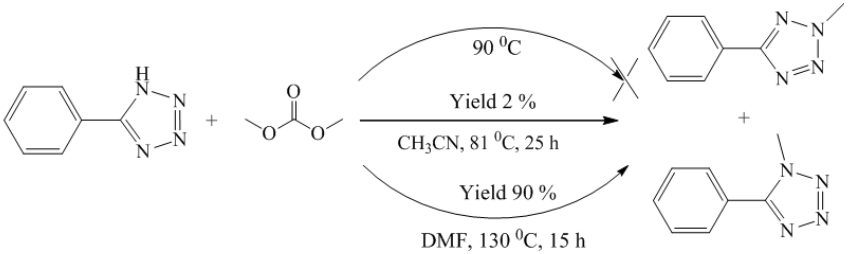
In recent years, dimethyl carbonate has gained an increasingly important role in the chemical industry, mainly due to its versatility as an environmentally friendly solvent and methylating agent. Dimethyl carbonate is suitable replacement for toxic dimethyl sulfate and methyl halides, which are widely used in organic chemistry [1]. Using 5-phenyltetrazole as an example, we have studied the possibilities of using dimethyl carbonate as a methylating reagent for NH-unsubstituted tetrazoles. It was found that heating of dimethyl carbonate solution of 5-phenyltetrazole under reflux does not lead to the formation of methylated products. When the reaction was carried out in boiling acetonitrile in the presence of K_2CO_3, after 25 hours of the process a trace amounts of a mixture of 1- and 2-methyl-5-phenyltetrazoles was isolated (15 : 85). The best results are achieved when the process is carried out in dimethylformamide at 130 ° C in the presence of K_2CO_3. As a result, a mixture of 1- and 2-methyl-5-phenyltetrazoles is formed with a yield of 90%, containing 13% of 1-methyl-5-phenyltetrazole and 87% of 2-methyl-5-phenyltetrazole.



The individual 1-methyl- and 2-methyl-5-phenyltetrazoles from the resulting mixture of isomers can be isolated by liquid column chromatography.

Acknowledgment

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Direct synthesis and crystal structure of metal(II) thiocyanate complexes with 1-alkyl-1,2,4-triazoles

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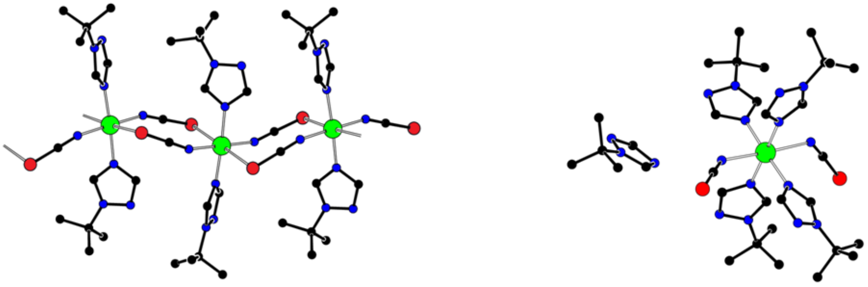
In continuation of our previous studies in coordination chemistry of 1,2,4-triazoles [1,2], here we report direct synthesis and characterization of metal(II) thiocyanate complexes with 1-*iso*-propyl-1,2,4-triazole (ptr) and 1-*tert*-butyl-1,2,4-triazole (btr). These triazoles were found to interact with metal powders and ammonium thiocyanate in organic solvents (DMSO, toluene, acetonitrile, alcohols) under heating to give crystalline complexes $[M(ptr)_4(SCN)_2]$, where M = Co, Ni; $[M(btr)_4(SCN)_2]\cdot btr$, where M = Cu, Ni; $[Cu(btr)_2(SCN)_2]_n$ and $[Cu(btr)_3(SCN)_2]$.

Single crystal X-ray analysis showed that ptr and btr acted as monodentate ligands coordinated by metal cations *via* the heteroring N^4 atoms in all obtained complexes. Complex $[Cu(btr)_2(SCN)_2]_n$ was found to be 1D coordination polymer, formed due to bridging thiocyanate anions (Fig. 1*a*). Other compounds are mononuclear complexes, in which thiocyanate anions are coordinated by metal only through the nitrogen atoms. In complexes $[M(btr)_4(SCN)_2]\cdot btr$, their crystal lattices include also non-coordinated triazole molecules (Fig. *b*).



a *b*

Fig. *a*) Coordination polymeric chain in the crystal structure of $[Cu(btr)_2(SCN)_2]_n$; *b*) complex molecule together with non-coordinated triazole molecule in the crystal structure of $[Cu(btr)_4(SCN)_2]\cdot btr$. All hydrogen atoms are omitted for clarity.

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Liposomal murrayafoline a modified with chitosan-folic acid conjugate

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Murrayafoline A (MuA), isolated from Murraya koenigii in Vietnam, is a carbazole derivative that shows biological activity as cytotoxic agent [1, 2]. Liposomal form of MuA (L-MuA) modified with chitosan-folic acid conjugate [3] (Ch-FA) can be used to reduce the drug toxicity, improve its bioavailability and create the drug delivery system.

Liposomes were prepared from the mixtures of egg phosphatidylcholine (PC), cholesterol (Ch) and MuA (16:4:1 wt.) in chloroform using combination of the thin film hydration and sonication methods. Surface modification of negatively charged liposomes (-42.2 mV) by positively charged chitosan-folic acid conjugate (27.3 mV) was performed by mixing liposomes with polymer solution up to final Ch-FA concentrations of 0.05-2.00 %. The mean diameter (d) and ζ-potential, measured using dynamic light scattering, were in the range from ~ 148 to 361 nm and from –42.20 to –23.8 mV for different formulations respectively (Table).

Table. Characteristics of L-MuA, Ch-FA and L-MuA/Ch-FA.

Formulations	d, nm	ζ, mV
L-MuA	148±21	-42.2±1.6
L-MuA/Ch-FA0.05%	289±43	-38.1±2.2
L-MuA/Ch-FA0.5%	298±45	20.6±1.7
L-MuA/Ch-FA2%	361±60	23.8±0.6
Ch-FA	300±44	27.3±0.7

ζ-potential of unmodified liposomes was negative owing to negatively charged phosphate groups of phospholipids. ζ-potential of Ch-FA-modified liposomes shifted to positive with increasing Ch-FA concentration. Due to the process of the surface modification the mean diameter of L-MuA/Ch-FA was higher than for L-MuA and increased for formulations containing 0.05 – 2.00 % of conjugate. Thus, it was obtained and characterized liposomal Murrayafoline A modified with chitosan-folic acid conjugate that can be used in biomedicine.

Acknowledgment

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Creating new agrotextile with nourishing properties

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The development of modern analytical methods has exposed a huge problem of environmental pollution, especially food. Currently, a search is underway for technological solutions that provide similar production efficiency, but are safe for the environment. The solution can be modern agrotextiles based on biodegradable materials that do not generate waste [1, 2].

In our research, an attempt was made to create a new agrotextile with nutritional properties and water retention in the soil. To ensure the competitiveness of this solution, were used cheap and commercially available materials such as starch, borax and glycerin. All substances used are biodegradable and do not have any harmful effects on the environment. Moreover, they are an ecological fertilizer. The mechanical properties, the ability to swell, biodegradability, the process of thermo-oxidative aging, and others have been investigated.

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Concentration of PAHs from exhaust gases

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The study of the chemical composition of waste gases has a scientific and applied value, since it allows one to determine both the dependence of the component composition of a mixture of polycyclic aromatic hydrocarbons (PAHs) on the pyrolysis conditions and the degree of toxicity of the waste gases of pyrolysis plants. A quantitative analysis of PAHs in gaseous pyrolysis products of a propane-butane mixture during carbon nanomaterials synthesis has shown that at sampling with a small amount of Supelpak-2 adsorbent, widely used in international and domestic methods [1-2], efficient capture of multinuclear aromatic hydrocarbons is not ensured. Therefore, an important research issue is the development of a simple and effective method for sampling PAHs with their subsequent GC/MS analysis. The principal essence of the technique is to minimize the size of the cartridge, which is achieved by impregnating two glass fiber filters with organic low-volatile solvents – diethylene glycol, tetraethylene glycol or dimethyl sulfoxide [3]. The latter is characterized by the highest extracting capacity in relation to PAHs.

The developed technique makes it possible to minimize the size of the cartridge and increase the capture efficiency of multinuclear aromatic hydrocarbons (from four rings in a molecule) up to 96–98% in comparison with the solid adsorbent under equal conditions, where the capture efficiency is 1–5%. The established values of the capture efficiency of the measured components are explained by the high extraction ability of DMSO to multinuclear aromatic hydrocarbons.

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Correlation of different bioindicators in the analysis of the toxic effects of various aluminum salts

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Currently, the methods of bioassay do not have a generally recognized and standardized system of biological analysis, there are no unambiguous requirements that an indicator system should meet. The relevance of studying the toxicity of aluminum salts is determined by the fact that aluminum cation is contained in drinking water, artificial dyes and additives (E173, E520, E521, E523, E554, E555, E556, E598), and there is also a correlation between the concentration of aluminum ion in brain tissues and the clinical manifestations of Alzheimer's disease[1]. Purpose of the research was quantitative determination of the toxic effect of aluminum salts (chloride, sulfate, and nitrate) on various biological organisms and correlation analysis of bioindicators among themselves.

Dero furcata and plants (*Phaseolus, Lepidium sativum*) were studied as test organisms [2]. Solutions with different concentrations of the Al^{3+} ion in the range from 1 to 0.00001 mol/l were taken for the experiment. The test organisms were introduced into Petri dishes in three parallel ones for different concentrations and for each of the salts, as well as three parallel ones with the settled water for control. The study was conducted according to standard methods [3]. Toxicity (TLV) for plants was determined by calculating the percentage of sprouted seeds and that for *Dero furcata* – by the time of formation of conglomerates. A mathematical statistical analysis of the obtained results was carried out, statistically significant values of TLV and Cl50 were calculated, and a correlation with the ionic strength of solutions and the activity coefficients of the Al^{3+} was established. In the cress experiment, the following TLV values were calculated for aluminum sulfate, chloride, and nitrate: 3.42 mg/dm^3; 1.34 and 2.61, respectively. Similar TLV values were calculated for *Phaseolus*: 3.55 mg/dm^3; 1.38 and 2.66, respectively. The experiment with *Dero furcata* showed similar data. This allows us to use the studied organisms as reliable bioindicators.

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Hydroxyalates of γ-aminopropylsilanes as potential growth regulators of plants

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Hydroxyalates of γ-aminopropylsilanes have growth-regulating activity and show a stimulating effect on the morphophysiological parameters of growth and development of wheat (*Triticum aestivum* L.), radish (*Raphanus sativus* L.), lupine *(Lupinus angustifolius* L.), peas (*Pisum sativum* L.), watercress (*Lepidium sativum* L.). Hydroxyalates of γ-aminopropylsilanes were obtained by reaction of equimolar amounts of y-aminopropylsilanes with oxalic acid in an organic solvent. The corresponding γ-aminopropylsilanes were obtained by a hydrosilylation reaction catalyzed by H_2PtCl_6. Hydrosilylation of allylamines was carried out by heating reagents without a solvent both at atmospheric and at high pressure in sealed glass ampoules. Several variants of the reaction were used: heating the reaction mixtures at the temperature of 180 °C during 6 days for 4 hours daily; heating the reaction mixtures in glass ampoules at the temperature of 120 °C (1 hour), 140 °C (1 hour), 160 °C (1 hour), 180 °C (12 hours); heating the reaction mixtures at atmospheric pressure and the temperature of 170 °C during 4 days for 1 hour daily. In all cases, the hydrosilylation products were mainly the products of addition according to the Farmer's rule (Figure):

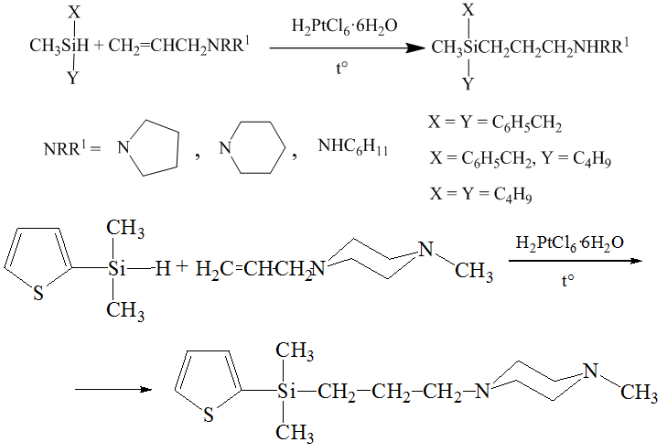

Fig. Hydrosilylation of allylamines by hydrosilanes

Influence of DMSO addition on swelling of chitosan lactate films

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The study of the properties of the films of chitosan with dimethyl sulfoxide (DMSO) additive is determined by the interest in the properties of this substance and its widespread use in pharmacy. There are a number of inventions in which DMSO is used in combination with chitosan for the formation of film membranes [1], plates [2], rods [3] to provide hemostatic, wound healing, anti-inflammatory action in medical practice. Such dosage forms have a prolonged therapeutic effect, sorption activity.

In this work, films of chitosan lactate in the presence of DMSO were obtained. The concentration of chitosan lactate in the solution mixture was varied from 1 to 2 wt.% The concentration of DMSO in the solution was also varied up to 30 vol.%. The concentration of glycerol was - 10 vol.%. The films were formed by casting of mixed solution and subsequent drying in an oven at 50 ºC.

It was found that chitosan lactate films with DMSO showed the ability to swell significantly in saline. With increasing concentration of DMSO swelling increases from 400% at 5 vol.% to 1200% at 20 vol.% of DMSO. Swelling ability also increases with the rise of chitosan concentration. It was found that films based on chitosan lactate with DMSO at concentrations of the latter above 5 vol.% become insoluble. The swelling of the obtained films didn’t decrease upon 3 days of experiment. These results are consistent with the X-ray diffraction data of [4], which showed that the presence of a high concentration of organic solvent leads to a change in the crystal structure of the resulting chitosan acetate films and makes them insoluble in water. Thus, the addition of DMSO to a solution of chitosan lactate, followed by film formation leads to a change in the properties of the films, changing their solubility and allows you to exclude the introduction of a crosslinking agent in this case.

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Modified epoxy coatings with aminoimide-containing oligomers

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Epoxy materials have superior performance properties, so they have been used to produce high quality coatings. Coating materials based on epoxy oligomers are used to prepare responsible coatings for various purposes, chemical-resistant, water-resistant, heat-resistant and insulating coatings. They are characterized by high adhesion to metallic and non-metallic surfaces, resistance to water, alkalis, acids, ionizing radiation, low porosity, small moisture absorbability and high dielectric properties. However, there are a number of outstanding issues to improve the barrier properties of paints based on epoxy resins, which limit their wider use in aeronautical engineering as well as in engineering and shipbuilding. Chemical structure of epoxy resins provides opportunities to control their properties by introducing modifying additives, to achieve maximum compliance with the requirements of the resulting material.

The aim of this study was to investigate the effect of reactive aminoimide–containing oligomeric modifiers on the physicomechanical and protective properties of coatings formed on the basis of epoxy varnishes. The choice of aminoimide containing oligomeric modifiers was determined by the presence of reactive maleimide and amino groups in their structure and the bulky structure of macromolecules.

The object of the study was commercially produced epoxy resin E−41 in solution (E−41 r) (TU 6-10-607-78) , which is a solution of the resin E−41 with a mass fraction(66 ± 2) % in xylene (GOST 9410-78, GOST 9949-76) with acetone (GOST 2768-84) at a ratio of 4 : 3 by weight. Resin solution E−41 in a mixture of xylene and acetone (resin E−41 r) is used for the manufacture of paints for various purposes. Paint application is one of the most common and reliable ways to protect metal surfaces from corrosion and give a decorative surface finish. It is known that the testing of protective properties of the coating in an operational environment takes a lot of time, that does not comply with any developers or manufacturers. Rapid tests provide information about the resistance of the coating under its compulsory destruction simulating natural mechanism of aging in a short time. Electrochemical methods are used as these accelerated test methods. Chemical structure of epoxy resins provides opportunities to control their properties by introducing modifying additives, to achieve maximum compliance with the requirements of the resulting material (inhibits the process of underfilm corrosion of the substrate and increases the protective effect of the anticorrosive coating).

Fabrication of polysaccharide-based multilayer films with antibacterial properties

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Nowadays, one of the serious problems in regenerative medicine is implant-related infection originating from pathogenic microorganisms which adhere to the implant surface and form biofilm preventing penetration of antibiotics to the bacterial cells [1]. To solve this problem the surface of implants might be covered by antibacterial coatings [2]. A perspective technique for creation of multilayer films with tailored characteristics is layer-by-layer (LbL) assembly [3].

The aim of this study was to design ultrathin antibacterial coatings based on polysaccharides (pectin, chitosan) and their Ag-containing nanocomposites (pectin-Ag, chitosan-Ag) suitable for implant modification. Multilayer films were fabricated by LbL assembly and the process of their buildup was monitored by quartz crystal microbalance with dissipation [3]. To establish the influence of film compositions and physical-chemical properties on their antibacterial effect, the assembly of the different polycation/polyanion combinations yielded four chemically different multilayer: (chitosan/pectin)$_{10}$, (chitosan-Ag/pectin)$_{10}$, (chitosan/pectin-Ag)$_{10}$, (chitosan-Ag/pectin-Ag)$_{10}$, has been prepared.

The prepared multilayers showed high antibacterial activity against *E. coli* due to the antiadhesive and/or bactericidal behavior. Almost two-fold decrease in the number of the adhered *E. coli* was revealed for pectin-terminated LbL films. We observed a significant enhance in antibacterial activity for pectin-Ag-terminated coatings: the number of adhered *E. coli* was in 3–7 times lower compared with uncovered surface. A lot of damaged *E. coli* cells with irregular shape and cytoplasm leaking (from 47 to 89%) were observed on the surface of LbL films. At the same time, the multilayers showed a mild activity against *S. aureus* predominantly due to the antiadhesive effect. So, the prepared ultrathin LbL films based on chitosan, pectin and their nanocomposites with silver nanoparticles look as perspective materials for covering the surface of medical implants in order to reduce their bacterial contamination.

Acknowledgment

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Structure activity relationship studies on KasA: aldonamides' affinity to receptor in context of TB drug design

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KasA is a key enzyme involved in the synthesis of mycolic acids. The latter, being the fragments of *M. tuberculosis* cell wall, protect bacteria from the action of acidic environment, thereby allowing them to persist in the human body. Inhibition of this enzyme leads to disruption of the FAS-II system, preventing the build-up of the fatty acid chain [1]. This mechanism underlies the action of few TB drugs, including the legendary isoniazid.

We have studied the series of more than 50 open-chain aldonamides in context of the influence of their relative configuration and functionality on affinity to KasA receptor. The receptor choice (2WGF Transferase: chain A [1]) is based on the comparison of SAR obtained both *in silico* and *in vitro* experiments for free-hydroxy and acylated isonipecotamides synthesized previously [2]. To design open-chain derivatives we have chosen monose derivatives which are structurally and functionally isosteric to isonipecotamides and possessing all possible relative configurations. Structure design includes monose skeleton modification by introduction of the substituted amide and amino groups (both transformations are available from the classical sugar chemistry). The *in silico* study was carried out in [3] by using the semi-empirical PM6 and the MMFF94 geometric optimization techniques for pH=7. To find the energetically optimal conformations for labile open-chain aldonamides we have proceeded every docking for at least 100 runs. L-altro- and D-gluco- configuration-based derivatives showed the highest affinity to receptor. After variation of substituents in amide fragment and replacement of hydroxyl with amino group we have found the highest affinity for N-tert-butyl L-4-deoxy-4-aminoaltrosamide (-10.93 kcal / mol), N-benzyl L-4-deoxy-4-amino-altrosamide (-11.48 kcal / mol) and N-benzyl D-gluconamide (-10.01 kcal / mol), The SAR analysis showed these structures form conformations with the maximum number and the optimal geometry of intramolecular hydrogen bonds, as well as hydrophobic interactions. The latter can be discussed in terms of multiple interactions between N-alkyl substituted amide group and protein hydrophobic side chains (Pro and Ile in protein studied). Based on the data obtained, a pharmacophore was proposed with the L-altro- or D-gluco- configuration, bulky hydrophobic N-substituted amide group and possible amino group at 4th C-Carbon.

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Influence of functionality and stereochemistry on the solubility of mono- and heterofunctional oxo-compound

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The oxo group affects significantly the physicochemical properties of heterofunctional substances to which most drugs belong. The introduction of an oxo group into a molecule of an organic substance makes it more hydrophilic; in the case of drugs, this factor contributes to an increase in the bioavailability of the formulation. At the same time, unlike hydroxyl and amino groups, which also increase significantly hydrophilicity, the introduction of an oxo group does not affect the lipophilicity of the substance. At present, the increase in hydrophilicity upon the introduction of the oxo group is explained by the formation of intermolecular hydrogen bonds of the substance with water via participation of two lone electron pairs of the carbonyl group. However, this explanation cannot fully explain the fact that the oxo group increases the hydrophilicity of the molecule to the same extent as the hydroxyl group (which has a polarized OH bond), without affecting the lipophilicity of the molecule. The study of the factors that affect the dissolution of substances containing the oxo group will allow to understand the real mechanism of the growth of hydrophilicity due to the carbonyl group [1]. This, in turn, makes it possible to plan a targeted modification of biologically active substances to increase their bioavailability [2].

We have studied the series of monofunctional and heterofunctional compounds containing oxo-group including monose cyclic hemiacetal forms. For monofunctional derivatives the correlation between the formation of hydrates and solubility was found. The unexpected the higher solubility of cyclohexanone compared to acyclic analogues can be explained in terms of the thermodynamic parameters for oxo- distorted and geminal diol “pure” chair conformations. Comparison of experimental and literature data showed the ratio of constitutional (cycle size) and configurational (anomer ratio) isomers in solution, as well as competition between the possible formation of intra- and intermolecular hydrogen bonds are the main factors affecting the monose solubility. It was also found that 50% water-mannose and water-glucose solutions make it possible to obtain more concentrated *Ibuprofen* solution compared to “pure” aqueous solutions. It makes monose-water mixtures promising bi-component systems for increasing the concentration of substances, including active drugs, in solution.

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Nanoporous support for automated synthesis of cyclooctyne oligonucleotides and further solid-phase copper-free modification

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Recently modified oligonucleotides have appeared in focus of researchers as new generation therapeutic agents[1]. Because of their high molecular weight and low therapeutic dosage, the targeted delivery and facilitated cell penetration is a special concern of gene therapy [2]. Modifications, either targeting, stabilizing, or reporter can be introduced to synthetic RNA/DNA oligonucleotides during automated solid phase synthesis with phosphoramidite reagents or modified solid supports. However, sometimes the more convenient way is to synthesize the oligos with reactive groups for click-chemistry with further modification thereof.

Here in we report a convenient approach for solid-phase preparation of oligonucleotide conjugates with ligands for targeted delivery: biotin, cholesterol, mannose and N-acetylgalactosamine (GalNAc) [2,3]. The approach is based on using a new cyclooctyne modified support (**1**), which was obtained by treatment of aminated control pored (50 nm porous diameter) glass (CPG) material with reagent **2**. Support **1** allows to synthesize alkyne-modified oligonucleotides and then to conjugate them with azide-bearing ligands on the solid phase by copper-free strain-promoted [3+2] azide-alkyne cycloaddition (SPAAC).

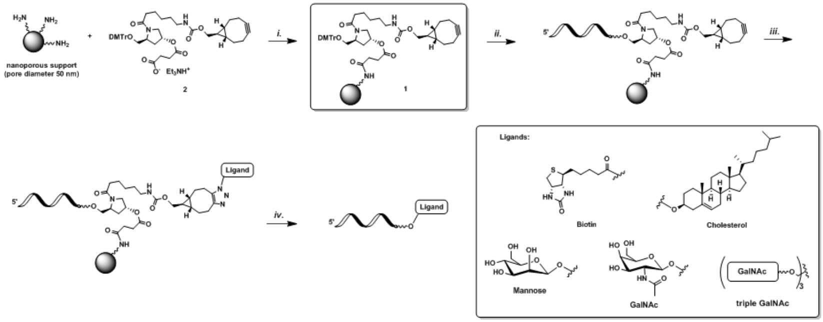

Fig. Solid-phase SPAAC modification of alkyne-modified oligonucleotides:
i. – treatment of the amino-CPG support with reagent 2; *ii.* – automated oligonucleotide synthesis; *iii.* – modification of cyclooctyne oligonucleotides with azide-bearing ligands on solid support; *iv.* – deprotection and cleavage from the support.

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Raman spectroscopy of activated carbons of various origins

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Activated carbons of different origins have been studied by Raman spectroscopy: disintegrated activated carbon fabric OUT-MI, mineral charcoal SILCARBON TH-90G, charcoal OU-A, the experimental mesoporous activated carbon obtained from the hydrolysis lignin by carbonization and chemical activation (AC), as well as the same activated carbons modified by cellulose sulfate acetate sodium salt (Na-CAS) in the amount of 0.08 g of polymer/g of coal. The structural parameters of the studied samples obtained from the Raman spectra are presented in the table. All the samples have two obvious D and G bands, which are assigned to the disorder of carbon atoms in the graphene layers, crystalline lattice defects and the graphitic structure of carbon materials, respectively [1,2]. Two prominent peaks appear at approximately 1350 cm^{-1} (D band) and 1600 cm^{-1} (G band), which are typical for spectra of carbon materials. The value of R (I_D/I_G) is defined to characterize the disordering degree of carbon materials. According to literature data, while the G-band is characteristic of graphite, the D-band is associated with defects, curved graphite sheets and lattice distortions in carbon structures. Reducing the intensity ratio I_D/I_G for modified samples may indicate a decrease in the number of defects and correlates with the adsorption properties: the value of Gibbs adsorption for methylene blue dye increases when R decreases.

Table. Raman Spectra parameters and specific adsorption for the activated carbon samples

Sample	Peak Intensity Frequency, v_x, cm^{-1}		$R=I_D/I_G$	A, mmol*g^{-1}
	G band	D band		
AC	1587	1357	0,988	1,40 ± 0,03
AC- Na-CAS	1592	1360	0,915	1,63 ± 0,03
OUT-MI	1596	1314	1,055	0,86 ± 0,02
OUT-MI- Na-CAS	1592	1313	1,012	1,33 ± 0,03
OU-A	1592	1316	0,931	0,94 ± 0,02
OU-A- Na-CAS	1591	1336	0,908	1,42 ± 0,03
SILICARBON	1587	1357	0,971	1,18 ± 0,02
SILICARBON- Na-CAS	1589	1344	0,959	1,49 ± 0,03

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Thermodynamics of polymer solutions in the entropy-fractal approach

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As a statistical theory of open systems, only entropy has a set of properties that allows it to be used in quantitative statistical uncertainty in microstates, natural polymers (hyperbranched structures, dendrimers, lignins, biological systems, dendrites, systems of internal organs, blood vessels, etc.). In the entropy-fractal approach, the Renyi entropy Rn [1] effectively "works" for equilibrium systems and the Tsallis entropy Ts [2] for open systems.

A functional relationship has been established between entropies S and the fractal dimension d – the most important characteristic of real objects, including natural polymers: $S \approx ln\varepsilon^{-d}$, where is the coating element of a fractal object (polymer). In this communication it is shown that the generalized non-ideality factor of systems (GNF) [3] can be introduced into the equations of informational entropy of Renyi and Tsallis and new expressions of informational and thermodynamic entropy can be obtained with a moment of order g_{th} . Equations in the Renyi

$$S_{g_{th}}^{M-Rn} = \frac{R}{g_{th}} ln\left(\sum_{i=1}^{N} p_i^{g_{th}-1}\right) \qquad (1);$$

$$(S_{g_{th}}^{M-Ts}(p) = \frac{R(1- {}_{i}^{N(\varepsilon)} p_i^{1-g_{th}})}{g_{th}}, \qquad (2)$$

describing self-organized structures of equilibrium (1) substantially nonequilibrium (2) systems. These equations can be used to study the thermodynamic properties of solutions of high molecular weight compounds.

$$\text{GNF: } g = 1 + \langle -\beta_{ord} + \alpha_{nord} \rangle = 1 + \langle -p_i(\beta) + p_i(\alpha) \rangle, \qquad (3)$$

where $\beta_{ord} \equiv 1/n\sum_i^n \beta_i$ and $\alpha_{nord} \equiv 1/n \ {}_i^n \alpha_i$ – relative average characteristics (p_i is statistical probabilities) of opposite processes. The thermodynamic factor g_{th} varies in the range $0 \leq g_{th} \leq 2$ and depends on which of the competitive processes prevails.For example, dioxane lignin DL_{pin} of pine in the dioxane with fractal dimension d = 2,50 ± 0,08 and $g_{th} = 0.83$ at T = 298 K enthalpy of mixing ΔH_{mix} = –0.055 kJ/mol andΔG_{mix} = –18.55 kJ/mol. For a polyelectrolyte in the system: dialyzed lignosulfonate DLS with d=2,44 ± 0 and $g_{th} = 0.79$ ΔH_{mix} practically equal to zero show that ΔG_{mix} = –17.35 kJ/mol. Thus, the conformational behavior of DL_{pin} in dioxane and DLS in a buffer solution determines the thermodynamic factor TΔS.

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MOF-199 as a storage matrix for diphenylamine.

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As researchers have focused on finding new substitutes for traditional inhibitors to solve different problems, nanostructured systems can play a vital role among various alternatives [1].

Application of diphenylamine to MOF-199, which is considered a corrosion inhibitor in the literature, has a positive effect on corrosion resistance. MOF-199 itself , a mixed-type inhibitor, was synthesized using a well-known technique [2] to obtain samples of a microporous structure (Fig.).

The sorption capacity with respect to diphenylamine is 303 mol/d. The chromatographic retention time of diphenylamine was determined using methanol, acetonitrile, and tetrahydrofuran as eluents. The temperature control was performed at 25 °C with an eluent velocity of 1.25 ml/min. The best retention time was observed in methanol at 25 °C and was 0.83 seconds. In acetonitrile and tetrahydrofuran, the contact time is reduced to 0.57 s and 0.77 s accordingly.

Thus, the best fusion of diphenylamine with the MOF-199 surface is provided by an alcohol solution.

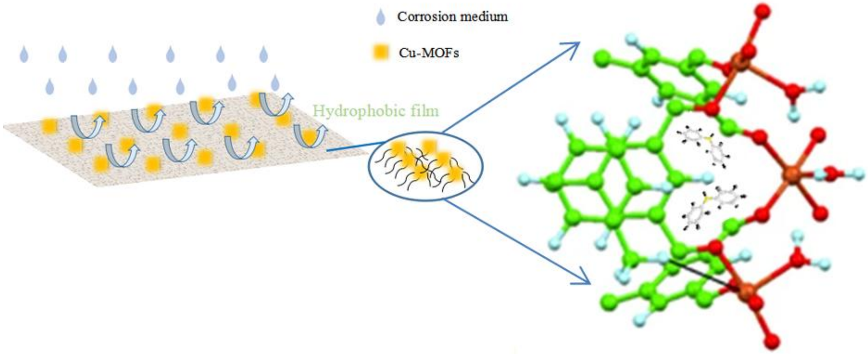

Fig. Composite inhibitory behavior model

Acknowledgement

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Pro/antioxidant effect of non- and proteinogenic amino acids on $Cu^{2+}(Fe^{2+})$-mediated fragmentation of phosphatidylglycerol

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In the polar moieties of glycerophospholipids the reaction of free radical fragmentation, proceeding through $H_2C(Y)\text{-}C^{\cdot}(OH)\text{-}H_2C\text{-}OP(O)O_2R^{-}$ radicals formation, can occur [1]. The fragmentation leads to the rupture of the phosphoester bond in lipid molecules and the formation of phosphatidic acid. Amino acids (AA) play an important role in the regulation of various signaling pathways, oxidative stress, apoptosis, and autophagy in biosystems. The aim of this work was to study the effect of non- and proteinogenic AA on $Fe^{2+}(Cu^{2+})$-mediated fragmentation of dimyristoylphosphatidylglycerol (DMPG) with the formation of dimyristoylphosphatidic acid (DMPA). Preliminarily, before studies in liposomal membranes, photometric monitoring of the ability of β-alanine, taurine, hypotaurine, α-alanine, histidine, glycine, methionine (in a wide concentration range of 0.05-20 mM and in the presence of various biologically active substances) to regulate the fragmentation of $H_2C(OH)\text{-}C^{\cdot}(OH)\text{-}H_2C\text{-}OP(O)O_2H^{-}$ and $H_2C(OH)\text{-}HC(OP(O)O_2H^{-})\text{-}C^{\cdot}H(OH)$ $\{HC^{\cdot}(OH)\text{-}HC(OP(O)O_2H^{-})\text{-}CH_2(OH)\}$ radicals was carried out. It has been found that, in the presence of $Fe^{2+}(Cu^{2+})$ ions, the effect of the studied AAs on the fragmentation of phospho-derivatives of glycerol with the rupture of phosphoester bond can be neutral, pro/antioxidant, or inversed. So, in the presence of Cu^{2+}, β-Ala in large amounts ($AA:Cu^{2+}>10:1$) has an activating effect, which decreases in the presence of effective $HO^{\cdot}$-acceptors (Figure). This may be the mechanism of action of β-Ala in the development of oxidative stress and apoptosis observed in mitochondria containing diphosphatidylglycerol [2].

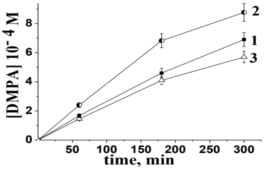

Fig. DMPA accumulation in DMPG-liposomes (20 mM) incubated with $CuSO_4$–H_2O_2 (0.1/0 mM) at 37 ° C, 1 - without additives; in the presence of 2 mM β-Ala: 2 - alone, 3 - mixed with 1 mM NaN_3

Acknowledgement

This work was supported by the State program of scientific research of Belarus «Chemical processes, reagents and technologies, bioregulators and bioorganic chemistry», project 2.2.03.04.

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Optimization of sorption properties of cation exchanger FIBAN K-6

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With the development of chemisorption technologies, selective and inexpensive fibrous sorbents obtained from available raw materials acquire great importance for solving environmental problems. Aminocarboxyl cation exchanger FIBAN K-6 developed at the IPOCh of NAS of Belarus on the basis of polyacrylonitrile fiber is promising for use in purification of technical and drinking water from copper, lead and cadmium cations [1].

The effect of crosslinking and conditioning on the physicochemical and sorption properties of this sorbent has been investigated. Epichlorohydrin was applied as a crosslinking agent. Conditioning was carried out by alternate triple treatment of the cation exchanger with 0.5 M NaOH, H_2O and 0.5 M HCl.

It was found that the use of epichlorohydrin as a crosslinking agent reduced swelling of FIBAN K-6 samples and contributed to the stability of the fiber geometric shape. Samples of cross-linked cation exchanger FIBAN K-6M provide 1.5 times higher dynamic capacity before slipping of MPC of copper and lead ions as well as 2-3 times higher volumes of treated water (Table).

Samples of FIBAN K-6 and FIBAN K-6M	Number of column volumes of water, purified from cations to the MPC level					
	Cu^{2+}	Pb^{2+}	Ni^{2+}	Co^{2+}	Cd^{2+}	Zn^{2+}
Non-cross-linked, non-conditioned	828	993	<497	331	745	497
Cross-linked, non-conditioned	1108	1385	277	<277	554	277
Cross-linked, conditioned	2367	3943	<592	<394	1183	592

Conditioning of cation exchanger FIBAN K-6M leads to an increase in the exchange capacity of the exchanger by carboxyl groups with a simultaneous decrease in the amino group content, and also improves the dynamic sorption capacity by more than 2 times compared to the non-cross-linked sample of FIBAN K-6. The amount of purified water increases by up to 4 times.

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Preparation of complexes based on chitosan-Ag nanocomposite and cephalosporin antibiotics

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Bacterial drug resistance is a global problem of modern society. It is known that the resistance of microorganisms to metal nanoparticles and their oxides, in contrast to traditional antibiotics, is rarely occurred. In order to improve the biocompatibility and aggregative stability of nanoparticles, it seems promising to use polysaccharides in their synthesis, which can be used simultaneously as reducing agents and stabilizers [1]. Recent studies have shown that combining nanoparticles with antibiotics not only reduces the toxicity of both agents towards human cells by decreasing the requirement for high dosages but also enhances their bactericidal properties [2]. Combining antibiotics with nanoparticles also restores their ability to destroy bacteria that have acquired resistance to them.

In this work the effect of the mass ratio of chitosan-Ag : antibiotic in the reaction mixture on the physicochemical properties of complexes was established. Chitosan-Ag nanocomposite in aqueous solutions were synthesized by a facile hydrothermal method. Antibiotics of the third-generation cephalosporin group (ceftriaxone and cefotaxime) have been used to form complexes with chitosan-Ag nanocomposite. It was shown that when the mass ratio of ceftriaxone:chitosan-Ag in the reaction mixture changes from 0.5 to 1.25, the efficiency of antibiotic binding to nanoparticles increases 10 times: from 7.2 ± 0.2 to 71.7 ± 0.2 %. A further increase in the concentration of ceftriaxone during the synthesis leads to a gradual decrease in the efficiency of its binding to 14.2 ± 0.3% (with an 8-fold excess in relation to chitosan-Ag). In the case of cefotaxime, with a change in the mass ratio of antibiotic: chitosan-Ag in the reaction mixture from 0.5 to 10.0, a smooth decrease in the efficiency of its binding from 66.2 ± 1.5 to 13.0 ± 0.7% was observed. It was found that the maximum content of ceftriaxone and cefotaxime in the synthesized complex was 1.06 ± 0.01 and 1.29 ± 0.03 mg / mg chitosan-Ag, respectively.

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Creation of systems of controlled release of biologically active substances for cosmetic

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In modern pharmacology and cosmetology, the solution to the problems of targeted use of drugs is associated with the creation of new forms of delivery of biologically active substances (BAS). The use of carriers for biologically active substances allows us to obtain dosage forms with improved compatibility with biological fluids, controlled time of entry into the body, high storage stability and so on. By creating composites that would provide the necessary content of BAS and their controlled release, we can reasonably hope to achieve positive results in this direction. This paper proposes the creation of composites based on clay minerals and zeolites, which provide various forms of inclusion of the active substance by optimizing the composition and improving the methods of formation. Significant hydrophilicity of clays increases the moisture content in materials and, as a consequence, allows one to increase the content of BAS.

The release of chlorophyll A and B, carotenoids, anthocyanins and vitamin C from plant raw materials and clay / zeolite / plant raw materials composite was studied by UV spectroscopy [1]. The level of safety of the obtained materials and plant raw materials was assessed using the program "Rana" [2]. All indicators were not more than 33, composites are hypoallergenic. The proposed composite materials are clay / zeolite / vegetable raw materials. Indicators of the level of safety of components and composite materials are studied. The possibility of their use in cosmetics is substantiated. The hypoallergenicity of the studied systems is confirmed. Kinetic studies of biologically active substances can be used as a factor in regulating the direction of preventive action of shampoos, masks and supplements.

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Development of targeted cosmetic products based on clay / diatomite / vegetable raw composite materials

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A wide range of therapeutic and prophylactic properties of clay minerals creates the preconditions for their inclusion in cosmetics, in particular shampoos, in the development of new recipes. In the last few years, well-known cosmetic companies have introduced innovative developments-shampoos with clays, which, thanks to the presence of the latter, strengthen the hair follicles and prevent their brittleness and loss. To increase the effectiveness of the clays that are part of the shampoo, it is advisable to use their compositions with vitamins and other biologically active substances (BAS). Clay / diatomaceous earth / vegetable raw material samples were obtained by mechanochemical activation.

The release of chlorophylls A and B, and carotenoids from plant raw materials and composite materials was studied by UV spectroscopy. To assess the level of safety of the obtained materials there was used software product "Rana" - information system designed for storage and systematization of composition data and calculation of the development of cosmetics or fillers, determining their level of safety in terms of the composition of the final mixture . Safety is assessed on three indicators - Cancer, Developmental & Reproductive Toxicity, Allergies & Immunotoxicity. Composite materials based on clays and various biologically active substances are proposed. The hypoallergenicity of the studied systems has been confirmed. Kinetic studies of biologically active substances can be used as a factor in regulating the direction of the preventive action of shampoos.

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Design and structure analysis of fusion proteins of bovine DNA exotransferase and *E. coli* SSB protein

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This work aimed to design a model of a fusion protein from bovine DNA exotransferase and single-stranded DNA-binding protein from *E. coli* (EcSSB), choose the orientation of domains, find out optimal linker between two protein genes, and test stability of the fusion protein. The hypothesis of the study is that an additional DNA-binding domain attached to TdT will provide an increase in the activity and stability of the enzyme, as well as create new ways of controlling exotransferase activity *in vitro*, which is of particular importance for the creation of an enzymatic method for *de novo* DNA synthesis.

At the first stage, we modeled fusion proteins with the addition of EcSSB at the N and C terminals of the enzyme. As a result of the study, it was proved that EcSSB at the N terminal of the enzyme does not interact with DNA passing through the DNA-affinity domain of the enzyme and, will practically does not effect on enzyme activity (Fig.). In this case, the addition of EcSSB at the C terminal of the enzyme probably has a positive effect on the enzyme activity.

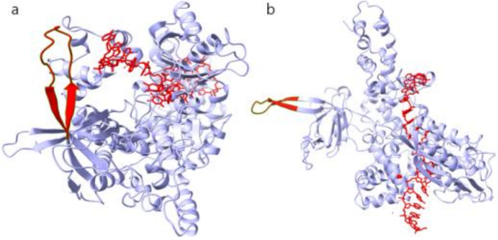

Fig. Model of fusion protein, the DNA and DNA-affinity domain of EcSSB are highlighted in red: a – fusion at the C terminal of the enzyme; b – fusion at the N terminal of the enzyme

Further we designed fusion proteins with various linkers, which are most often used to create fusion polymerases [1, 2]. The primary validation of the obtained models was carried out using the Ramachandran map and the QMEAN index. Further validation of the models was carried out by the molecular dynamics method. According to the results research we found out that the linkers GGGGSGGGSGGGGS and GGGSGGGS have the best stability indicators (minor fluctuations of RMSD and the total number of hydrogen bonds), as well as the smallest gyration radius (6.0 angstroms), coupled with high mutual mobility of DNA-affinity domains of proteins.

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Adsorption of serum proteins on LbL films based on chitosan graft copolymers with polyvinyl alcohol and dextran sulfate

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Layer-by-layer (LbL) films of polyelectrolytes modified with side chains of hydrophilic polymer is a promising way to improve surface biocompatibility and resistivity to protein adsorption of films and nanoparticles. The coating obtained by electrostatic adsorption of chitosan (CH) grafted with poly(ethylene glycol) (PEG) or dextran of low molecular weight and dextran sulfate (DS) has been shown to decrease adsorption of fetal bovine serum (FBS) proteins [1].

Poly(vinyl alcohol) (PVA, 2.0 kDa) was synthesized by radical polymerization of vinyl acetate in the presence of chain transfer agent followed by acid-catalyzed hydrolysis [2]. Copolymers of CH (450 kDa) with PVA (CH-PVA) were obtained using EDC as a crosslinker [1]. The degree of substitution (χ) was controlled by varying the PVA/CH mass ratio in the reaction mixture. The wet mass of (CH-PVA/DS)$_n$ films was evaluated using a quartz crystal microbalance. The dry mass was recalculated from absorbance at 497 nm of the LbL film of FITC-labeled copolymers [1]. The L/2R$_g$ parameter was calculated using experimental surface distance between PVA chains and the radius of gyration of PVA (1.1 nm).

The thickness of a CH-PVA/DS bilayer is 1.1±0.2 nm and almost independent of χ. The mass of FBS protein adsorbed on the (CH-PVA/DS)$_{5.5}$, χ=0.33 films decrease by 50% as compared with unmodified CH. The protein resistance of the LbL films is reciprocal to L/2R$_g$. The protein resistance efficacy of LbL films based on CH-PVA graft copolymers is comparable with that of PEG-based ones.

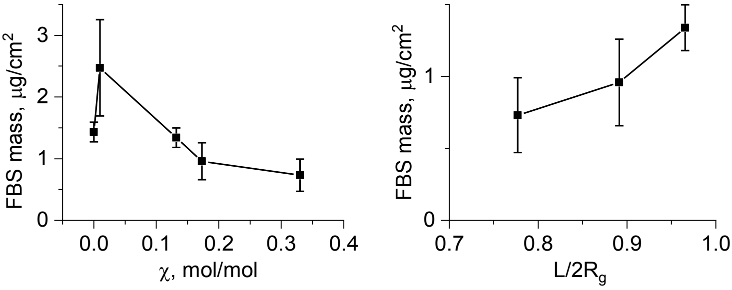

Fig. Protein resistance of (CH-PVA/DS)$_{5.5}$ films

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The process of obtaining polyacrylamide-based polymers via frontal polymerization in continuous mode

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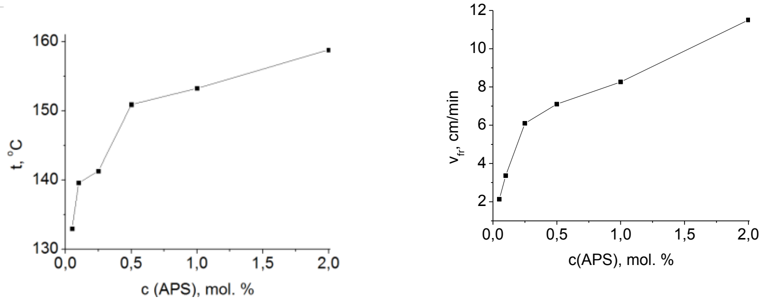
Polyacrylamide-based polymers are widely used in agriculture, medicine, for sewage cleaning, contact lenses production and some other fields [1]. The main way of obtaining polyacrylamide-based polymers is free-radical polymerization. The less common way of obtaining such polymers is frontal polymerization (FP). It is a simple and convenient method of polymerization [2]. One of the main advantages of FP is low energy consumption since FP reactions are highly exothermic and self-sustained. Also it is perspective for polymers and hydrogels obtaining. Hydrogels are three-dimensional polymer networks consisting of water-soluble polymers. Continuous mode of FP has been studying for a long period of time [3]. In the present work FP in continuous mode was used for acrylamide (AA) polymerization in dimethylsulfoxide (DMSO) at equal molar ratio of AA and DMSO. Ammonium persulfate was taken as an initiator.

We have shown that acrylamide polymerization by means of FP in continuous mode is possible to carry out at the minimum initiator concentration of 0,25 mol. %. The macrokinetics of FP in continuous mode has been studied (Figure).



a

b

Fig. The dependence of temperature (a) and front rate (b) on the APS concentration

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Conformation and thermo-responsive properties of polymethacrylate molecular brushes with oligo(ethylene glycol)-block-oligo(propylene glycol) side chains and homopolymer

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Polymer micelles formed by amphiphilic block copolymers, brushes with side chains of block structure form stable monomolecular micelles of cylindrical shape which do not break up under very strong dilution. The synthesis of polymer molecular brushes based on five novel diblock macromonomers (methoxy [oligo(ethylene glycol) e - block -oligo(propylene glycol) p] methacrylates, OEG e OPG p MA) with different lengths of oligo(ethylene glycol) (e) and oligo(propylene glycol) (p) moieties. e = 7.0, p= 10.3 (E7P10), and brushes E7P10-DMAPMA differenced by composition has been studied.

Samples	*dn/dc* cm^3/g	$M_w \times 10^{-3}$ g mol^{-1}	R_{h-D} nm	[η] cm^3/g	k´	R_{h-f} nm	$R_{h-\eta}$ nm	A_0
E7P10	0.225	49	4.3			4.5	-	3.2
	0.035	54	4.2	12	0.55	4.5	4.3	3.2
E7P10-DMAPMA 80:20	0.168	65	5.9	-	-	4.2		
	0.05	69	3	14.4	1.12		5.4	3.1
E7P10-DMAPMA 90:10	0.121	80	5	-	-	4.8	-	-
	0.041	80	3-5	14.5	0.97		5.8-	3.2
E7P10-DMAPMA 95:5	0.134	87	4.7	-	-	4.2	-	
	0.04	70	5	15.9	0.88	4.2	5.6	3.2

Conclusions: Conformation of copolymers was close to coil in good solvent. The polymers have a critical solution temperature in the range from 34 to 71°C.

Acknowledgment

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NMR studies of steroids with heterocyclic rings in the side chain and their reductive derivatives

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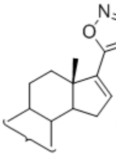
The method of NMR correlation spectroscopy is widely used today in molecular design, studying molecular complexes, organometallic compounds. As part of our heterocyclic steroid derivative studies, the steroidal compounds containing isoxazole (**1**-**5**), dihydrofuran (**11**), tetrahydrofuran rings (**9**-**10**) or β-dicarbonyl fragment (**6**-**8**) in the side chain were prepared. The structure of products and configuration of newly formed chiral centers were confirmed by NMR correlation spectroscopy. Application of modern HSQC, COSY, HMBC, TOCSY and NOESY technics of NMR spectroscopy allowed us to complete full assignment of signals in the NMR spectra of studied compounds and to elucidat their structure comprehensively.



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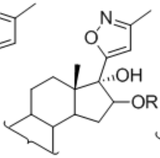
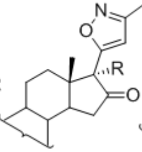
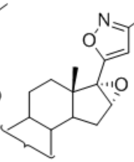


2 R=16α-H,16α-Ac, 16α-Bz,16β-Ac



3 R=H, OH



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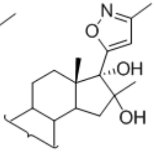
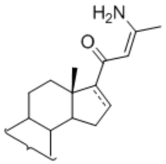
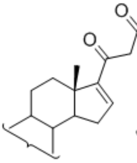


5 16α-OH, 16β-OH



6 double bond
7 single bond



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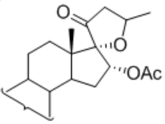
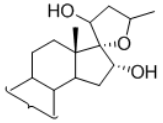
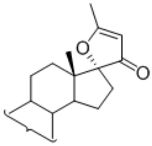


9 (*5′R*)-Me, (*5′S*)-Me



10 (*3′R*)-OH, (*3′S*)-OH, (*5′S*)-Me, (*5′R*)-Me



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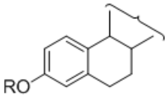

R=H
R=Me

Thermodynamic properties of 1-benzyl-4-phenyl-1H-1,2,3-triazole

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The results of complex thermodynamic study of 1-benzyl-4-phenyl-1H-1,2,3-triazole in crystalline and gaseous states are represented. The substance was synthesized by Huisgen [3+2] cycloaddition reaction between phenylacetylene and benzyl azide. Reaction proceeds smoothly under mild conditions at room temperature in THF with 5 mol.% of the product of copper(ll) poly-5-vinyltetrazolate thermolysis as a catalyst. The temperature dependence of 1-benzyl-4-phenyl-1H-1,2,3-triazole heat capacity in the range (80–370) K was obtained using adiabatic vacuum calorimeter TAU-10 (Termis, Moscow, Russia) [1]. The relative expanded uncertainty of the measurements was determined to be 0.4 %. There were no anomalies on the heat capacity curve (Fig.). Standard thermodynamic functions, such as heat capacity, entropy, reduced enthalpy and reduced Gibbs energy, were calculated from the received data. The values of these functions at 298.15 K were (276.1 ± 1.1), (212.0 ± 0.8), (131.8 ± 0.5) and (80.18 ± 0.32) $\text{J·mol}^{-1}\text{·K}^{-1}$ respectively. Standard internal energy and enthalpy of combustion at 298.15 K of the substance in condensed state were obtained using bomb combustion calorimeter B–08–MA [2]. The values were determined to be $\Delta_c U^o = -(8075.68 \pm 2.86)$ kJ·mol^{-1} and $\Delta_c H^o = -(8080.02 \pm 2.86)$ kJ·mol^{-1} respectively. The standard formation enthalpy of the 1-benzyl-4-phenyl-1H-1,2,3-triazole in condensed state at 298.15 K was $\Delta_f H^o = (319.42 \pm 3.47)$ kJ·mol^{-1}. Standard thermodynamic functions of the substance in gaseous state were calculated using the statistical thermodynamics approach. Standard formation enthalpy of the 1-benzyl-4-phenyl-1H-1,2,3-triazole in gaseous state was calculated in the framework of the isode

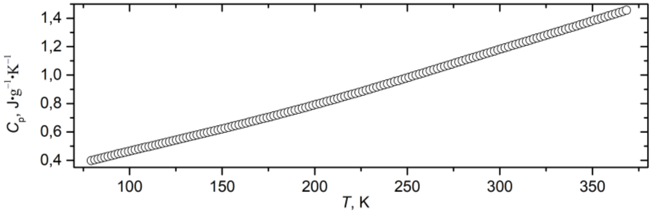

Fig. The heat capacity temperature dependence of the 1-benzyl-4-phenyl-1H-1,2,3-triazole

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Thermodynamic parameters of temozolomide

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Temozolomide is an orally administered alkylating agent, which causes DNA damage leading to tumor cell death, and it is used largely in the therapy of glioblastoma [1]. The results of complex thermodynamic study of temozolomide are represented in this work. The sample contained 99.6 mas. % of the compound. Heat capacities of temozolomide in crystalline state at saturation pressure in the range of (80 – 370) K (Fig) were determined in TAU-10 vacuum adiabatic calorimeter [2]. Relative expanded uncertainty of the heat capacity measurements was determined to be 0.4 %. Standard thermodynamic functions of the compound in condensed state in range of (80 and 370) K were calculated from the received data and the values of heat capacity, entropy, reduced enthalpy and Gibbs energy at $T = 298.15$ K were determined to be (212.3 ± 0.8), (175.4 ± 0.7), (108.1 ± 0.4) and $-(67.29 \pm 0.82)$ J mol^{-1} K^{-1} respectively. Standard thermodynamic functions of temozolomide in gaseous state in the range of (0 – 1500) K were calculated using statis

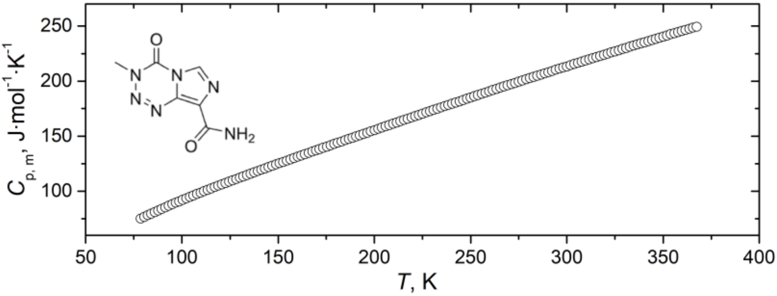

Fig. The heat capacities of crystalline temozolomide

Standard combustion energy of crystalline temozolomide at 298.15 K was determined in a combustion calorimeter B–08–MA [2]. Standard enthalpies of combustion and formation of crystalline temozolomide at 298.15 K were obtained to be $\Delta_c H^\circ = -(3154.46 \pm 0.56)$ kJ·mol^{-1} and $\Delta_f H^\circ = -(64.11 \pm 0.97)$ kJ·mol^{-1}. The method of isodesmic reactions was proposed to calculate the gas-phase formation enthalpies of temozolomide. Sublimation enthalpy was calculated in the framework of electrostatic potential model.

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Synthesis, structure and properties of polyaldehyde dextran

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Dialdehyde dextran is being actively studied as a potential carrier of biologically active substances due to its biocompatibility and ability to prolong the action of low molecular weight substances.

The purpose of this work is to obtain polyaldehyde dextran by oxidation of dextran with a sodium periodate aqueous solution, to study the structure and physicochemical properties.

The effects of the $NaIO_4$: glucopyranose units (GPU) molar ratio, solution pH (2,6 - 6,9), duration reaction (5 – 180 min) and reaction temperature (0 – 30 °C) on the composition, the homogeneity of substitution and the rate of dissolution of oxidized dextran were studied. It was found that as the molar ratio increased (more than 10%), the limiting oxidation degree of dextran increased and hemiacetals formed; also, the parallel reaction of dextran oxidation occurred with the release of formic acid, i.e. a polymer is formed containing three types of oxidized units (Figure)

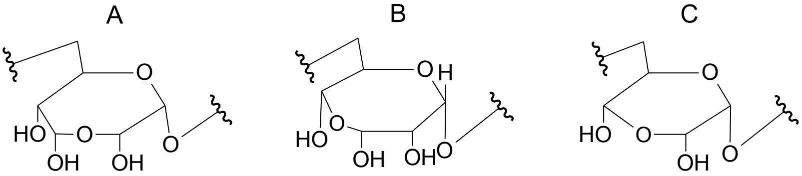

Fig. Supposed structures of oxidized units

The presence of structures in dialdehyde dextran under the indicated reaction conditions is confirmed by IR spectroscopy data.

Table. Reaction conditions and composition of oxidized dextran depending on the content of sodium periodate in an aqueous solution (T   20 °C, t 1,0 h, pH 2,67)

Molar ratio of $NaIO_4$: GPU	OD	Number of oxidized units		M_w, Da
		2,4	3,4 and 2,3	
0,10	8	0	8	62900
0,20	15	6	9	58700
0,48	41	14	27	47300

Note. The oxidation degree (OD) is the total number of oxidized units per 100 GPU of dextran.

As a result of studying the regularities of the oxidation reaction, the optimal conditions for obtaining the most homogeneous on composition samples of dialdehyde dextran with the oxidation degree in the range of 20–50 were determined: molar ratio 20–50; temperature 20 ^{0}C; reaction time 1 hour.

«Click»-synthesis of 1-benzyl-4-phenyl-1*H*-1,2,3-triazole facilitated by copper(II) complex of 1-*tert* -butyl-(benzoylamino)-1*H*-tetrazole

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1*H*-1,2,3-triazoles are promising and important N-heteroaromatic compound, having tremendous application in various research fields, including synthetic organic chemistry and pharmaceutical synthesis. 1,4-Disubstituted derivatives of this compounds exhibit a wide range of biological activity: antitumor, antiviral, anti-allergic and fungicidal, thus gaining a lot of attention from medicinal chemists as a source for new potential therapeutic agents.[1,2]

The present paper we report of the implementation of copper(II) complex of 1-*tert*-butyl-5-(benzoylamino)-1*H*-tetrazole as a catalyst for Huisgen [3+2] cycloaddition synthesis of 1-benzyl-4-phenyl-1*H*-1,2,3-triazole (Fig. 1). The optimal condition of the reaction (THF as a solvent, reflux for 4 hours, aerial conditions, 5 mol.% catalyst loading) allowed us to obtain the target triazole in excellent yield – 92 %.

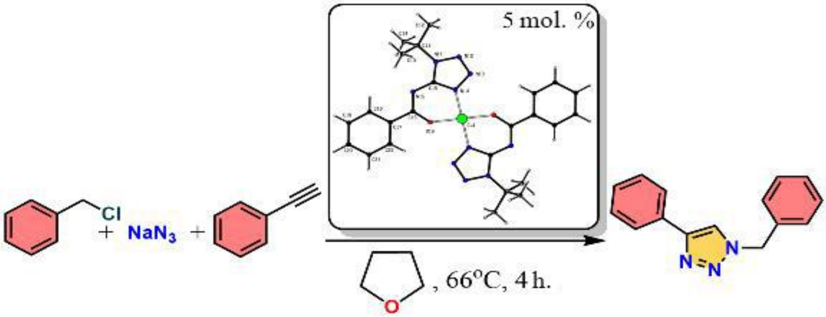

Fig. Scheme of "click"-synthesis of 1-benzyl-4-phenyl-1*H*-1,2,3-triazole

The structure of the catalyst and the target product were confirmed by IR, ^{1}H and ^{13}C NMR spectroscopy, and X-ray diffraction analysis.

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The students´ protagonism on the learning of chemical or physical transformations: contributions of media literacy

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Today, many teachers try to improve their students' learning by using videos, software and other digital resources to enhance their classes and make them more engaging experience. Besides, such technologies permeate students' lives; this type of approach can motivate them in class, arouse students' curiosity and stimulate fruitful discussions [1]. In this sense, the expression of scientific knowledge requires a sophisticated development of reasoning [2]. The possibility of employing various semiotic modes to express this complex knowledge favours the discussion of the topics by the whole classroom in a peer process accomplished with teacher mediation and, therefore, should facilitate and enhance the learning process. In this context, the present article reports the results of an investigation related to the audiovisual productions of High School students of a public school situated in the metropolitan area of São Paulo City (Brazil). The data presented here came from the analysis of the information gathered during the implementation of a teaching-learning sequence (TLS) concerning the transformation of materials. This TLS aimed to stimulate cognitive conflict situations involving common sense and science knowledge, leading the students to elaborate arguments to answer to everyday problems from their world [3]. In general, the data show that the students focused on macroscopic scale descriptions of the phenomena when their explanations are restricted only to written registers. This approach enabled the students to express dynamic aspects of their mental particle model concerning the material changes during iodine physical state transformation. This approach promotes the involvement of many cognitive processes: in addition to digital integration, the students can use visual resources to communicate their knowledge and thus collectivize their ideas and productions with other students and the teacher, thus facilitating the learning-teaching processes by becoming protagonists of their learning process. A multimodal process approach should lead to the expression of students' knowledge. In this process, the teacher offers its students several ways to socialize their mental models to build a common one.

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Progress in chemistry and scientists' responsibility for the continuity of the educational system

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By Sant-Exupery “The man is not a simple word of the vocabulary, the Man is that of he is responsible”. As a general rule, most research in any field should correlate with the global realities of worldwide economic development and should base on existing progressive and valuable advanced trends. Faced with contemporary scientific challenges and the conceptual principles of educational and institutional reforms in Country, our group of scientists work not only in the field of researches of new materials for advanced technical domains but also to keep the continuity of the educational system accomplished during decades[1,2]. To achieve this goal within our University/Institute a group of scientists has organized the Educational and Training Center “RATIO”. Several open lessons and numerous training courses have been organized, quite a few educational steps in the ecological field have already taken place. Then, Seminars and International Conferences were organized with the participation of scientists that are researchers from Georgia and various foreign countries. It should be emphasized - with the involvement of students of educational establishments, including not only Institutes and Universities, but also by the inclusion of learners of institutions for disabled people.

Faced present-day defies and challenges due to the pandemic and the rather difficult situation in the educational field our training course was called “Modern learning process and interactive forms of education by implementation of telework method”. The basic point of our work was the implementation of continuity of education on the chemical and ecological domains. Our training lectures include various new achievements in chemistry, in ecology fields VS the responsibility of scientists. It can be introduced in the lyceums, colleges and higher education institutions This experience of exercising was acquired several times before. This teaching should be done in a new way with various interesting audio-video films, it can be also supported by special training software, especially in distance learning conditions in the current pandemic situation.

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New approaches to organization of on-line education and examination on the example of analytical chemistry at the Belarusian State Medical University

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Now the organization of on-line forms of education is becoming especially actual, taking into account quarantine measures, or the influence of natural factors. The involvement of computer technologies in the assessment of knowledge can significantly reduce the influence of negative factors. BSMU uses Learning Management System Moodle (modular object-oriented learning environment), which is an open source, free to download, flexible user-friendly e-Learning platform, supported by a global community. Within the framework of this system, an electronic educational methodological complex (EEMC) was developed for each subject. The structure of the EEMC for each subject contains such sections as the normative documents of the discipline, a lecture course, a description of laboratory classes, methods of knowledge test control, general criteria assessments of knowledge on tests and exams, a list of basic and additional literature. This system allows us to control knowledge at each classes [1]. The created approach was useful in organizing distance learning for students. In fact, we can talk about the on-line form of teaching. In the latter case, feedback is carried out between the lecturer and the trainees. In preparation for distance teaching, virtual classrooms were created. Working in a virtual classroom made it possible to conduct a video conference or chat. Thus, learning becomes interactive, which is based on psychological mechanisms for enhancing the influence of the group on the process of assimilation by each participant of the experience of mutual learning and interaction. Thus, they can be characterized as methods of encouraging students to interact with each other under the supervision of a teacher. Since the distance learning system was introduced at the end of the spring semester, in fact, the basic practical skills have already been largely acquired. From the point of view of practice-oriented education at BSMU, a scientific-practical conference of young scientists with international participation "Actual problems of modern medicine and pharmacy" is held annually. The adopted approaches to the organization of the educational process and research work at BSMU significantly expand the horizons of students, contribute to increasing motivation to study specialized and special disciplines and the formation of solid knowledge in the subjects studied.

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Professionally oriented profile teaching of chemistry in the system of continuing education

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The choice of a chemical profession is an actual and difficult problem for learners in the modern world. The problem is not the lack of information about the professions and the ways to obtain them, but the lack of learners' skills to analyze information, correlate their interests, needs and opportunities, to be responsible for their choices. The ability to consider similar and alternative options for getting a profession is no less important when choosing a chemical specialty, a group of related specialties of study at the University. The enrollee will be able to make the right choice if he has vocational skills to act effectively in situations with a high degree of uncertainty.

Therefore to prepare pupils for future choice of chemical profession is an important part of the pedagogical activity of a chemistry teacher in a modern profile school. It involves the convergence of the goals, content, process and results of chemistry learning and the orientation of pupils to the chemical professions by educational environment.

Training pupils for a conscious choice of a chemical profession includes identification and updating of the vocational guidance component of the content of chemical education; educational excursions to chemical production, solving problem situations with production content; performing competence-oriented tasks in chemistry with a professional context, etc. Clarification of professional choice in chemical classes involves the choice of a profession by pupils in the areas of technological, scientific or pedagogical profiles of the work of chemists, as well as ways of mastering them. In the educational process, this is facilitated by the pupils's practical experience in all the indicated areas, understanding the image of the professional future, analyzing the results of educational activities, situations of choice, professional tests (based on mutual assessment, self-assessment, SWOT-analysis).

Thus, professionally oriented profile teaching of chemistry can contribute to the vocational guidance of learners in the conditions of the information society and plays an important role in preparing learners for the choice of a chemical profession and ways to get it in the system of continuing chemistry education. For its effective implementation, it is necessary to improve the qualifications of chemistry teachers on the issues of systemic orientation of pupils to chemical professions in the conditions of profile education.

Opportunities for the development of research competencies of students by means of a modern chemical experiment at school

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Central modernization carried out in Belarus in 2015-2020 made it possible to providematerial and technical resources tochemistry rooms at the school. As a result, the teacher havegotlearning tool (LT) combining the characteristics of a classic device and IT technologies one such LT is the hardware and software complex with a set of sensors [1]. However, the teacher was not ready to use such LT since there was no experience with him, there were no methodological recommendations for its use, but there was a desire to work with this LT, this is due to the relevance of our scientific research. Combination of personal activity, competent, systems-structural and integrative approaches, as well as principles (science, humanization, systematics, historicism, the connection of learning with life) and the theory of personal development determined the methodological apparatus of our scientific research.

We have developed didactic tool based on uses the hardware and software complex with a set of sensors – demonstration chemical experiment on topics: "Theory of electrolytic dissociation", "Thermodynamics", "Chemical kinetics"; heuristic tasks (cognitive, creative, organizational) for the experiment, allowing you to organize a heuristic conversation; theoretical model of development of research competencies of school students (comparison, analysis, synthesis, abstraction, generalization, systematization and others). This is the theoretical novelty of our research, practical novelty of our research is the testing of the experiment [1] and introduction of the developed experiment into the educational process of schools implemented in 2018 – 2020 at national seminars, in articles of periodicals, on the website of the National Educational Portal of the Republic of Belarus. The contradiction identified by us as a result of our scientific research has been eliminated.

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Information and communications technologies as methodological support of the practical training in Inorganic Chemistry

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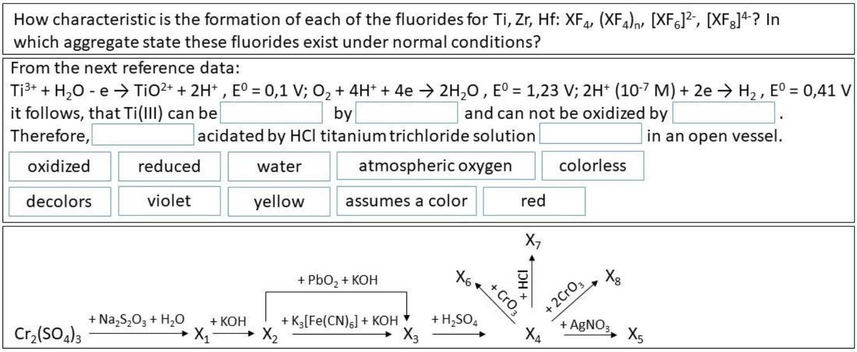
Practical training of the students in a system of Higher Chemistry education along with the laboratory work utilizes solving of calculation and logical tasks. The epidemic situation that formed in 2020-2021 provoked massive transfer to remote conducting of the classes. And therefore, the essential expansion of the use of information and communication technologies in the teaching of the Chemistry disciplines occurred. The tasks embodied by information and communication technologies help to individualize the teaching process, make it more interactive and attractive for students. But on the other side, information technologies demand altering not only the manner of the tasks but their matter as well.

At the Chemistry Faculty of the BSU the remote practical teaching the Inorganic Chemistry implied training of the students by the tasks with the different level of the cognitive activity. The first level tasks (reproductive) requested following the example, completing tasks on the analogy, and the search for the ready-made answers in the textbooks. The second level (reconstructive) required using the known ways of solving the problem but in new situations with the self-constructed decision course. The third level (exploratory) tasks counted on the students' individual solutions in the absence of the ready algorithm. An example of the task, which contains the reproductive question, drag-and-drop reconstructive task, and exploratory transformation chain, is presented in Figure.



How characteristic is the formation of each of the fluorides for Ti, Zr, Hf: XF_4, $(XF_4)_n$, $[XF_6]^{2-}$, $[XF_8]^{4-}$? In which aggregate state these fluorides exist under normal conditions?

From the next reference data:
$Ti^{3+} + H_2O - e \rightarrow TiO^{2+} + 2H^+$, $E^0 = 0{,}1$ V; $O_2 + 4H^+ + 4e \rightarrow 2H_2O$, $E^0 = 1{,}23$ V; $2H^+ (10^{-7}$ M$) + 2e \rightarrow H_2$, $E^0 = 0{,}41$ V
it follows, that Ti(III) can be ______ by ______ and can not be oxidized by ______ .
Therefore, ______ acidated by HCl titanium trichloride solution ______ in an open vessel.

oxidized | reduced | water | atmospheric oxygen | colorless
decolors | violet | yellow | assumes a color | red

Fig. An example of the task in a remote mode for the topic "Metals of the IV-VIB groups"

The combination of the split-level tasks with information and communication technologies provides intense interest from the students and better educational outcomes.

Using the MOODLE platform in teaching chemical disciplines

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Various options for distance learning are dynamically developing at present. This process is primarily due to the urgent demand of the society for the opportunity to live, work and study without the reference to geolocation. Modern means of communication and information exchange allow the society to gain a new level of communication. The COVID-19 pandemic has played an important role in a distance communication development.

To some extent, it is more difficult to organize distance teaching of disciplines that require obtaining practical skills in specially equipped laboratories. These disciplines include chemistry. We have gained experience in using the MOODLE educational platform for full-time and part-time students in order to organize the educational process. The obtained results can be very clearly presented for part-time students. Theoretical and practical material was prepared and systematized for the organization of distance teaching of the discipline «Physical and Colloidal Chemistry». This material includes interactive lectures, lectures-presentations (1 in Fig. 1), virtual laboratory work (2), a set of tasks with explanations and tasks for self-fulfillment (3). This block provided students with the necessary knowledge in terms of distance learning. The activity of its study is shown in Fig. 1. After mastering it, the students passed training testing (4), and then the final testing, the results of which are shown in Fig. 2.

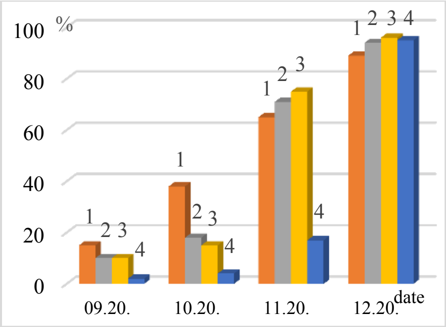

Fig. 1 Activity of passing the theoretical block

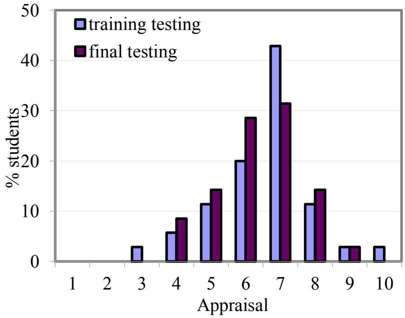

Fig. 2 Comparison of the test results

The analysis of the results presented in Fig. 1 and 2 shows that the overwhelming majority of part-time students have fully mastered the theoretical block by the end of the semester. A good level of self-preparation was reflected in the test results. About 80% of students have successfully passed the intermediate control.

The problem of adaptation of first-year students to conditions of self-isolation

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Adjustment of former school students to studying at the university is a complex and ambiguous problem. A first-year student is affected by a range of factors, the successful adaptation to which depends on the person’s psychological stability. This academic year to the difficulties of getting used to the new conditions has been added the factor of distance learning. An unusual nature of the phenomenon of self-isolation has a strong impact on students. The forced transition to distance learning presents a lot of difficulties and causes a certain amount of stress to all the participants of the educational process.

Firstly, quarantine proves hard for those first-year students who are not used to self-discipline and self-control. Many freshmen believe that attending classes that are held online is not necessary, since the subject is either not interesting to the student, challenging or can be viewed in recording. Moreover, studying which consists of virtual imitation of experimental work accompanied by a video demonstration is in itself passive. Freshmen feel a lack of personal contact and do not form an adaptation to student life.

Secondly, in addition to the problems with the self-organization, there appear to be complications with the technical part of the educational process. Not every student possesses the equipment for e-learning such as desktop computers or the necessary headset (headphones, microphones, high-resolution cameras). Though listening to the lecture material is possible on most devices, practical classes pose a problem and conducting them in this format can be inconvenient. Virtual laboratory allows students to remotely do an experiment, but the simulation can only be run on a desktop computer or a laptop and is not supported by some of the browsers. Besides that, while conducting online classes there appear to be technical problems such as inadequate internet connection or bad sound quality.

In conclusion, it can be said that the problem of adjustment to conditions of self-isolation is a process which is formed long and slowly. That’s why it’s all the more difficult for the first-year students, whose adaptation to the quarantine conditions is complicated by the social adaptation.

An experience on the analysis of visual representations in simulators for teacher training

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The present work is framed in a proposal for the analysis of models and their representations in simulators for student teachers in chemistry. Among the ICT resources are simulators, which are software tools that allow simulating physical-chemical processes represented on a graphic screen. In general, all simulations present some possibility of modifying the simulation parameters in order to observe and analyze the consequences that these changes have on the process under study [1]. Simulators are an instructional resource that began to be widely used during the pandemic and virtualization of science teaching. Such simulators consist of animations containing different levels of representation of the subject matter: (1) sensory or perceptual level (macroscopic level), (2) particle level: atoms, molecules or ions (microscopic or submicroscopic level) and (3) symbol level, formulas and equations (symbolic level) [2]. There is great difficulty in trainee teachers in interpreting, applying, and moving between the different representational levels. With the aim of promoting these skills, we generated a research space to analyze different types of representations and models. In the first instance, the students carried out an extensive search of images in different simulators for different chemistry topics. Only simulations that had a high conceptual content and sought the construction of a mental model of the phenomenon were selected. The analysis of the different levels of representation of matter in the images, as well as the analysis of the concepts and models represented, allowed teachers to develop skills for: i) critical evaluation of resources, ii) selection criteria for simulations and iii) design of images for educational materials.

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Monitoring of productive skills formation and development in teaching chemistry

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Until nowadays, the quality of the educational process was mainly assessed in the final student certification that always took place at the end of the academic term. The constant process of forming awareness and skills was totally ignored. Despite this, not being considered at the right time of learning, the exactly identified anticipated difficulties will provide the further changes for students, taking into account the individual circumstances that will definitely lead to higher academic results.

According to the Federal Educational Standard of Russia, students of all grades must develop the meta-skills (cross subject skills). Students are expected to be able to solve the problems among disciplines. The productive skills formation still remains to be the essential part of learning. It allows students to follow the previously anchored patterns. Also helps to apply the same procedure in newly occurred learning situations and successfully solve cognitive, creative tasks.

The purpose of the work: is to develop a digital toolkit that allows to track all the stages of productive skills formation based on the given chemistry algorithm in high school.

The work is based on the hypothesis that monitoring the productive skills formation process will increase the mobility of the feedback and determine the "zone of proximal development" for each student. It will be beneficial in the majority of the aspects: to build up the individual academic tracks; to ensure the individual approach whilst teaching chemistry at all stages; to promote awareness of the studied subject; to encourage students to solve high-level creative problems.

To achieve these goals, the digital toolkit was developed and tested. The toolkit allows to monitor each algorithmic component formation process; allows to determine the productive skills formation for solving further complex problems; and, to increase the usage of the feedback to make the learning process more efficient.

Acknowledgment

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Taking the traditionally taught classroom to the inquiry-based online learning model

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With universities, teacher education institutions, and high schools gearing up heavily in online course delivery in every discipline, science educators specifically are asking themselves «How do we provide this access to our students and still maintain our pedagogical integrity in science instruction? [1]. This question seems to be at the heart of a national discussion. The shift to online learning has created apprehension among academics throughout education at all levels. This new pedagogy is creating a myriad of myths about teaching online. Online learning or E-learning offered over the internet, is contrasted with traditional courses taken in a brick-and-mortar school building [2]. Online learning environments provide a greater degree of flexibility than traditional classroom settings in presentation mode. They can be a hybrid model that combines face-to-face and online instruction, which has two modes: asynchronous and synchronous [3]. With this shift in teaching and learning methodologies, instructors and students may have different perceptions about their responsibilities in online courses. This presentation contends that instructors need to be actively involved with providing direction and support to enhance student learning in online courses. At the same time, responsibility for knowledge and skill development also rests with the students [4]. Suggestions are offered for curriculum developers how on to enhance the quality of course content and improve communication that will strengthen the learners' experience for success [5].

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Structure of the subject competence in chemistry

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The introduction of a competence-based approach in the educational process contributes to improving the quality of training of future specialists. In this regard, considerable attention is paid to the issues of the content of competencies, their development, and the search for means of measurmeant and evaluation of their formation in students. We have proposed the structure and content of the subject competence in chemistry for the students of the specialty “Biology and Chemistry” as future teachers of chemistry. There are different approaches to determine the structure of subject competencies. We adhere to the approach according to which the chemical competence model has three components: content, process, and control and evaluation [1]. We consider this approach appropriate, since the most important didactic questions are: “What to teach?” (the content component), “How to teach?” (the process component), “Have the learning objectives been achieved?” (the control and evaluation component). In the content component of the chemistry subject competence, we have identified the following modules: “Chemical element”, “Simple substance”, “Complex substance”, “Chemical experiment”, “Mathematical calculations” [2]. In the process component, it is expedient to distinguish the modules “Forms of training”, “Types of training”, “Training Methods”, “Training Tools”, in the control and evaluation component – the modules “Pedagogical control” and “Self-assessment” (Scheme).

<table>
<tr><th colspan="3">Chemistry subject competence</th></tr>
<tr><td>Content component</td><td>Process component</td><td>Control and evaluation component</td></tr>
<tr><td>Chemical element
Simple substance
Complex substance
Chemical experiment
Mathematical calculations</td><td>Forms of training
Types of training
Training methods
Training tools</td><td>Pedagogical control
Self-assessment</td></tr>
</table>

Scheme. Structure and content of the subject competence in chemistry

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Graph theory approach in quantitative assessment of the efficiency of microstructuring of the course of Organic chemistry

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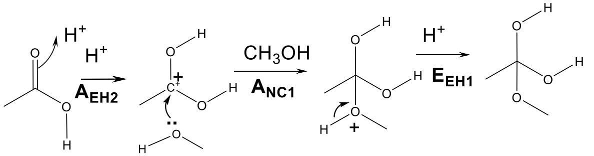
Earlier an original system of disciplinary didactic principles has been elaborated [1]. The system consists of original epystomology and didactics, moreover now we propose mathematical evaluation of the relevance of course construction based on Graph theory approach. Any of three principles proposed (structural adequacy principle, functionality principle, and mechanistic simplification principle) can be chosen for evaluation of the course relevance. The mathematic technique based on graph theory was proposed by Toldsepp [2] for macrostructuring. Here we assess the course of micro-structuring including the choice and sequence of reactions. We present course chapter as a graph in the form of the adjacency matrix. The matrix contains subcomponents which are in our case the chosen reactions. All the reactions from the chapter are formally divided into elemental stages of addition and elimination (the didactic adaptation of the reaction step by step mechanistic presentation), taking also into account the type of reagent/leaving group, the type of the atom coupling with the reagent, and finally, multiplicity of the bond.



E.g. **A_{EH2}** means “Addition (**A**) of Electrophile (**E**) to Heteroatom (**H**) belonging to a double (**2**) bond”; **A_{NC1}** means “Addition (**A**) of Nucleophile (**N**) to Carbon (**C**) belonging to a single (**1**) bond”; **E_{EH1}** means “Elimination (**E**) of Electrophile (**E**) from Heteroatom (**H**) to leave a single (**1**) bond”. The relevance of microstructuring is associated with the presence of the same elemental stages in reactions as well as with the distances between them. Mathematically it can be calculated as two indicators. The summary distance from the main diagonal of the matrix can be associated with the didactic principle of content compactness: the smaller the parameter’s value, the shorter the time lags between learning different subcomponents of a teaching material. The sum of the elements on the diagonal adjacent to the main diagonal is associated with the principle of continuity of a teaching material. Supposing, every new structural element ideally ought to be built on the previous one, and then the value has to be maximal for a given matrix.

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Improvement of practice-orientation of organic chemistry for pharmaceutical students

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The traditional education is based mainly on mastery of content, neglecting the training of inquiring attitudes. Such system of education is teacher-centered, the students getting the information from a teacher about the known facts. In contrary, process-oriented, self-directed, creative and interdisciplinary learning which is referred to constructivist paradigms should be used in academic education. The inquiry technology is aimed on learning content as a means to develop problem-solving skills, students being the participants of the projects.

The academic process at medical Universities is traditionally practically oriented and includes only a few elements of scientific technologies. For pharmaceutical education this is often associated with the pharmacy assistant counter work; though pharmaceutical University educations includes much wider range of professional activities. We have improved the Organic Chemistry curriculum for pharmaceutical students in context of more practice-oriented teaching with the aid of modern educational technologies. We have modified the traditional modules ("Modern Synthesis in the preparation of pharmaceutical drugs", "Small molecules in biological processes" etc.) and added the new module "Molecular modelling in rational drug design". The new module consists of theoretical and practical parts. The latter includes lab classes where the students design structure and simulate molecular properties with the aid of ChemOffice application, followed by the molecular docking in online resources, e. g. [1]. The knowledge and skills obtained can be improved within the framework of Student research [2]. We propose students the projects concerning the search and primary investigation of biological activity of organic substances as potential pharmaceutical drugs, molecular docking being the key element of the research project. The research includes also the literary review and drug analysis (Journals, drug databases), the choice of the possible substrates (protein databases), the evaluation *in silico* the model based on a set of substances synthesized earlier and tested *in vitro* on biological activity, design of new drug-candidates and the assessment of their activity *in silico*. The results obtained are valid and correlated with the data from previous scientific researches, being presented in student conferences and, finally, published. Student research motivates students to study professionally oriented topics, trains their skill in the field of pharmaceutical chemistry and molecular biology, as well as helps the faculty to find the candidates for entering the Master and PhD programs.

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Online chemistry teaching at BSTU during the coronavirus pandemic

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The study is aimed at analyzing the experience of using information and communication technologies in the process of teaching chemical disciplines at the Belarusian State Technological University during the coronavirus pandemic. In a very short time, teachers were forced to adapt the educational process to online learning. The results of the implementation of information technologies at the Department of Chemistry, Technology of Electrochemical Production and Electronic Engineering Materials are considered.

To implement distance learning technologies at the University there is a Learning Management System; it is based on Moodle, where students can access learning materials and feedback from teachers. The main purposes of applying the Distance Learning System at the University were creating opportunities for quality educational services, involving effectively the variety of IT means in the educational process, developing students' motivation to learning, and continuous self-education via modern information and communication technologies. We analyzed learners' perceptions of online learning, their ability to absorb information and use e-learning platforms. An anonymous online survey of students was conducted using the Google Questionnaire Forms service. Data was collected from 132 students (Fig.).

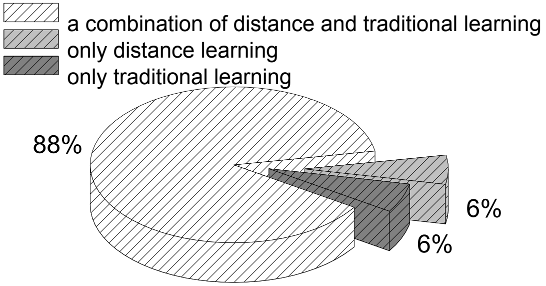

Fig. Respondents' answers to the question:
Do you think distance learning is the necessary form of the educational process?

According to students, the most effective use of information and communication technologies is through colloquia (75%), seminars (56%) and lectures (43%). The degree of correlation between the students' examination score of and the students' rating score based on the results of distance learning is very high. Online learning technologies have proven to be indispensable in organizing the educational process with students of the Faculty of Extramural Studies.

Tools for the formation and evaluation of the competencies of future teachers in the development of the discipline «Methods of teaching chemistry»

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Teaching a student of the pedagogical direction of training involves arming him with a large set of competencies. We are convinced that when mastering the discipline "Methods of teaching Chemistry", subject-methodical competencies are priority. They include chemical knowledge and skills, as well as the ability to plan and organize the process of teaching chemistry in accordance with regulatory requirements and educational prospects.

In addition to the formation of students set of competencies, the task of evaluating the effectiveness of the educational process arises. As a part of the development of methods of teaching subjects, the most important tool for the formation and evaluation of students competencies are tasks for the creation of educational and methodological products [1]. Systematic work on such tasks, followed by demonstration, discussion and correction of the results, is the essence of the formative assessment.

One of the approaches to creating a bank of tasks for the development of educational and methodological products can serve as a "didactic" approach, which is based on the isolation of step-by-step actions of a chemistry teacher in the preparation and conduct of different types of lessons. Tasks vary in scale and complexity. For example, before students receive a task to develop a summary of a combined lesson, they are asked to: analyze the content of the chemistry lesson and formulate its goals; develop options for a combined survey when checking homework; give examples of tasks for the formation of sign-symbolic universal educational actions among schoolchildren; describe various forms of combining a word with a demonstration experiment, etc. Generalized criteria for evaluating the created methodological products are: their quality, degree of independence and the time of presentation. The quality criteria for each type of methodological products are different.

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Methodology of chemistry teacher work on developing students' skills for self-management of educational activities

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The results of many years research of the author have shown that methods of chemistry teacher work on development students' skills for self-management of educational activities include the following aspects.

- ·Principles of organization functional development by students, which are motivation, personal goal-setting of the student, self-determination, individualization, communicative complementarity, controllability.
- Metacognitive (organizational and activity) methods of forming self-management skills of students' educational activities, that include goal-setting, planning, forecasting, self-control, self-assessment, reflection, the method of working with text, etc., and are based on the development of theoretical knowledge, performing a chemical experiment, carrying out quantitative calculations in chemistry.
- Types of tasks in chemistry, that contribute the formation of a whole complex of student's skills for self-management of educational activities.
- Main provisions of the relationship between management and self-management of educational activities in the process of mastering theoretical knowledge in chemistry by students, that have to ensure the control function of previously acquired theoretical knowledge, to identify structural and meaningful components and connections in newly studied objects, to use methods of chemical science and methods of scientific thinking, schematization of structurally meaningful and relationships in the system of knowledge under consideration, the solution of new practical problems on the basis of the identified and generalized system of knowledge, and the acquired system of educational actions.
- Groups of tasks of an experimental nature in a form of real, mental and virtual chemical experiment which are presented by different methods, such as drawings of devices and installations, description of the properties of substances, requirements for the recognition of substances, and which differ by the method of implementation such as home experiment, self-preparation for practical work and test self-control, animation modeling, research work [1].
- Methodological techniques for transforming the conditions of computational problems in various ways, that are using algorithms, drawings, drawing up structural and logical diagrams, using data tables, extracting information presented in graphical form, visual modeling of processes [2].

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Modern educational technologies in teaching chemical disciplines at a pedagogical university

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Innovations in education are primarily associated with information and communication technologies (ICT) and e-learning today. Until now, distance learning has been seen as an addition to full-time learning. The 2020 pandemic has shown the need to adapt all educational actors to distance learning using modern ICT capabilities without losing quality.

The achievement of high educational results is greatly influenced not only by the equipment of technical means, but also by the organization of the educational process.

Learning Management System Moodle is used to provide distance learning at the Belarusian State Pedagological University Named After Maxim Tank. This system offers extensive tools for presenting teaching materials, conducting lectures, seminars and practical classes.

The organization of effective remote training requires teachers to expand their competencies. It is necessary to select carefully the didactic material, organize feedback with students, create to test for examinations. We have developed interactive electronic educational and methodological complexes for such academic disciplines as "General and Inorganic Chemistry", "Organic Chemistry", "Analytical Chemistry", which meet the above requirements. The outcome of training also depends directly on the motivation, independence, abilities and self-discipline of students.

Thus, distance learning is effective when a teacher organizes students' personal knowledge engineering activities. This approach involves the integration of information and pedagogical technologies, ensuring the interactivity of educational actors and the productivity of the educational process. However, a laboratory workshop plays an important role in the study of chemical disciplines.

Video recordings of the experiment, even with the most detailed comments, are an unequal replacement for work in the laboratory. Interactive learning packages based on electronic learning systems can be used to expand the capabilities of traditional face-to-face learning.

Natural science education as an aspect of the roadmap for addressing sustainable development issues

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The process of Ukraine's accession to the European space and the signing of the Bologna Convention provides for the modernization of the higher education content, a change in its philosophy. The higherchool faces the task of training a new generation of professionals who should meet today's requirements. Natural science education has great potential to directly address sustainable development issues and environmental issues.

The purpose of research is the creation of an effective didactic system through the integrated approach of a natural education for example of water security course with a special emphasis on professional orientation. Methods of the analysis, synthesis of knowledge, educational experiment, and mathematical statistics were used for the fulfillment of the purpose.

The study is implemented by Programme EU Erasmus+ Jean Monnet Activities as part of the interdisciplinary European studies in Petro Mohyla Black Sea National University. The effective didactic system of interdisciplinary knowledge of natural-science courses, namely the water security course, was created.

The teaching course for Master's students in Environmental Science covers the main topics, such as water resources, water quality, climate change, integrated water management, water policy and law issues. The course constructs on the interdisciplinary basis and covers key elements of the strategy for sustainable development and European experience in the field of the environmental water recourses policy. The course is interdisciplinary and connects the policy and tools of water monitoring and management, principally addressing EU and Ukraine practices of water quality, water resources, biodiversity, and fisheries, and their progressive integration.

In the process of forming students' knowledge, the tendency to increase their educational activity, interest in carrying out independent scientific research, in expressing original views on environmental issues discussed during classes was determined. The coefficient of completeness of knowledge was evaluated. It is proved that the selected educational material is quite fully assimilated by students, as evidenced by the average coefficient of 0.85.

The prospect of further research activities is to improve the theory and practice of the integrated study of natural courses based on the developed conceptual provisions of the education content integration, and also to improve the methodology of assessing the quality of students' knowledge during the study of integrated courses.

Pedagogical system of formation and development of the methodological culture in the training course at the Department of Inorganic Chemistry of BSU

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The report is devoted to the history and methodology of the development of a pedagogical system for the formation and development of methodological culture among teachers and students of Chemistry at the Department of Inorganic Chemistry of BSU. The beginning of this system was laid in the mid-60s of the twentieth century by the head of the Department of Inorganic Chemistry V. V. Sviridov. It was developed in the works of his colleagues and followers. Historically, the following components of the pedagogical system of forming the methodological culture of the teachers and the students have been developed.

1. Methodological seminar for lecturers and researchers of the Chemistry Faculty. The problems of the seminar had two directions. The first was a discussion of the methodological problems of chemistry that have arisen in connection with the intensification of chemical research, the emergence of new areas, approaches, and methods in them. The second was a discussion of possible ways to project the new state of science on the content and organization of university chemical education. Subsequently, this seminar took the form of an international conference on chemistry and chemical education, which was called "Sviridov Readings".
2. Laboratory practice in Inorganic chemistry and course project. They are organized on the basis of the training and research approach, which was developed at the department.
3. Educational and methodological complex for the course "Methodology of chemistry" for students studying in the direction of scientific and pedagogical activity. The purpose of this course is to introduce future chemistry teachers to the necessary minimum of methodological knowledge and to demonstrate methodological techniques for organizing training based on the teaching and research approach.
4. The system of methodological support for the development of school chemical education using the research method of teaching.
5. Operation of the scientific and methodological journal "Chemistry: problems of teaching" (currently "Biology and Chemistry"). The journal acts as an intermediary between the educational process and cutting edge science, promotes the integration of education and science, reduces the gap between the content of education and the needs of a rapidly changing society, and paves the way for the future.

Prospective chemistry teachers' views about the use of Kahoot in the nuclear chemistry course

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Most of the chemistry classes are conducted online at university levels due to Covid-19 currently. One of such courses conducted at Balıkesir University was Nuclear Chemistry. The course is intended to provide the prospective chemistry teachers (PCTs) with the fundamental nuclear chemistry knowledge necessary to teach in their future high school chemistry class, give them an awareness and understanding of the expose of radiation and radioactivity in everyday life. This course is also aimed to educate the PCTs as scientifically literate people and to gain skill them to be able to manage social-scientific discussions concerning everyday radiation, nuclear power, and radioactive waste. On the other hand, the studies have shown that the students hold a series of misconceptions concerning both the concepts related to nuclear chemistry [1, 2] and the prerequisite knowledge for essential to learn nuclear chemistry [1, 3]. For this reason, it is critical to identify whether the PCTs had any misconceptions in their previous learning at the beginning of the lesson, and measure their knowledge frequently during the lessons and shape the teaching accordingly to be able to provide meaningful learning. Furthermore, increasing the motivation of students and provide their cognitive engagement in the lessons are the other most important challenges in online courses. All these challenges can be achieved by activating students in the lessons. Kahoot! is a game-based learning platform [4] used to include students in the lesson, motivate and measure learning. In this study, the Kahoot was used as a formative measurement during the online Nuclear Chemistry course which was the 7th-semester course, and the views of the PCTs about the applications were taken. The study group consists of 12 PCTs, seven female and five male. A total of 4 Kahoot applications were carried out, one of which was designed to assess the pre-existing knowledge of the PCTs at the beginning of the lesson. The data for the PCTs' views were collected with a Google form with 10 open-ended questions.

Within the scope of this study, firstly, the findings of the PCTs' views on the use of Kahoot will be presented. Besides, it will be explaned how the Kahoot application was performed in the lesson and the observations of the instructor on how the use of Kahoot affects the PCTs' motivation and cognitive participation will be given.

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Methodology of students' constructive learning activities in teaching the theme of chemical equilibrium

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One of the problems in the teaching process of chemistry is the process of working out new teaching methods that meet the learning difficulties in the field of chemical kinetics. Proper mastery of chemical kinetics requires students to have a conceptual understanding of the dynamic side of chemical theory, and constructive learning contains its basis. The following principles should be used in the teaching process: knowledge must be acquired and mastered independently, productively and creatively; logical, critical and creative thinking, as well as problem-solving and decision-making skills should be formed. We illustrate this on the example of chemical reactions proceeding in both directions (straight and reverse). Under certain conditions, a chemical equilibrium occurs. For example:

$$CH_3COOH + CH_3OH \leftrightarrow CH_3COOCH_3 + H_2O \qquad (1)$$

Chemical equilibrium is a continuous and time-independent state of a reaction system which is characterized by a constant at a given temperature.

For a general chemical reaction $aA + bB \Leftrightarrow cC + dD$

$$\frac{[C]^c \cdot [D]^d}{[A]^a \cdot [B]^b} = K_C \, [(mol/l)^{\Delta v}]; \qquad \frac{p_C^c \cdot p_D^d}{p_A^a \cdot p_B^b} = K_p \, [kP_a^{\Delta v}] \qquad (2)$$

$$\Delta v = (c + d) - (a + b) \qquad (3)$$

where we used molar concentrations (C, D, A, B), reactions coefficients (a, b, c, d) and partial pressures (p_C, p_B, p_A, p_D).

During the chemical equilibrium with $\Delta v = 0$, the amount (mol) of all the substances involved in the reaction can be written according to the law of mass action. The law of mass action equations can be derived from kinetics and thermodynamics. According to the equation (1)

$$K_C = \frac{[CH_3COOCH_3] \cdot [H_2O]}{[CH_3COOH] \cdot [CH_3OH]}; \qquad K_C = \frac{v[CH_3COOCH_3] \cdot v[H_2O]}{v[CH_3COOH] \cdot v[CH_3OH]}$$

But for the equation $N_2 + 3H_2 \Leftrightarrow 2NH_3$:

it will be: $K_p = \frac{P^2(NH_3)}{P(N_2) \cdot P^3(H_2)}$

We came to a conclusion that, methods for developing constructive abilities, which form the basis of learning theory in students in the direction of teaching and understanding the relationship between quantitative and qualitative aspects of chemical kinetics, must be carefully elaborated.

Teaching the course "Chemistry" at RUDN University in the context of distance learning

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The coronavirus pandemic has affected all areas of public life. The need to conduct classes outside the walls of universities in a distance learning mode forced the faculty to revise all the teaching methods developed over the years and contributed to the search for new education methods. At RUDN University, Chemistry is taught at the Faculty of Physics, Mathematics and Natural Sciences (Faculty of Sciences). In addition to the students of chemical specialties at the Faculty of Sciences, the Faculty provides training to the students of the Faculty of Ecology, Agrarian-Technological and Medical Institutes, and the Engineering Academy. This publication discusses the problems of teaching the course "Chemistry" for non-chemical specialties. Despite the fact that the electronic forms of education have always been actively introduced at RUDN University and some of the exams and tests have been conducted via a telecommunication educational and information system (TUIS), using a bank of questions for online assessment on various topics created for this purpose, nevertheless, when the pandemic broke out the chemistry teachers faced a number of significant difficulties. Teaching such a rather complex subject as "Chemistry" for a wide contingent of students from 139 countries of the world (the percentage of foreign students is about 70%) is not easy. The level of the students' initial training is very different, there is also a language barrier. Usually, studying Chemistry is carried out in the 1st year, and for the vast majority of students of non-chemical fields, the study of chemistry is limited to this. Also, doing the Chemistry course must be accompanied by an experimental part, but the laboratories turned out to be inaccessible. In the distance learning mode, teaching was carried out using the TEAMS platform. When conducting lectures and seminars, it turned out that the demonstration of presentations, even if competently prepared, gives very low results. Using graphic tablets and videos proved much more effective in explaining the material. Lectures were recorded and then uploaded to TUIS, where the students could view them again. When conducting laboratory exercises, an integrated approach was used: the demonstration of the experiments was followed by filling out laboratory journals and using a virtual laboratory. The Faculty of Science is planning to introduce the so-called "zero course" - "Digital Preparatory Faculty" in chemistry for students who have "poor" training in this subject. The introduction of such a course, conducted in the first month of study, would facilitate the early adaptation of first-year students to mastering the material in chemistry according to the higher school curriculum.

Non-formal education: past or future?

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The formation of the educational sphere at the initial stage was carried out by informal methods, the senior taught the younger, which made it possible to achieve a thorough introduction of socially acceptable norms, values, and ideas into the personal sphere of a person, and also effectively implemented the most important principles of training: differentiation and individualization. With the formation of an industrial society, there were also inconsistencies in this approach to education with the needs of society: the uncertainty of the scope of application of the acquired knowledge, teaching is eclectic, without programs that take into account the full breadth of the needs of society, a narrow circle of trainees, high cost of training. Formal education, which was widely developed in the industrial era, ensured the standardization of the content of education, the unification of didactic systems. This led to a greater involvement of the state in educational processes. Formal education provides state control and orders for specialists in various fields. the presence of specially designated premises, material support, specially trained personnel, unified programs in subjects, training in a team, among equals. Teaching chemistry, as one of the most ancient sciences, has passed all the stages of formation: informal, formal, modern. At the stage of entering the post-industrial, information society, the need for individual training again attracts attention due to the ever-increasing need for continuous education, self-education, without which it is impossible to meet the level required for an employee. For example, manufacturing, IT, communications, transport, etc. The international direction is "life - wide education" (lifewide learning), which emphasizes not only the consistency of the learning process, but also the diversity of its forms-formal, informal and informative.

Study of the discipline «Chemistry» using ICT by students of agricultural specialities

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Chemistry is theoretical basis of agronomic sciences, the purpose of its teaching which is to prepare students to study disciplines related to the formation and conversion of compounds in the nature. To date, the task of learning chemistry is possible to implement only taking into account the trends in the informatization of the high-er education system. It is a qualitatively developed and affordable electronic educa-tional and methodical complex that can be a key to raising the level of education and professionalism of students. Currently, the development of a computer shell Eumk is made using software packages such as Adobe Dreamweaver, Toolbook, Courselab, Quiz Force, Power Point Force, MS Office, LMS Moodle, etc. [1,2]. At the Department of Chemistry, an electronic chemistry course was developed for specialties of *Zooengineering* and *Industrial fish farming* on the basis of LMS Moodle, containing the materials necessary for implementation within the disci-pline of all planned types of work and achieve all planned learning outcomes. Text, graphic, multimedia files of various formats are prepared, as information support and professional-oriented material learning a list of references, reference catalog to extensive Internet resources. Functional blocks contain educational and methodological materials, interactive elements and static resources of the Moodle system: lectures, glossary, test tasks, reference materials, web pages and Wiki [3]. To verify the assimilation of the material passed, various control options are possi-ble, including the scheme and criteria for the current and final estimation of topics, laboratory sessions of independent work and individual tasks, as well as obtaining a final assessment on discipline. Evaluation of the knowledge and skills acquired when performing experimental work was carried out by testing in the electronic training environment Moodle. To enable the student to access courses using a mo-bile device, you need to install the application, enter the address of the distance learning site (him.moodlecloud.com), your username and password.

Thus, the use Moodle of allows the teacher to improve the quality of education of full-time students at the expense of a built-in system for monitoring their knowledge for each topic.

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Promising directions for improving the quality of students' knowledge on the subject "Chemistry»

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In the traditional system of teaching the discipline "Chemistry" in a technical university, the passive method of teaching is used as a method of transmitting information. Currently, the main methodological innovations in the presentation of the discipline of "Chemistry" are associated with the use of interactive methods, case studies, business games, etc. [1]. The above-mentioned educational methods often ignore the development of students personal components: motivation, leadership, communication skills, ability to cooperate, etc. The old motivational schemes in modern life are no longer working. The world around us is changing rapidly. Therefore, when studying the discipline "Chemistry", it is necessary to use new directions. One of these areas is gamification. Gamification is the process of using the dynamics of games and game thinking in non-game processes to increase the audience's enthusiasm for solving applied problems, acquiring knowledge, skills and abilities [2]. Gamification allows students to develop their personal and communication skills in a harmonious way. It is useful to combine traditional forms and methods of teaching students with elements of gamification. The techniques and principles on which the games are built can also be used in the study of the discipline "Chemistry" . The assimilation of information or the performance of any actions in a playful way, with increased emotional involvement, is much faster and better. Elements of gamification in the study of the discipline "Chemistry» are the following: a) splitting information into "levels"; b) access to a new level, only after mastering the previous material; c) visual display of success-points, badges, graphics; d) competitive element, etc. The use of these and other elements in video games allows you to consolidate and develop knowledge, give the necessary practical experience, makes the learning process more interesting and exciting. The use of gamification in the study chemistry will ensure safety and reduce costs because chemical reactions and processes will take place in a virtual environment. According to Russian experts, in the coming years, gamification will be one of the main educational directions not only in Russia, but also in the world [3].

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Assessment and supervision of students' independent work in chemistry at higher school

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In practice organization of students' independent work does not correspond to present requirements; and experience of its traditional educational modal cannot be used. Present-day methods of students' independent activity assessment are not synonymous in assessment parameters. Even more than that, they are very time-taking at the stage of mathematical processing their results. Solving of the problem should be found in theory of gnoseology, methodology of cognition. All the investigations carried out were performed on the methodological bases of theory of activity. In the process of practical realization of this methodological approach to the essence of independent work the missed member reveals itself: it is insufficiently elaborated theoretical foundation that could become the basis of effective students' independent work in a subject teaching, including chemistry. New approach to independent work is possible along with developing theory of independent work on the basis of interdependence methodology of integrative-differential approach to the process of teaching.

Examining of independent work from the point of view of correlation of integrative / differential approach to teaching chemistry at high school puts it into a new category level and promotes for the development of its theory expressing its integrative / differential essence. However, taking into consideration essence of chemical knowledge, special attention should be paid to means and mechanism of mastering them in the process of students' independent work. In this respect it is necessary to investigate differention / integration processes from the point of view of universal law of development. Many-level system of organizing assessment and control of students' independent work while teaching chemistry at high school is created on the basis of differention/ integration theory of development.

The methodic system proposed by us includes assessment system of independent work itself in contrast to traditional assessment of only its (final) product – knowledge and skills in the subject. Requirements to types of independent work as well as parameters and criteria of their assessments are elaborated in compliance with engineering-ecologic profile on the given discipline. This created system of students' independent work assessment and control provides not only landmarks for individual activity but also possibilities for its more objective self-estimation and self- control.

The role of pedagogical practice in the formation of professional and methodological competence of the future chemistry teacher

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Pedagogical practice is an important part of practical training of the future chemistry teacher at the pedagogical university. During the practice students model their professional activity, deepen and systematize theoretical knowledge, gained in the study of chemical disciplines, develop skills of preparing and conducting scheduled, optional and extracurricular activities in chemistry. At the same time, precisely pedagogical practice highlights the problem of discrepancy between the traditional chemical and methodological training of students at the pedagogical university and the ever-increasing requirements of modern school. The purpose of the research is to identify innovative capacity of pedagogical practice in the formation of professional and methodological competence of the future chemistry teacher. The main methods used in the research are: content analysis of scientific and methodological literature concerning the problem of the research; questionnaire of students and teachers; study and generalization of the experience of pedagogical practices at institutions of general secondary education. The analysis of the practitioners' questionnaires allowed to identify both positive factors and difficulties that students faced during the practice. As a result of the conducted research, the methods of improving the organization of pedagogical practice of the future chemistry teachers are proposed. Particularly, the propaedeutic stage of preparation for practice in the process and through lecture, practical, laboratory classes at the university in order to form personally and professionally significant competencies, including information technology and communication. In practical classes after students' pedagogical practice is necessary at school, it is effective to use the case method, that focuses on analyzing specific pedagogical situations, watching and discussing video lessons. The interactive form of training, sharing acquired experience, conducting of master-classes and training seminars by teachers to develop students' practical skills in various methods and technologies are relevant. The maximum use of the possibilities of pedagogical practice for the formation of professional and methodological competence of the future chemistry teachers will contribute to their rapid adaptation to teaching activity.

Organization of the educational process at the stage of pre-university training using electronic educational resources

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An important task of the modern education system is to create an information and educational environment that allows for operational changes in the educational process and requires a fundamentally new approach to its organization. The faculty of pre-university training of Vitebsk State Medical University being a stage in the system of continuing education of future specialists carries out the training of students and applicants for successful passing of centralized testing in chemistry and ensures the continuity of the formation of subject and key competencies which are necessary for students for further studies and self-determination. To this end the Department of Chemistry along with the traditional methods introduces interactive teaching ones that ensure the student in active communication. The department has accumulated experience in applying blended learning technology in the educational process which combines classroom instruction and online training. Guided self-directed work is an important aspect of this technology. To provide educational and methodological support for guided independent work the Moodle distance learning system is used which has ample opportunities for implementing the learning process in an e-learning environment. Educational lectures have been created on the basis of the interactive element of the Lecture course, presentation of lecture material in PowerPoint, converted into HTML5 format using the iSpring Suite program which makes it possible to improve the quality of educational content and supervise students' individual work. At certain stages of training online classes are held in the form of video conferencing, consultations using Zoom, Skype software. E-mail, chats in Viber, WhatsApp messengers are used as means of communication. The department actively uses e-learning technologies in particular the LearningApps.org online service which provides the development of electronic interactive tasks with elements of gamification which heighten interest in the subject. In their practice teachers adapt the online platform Plickers which provides mutual communication among participants in the educational process and allows them to assess immediately the students' answers using QR codes in practical classes. The electronic learning resources used make it possible to improve the skills and methods of independent activity, to develop the educational, cognitive and informational competences of students which contributes to their further successful study at a higher educational institution.

Methodological work at the Department of Inorganic Chemistry of BSU: traditions and innovations

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The Department of Inorganic Chemistry was organized at the opening of the Belarusian State University (BSU) in 1921. For many years, the department paid considerable attention to the selection of the content of chemical education and the implementation of its continuity at the stages of «school - university - postgraduate education»; improvement of teaching methods, and, in particular, the implementation of the teaching and research approach, control quality of education, training and advanced training of teachers. These trends continue and develop, enriching at the present time with new directions and approaches. The Department of Inorganic Chemistry supervises the teaching of fundamental chemical disciplines, disciplines taught by the decision of the Council of the Faculty of Chemistry, and courses at the choice of students. For these disciplines textbooks have been prepared and published, and educational materials presents at the educational portal (https://educhem.bsu.by/course/index.php?categoryid=8). The content of all courses reflects the results of scientific research carried out at the department and in other divisions of BSU. This makes it possible to realize the requirement of the advanced nature of the content of chemical education in relation to the needs of practice.

Systems of creative tasks have been developed, the implementation of which is primarily aimed at developing students skills: to search, process and systematize data, to understand tasks in various formulations and contexts, to transform and create information. These developments are aimed at enhancing the independent activity of students, allow them to realize the relationship between organized education and self-education and determine the trajectory of individual work for each student, taking into account the level of his previous training. Teachers of the department widely use a rating system for assessing knowledge, active and innovative teaching methods, such as ICT, heuristic and project-based learning, the case method, stroritelling, business games etc. Much attention is paid to the formation of communication competencies in the special academic discipline «Professional Communication in Chemistry».

The development of practice-oriented and professionally significant competencies is carried out, among other things, by involving students in research work in the student research laboratory. The students are involved in the creation of laboratory works based on scientific developments of the department, multimedia educational presentations and blogs, as well as in the organization of classes with schoolchildren at the Faculty of Chemistry.

Evaluation of teaching activity as a component of internal quality assurance in higher education

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Modern higher education in Ukraine is focused on quality standards set by the parameters of the Bologna process. "Over the last 20 years, the main mission of the Bologna Process and the main goal of structural reforms has been to ensure and improve the quality and relevance of teaching and learning" [1]. According to the Law of Ukraine "On Higher Education", the quality assurance of higher education should be understood as “compliance with the conditions of educational activities and learning outcomes to the requirements of legislation and standards of higher education, professional and / or international standards (if any) as well as stakeholder and society needs, provided by internal and external quality assurance procedures." [2, Article 1].

One of the factors of internal quality assurance in higher education is the level of scientific and pedagogical workers’ professional activity. Currently, in Ukraine, the most common procedure for its evaluation is a teacher personal rating based on the results of the academic year. The results of the ratings can be used for the annual identification and reward of the best in the profession, applied by the authorities of higher education institution for managerial and forecasting purposes, and serve as an effective motivator for improving scientific and pedagogical workers’ professional activities.

Evaluation of teaching activity is a longer and more comprehensive process than teacher ratings. Procedurally, it consists of collecting and analyzing the results of teachers' activities, forming judgments about their activities, revealing the factors that influenced the results, and making management decisions.

Evaluation of scientific and pedagogical workers’ activities is a multi-subjective process. Special attention should be paid to the assessment of teachers’ activities by seekers of higher education themselves. It allows obtaining objective characteristic of the education quality to make timely specific decisions regarding the scientific and pedagogical workers’ teaching activity.

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Extraction-photometric analysis in a laboratory experiments of chemical disciplines

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In the state standards of higher education of natural science and technical areas of training, as well as in a number of relevant professional standards, competence in the field of analytical chemistry is indicated as one of the main qualification characteristics of a university graduate of the corresponding profile. This is due to the interdisciplinarity of analytical chemistry and a wide range of applications of analysis methods, which are used not only directly in chemical production, but also in energy, construction, metallurgy, materials science, standardization, certification and many other areas.

One of the popular methods of chemical analysis in industrial and scientific laboratories is the extraction-photometric method of quantitative analysis, for example of higher carboxylic acids. We have developed a new rapid, accurate and inexpensive method for the determination of such acids with the cationic dye pyronine G.

Based on our experimental data, we have developed laboratory experiments that will allow students to get acquainted with the extraction, learn how to work with a UV spectrophotometer, decode spectra, build calibration plots, and determine higher carboxylic acids in real samples.

The main advantages of using extraction-photometric analysis in the educational process are immediately visible. It makes it possible to simultaneously study and apply in practice both methods of extraction and concentration - extraction, and optical methods of analysis - molecular photometry. After completing the work, students gain experience in combining various methods to obtain the final result, which allows them to expand their horizons and move to a qualitatively new level of research and analysis. The laboratory experiments developed by us have been introduced into the laboratory practice in the disciplines "Analytical chemistry", "Modern methods of obtaining and research of substances" for students of a pedagogical profile (BSPU named after M. Tank), it is also possible to use it for students of agricultural, medical and technical profiles.