



XXII MENDELEEV CONGRESS  
ON GENERAL AND APPLIED CHEMISTRY

# BOOK OF ABSTRACTS

IN 7 VOLUMES

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**XXII MENDELEEV CONGRESS  
ON GENERAL AND APPLIED CHEMISTRY**

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

**BOOK OF ABSTRACTS**

**Volume 6**

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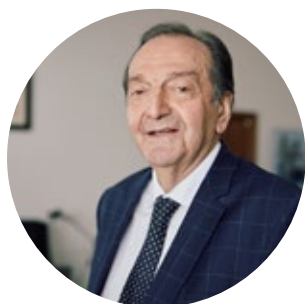
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An abstract visualization of a molecular structure, possibly a protein or a complex polymer, rendered in a vibrant, multi-colored point cloud or surface representation. The structure is composed of numerous small spheres (atoms) in shades of blue, green, yellow, and red, connected by lines representing bonds. The overall shape is complex and irregular, with many protrusions and indentations. The background is a solid, deep blue.

Section 1

# FUNDAMENTAL BASES OF CHEMICAL SCIENCE



# COMPARATIVE SORPTION OF CR(VI) IONS BY CHELATING ION EXCHANGERS

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The patterns of sorption of Cr (VI) ions from solutions of potassium dichromate by chelating ion exchangers bis-picolylamine (AMP) and iminodiacetic (Amberlite IRC 748) functional groups were studied, and the corresponding parameters were calculated. The dependence of the sorption capacity of both ion exchangers for chromium (VI) ions on the pH of the solution is extreme, with a maximum at pH 5-6. With an increase in the pH of solutions from 2.5 to 5-6, the sorption capacity of ion exchangers for chromium ions increases, reaching a maximum value of 236 mgCr/g (AMP) and 186.4 mgCr/g (Amberlite IRC 748). Sorption by both ion exchangers is characterized by a convex isotherm, which indicates the preferential sorption of Cr (VI) on anion exchangers in OH<sup>-</sup>, Cl<sup>-</sup> and Na<sup>+</sup>-forms. AMP in the OH<sup>-</sup>-form sorbs less chromium (VI) than in the chloride form. A similar picture is observed during sorption with Amberlite IRC 748. The Na-form sorbs Cr (VI) ions more preferentially than the H<sup>+</sup>-form. It is known that the absorption of chromium can occur on ion exchangers both according to the classical mechanism and as a result of a redox reaction, with chromium (VI) being reduced to chromium (V) and then to chromium (III). Perhaps a similar process occurs on these ion exchangers. The increased sorption capacity of the studied ion exchangers for chromium (VI) ions is probably explained by the fact that, along with ion exchange, complexation also occurs anion due to the presence in their structure of nitrogen and oxygen atoms with lone pairs of electrons due to donor-acceptor interaction. When chromium is desorbed from the AMP anion exchanger with a 1-1.25 N NaOH solution partial destruction and a sharp change in the color of the exchanger are observed.

The sorption of Cr (VI) ions by both ion exchangers in a certain concentration range is described by the Langmuir, Freundlich and Temkin equations that have been proposed. The equilibrium and kinetic parameters of the processes were determined, and thermodynamic quantities were calculated based on these data. It is shown that with the release of heat and a decrease in entropy, the selectivity of the system is controlled by the enthalpy factor.

# SORPTION OF NON-FERROUS METAL-IONS BY STRONG AND WEAK CATION EXCHANGERS

**Gojayeva A.E.<sup>1</sup>, Mammadova F.S.<sup>2</sup>, Abbasov A.D.<sup>3</sup>**

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The equilibrium condition and kinetics of the sorption of  $\text{Cu}^{2+}$ ,  $\text{Zn}^{2+}$ ,  $\text{Co}^{2+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Cd}^{2+}$ ,  $\text{Pb}^{2+}$  ions with Diaion PK 208 ( $-\text{SO}_2\text{OH}$ ) and DiaionWK 100 ( $-\text{COOH}$ ) cationites have been studied. Thermodynamic parameters have been calculated on the basis of data obtained from the equilibrium and kinetic studies. Sorption isotherms have been built and relevant equations have been suggested. Kinetic and thermodynamic parameters have been calculated and it has been noted that heat release and entropy reduction are managed by enthalpy factor. Sorbents are respectively characterized by 1,2 meq/mL, 4,3 meq/g and 2,8 meq/mL, 9,0 meq/g -accordingly for Diaion PK 208 and Diaion WK 100 sorption capacities. Sorption isotherms of metal ions were taken in the interval of 0.25-2.50 gMe<sup>2+</sup>/L by changing concentrations method, and for mathematical processing of sorption isotherms sorption models of Langmuir, Freundlich, Temkin have been used. It was confirmed by calculations that isotherms obey Langmuir equation with certain deviations in all cases, and formulas relevant to Langmuir equation of isotherms were suggested. Even though in all cases the selectivity of sorption is considerably higher in the low concentrations, it drops sharply by the increase of the molar share in the sorbent phase of ions. In all cases the value for diffusion coefficients for  $\text{Cu}^{2+}$  was higher than the values for other ions. The linear dependence of  $F$  from  $t^{1/2}$  within the interval of  $F=0.4-0.42$  values, the increase in the speed of the processes after temporary suspension, which is explained by the “kinetic memory” as well as the characterization of Bio criteria by  $\text{Bio}>50$  values confirm that the processes are under the control of internal diffusion within the selected concentrations. By using the diffusion coefficients and activation energy the values of activation entropy were calculated by R.Barrer equation:  $D_0 = d^2(ekT/h)\exp(\Delta S/R):ekT/h=1,69.10^{13}\text{sec}^{-1}$ ,  $d=0.5\text{ nm}$ . The calculated values of activation entropy have negative values in all cases. Experimental data confirm the tendency of reduction of the entropy with increasing of sorption selectivity in the systems studied. In all processes studied with heat release and reduction of entropy in the system, the selectivity is controlled by enthalpy factor. The lowest values of the calculated activation energy and other thermodynamic parameters are obtained in the system of  $\text{Cu}^{2+}$ -Diaion WK 100.

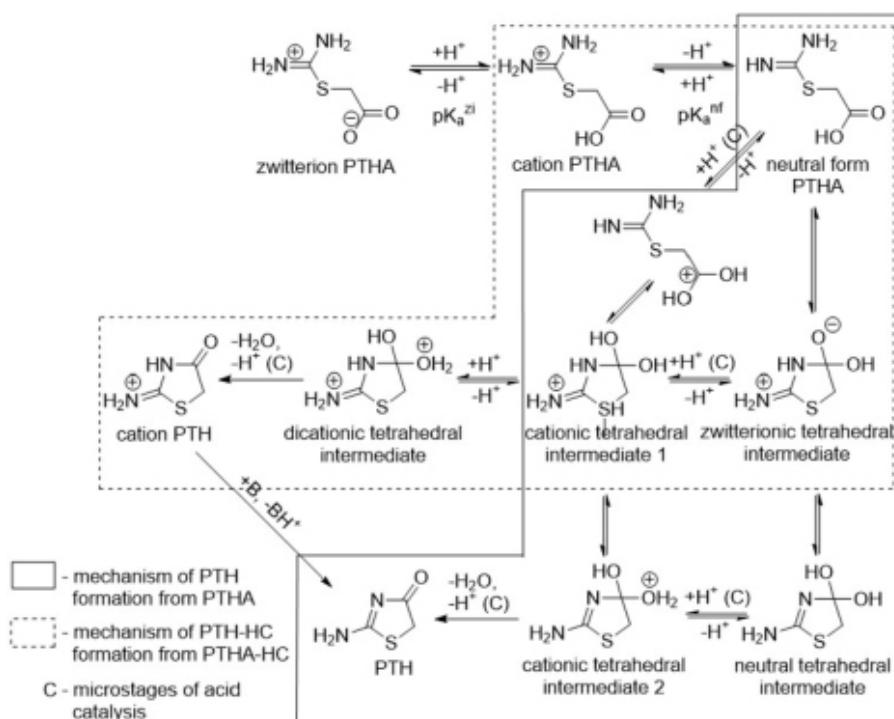
# MECHANISM OF PSEUDOTHIOHYDANTOIN FORMATION

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The previously proposed mechanisms for the cyclization of pseudothiohydantoic acid (PTHA) to pseudothiohydantoin (PTH) and its hydrochloride (PTHA-HC) to pseudothiohydantoin hydrochloride (PTH-HC)<sup>1,2</sup> are not complete and not entirely accurate. Detailed cyclization mechanisms consistent with experimental data are presented.

Only the minor<sup>2</sup> neutral form of PTHA cyclizes into PTH. PTHA-HC cyclizes into PTH-HC also through this form.



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*The work was carried out with the support of the Ministry of Education and Science of the Russian Federation (FSEN-2023-0002).*



# INFLUENCE OF THE NATURE OF THE SOLVENT ON THE REACTION OF NUCLEOPHILIC SUBSTITUTION OF A CHLORINE ATOM IN THE AROMATIC SERIES

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The reaction of nucleophilic substitution of the chlorine atom in 2,4-dinitrochlorobenzene to an amino acid residue was studied to obtain 2,4-dinitro- *N*-acetylaniline.

The approach to selecting a solvent for carrying out a nucleophilic substitution reaction is determined by its ability to reduce the free energy of the activated complex. The decrease in free energy is due to a change in the polarity of bonds, which can be influenced by the selection of solvent based on parameters such as donor number (DN) and acceptor number (AN), proposed by the Gutmann school.<sup>1</sup> The half-sum of these numbers reflects the real picture of the interaction of the solvent with the partially negative nucleus of the molecule in the transition state and the partially positive nitrogen atom in the aliphatic part of the molecule.

During the study, the following patterns of reaction were identified depending on (DN + AN)/2 solvent used (Table 1).

Solvent	DN	AN	(DN+AN)/2	Start time of HCl release, min	Product yield, %
Ethanol	19.2	37.1	28.15	4	>80
DMF	26.6	16.0	21.3	6	>80
Acetonitrile	14.1	18.9	16.5	10	>80
1,4-Dioxane	14.8	10.8	12.8	12	<80, >50
Butyl ether	19.2	3.9	11.5	13	<50
THF	20.0	8.0	14.0	14	<50

**Table 1.** Effect of solvent on the reaction of nucleophilic substitution of a chlorine atom in 2,4-dinitrochlorobenzene to an amino acid residue

The data obtained indicates selective stabilization of the transition state with an increase in the donor-acceptor force of the solvent due to the formation or localization of a negative charge.

## References

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# ANODE POLARIZATION OF Pb-Ag-Sb ALLOYS IN THE KCl-PbCl<sub>2</sub> MELT

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Technologies of alloys separation in molten chloride systems are based on the understanding the mechanisms of the processes in the molten salt electrodes. The present research is devoted to the study of the anode processes on the liquid metal surface of the Pb-Ag-Sb ternary alloys to determine the sequence of lead, silver and antimony dissolution from the melt to the chloride KCl-PbCl<sub>2</sub> melt.

Anode dissolution of the Pb-Ag-Sb alloys was studied by the current switch-off method from the stationary state under galvanostatic regime using a galvanostat-potentiostat Avtolab 302N (Metrohm, Holland). Polarization was measured at the moment of the current switch off, the constant current pulse amplitude varied from 0.001 to 1 A, the polarization time was 7-8 seconds.

The analysis of the polarization curves of individual metals and their alloys demonstrate that the anode process of liquid metal alloys has a diffusion nature in the KCl-PbCl<sub>2</sub>(50-50 mol. %) melt. The dissolution mechanism may be as follows. At small deviations of potential from the equilibrium values metallic lead dissolves according to reaction:



An increase in the anode polarization is associated with the lack of lead in the diffusion layer from the alloy side, which appears due to the insufficient rate of the electronegative Pb-Ag-Sb alloy component transfer toward the reaction region from the alloy volume. The anode potential value shifts to the positive side, which provides conditions for antimony dissolution according to reaction:



An increase in the anode polarization is explained by the lack of antimony in the diffusion layer from the alloy side. The concentration of silver increases at the metal alloy/molten salt interface. The anode potential value shifts to the positive side, which results in silver dissolution according to reaction:



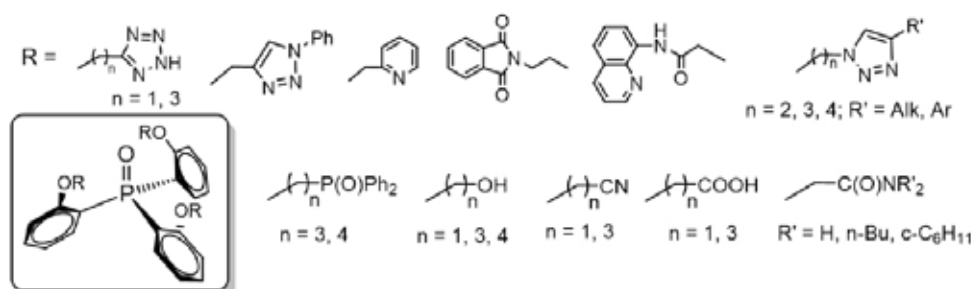
The obtained data on the alloys polarization demonstrate that the efficient lead separation from the alloys is possible even at the potentials close to the electropositive component extraction. The technology of electrochemical separation of lead from antimony and bismuth has been successfully implemented in the laboratory-scale tests.

# FUNCTIONALIZED TRIARYLPHOSPHINE OXIDES

**Baulina T.V., Kudryavtsev I.Y., Bykhovskaya O.V., Matveeva A.G.,  
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New tripodal phosphine oxides modified by functional groups promising as O,N ligands for *d*- and *f*- elements have been synthesized. Complexes of the compounds with lanthanides and actinides have been prepared. The structure of the ligands and their complexes in solid state and solution has been studied.



Extraction properties of the ligands toward *d*- and *f*-block elements have been studied. Biological activity and fluorescent properties of certain complexes of the prepared phosphine oxides have been examined.

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# CITRATE AND XYLO-TRIHYDROXYGLUTARATE COMPLEXES OF GADOLINIUM(III)

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The study of polynuclear complexes of gadolinium(III) with polyfunctional  $\alpha$ -hydroxy acids is of independent scientific interest and is of some value from a biochemical point of view. To date, we have obtained new information about the complexation of gadolinium(III) with trihydroxyglutaric and citric acids.<sup>1</sup>

In particular, we have developed a method for the synthesis of trihydroxyglutaric acid from D-xylose, which allows us to obtain the target product suitable for studying complexation. To the existing methods, additional stages of purification of trihydroxyglutaric acid have been introduced, which consist of washing with diethyl ether and acetone, as well as the use of ion exchange to remove traces of calcium ions.

By combining the methods of pH-metry, proton magnetic relaxation and mathematical simulation, complex formation in the systems gadolinium(III)—citric acid and gadolinium(III)—xylo-trihydroxyglutaric acid was studied. General patterns of complex formation were identified: in both systems, processes of formation of polynuclear complexes occur, starting from the acidic pH region, which dominate almost the entire pH range studied.

For the first time, binuclear *bis*-  $\text{Gd}_2(\text{HCit})_2^0$  and  $\text{Gd}_2\text{Cit}_2^{2-}$  hexanuclear *hexakis*-  $\text{Gd}_6(\text{OH})_2\text{Cit}_6^{8-}$  and  $\text{Gd}_6(\text{OH})_3\text{Cit}_6^{9-}$  citrate gadolinium(III) complexes were described, the formation of which can be considered typical for  $\text{M}^{3+}$  ( $\text{Al}^{3+}$ ,  $\text{Ga}^{3+}$ ,  $\text{In}^{3+}$ )—citric acid systems.

In the gadolinium(III)—xylo-trihydroxyglutaric acid system, polynuclear complexes of the composition  $\text{Gd}_2(\text{H}_3\text{Thgl})(\text{H}_2\text{Thgl})^+$ ,  $\text{Gd}_4\text{HxThgl}_4$  and  $\text{Gd}_4\text{HxThgl}_8$  were identified for the first time. The formation of mixed-ligand hydroxo—trihydroxyglutarate complexes of gadolinium(III) was not detected, which is apparently due to the large number of donor groups.

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*This paper has been supported by the Kazan Federal University Strategic Academic Leadership Program.*

# REGULARITIES OF THE ELECTROOXIDATION PROCESS OF THE METHIONINE ANION ON PLATINUM

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Establishing the relationship between the nature of the metal electrode, structural isomerism and the number of functional groups in organic molecules and their adsorption and electrochemical behavior is necessary to identify the mechanism of electrode processes involving organic substances and their effect on the speed of other processes at the metal|electrolyte interface. Thus, the purpose of this work is to establish the kinetic patterns of electrooxidation of the methionine anion on the Pt(Pt) electrode.

The patterns of the anode process were established using the method of linear voltammetry, a rotating disk electrode, and supplemented with coulometric measurements followed by spectrophotometric determination of the concentration of amino acids in solution. The working electrode is a platinum-plated platinum grid, the background electrolyte is a 0.1M NaOH solution, into which a certain aliquot of an amino acid solution was injected before the experiment.

It is established that the process of anodic oxidation of the methionine anion on the Pt(Pt) electrode proceeds in the area of potentials of oxygen adsorption, which corresponds to the maximum current. The fact of electrooxidation at the corresponding maximum potential is confirmed coulometrically. It was determined that two electrons participate in the process of electrooxidation, and the main product of the anodic process is methionine sulfoxide.

Quantitative processing of the results was carried out within the framework of the theory of linear voltammetry for a heterogeneous Red-Ox reaction, not complicated by liquid-phase diffusion, not accompanied by non-dissociative substitutive co-adsorption of the reagent and product<sup>[1]</sup>. It has been established that the limiting stage of the anodic process is the charge transfer stage proceeding from the adsorbed state, and the adsorbed form is actually the methionine anion. The rate of the anode reaction is determined by the rate of "separation" of the first electron, and the process of electrooxidation is kinetically irreversible.

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# THE T-FACTORS REVEALING WHEN ISOLATING Nu-PARTICLES

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The new aspect of a stable nuclide (S) and a radionuclide (R) is described, its consequences are important<sup>1-3</sup>. The new model (M) is based on a limitation (L) of time of looking ( $t_L$ ) after R-nuclei ( $\tilde{N}$ ) of an element (E), on a substitution of nuclei  $\tilde{N}$ , which didn't decay during a certain  $t_L$ , by nuclei-equivalents (NE). R doesn't have NE-decays even during  $t \gg t_L$ : the NE-nature is other. There is a conclusion by Prof. M. Bunge<sup>2</sup> about a benefit of such M, theories. There is a visual process (P) with L in  $t=t_2$  for simple R-particles (A) in the chamber (it isn't for R with ultra-little  $T_{1/2}$ , but it's for all E):  $t_0=0$  – a start of ionization of  $A^0$  by a flow, its source's automatic shutdown,  $t_1$  – a start of recombination  $A^+ + e^-$ ,  $t_2$  – its finish, an automatic start of a new stage. For  $t=t_2$  the sum of A in P is  $s_0 = s_1 + s_{1-2} + \Delta s$ :  $s_1$  – with  $\tilde{N}$  which decayed during  $t_1$ ,  $s_{1-2}$  – during  $(t_1; t_2]$ , there is no decay in  $\Delta s$  during  $t_2$ . So A in  $s_1$ ,  $s_{1-2}$  are with  $\tilde{N}$ , in  $\Delta s$  – with their NE. For  $t < t_0$  it's an exact prognosis of P. "The statistics increases" by a large k of parallel P:  $s_0 = s_{0,1} + \dots + s_{0,k}$ , etc. Further,  $\tilde{N}$ , its NE are collectives of  $p^+$ ,  $n^0$ . Their charges are  $Q=Z+q$ . Z is a total charge of "real R-" (RR)  $p^+$  of a collective (they are able to get a changed collective (CC) or to be transformed), q – of "equivalent R-" (ER)  $p^+$  of it (they are able neither the first nor the second). All  $p^+$  of  $\tilde{N}$  are RR:  $q=0$ ,  $Q=Z$ ; all  $p^+$  of its NE are ER:  $Z=0$ ,  $Q=q$ . Further, for  $t=t_2$  R with little  $T_{1/2}$  have  $s_1 + s_{1-2} > 0$ . Thus, A-mass of  $^{25}\text{N}$  consists of A with  $\tilde{N}$  ( $Q=Z=7$ ), A with NE ( $Q=7$ ,  $Z=0$ ). A in  $s_1 + s_{1-2}$  consist of nitrogen atoms, A in  $\Delta s$  – of Nu(-a) – of nullbecquerelium atoms (Nu is a symbol of the E with 0 Bq,  $Z=0$  is its sign): Nu-a, which are so isolated from  $^{25}\text{N}$ , have electrons and chemistry (EC) of N, Nu-a from  $^{30}\text{F}$  have EC of F, etc. Nu-positions (Nu-p) from  $^{25}\text{N}$  are in gr.15, in periods 1-7. Nu-p in PT are minor<sup>1,3</sup>. R with not little  $T_{1/2}$  have  $s_1 + s_{1-2} \approx 0$ . Their A in  $\Delta s$  consist of Nu too. So Nu is from all E in view of T-factors ( $t_L, T_{1/2}$  of R).

$Q=Z+q$  is true for S: its "real S-"  $p^+$  can't get CC, can't be transformed,  $Q=Z$ , there are no NE, Nu. Nu covers all PT<sub>IUPAC</sub>-cells, so for its P-zone<sup>2</sup> [ $Z=1$ ;  $Z=56$ ]:  $G_{(\text{passed groups in a period})} = Z + D_{(\text{passed rel. positions})} - 18N_{(\text{group repeated passages})}$ . Professors N.F.Stepanov<sup>1</sup>, V.A.Funtikov<sup>4</sup>, J.P.Cid Ugalde et al. recognized it as innovation.

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# ON SOME PROPERTIES OF FERRATES

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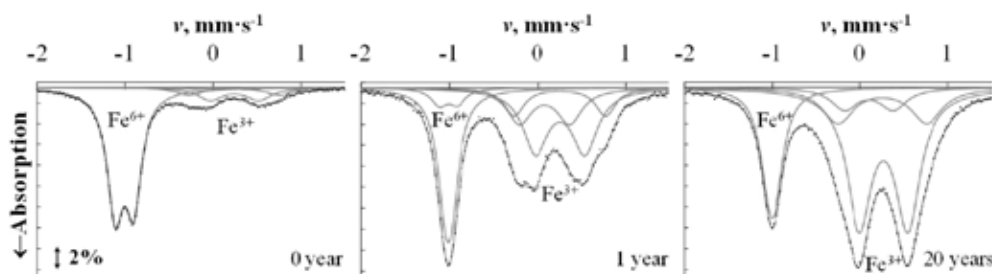
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Iron is one of the most abundant elements on Earth. It plays a crucial role in both human development and the existence of life. Its ability to exist in different oxidation states, which are not found in nature, has been known since the 19th century. However, there are still gaps in our understanding of chemistry regarding such compounds.

For example,  $K_3Na(FeO_4)_2$ , which is formed by crystallizing from a solution, decomposes into  $K_2FeO_4$  when it is in the solid state at room temperature. The decomposition<sup>1</sup> results in the formation of  $K_2FeO_4$ , which remains stable more than 20 years. Thus, decomposition does not occur due to the instability of hexavalent iron. It is caused by the structural instability of the substance.



**Figure 1.** Room-temperature Mossbauer spectra of a sample of  $K_3Na(FeO_4)_2$  at three stages of its decomposition.

Another way of decomposition is shown by the solid  $Na_4FeO_4$ , which disproportionates at room temperature<sup>2</sup>. This should be taken into account in the solid-state synthesis of ferrates(VI): Over the years of research on the solid-state oxidation of iron, we have not been able to obtain ferrate(VI) without the admixture of iron(III).

When added to water, freshly prepared ferrates(IV) and (V) may not produce the wine-colored  $FeO_4^{2-}$ -ion. However, the color may appear if the solids are kept at ambient temperature for a certain amount of time. This is important for the use of ferrates in water treatment<sup>3</sup>.

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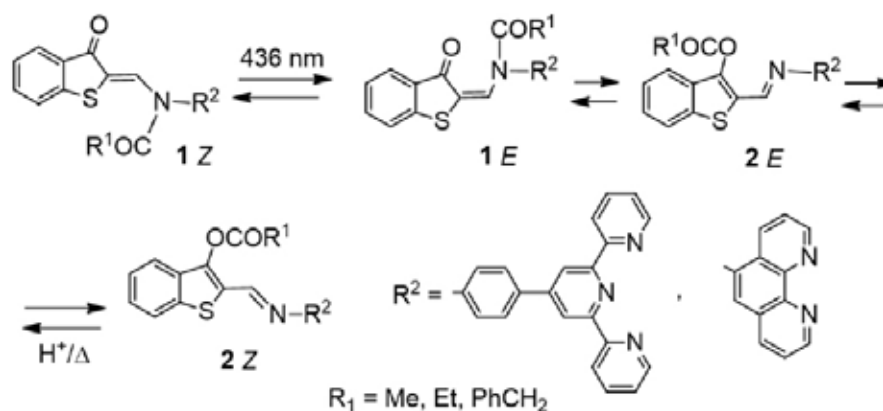
# PHOTO- AND IONOCROMIC ACYLOTROPIC SYSTEMS

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Photoacylotropic enaminketones of the benzo[*b*]thiophene series containing terpyridine and phenanthroline groups have been synthesized. They represent polyfunctional on-off-on switches of optical and fluorescent properties.<sup>1,2</sup>



The three-step mechanism of photoinitiated rearrangement has been characterized in detail by IR, <sup>1</sup>H and <sup>13</sup>C NMR spectroscopy, HRMS, XRD analysis and DFT calculations. The emission modulation is realized by sequential exposure to light/H<sup>+</sup> or by sequential addition of Fe<sup>2+</sup>/AcO ions.

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# LONG-GOING PROBLEMS OF SYNTHESIS OF POLYHEDRAL CLUSTERS $B_nH_{n-2}$ ( $n > 12$ ) AND $P_n$ ( $n > 4$ ): POSSIBLE SOLUTIONS

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Polyhedral borohydride anions  $B_nH_n^{-2}$  ( $n = 6-12$ ) were synthesized in the early 1960s and studied in thousands of works. According to calculations, their analogues are stable at  $n > 12$ ; the cluster  $n=15$  is part of framework borides of the  $YB_{50}$  type. But  $B_nH_n^{-2}$  ( $n > 12$ ) have not yet been synthesized. Attempts to synthesize  $B_{21}H_{21}^{-2}$  by reducing  $B_{21}H_{18}^{-1}$  were unsuccessful. Recently, carborane analogues  $B_{n-2}H_{n-2}C_2R_2$  up to  $n=16$  were synthesized by successive treatments of Na and  $HBBR_2(SMe_2)$ , but this approach is not applicable to  $B_nH_n^{-2}$  because  $B_{12}H_{12}^{-2}$  is not reduced by sodium. It can be assumed that for silaboranes  $B_{n-2}H_{n-2}Si_2R_2$  the size  $n$  can be increased in the same way as for carboranes. However, Si atoms, unlike C atoms, can then be removed from the cluster by the action of HF or alkalis, followed by the completion of the nido-cluster to the closo-one by the action of  $BH_4^{-1}$  or other known ways. Since the framework structure of  $BeB_3$  includes 15- and 16-vertex deltahedra, the highly coordinated positions of which are replaced by Be, it should be expected that reactions of Be hydrides or borohydrides with salts  $BH_4^{-1}$  or  $B_3H_8^{-1}$  in suitable combinations can give similar beryllium interstitial compounds into the cluster - for example, the following:  $M_4[B_{12}H_{12}(BeBH_4)_2]$ ,  $M_5[B_{12}H_{12}(BeBH_4)_3]$ ,  $M_4[B_{12}H_{12}(BeBH_4)_4]$ ,  $M_2\{Be_2B_{12}H_{12}\}$ ,  $M_2\{Be_3B_{12}H_{12}\}$ , where M is an alkali metal. Since it is known that beryllacarboranes of the type  $LB_eB_9H_9C_2H_2$  are very easily hydrolyzed, Be atoms can be removed by mild solvolysis followed by completion to closo balance by the action of  $BH_4^{-1}$ , up to the production of  $B_nH_n^{-2}$  ( $n=14-15$ ) or  $B_{16}H_{16}$ . This is a rare case when the irreplaceable properties of beryllium may be more important than its toxicity.

$P_n$  ( $n > 4$ ) molecules have been studied in detail by theorists, but have not yet been synthesized. It should be expected that the simplest path to them leads through the reactions of long-prepared cluster phosphides containing the  $P_7^{-3}$  and  $P_{11}^{-3}$  anions, or their derivative phosphanes  $P_7H_3$ ,  $P_{11}H_3$  with trihalides of P in the cavities of zeolites or other typical conditions that prevent polymerization.

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# ACTIVE THERMOSTABLE RUTHENIUM CATALYST FOR PHOTOINDUCIERED WATER OXIDATION IN ARTIFICIAL PHOTOSYNTHESIS

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An effective way of solar energy (SE) storage is artificial photosynthesis (APS). In nature, the catalyst for the process of water oxidation is the manganese cofactor  $\text{Mn}_4\text{O}_5\text{Ca}$ . In APS other transition metals, such as Co, Ni, Fe, including Ru, can perform the function of the manganese cofactor. All the ruthenium complexes are ineffective because of the presence of organic ligands, which undergo oxidation faster, than water and low stability for presence of labile Ru-O-Ru bonds resulting in catalyst degradation. To design active and stable ruthenium catalyst, we studied in this work the following approaches: 1) replacement of organic ligands in complexes by inorganic ligands; 2) replacement of oxygen bridge between ruthenium nuclei by nitrogen one; 3) use  $\text{Li}^+$  as counter cations in the catalyst synthesis.

In this communication we studied by X-ray spectroscopy the structure of a new complex  $\text{Li}_3[\text{Ru}_2(\mu\text{-N})\text{Cl}_8 \cdot 2\text{H}_2\text{O}]$  (**1**), and photocatalytic water oxidation reaction in the presence of electron acceptor  $\text{K}_2\text{S}_2\text{O}_8$ , photosensitizer (bpy) $_3\text{RuCl}_2$  and **1**. The Ru-N distance in this complex is shorter (1.72 Å) than Ru-O distance (1.86 Å) in its oxygen analog  $\text{Li}_4[\text{Ru}_2(\mu\text{-O})\text{Cl}_{10} \cdot 2\text{H}_2\text{O}]$ . Complex **1** is stable in acidic solutions. In IR spectrum of **1** the maximal peak with  $\nu = 1075 \text{ cm}^{-1}$  (Ru-N-Ru) persists for several days.

The initial rate of the process  $w_0$  versus the concentration of complex **1** described by the parabolic law. This indicates that the catalytically active species is formed from two complexes **1** and is a tetranuclear ruthenium cluster. In the ESI-mass spectrum for the products of the photocatalytic oxidation of water, has the highest peak at  $m/z = 512.28$ , which corresponds to the cation  $\text{Ru}_4\text{N}_2\text{O}^{5+}$ . This cation is catalyst for four-electron oxidation of water to  $\text{O}_2$ :  $2 [\text{Ru}^{\text{IV}}\text{-N-Ru}^{\text{IV}}] + 2 \text{H}_2\text{O} = 2 [\text{Ru}^{\text{III}}\text{-N-Ru}^{\text{III}}] + \text{O}_2 + 4 \text{H}^+$ . Maximal catalyst turnover number  $\text{TON} = 360$ , quantum yield  $\text{O}_2$   $\Phi = 0.51$  higher in its oxygen analog  $\text{Li}_4[\text{Ru}_2(\mu\text{-O})\text{Cl}_{10} \cdot 2\text{H}_2\text{O}]$  ( $\text{TON} = 240$ ,  $\Phi = 0.2$ ). The mechanism of the photoreaction is discussed.

*This work was supported by the Ministry of Science and Higher Education of the Russian Federation (project no 124020200104-8).*

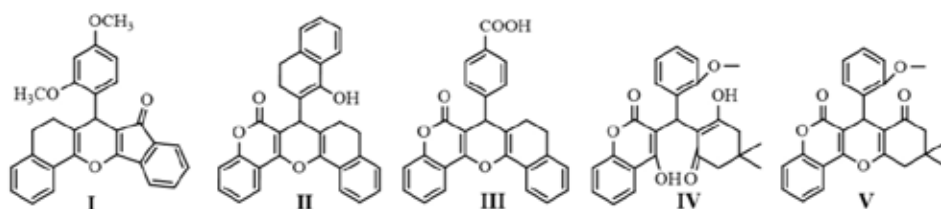


# ELECTROCHEMICAL METHOD FOR S-(RE-)CYCLIZATION OF 2H-CHROMEN-2-ONES USING OXIDATIVE ACTIVATION OF HYDROGEN SULFIDE

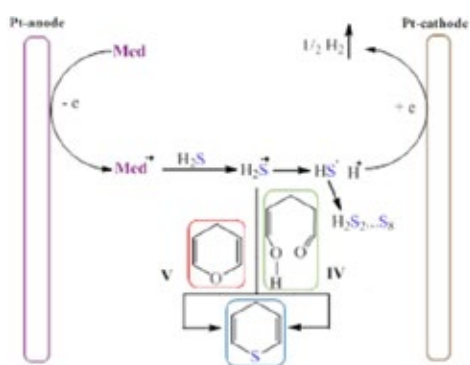
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Interest in multifunctional heterocyclic compounds is due to their pharmacological activity towards various biological targets of a living organism, which makes it possible to create multi-purpose drugs based on them.<sup>1,2</sup> Electrosynthesis is a convenient and simple way to replace a heteroatom in the cycle with sulfur using activated hydrogen sulfide. In this study, we selected polycarbonyl compounds with chromene moiety **I-V** to study the interaction with  $H_2S$  under electric current.<sup>3</sup> The oxidized form of  $H_2S$  fragmented into a thiyl radical and a proton during electrosynthesis, by that creating an acidic environment during the electrode process.



As a result, products of S-(re-)cyclization of substrates were obtained in quantitative yields of up to 51-82%,



depending on the structure of the starting compound and the method of activation (direct and indirect). Electrosynthesis was carried out in a diaphragm-less electrochemical cell at 25 °C. Anodic activation of  $H_2S$  was carried out on a Pt-anode, and mediators (Med) of various natures were used for indirect oxidation of the reagent: tetrabutylammonium bromide, DABCO, tri-*p*-tolylphosphine. With an increase in the duration of electrosynthesis, the resulting substituted thiochromenes are

converted into thiochromilium salts. In the case of indirect oxidation of  $H_2S$ , the reduction in energy consumption was 0.5-0.8 V compared to direct electrosynthesis. The proposed synthetic method is environmentally friendly due to the absence of catalytic amounts of strong acids.

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# FEATURES OF OBTAINING NITRO-SUBSTITUTED 6H-INDOLO[2,3-B]QUINOXALINES

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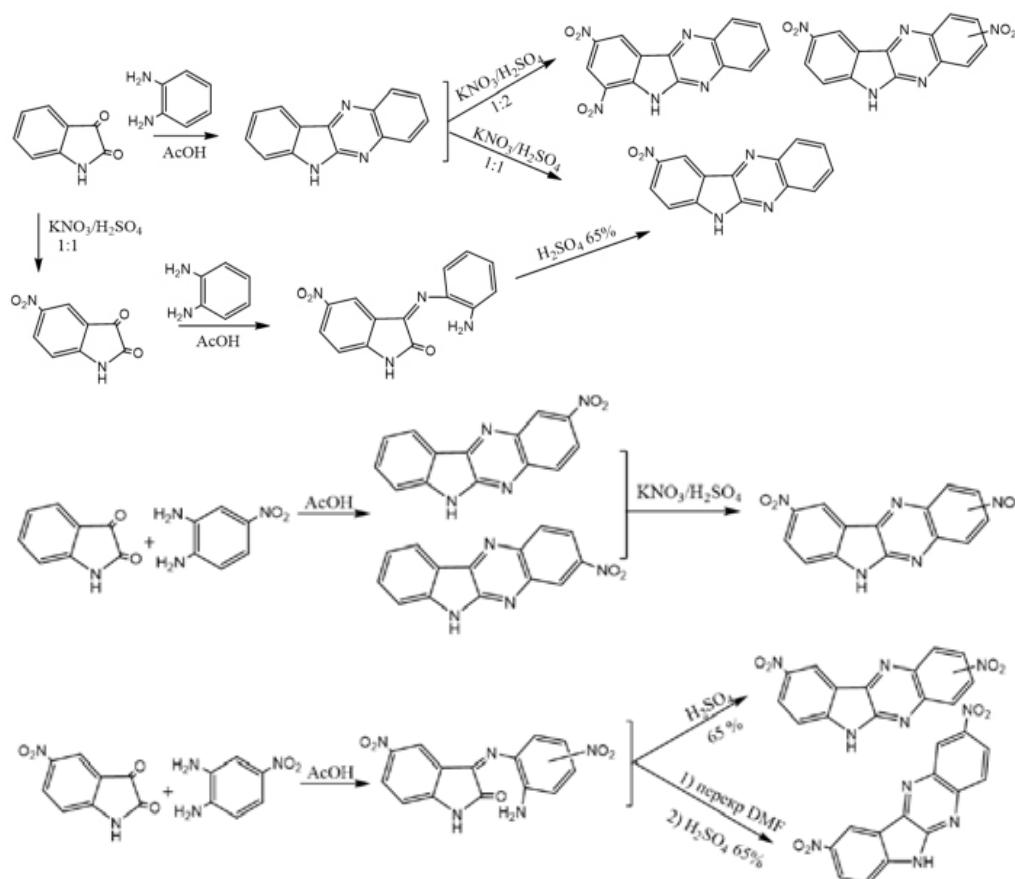
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The conditions for the preparation of nitro-substituted 6H-indolo[2,3-b]quinoxaline derivatives, which are valuable precursors in the synthesis of the corresponding amines containing the 6H-indolo[2,3-b]quinoxaline fragment, have been studied and optimized. Amines obtained by reduction of nitro compounds synthesized in this work can be used in the synthesis of new classes of organic dyes and compounds with semiconductor properties.



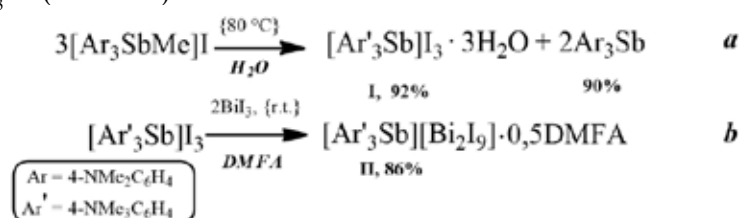
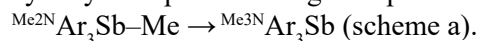
The work was carried out with the financial support of the Russian Science Foundation, project 03-01-00001.

THE FIRST EXAMPLE OF THE (Sb-Alk→N-Alk)  
TRANSALKYLATION REACTION IN A SERIES  
OF ARYLALKYLANTIMONY DERIVATIVES

**Grinishak I.P., Egorova I.V.**

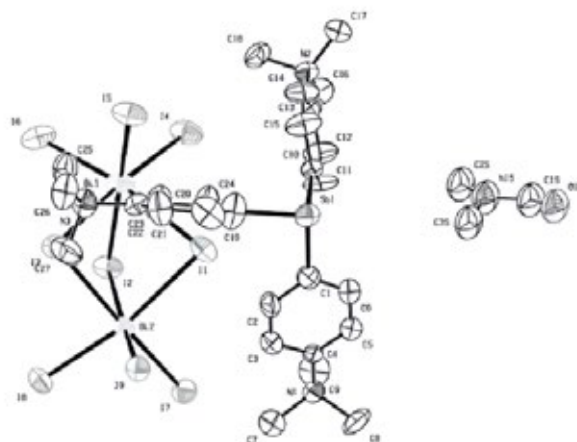
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Functionalization of aromatic rings of organoantimony compounds determines the possibility of constructing complex organic structures based on them. The selective activation of reactive centers of such compounds is of particular interest.<sup>1</sup> For organoantimony compounds, we have demonstrated for the first time the possibility of rearrangement of the arylalkyl compound through the path:



The structure of compound **I** is confirmed by elemental analysis, infrared spectroscopy (IR), and the results of nuclear magnetic resonance (NMR) experiments:  $^1\text{D}$ :  $^1\text{H}$ ,  $^{13}\text{C}\{^1\text{H}\}$ ,  $^{13}\text{C}$ ;  $^2\text{D}$ :  $^1\text{H}$ ,  $^{13}\text{C} - \text{HSQC}$ ,  $^1\text{H}$ ,  $^{13}\text{C} - \text{HMBC}$ ,  $^1\text{H}$ ,  $^1\text{H} - \text{COSY}$ ,  $^1\text{H}$ ,  $^{15}\text{N} - \text{HMBC}$ .

In order to establish the structure of the cationic part of compound **I**, complex **II** was synthesized (scheme *b*).



**Figure 1.** ORTEP representation of the structure of complex **II** in the crystal ( $p = 0.3$ ).

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# TRIS(2,6-DIMETHOXYPHENYL)BISMUTH. SYNTHESIS, STRUCTURE, PROPERTIES

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Organobismuth compounds exhibited anticancer, antileishmanial, and some extent of antifungal and other medicinal properties.<sup>1</sup> They are used in analytical practice and have great synthetic potential.

Synthesis of *tris*(2,6-dimethoxyphenyl)bismuth, is based on the reaction of bismuth (III) chloride with 2,6-dimethoxyphenyllithium obtained from 1,3-dimethoxybenzene and phenyllithium, which is less pyrophoric than *bu*-tyllithium used in a study by Wada and co-workers.<sup>2</sup>

To determine the spatial structure of the compound by slow crystallization from chloroform, single crystals of *tris*(2,6-dimethoxyphenyl)bismuth suitable for X-ray diffraction analysis were obtained.

Compound  $[2,6-(\text{MeO})_2\text{C}_6\text{H}_3]_3\text{Bi}$  crystallizes in the monoclinic syngony. According to the X-ray diffraction data in  $[2,6-(\text{MeO})_2\text{C}_6\text{H}_3]_3\text{Bi}$ , the Bi–C interatomic distances are 2.256, 2.257, 2.274 Å. The values of the CBiC bond angles are 95.97, 100.90, 100.45°.

Tri-*p*-tolylbismuth perchlorate and  $\mu$ -oxo-bis[(perchlorato)tri-*p*-tolylbismuth] were synthesized by the reaction of tri-*p*-tolylbismuth dibromide with silver perchlorate and its hydrate.<sup>3</sup> The reaction of silver perchlorate with other organo-bismuth compounds remains a poorly studied method for the synthesis of bismuth perchlorates. We studied the reaction of *tris*(2,6-dimethoxyphenyl)bismuth dibenzoate with silver perchlorate in chloroform. *Tris*(2,6-dimethoxyphenyl)bismuth dibenzoate was obtained by the oxidation of *tris*(2,6-dimethoxyphenyl)bismuth with benzoyl peroxide in benzene (at the ratio 1:1).

The IR spectrum of *tris*(2,6-dimethoxyphenyl)bismuth diperchlorate contained the absorption bands with maximums at 1099 [ $\nu_{\text{as}}(\text{ClO}_2)$ ], 1016 [ $\nu_{\text{s}}(\text{ClO}_2)$ ], 891 [ $\nu_{\text{s}}(\text{ClO}_2)$ ], 623 [ $\nu_{\text{s}}(\text{ClO}_2)$ ]  $\text{cm}^{-1}$ .

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# SYNTHESIS OF 1,3,4-OXADIAZOLES BASED ON THE TRIPLE BOND OF DIALKYL CHLOROACETYLENE PHOSPHONATES

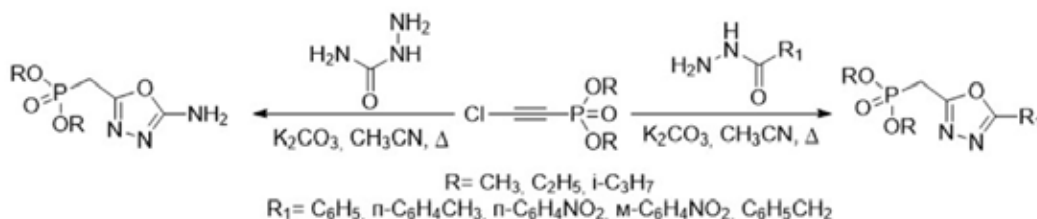
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The presence of 1,3,4-oxadiazoles in a wide range of biological activity<sup>1</sup>, including anti-inflammatory, antibacterial, antituberculous and antimalarial, makes it possible to use the latter as effective pharmacophore fragments in the composition of many drugs, the medical effects of which are simultaneously directed at various targets. For this reason, the development and modernization of approaches to the synthesis of 1,3,4-oxadiazoles is of particular interest

In this paper, a new non-catalytic method is considered that allows one-step, under mild conditions, to form a 1,3,4-oxadiazole cycle during the reaction of acid hydrazides with dialkyl chloroacetylene phosphonates. that the reaction proceeds under mild conditions, chemo- and regioselectively and leads to the formation of phosphonylated 1,3,4-oxadiazoles, yields of which varied in the range of 85-90% (figure 1).



**Figure 1.** Reaction of dialkyl chloroacetylene phosphonate with semicarbazide and acid hydrazides

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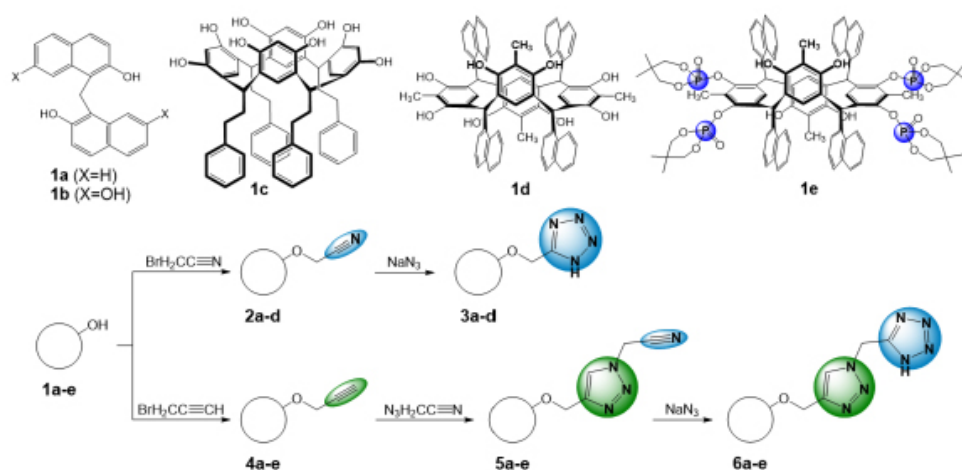
The research was carried out at the expense of a grant from the Russian Science Foundation No. 23-13-00224, <https://rscf.ru/project/23-13-00224> / using the equipment of the Engineering Center of the St. Petersburg State Institute of Technology

# FORMATION OF POLYCYCLIC AZOLE SYSTEMS ON THE 1,1'-DINAPHTHYLMETHANE AND CALIX[4] RESORCINARENES PLATFORMS

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The pathways for successive modification of 1,1'-dinaphthylmethanes **1a,b**, *rccc* tetra-C-phenethyl-calix[4] resorcinarene **1c**, *rctt* tetra-C-naphthyl-calix[4]resorcinarenes **1d,e** were developed. In the result of their implementation the series of new polyazole derivatives differing in structure of polycyclic platform and containing some functional branches oriented in a certain way in space with tetrazole, triazole<sup>1</sup> or triazole-terazole moieties was synthesized.



Using UV spectrophotometric titration, the effect of structural features of ligand, the nature and orientation of functional groups on the complexing abilities of synthesized homo- and heterofunctionalized derivatives **3a-d**, **6a-e** toward *d*- ( $\text{Cu}^{2+}$ ,  $\text{Ag}^{+}$ ) and *f*- ( $\text{Tb}^{3+}$ ,  $\text{Yb}^{3+}$ ) metal cations was studied.

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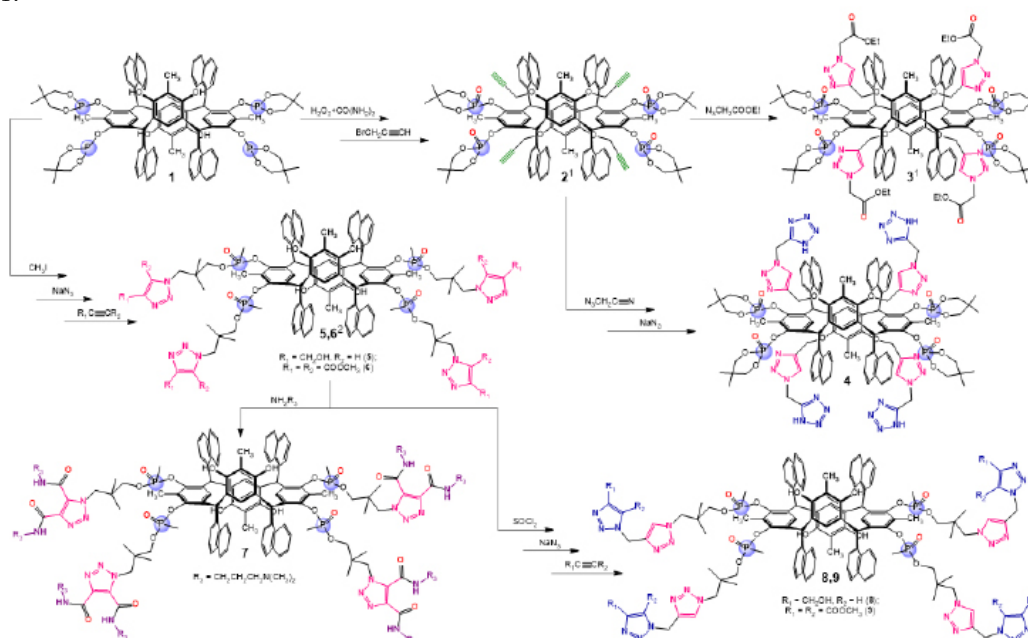


# REGIODIRECTION SYNTHESIS OF POLYTOPIC RCTT TETRANAPHTHYL-CALIX[4]RESORCINARENES

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The approaches for synthesis of polytopic derivatives of *rctt* *ortho*-methyl-tetra-*C*-naphthyl-calix[4]resorcinarene **1** containing active functional sites with predefined orientation relative to the macrocycle core were developed. Both considered routes based on use of bifunctional reagents with terminal groups capable of transformation at each of the subsequent stages.



Note that further transformation of compounds **8,9** can be continued both in horizontal (due to active terminal groups) and vertical (due to free OH groups) planes.

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1. Serkova O.S., Glushko V.V., Toropygin I.Yu., Maslennikova V.I. *ChemistrySelect*, 2020, **5**, 12168.
2. Serkova O.S., Glushko V.V., Toropygin I.Yu., Maslennikova V.I. *Russ. Chem. Bull.*, 2021, **70**, 1328.

# THE EFFECT OF SEPARATION OF BLOCKS ON THE CRYSTALLIZATION KINETICS AND PHASE COMPOSITION OF POLYBUTYLENEADIPATE IN THERMOPLASTIC POLYURETHANES

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The influence of the hard segment nature on the crystallization kinetics of medical grade thermoplastic polyurethanes (TPU) containing polybutyleneadipate (PBA) as a soft segment was investigated.

Using a combination of instrumental methods, important fundamental results in the physics of block-copolymers have been obtained in this work, explaining the relationship between phase separation of blocks in the amorphous state and crystallisation of one of the blocks on the example of thermoplastic polyurethanes based on biodegradable polyester PBA. It is shown that for TPUs with cycloaliphatic and aromatic urethane blocks, slow crystallisation of the polyester block stimulates phase separation and the phase composition is close to the initial polyester. Polyurethanes with aliphatic urethane blocks with good phase separation are characterised by fast crystallisation of the polyester block with the formation of a thermodynamically stable phase. Increase of cooling rate from the melt up to 30,000 K/min leads to suppression of phase separation of blocks and crystallisation from isotropic melt with corresponding change of crystalline phase of polyester block.

The possibility of obtaining polymorphic modification of a specific polyester block structure leads to a tool for tailoring the mechanical, thermal and biodegradable properties of adaptive materials.

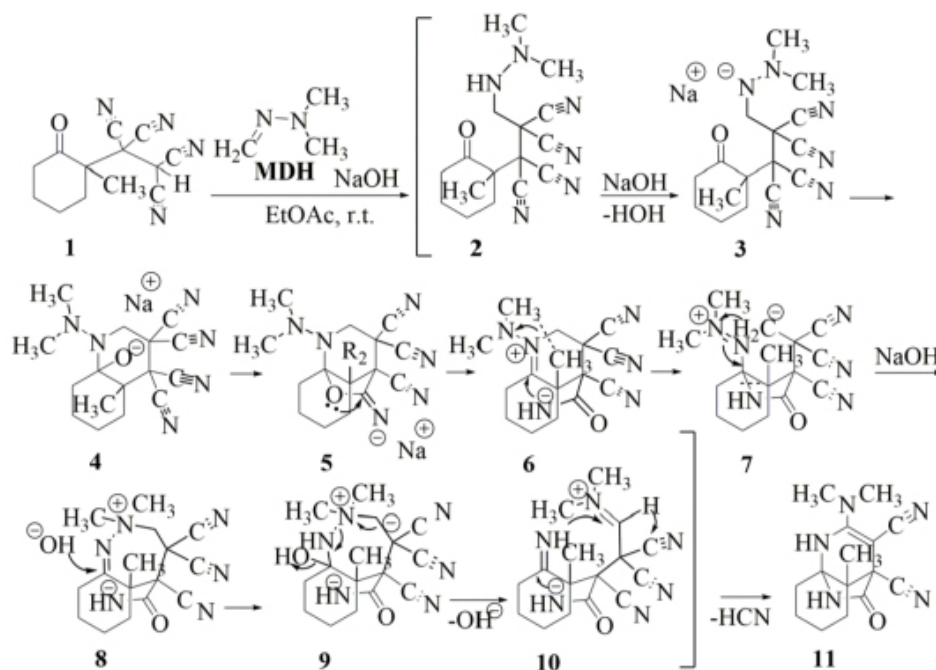
*This research was funded by state support with the K1-2022-035 project in the frame of the strategic academic leadership program «Priority 2030». This work was performed in accordance with the state task FFSG-2024-0010, state registration № 124013000757-0.*

# INVOLVING UTILIZATION INTERMEDIATE OF ROCKET FUEL HEPTIL INTO FINE ORGANIC SYNTHESIS

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As an alternative to the utilization of rocket fuel, Heptil (asymmetric dimethylhydrazine, UDMH),<sup>1</sup> instead of incineration, we propose the introduction of its methylene derivative (MDH)<sup>2</sup> into fine organic synthesis. The reaction of MDH with tetracyanoethylated ketone (TCK) **1** based on 2-methylcyclohexanone, yielded a tricyclic derivative **11** in one stage. We assume the formation of product **11** through several rearrangements catalyzed by alkali,<sup>3,4</sup> according to the scheme presented below (Figure 1):



**Figure 1.** The proposed synthesis scheme is 8a,4-(epiminomethano)quinoline-3,4-dicarbonitrile

## References

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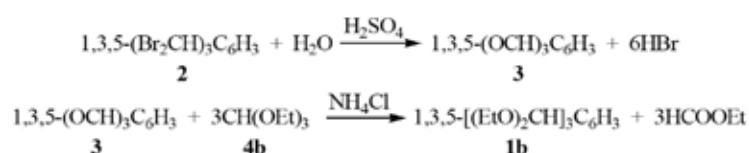
*The research was conducted with the financial support of the RSF, project 23-23-00656.*

# NEW METHODS FOR SYNTHESIS OF 1,3,5-BENZENETRICARBALDEHYDE AND ITS ACETALS

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Shaikhutdinova L.R., Karimova R.F., Ibragimov Sh.N., Nuriakhmetov B.D.**

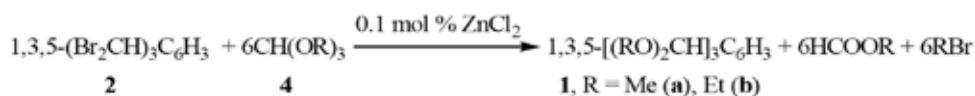
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Aromatic polyaldehydes and their acetals are used in the preparation of bactericidal compositions for disinfection and sterilization. The work describes a two-stage method for the synthesis of 1,3,5-benzenetricarbalddehyde hexaethyl triacetal **1b**: 1) hydrolysis of 1,3,5-tris(dibromomethyl)benzene **2** into 1,3,5-benzenetricarbalddehyde **3** using an aqueous solution of sulfuric acid; 2) acetalization of aldehyde **3** with triethyl orthoformate **4b**.

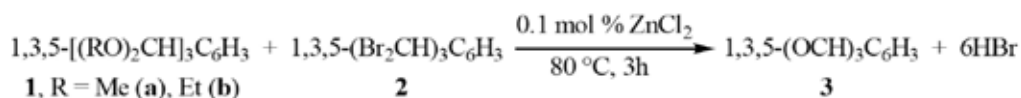


The disadvantages of the method are the use of sulfuric acid during the hydrolysis of hexabromide **2** and the evolution of hydrogen bromide. They corrode the equipment. The goal of this work is to develop methods for the synthesis of compounds **1** and **3** that do not have the above disadvantages.

Previously, we developed a method for producing acetals directly from benzalhalides<sup>2</sup>. We used this method to convert a hexabromide **2** to triacetal **1**.



Since the compounds **2** and **1** contain three dibromomethyl and three acetal groups, we assumed that when they interact with each other, trialdehyde **3** will be obtained. Indeed, when a mixture of **1** and **2** is heated in the presence of  $\text{ZnCl}_2$  at 80 °C for 3 hours, an aldehyde is formed.



## References

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# STUDY OF THE SOLUBILITY OF THE $Ca^{2+}, Na^{+} || CO_3^{2-}, SO_4^{2-} - H_2O$ SYSTEM AT 75°C

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The state of phase equilibrium in the  $Ca^{2+}, Na^{+} || CO_3^{2-}, SO_4^{2-} - H_2O$  system determines the conditions for processing liquid waste from aluminum production. Liquid waste, which is extracted during the production of aluminum at the plant (Tursunzade), contains carbonates, fluorides, sulfates and bicarbonates of calcium, sodium<sup>1</sup>.

The purpose of the study is to determine the ratio of the crystallization fields of equilibrium solid phases and the position of geometric patterns of concentration parameters. The experiment was carried out according to the pre-saturation method<sup>2</sup>.

The chemical analysis of the products was carried out using certain techniques<sup>3</sup>. The table shows all the data on the solubility of the four-component  $Ca^{2+}, Na^{+} || CO_3^{2-}, SO_4^{2-} - H_2O$  system at a temperature of 75°C.

№ points	Composition of the liquid phase, wt. %					Equilibrium solid phases
	Na <sub>2</sub> SO <sub>4</sub>	CaSO <sub>4</sub>	Na <sub>2</sub> CO <sub>3</sub>	CaCO <sub>3</sub>	H <sub>2</sub> O	
E <sub>1</sub> <sup>4</sup>	24,38	0,911	20,29	–	54,4190	Te+Gb+ Br
E <sub>2</sub> <sup>4</sup>	28,42	–	30,14	0,0058	41,4342	Na·1+ Br +Pr
E <sub>3</sub> <sup>4</sup>	15,19	0,824	–	0,0067	83,9793	5Ca·Na·3+Gp+Cc
E <sub>4</sub> <sup>4</sup>	16,98	0,783	21,18	–	61,0570	Gb+ Br +5Ca·Na·3
E <sub>5</sub> <sup>4</sup>	–	0,544	33,72	0,0091	65,7200	5Ca·Na·3+Cc+Pr
E <sub>6</sub> <sup>4</sup>	–	0,646	21,16	0,0053	78,1887	Br +Pr+5Ca·Na·3

**Table.** Solubility of the  $Ca^{2+}, Na^{+} || CO_3^{2-}, SO_4^{2-} - H_2O$  system at non-invariant points at 75°C

The results obtained during this work can be used as a reference material, as well as as a scientific basis for creating optimal conditions for processing natural and technical objects containing sulfates, sodium and calcium carbonates, in particular during the regeneration of salts from liquid waste from industrial aluminum production.

## Literature

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# INCOMING FLOW OF SCIENTIFIC AND TECHNICAL LITERATURE FOR THE FORMATION OF A THEMATIC FRAGMENT “CHEMISTRY” OF THE VINITI RAS POLYTHEMATIC DATABASE

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The polythematic abstract database of VINITI RAS on natural, exact and technical sciences is designed to provide scientific and information support and procuring for fundamental research and practical developments in priority areas of science, technology and engineering. Chemists of the Institute, execute analytical and synthetic processing of scientific and technical literature (STL) in chemistry, chemical technology and materials sciences, so we create a thematic fragment Chemistry, which is one of the 26 thematic fragments of the VINITI polythematic database.

The first and most important stage of work on the formation of a thematic fragment is the analysis of the incoming flow of STL. The aim of this analysis is to identify current and promising directions of research in the subject areas of Chemistry, Chemical technology, Materials science. Another task of the incoming flow analysis is the selection of documents for analytical-synthetic processing in accordance with the VINITI RAS Rubricator of fields of knowledge. VINITI RAS Rubricator (RVINITI) is built by deepening the Russian State Rubricator of Scientific and Technical Information (SRSTI).

The following types of analysis are used to process the input stream of NTL: descriptive, statistical, exploratory, and prognostic. Within statistical analysis, the structure of the incoming flow of STL in the field of chemistry, chemical technology and materials sciences is investigated by type (electronic, printed) and type of documents (serial publications, book-type publications, patents, etc.), years of publication, language and country of origin of the primary sources. The annual volume of analytical data is about 200,000 or more documents. In 2023, the incoming flow of the STL for the formation of the thematic fragment Chemistry predominantly contained documents received in electronic form (88%), in English (83.5%), from serial periodicals (92.5%), and publication year 2023 (71.1%). These indicators demonstrate the relevance of the information reflected in the thematic fragments on the chemical sciences.

*The work was carried out as part of the implementation of the State Assignment of VINITI RAS (FFFU-2022-0005)*

# EVALUATION OF ANTIOXIDANT PROPERTIES OF PYRROLIDINE DERIVATIVES WITH 2,6-DI-*TERT*-BUTYL- PHENOLIC FRAGMENT

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Antioxidant properties of 2-(3,5-di-*tert*-butyl-4-hydroxyphenyl)-4,7-dioxo-6-phenyloctahydro-1*H*-pyrrolo[2,3-*d*]-pyridazine-3-carboxylic acid (**1**) and methyl ester of 3-(3,5-di-*tert*-butyl-4-hydroxyphenyl)-5-(2-(2,5-dioxopyrrolidin-1-yl)phenyl)-1-methyl-4,6-dioxooctahydropyrrolo[3,4-*c*]-pyrrole-1-carboxylic acid (**2**) in comparison with BHT and Trolox.

Moderate activity against synthetic radicals was established: 2,2-diphenyl-1-picrylhydrazyl (33-36% inhibition), 2,2'-azino-bis(3-ethyl-benzothiazoline-6-sulfonic acid) (22-57% inhibition), as well as towards the natural radical of nitric oxide generated in a solution of sodium nitroprusside (27-38% inhibition), despite the presence of hydrogen atom transfer systems in the structure of the compounds **1** and **2**. The reducing capacity of compound **1** to participate in electron transfer reactions on Cu<sup>2+</sup> in complex with 2,9-dimethyl-1,10-phenanthroline (CUPRAC assay) and on Fe<sup>3+</sup> in the FRAP-assay is similar to that of the reference with Trolox, that activity is taken as 1.

In relation to the superoxide anion radical obtained in the enzymatic system xanthine/xanthine oxidase, a high utilization capacity of compounds **1** and **2** (26 and 37% inhibition) was shown, in contrast to the model system of non-enzymatic quinoid autoxidation of adrenaline, where the activity of the derivatives is only 13 and 24% inhibition, respectively. In the presence of Russian sturgeon sperm, an increase in the scavenging capacity of the compounds for the superoxide anion radical was found, which indicates their SOD-protective effect.

Based on the results obtained, we can conclude that 2-(3,5-di-*tert*-butyl-4-hydroxyphenyl)-4,7-dioxo-6-phenyloctahydro-1*H*-pyrrolo-[2,3-*d*]-pyridazine-3-carboxylic acid can be considered as a potential cryoprotector of sturgeon sperm with antioxidant action.

*This work was supported by the Russian Science Foundation under grant number 22-16-00095.*

# STUDYING THE TOXICITY OF A NUMBER OF HALOCHROMIC STILBENE DYES USING THE ALLIUM TEST METHOD

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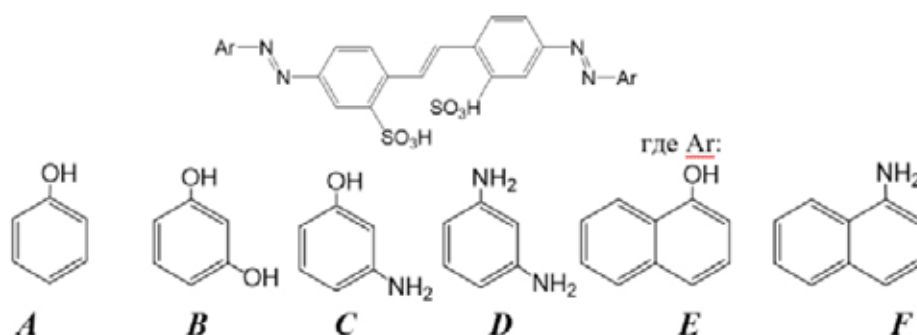
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Using the Allium test plant test system based on the Allium cepa plant - onion (Stuttgarten variety), the mutagenic, mitosis-modifying and toxic effects of textile materials dyed with a number of known and new stilbene halochromic dyes, obtained during the study, were studied, intended for the manufacture of diagnostic dressings.

The study was carried out in comparison with the dyes Diamond Green and Methylene Blue, used in medical practice. Undyed fibrous material (cotton wool) was used as a control sample



It was established that the toxicity, as well as the mutagenic and mitosis-modifying effects of all the studied dyes, with the exception of compounds **D** and **F**, are lower compared to the corresponding indicators for Brilliant Green and Methylene Blue. For compounds **D** and **F**, the identified indicators are comparable with the corresponding values obtained for Brilliant Green and Methylene Blue.

It was found that all materials painted with the studied dyes exhibit bacteriostatic properties.

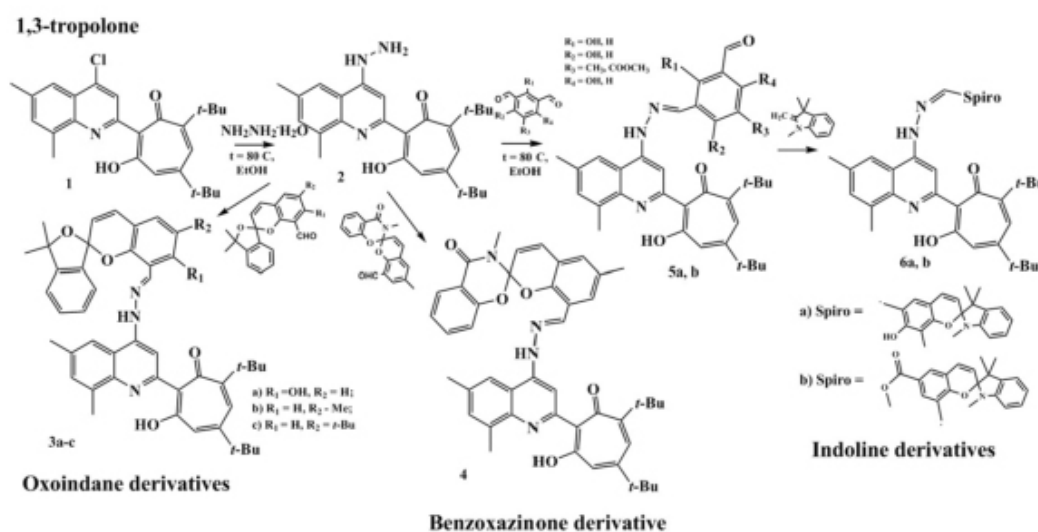
# SYNTHESIS OF MOLECULAR DYADS FOR THERANOSTICS BASED ON 1,3-TROPOLONE FUNCTIONALIZED WITH PHOTOCHROMIC OBJECTS

**Krasnikova T.A., Sayapin Yu.A., Ozhogin I.V., Bulanov A.O.,  
Makarova N.I., Tupaeva I.O., Gusakov E.A., Minkin V.I.**

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The targeted obtaining of medicines with therapeutic and diagnostic effects is an significant task of theranostics and set the challenge to chemists to synthesize molecular tandems based on photochromic and bioactive compounds.

Herein, photochromic compounds of spirocyclic nature act as photoswitch molecules for light control of pharmacological activity, and the 2-quinolin-2-yl-1,3-tropolone framework acts as a biologically active component. It has previously been found out that some 1,3-tropolone derivatives exhibit significant cytotoxic activity against many cancer cell lines<sup>1,2</sup>.



The structure of products 2-6 was established by physicochemical methods, including X-ray diffraction. Photochemical studies of the resulting systems were carried out.

## References

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2. Gusakov E.A., Topchy J.A., Mazitova A.M. et al. *RSC Adv*, 2021, 11, 8, 4555-4571.

*The work was carried out with the financial support of the Russian Science Foundation, project 21-73-10300.*

# SYNTHESIS OF CYCLOPROPANE-BASED NITROESTERS IN COMPRESSED 1,1,1,2-TETRAFLUORETHANE MEDIUM

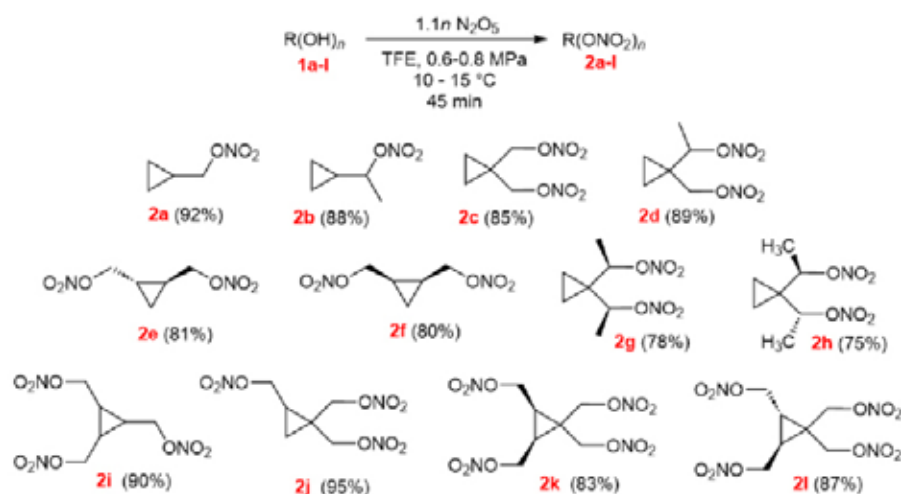
**Kuchurov I.V.<sup>a</sup>, Tretyakova E.A.<sup>b</sup>, Saigin D.I.<sup>c</sup>, Zharkov M.N.<sup>a</sup>,  
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Highly efficient, safe and sustainable procedure was developed for synthesis of cyclopropane-based nitroesters which is based on nitration of the corresponding alcohols with dinitrogen pentoxide in compressed 1,1,1,2-tetrafluoroethane (TFE, Freon R134a) medium.



The proposed approach shows significant advantages such as mild and clean reaction conditions, low operation pressure, procurable equipment, scalability and easiness of the fluid recycling which make it attractive for industrial implementation.



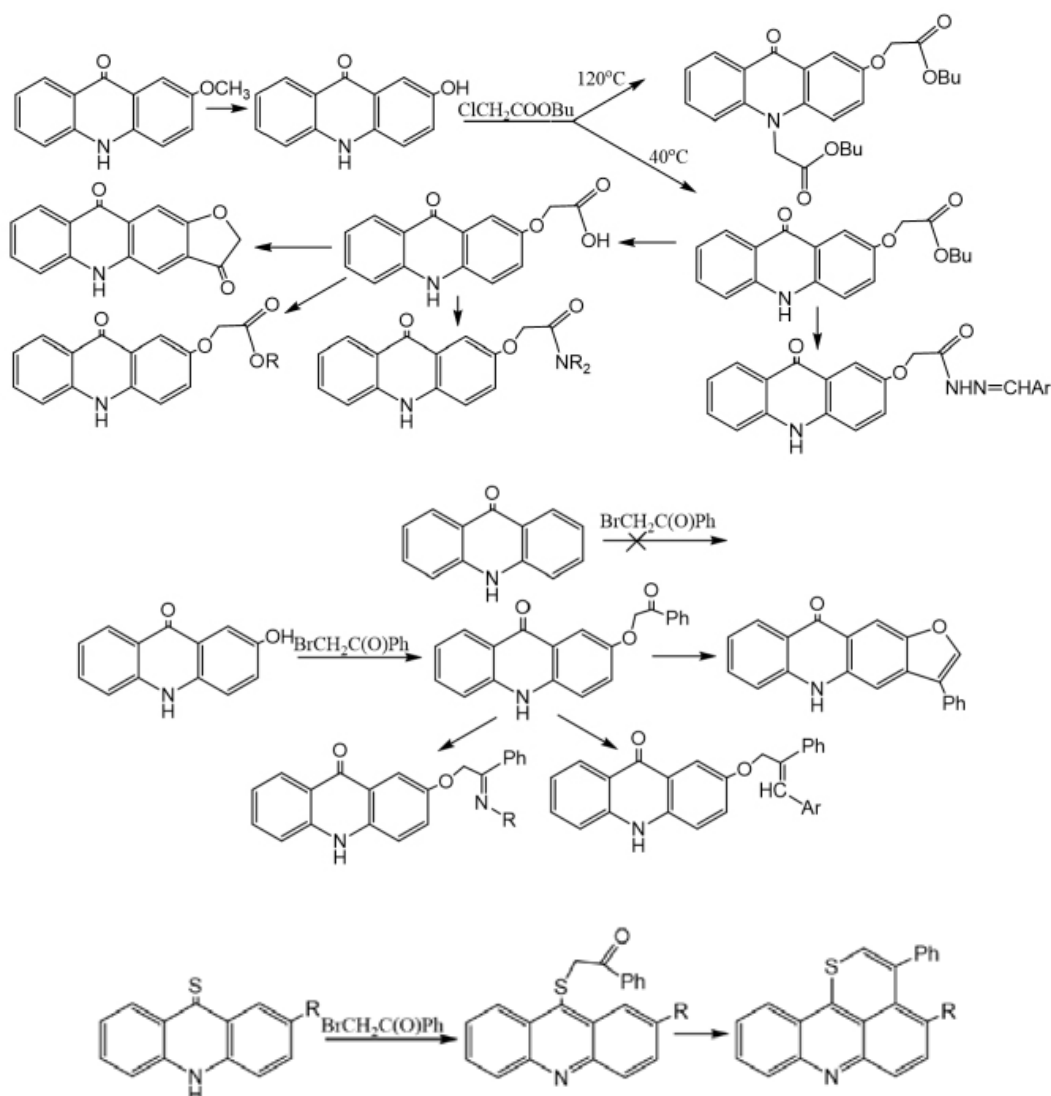
# FEATURES OF INTERACTION OF SOME 9-ACRIDANONE DERIVATIVES WITH ALPHA-HALOCARBONYL COMPOUNDS

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<sup>b</sup>Kursk State Medical University, 305041, Kursk, K. Marx st., 3

In order to synthesize new precursors for the production of biologically active compounds, the conditions for alkylation of 9-acridanone and its hydroxy derivatives, as well as 9-acridanone with butyl ester of monochloroacetic acid and phenacyl bromide were studied and optimized. For the obtained alkylation products, a number of derivatives were synthesized and their antibacterial activity in vitro was assessed.



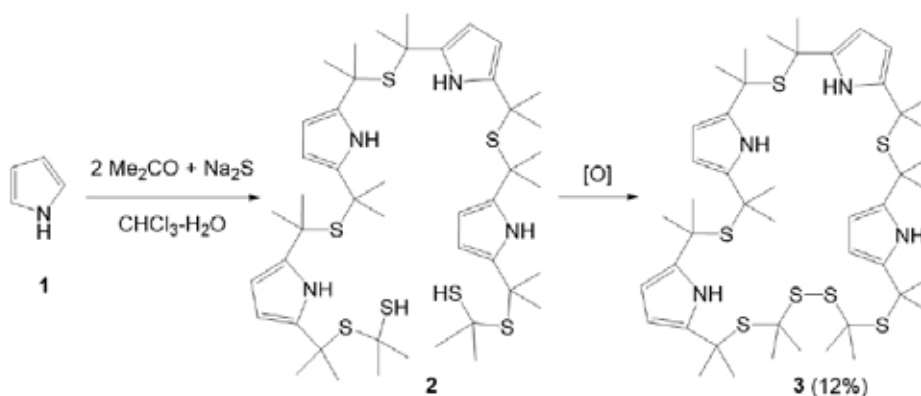
# MULTICOMPONENT POLYCONDENSATION OF PYRROLE WITH ACETONE AND SODIUM SULFIDE

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Porphyrin derivatives form supramolecular assemblies with proteins and are of interest as a therapy for cancer.<sup>1,2</sup>

We studied multicomponent cyclothiomethylation of pyrrole **1** in a *one-pot* mode. The use of a mixture of formaldehyde and hydrogen sulfide as a reagent in this reaction leads to tarring of the substrate due to the acidophobicity of pyrrole **1**. However, thiomethylation of **1** with the participation of acetone and sodium sulfide proceeds with regular self-assembly of molecules to form the target macroheterocycle **3**, formed during the oxidation of intermediate dithiol **2** in air.



The result was a mixture of poly(sulfanylpropan-2-yl)pyrroles with different chain lengths. HPLC-HRMS detected cyclic product **3** (12%), which was isolated by column chromatography and characterized by <sup>1</sup>H, <sup>13</sup>C NMR.

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# CHARGE CHARACTERISTICS BY MULLIKEN AND GEOMETRY OF STRUCTURALLY COMPLEX TITANOCENE

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Metallocene complexes of the titanium subgroup are promising precursors for catalysts for many organic syntheses, photo- and electroluminophores, phosphorescent and multifunctional materials. This is a class of compounds having rare ligand-to-metal charge transfer excited states, including unique phosphorescent ones.<sup>1</sup>

Determining the populations of orbitals and charge characteristics is a fundamental problem in photonics and the chemistry of coordination compounds that cannot be solved only experimentally. Modeling the geometry and excited states properties of non-classical compounds, especially organometallic compounds, is a difficult problem to solve. For the first time, the charge characteristics of a sophisticated organometallic complex were systematically assessed using 124 methods of different levels of theory and a conclusion was made on the reliability of the calculation results in the Mulliken approximation as the historically most important method.<sup>2</sup> It has been shown that the analysis of orbital populations according to Mulliken gives very contradictory results. Thus, in a systematic series of 124 popular methods (HF, DFT), only 30 methods based on the high-level basis QZVP (some methods) and the Pople basis sets 6-311G\*\* and 3-21G provided an acceptable analysis of the charge characteristics of the target titanocene dicarboranyl  $\text{Ti}(\eta^5\text{-Cp})(\eta^1\text{-CpCMe}_2\text{CB}_{10}\text{H}_{10}\text{C})_2$  within the traditional Mulliken approach. Moreover, the vast majority of these methods describe well the molecular architecture and electric dipole moment of the complex.<sup>3</sup> It was shown that the target titanocene dicarboranyl has a large electric dipole moment (10–11 Debye), which is very rare for organometallic molecules.

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# LIGAND-TO-METAL CHARGE TRANSFER EXCITED STATES IN ORGANOMETALLIC COMPOUNDS

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Organometallic compounds are an important class of materials in many areas of science and technology. Many classes of organometallic complexes are regarded as rather unstable to air/water and, historically, this fact has drastically hampered development of organometallic photophysics and photochemistry. One of the key problems in photophysics and photochemistry of organometallic complexes is the assignment and characterization of their excited states (e.s.). In this regard, ligand-to-metal charge transfer (LMCT) excited states are rarest and least studied; the state of art in organometallic LMCT e.s. was for the first time generalized in 2022.<sup>1</sup> The present contribution will be a reflection of on-going systematic research<sup>2-8</sup> in the field of organometallic LMCT e.s.: the properties of frontier molecular orbitals and the electron transfer paradigm in the case of LMCT e.s. ( $E_h \propto \Delta E_{\text{redox}}$ ), the discovery and study of phosphorescent LMCT states based on group 4 metallocenes, triplet-triplet LMCT energy transfer, the relationship between the emission quantum yield and the excited state lifetime, triplet-triplet LMCT absorption, LMCT solvatochromism and estimation of the electric dipole moment of metal complexes (Lippert-Mataga approach and the combined approach based on Bakhshiev, Bilot-Kawski and McRae theories), and so on. The examples to be discussed will illustrate the rich variety of photophysical and photochemical behavior, exhibited by organometallic species in pure LMCT e.s. Current state of computational methods available for LMCT spectral assignments of group 4 metallocenes and validity of the data obtained will be briefly notified.

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# MONO-IMINOACENAPHTHENONE LIGANDS: RESEARCH TRENDS

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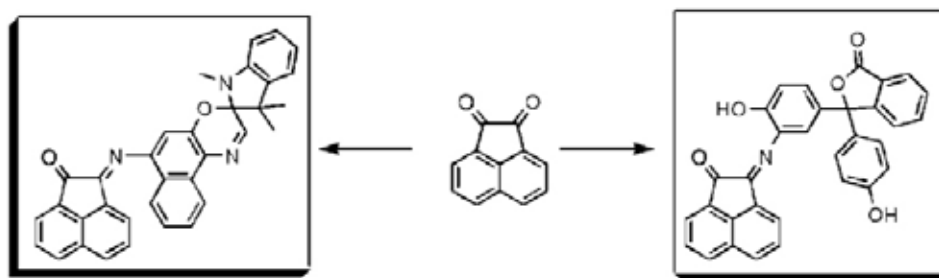
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Mono-iminoacenaphthenones (Ar-MIAN) have been shown to occupy an intermediate position between o-quinones and 1,2-bis-iminoacenaphthenes (Ar-BIAN). Their properties, primarily steric and redox, are intermediate in this series.<sup>1,2</sup>

The openness of the carbonyl carbon atom of Ar-MIAN leads to the possibility of coupling reactions due to the one-electron reduction of this type of ligands. Coupling occurs reversibly and is an option for stabilizing the radical anion form during reduction with certain reducing agents.

Catalytic processes are demonstrated using examples of hydroamination, hydroarylation, and ring-opening polymerization reactions.

A new direction in the research is the combination of a redox-active amino-acenaphthene fragment with pH-sensitive molecules, as well as with photosensitive dyes (Scheme).



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# CHANGES IN THE NANOCRYSTAL PROPERTIES WITH A DECREASE IN ITS SIZE OR WITH A CHANGE IN ITS SHAPE UNDER VARIOUS P-T-CONDITIONS

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The analytical method<sup>1</sup> (without computer modeling), which uses the paired Mie–Lennard-Jones interatomic interaction potential, studied the changes in the state equation ( $P$ ) and the baric dependences of gold properties during the transition from a macro to a nanocrystal of cubic or rod-like shape of 306 atoms.

Four parameters of the interatomic potential were determined by self-consistent method in work<sup>2</sup>. These potential parameters were tested when calculating the properties of the gold macrocrystal in the article<sup>3</sup>.

The following properties were calculated: Debye temperature ( $\Theta$ ), the first ( $\gamma$ ) and second ( $q$ ) Grüneisen parameters, elastic modulus ( $B_T$ ), thermal expansion coefficient ( $\alpha_p$ ), product of  $\alpha_p \cdot B_T$ , heat capacity ( $C$ ), specific (per unit area) surface energy ( $\sigma$ ), derivative of the  $\sigma$  function over temperature ( $\sigma'(T)$ ), and the melting point ( $T_m$ ). The pressure derivatives of these functions were also studied:  $\Theta'(P)$ ,  $B'(P)$ ,  $\alpha_p'(P)$ ,  $C'(P)$ ,  $\sigma'(P)$ , и  $T_m'(P)$ . When calculating the functions  $\sigma$ ,  $\sigma'(T)$  and  $\sigma'(P)$ , the method from<sup>4</sup> was used, and when calculating  $T_m(P)$  and  $T_m'(P)$  – the method from article<sup>5</sup> was used.

It was shown that under any  $P$ - $T$ -conditions the following functions decrease under isomorphic-isothermal-isobaric reduction of the nanocrystal size:  $\Theta$ ,  $q$ ,  $B_T$ ,  $T_m$ . In doing so, the next functions increase:  $\Theta'(P)$ ,  $\gamma$ ,  $\alpha_p$ ,  $|\alpha_p'(P)|$ ,  $C(P)$ ,  $|C'(P)|$ ,  $|\sigma'(T)|$ . It is shown that other properties:  $\alpha_p \cdot B_T$ ,  $B'(P)$ ,  $\sigma$ ,  $\sigma'(T)$ ,  $T_m'(P)$ , can change their size dependence when  $P$ - $T$ -conditions changed.

When the nanocrystal shape deviates from the most energy-optimal shape (in this case, it is a cube), the sized changes in the baric and temperature dependencies increase.

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# ON THE LINDEMANN PARAMETER FOR MELTING CRYSTALS AT DIFFERENT PRESSURES

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Based on the delocalization criterion of melting<sup>1</sup>, an expression for the Lindemann parameter has been obtained. For a single-component crystal with an Einstein vibrational spectrum, it has the form:

$$L_E(T_m) = \left[ \frac{(\langle u^2 \rangle)^{1/2}}{c} \right]_{T_m} = \frac{0.08185}{k_p^{1/3} [f_y(y_w)]^{1/2}}, \quad f_y(y_w) = \frac{2 [1 - \exp(-y_w)]}{y_w [1 + \exp(-y_w)]}, \quad (1)$$

where  $\langle u^2 \rangle^{1/2}$  is the root-mean-square deviation of an atom in a crystal,  $c = [6k_p V / (\pi N)]^{1/3}$  is the nearest-neighbor distance,  $k_p$  is the packing factor of the structure,  $V$  is the volume of the system,  $N$  is the number of atoms in it,  $T_m$  is the melting point,  $\Theta$  is the Debye temperature,  $y_w = 3\Theta / (4T_m)$ .

It was shown that for classical crystals (in which  $T_m / \Theta > 1.5$ ), the Lindemann parameter (1) is determined only by the crystal structure and does not depend on pressure, or size in the case of a nanocrystal. Calculations for various structures of classical single-component crystals have shown good agreement with the estimates of other authors.

For quantum single-component crystals (in which  $T_m / \Theta < 0.4$ ), the Lindemann parameter (1) is determined not only by the crystal structure, but also by density, as well as size and shape in the case of a nanocrystal. It was shown that for quantum crystals, the Lindemann parameter decreases with increasing pressure along the melting line. For quantum nanocrystals, the Lindemann parameter (1) increases with an isobaric decrease in the nanocrystal size. At this, the increase in the Lindemann parameter with size is more, the more noticeable the nanocrystal shape is deviated from the energy-optimal shape.

Thus, the Lindemann criterion can only be used to study the melting of classical crystals. The use of the Lindemann criterion to study the melting of quantum crystals (as they tried to do in work<sup>2</sup> when studying the melting of atomic metallic hydrogen) is incorrect.

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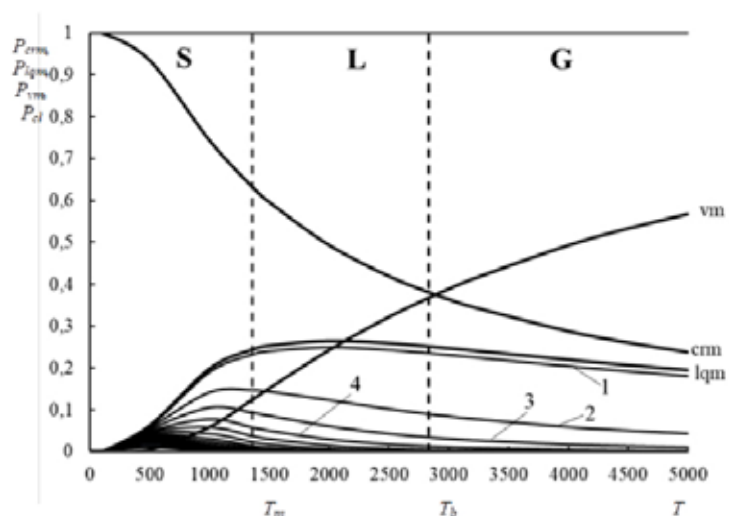
# STOCHASTIC PORTRAIT OF CLUSTERS IN THE INTERIOR OF SOLID, LIQUID AND GASEOUS STATES OF MATTER

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The structural approach in the research of clusters receives primary attention.

The random nature of these unstable formations has not been sufficiently studied. We have obtained a general picture of the relationship between clusters and the main aggregate states of matter as a special subclass of crystal-mobile particles identified for the solid state with equilibrium crystal lattice defects. In liquid and gas, they take the simplest rounded shape in comparison with structural total indicators – coordination numbers.



**Figure.** Temperature dependence of the fraction of crystal-mobile (crm), liquid-mobile (lqm), vapor-mobile (vm) and cluster (1, 2, 3, 4...) particles with a temperature shift of the maximum fraction of clusters.

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# SYSTEM OF EQUATIONS FOR THE DEVELOPMENT OF A STOCHASTIC APPROACH TO THE DESCRIPTION OF THE CLUSTERS STRUCTURE OF MATTER

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We have investigated next tools for stochastic development of clusters nature that follow: the Boltzmann distribution for the kinetic energy of chaotic (thermal) particle motion; the author's concept of chaotized particles consisting of three energy classes: from zero to the thermal melting barrier  $RT_m$  – crystal-mobile (*crm*-), from  $RT_m$  to  $RT_b$  (boiling barrier) – liquid-mobile (*lqm*-), above  $RT_b$  – vapor-mobile (*vm*-) particles; author's distribution of clusters by the number  $n$  of *crm*-particles included in them; theory of probability and theory of system stability; for the first time the mathematical theory of isomorphism in relation to establishing the equivalent of discrete and continuous distributions; the principle of superposition using to interconnect all shares of chaotized particles<sup>1</sup> –  $P_{crm}$ ,  $P_{lqm}$ ,  $P_{vm}$  and  $P_{cl}$ . Corresponding calculation formulas are proposed and their accuracy is assessed based on the ratio of the residual and total sums of the series.

$$\begin{array}{ll}
 1. P_l = \left( \frac{\Delta \varepsilon}{kT} - 1 \right) \exp \left( - \frac{i \Delta \varepsilon}{kT} \right). & 8. \sum_{l=1}^{\infty} P_{cl,n} = \frac{1}{A} \int_0^{\infty} (1 - P_{crm}) P_{crm}^x dx = P_{crm}. \\
 2. P_{crm} = 1 - \exp(-T_m/T). & 9. A = \frac{1}{P_{cl,n}} \int_{x=n-1}^{x=n} P_{cl,x} dx = \frac{P_{crm}-1}{P_{crm} \ln P_{crm}}. \\
 3. P_{lqm} = \exp(-T_m/T) - \exp(-T_b/T). & 10. P_{crm,m} = 1 - e^{-1} \approx 0,632. \\
 4. P_{vm} = \exp(-T_b/T). & 11. s = s_n + R_n. \\
 5. P_{crm} + P_{lqm} + P_{vm} = 1. & 12. \rho = \frac{R_n}{s}. \\
 6. P_{crm}^n + P_{crm} - 1 = 0. & 13. n_p = \ln \rho / \ln P_{crm}. \\
 7. P_{cl,n} = (1 - P_{crm}) P_{crm}^n. & 14. N_{cl,n} = N_A \sum_{n=1}^{\infty} (1 - P_{crm}) P_{crm}^n \cdot \text{mol}^{-1}.
 \end{array}$$

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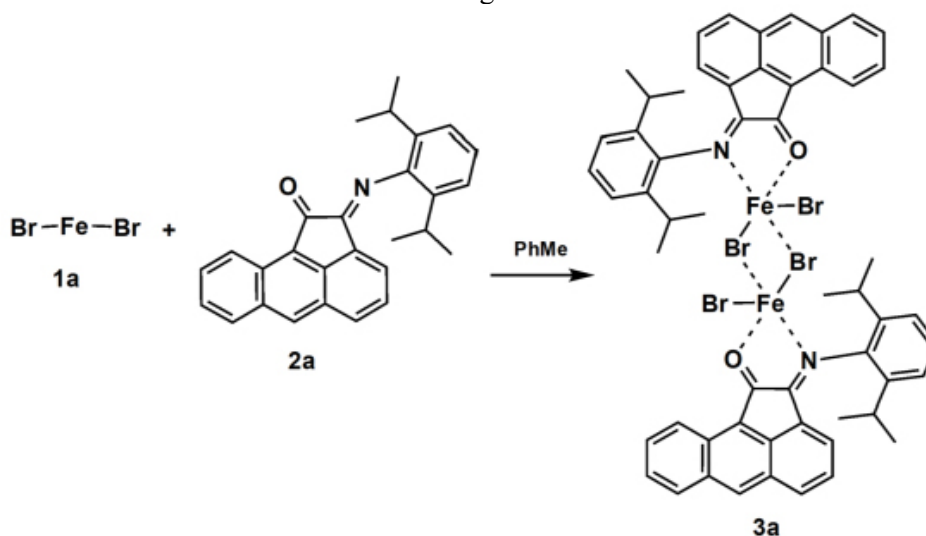
*This research was performed under financial support of the Ministry of Science and Higher Education of the Republic of Kazakhstan, project No. AR23483569/GF.*

# IRON(III) BROMIDE MONO(IMINO)ACEANTHRENONE COMPLEX

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Iron(II) bromide (**1a**) reacts with (E)-2-(2,6-diisopropylphenylimino)aceanthrylen-1(2H)-one (**2a**) in toluene at 423 K (in a sealed degassed ampoule no traces of moisture) to form dark red crystals. According to X-ray diffraction data, coordination complex bis((2-(2,6-diisopropylphenylimino)aceanthrylen-1(2H)-one)iron(II)dibromide) (**3a**) is formed, which has a dimeric structure due to the interaction of iron fragments.



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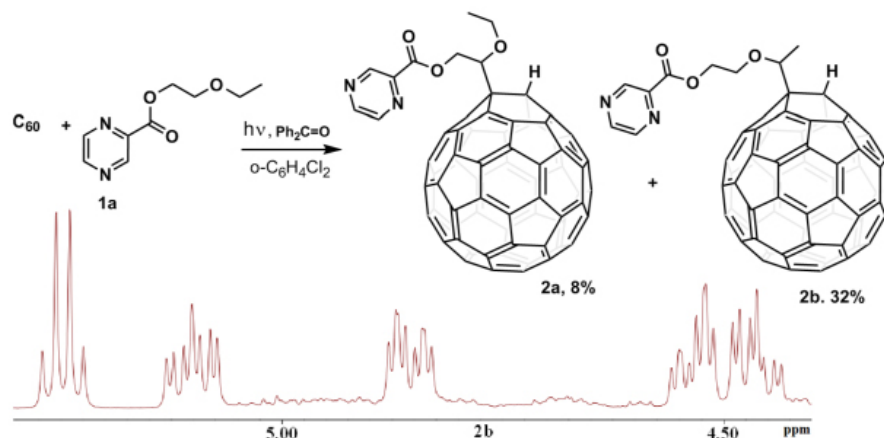


# FULLERENE 2-ETHOXYETHYLPYRAZINE-2-CARBOXYLATES

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$C_{60}$  reacts with 2-ethoxyethylpyrazine-2-carboxylate (**1a**) at the presence of benzophenone in o-dichlorobenzene at 293 K to form 1-(1-ethoxy-2-((pyrazine-2-carbonyl)oxy)ethyl)-1,2-dihydrofullerene (**2a**) and 1-(1-(2-((pyrazine-2-carbonyl)oxy)ethoxy)ethyl)-1,2-dihydrofullerene (**2b**). The  $CH_3$  signal of **2a** (t,  $\delta=1.56$  ppm) and **2b** (d,  $\delta=2.34$  ppm,  $J=6.3$  Hz) is shifted downfield compared to **1a** (t,  $\delta=1.19$  ppm,  $J=7.0$  Hz) in the  $^1H$  NMR spectrum ( $CDCl_3$ ). The signals of the  $CH_2$  groups and protons of the pyrazine ring in **2a** and **2b** under the acceptor influence of the  $C_{60}H$  fragment are also shifted downfield compared to **1a**. The singlet of the methine fullerene proton in **2a** lies in a weaker magnetic field (7.01 ppm) compared to **2b** (6.82 ppm) due to the acceptor effect of oxygen atoms. The signal of the methine proton of ester chain **2b** (quartet,  $\delta=5.25$  ppm) is in a stronger magnetic field compared to **2a** (dd,  $\delta=5.81$  ppm) due to the donor  $CH_3$  group. **2a** is less polar than **2b**, since it elutes first during chromatography on silica gel, which means that in **2a** the fullerene cage shields the polar pyrazine-2-carboxylate fragment more strongly. All reactions were performed in an inert atmosphere.



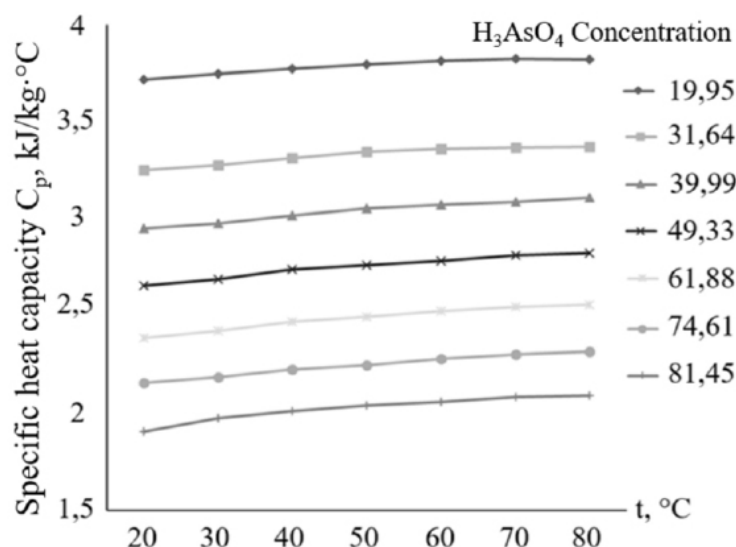
*The work was carried out use "Analytical Center of the IOMC RAS" and in the framework of the Russian state assignment.*

# HEAT CAPACITY OF SOLUTIONS IN $\text{H}_3\text{AsO}_4 - \text{H}_2\text{O}$ SYSTEM

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When optimizing the processes of electrolysis of arsenic acid solutions in order to isolate arsine, it is necessary to take into account the thermal properties of the solutions, first of all the heat capacity. The heat capacity values of solutions in the system  $\text{H}_3\text{AsO}_4 - \text{H}_2\text{O}$  are practically absent in literature. Therefore, to increase the yield of  $\text{AsH}_3$  at electrochemical production from arsenic acid aqueous solutions, it is necessary to study the thermal properties in the system  $\text{H}_3\text{AsO}_4 - \text{H}_2\text{O}$ . The measurements of the specific heat capacity of the  $\text{H}_3\text{AsO}_4 - \text{H}_2\text{O}$  solutions by adiabatic calorimetry are presented in this work.



**Fig. 1.** Dependence of the specific heat capacity  $C_p$  of arsenic acid solutions on temperature at different arsenic acid concentrations, mas. %.

It has been found that the  $C_p$  of solutions in the  $\text{H}_3\text{AsO}_4 - \text{H}_2\text{O}$  system increases with temperature increase and decreases with the increase of arsenic acid concentration. (Fig. 1).

The heat capacity of the solution with 19.95 mas. %  $\text{H}_3\text{AsO}_4$  increases as well as the heat capacity of water, which is characterized by a monotonic increase.

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# DITHIOCARBAMATES – PROMISING SYNTHONS OF BIOLOGICALLY ACTIVE SUBSTANCES

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Dithiocarbamates represent a wide class of sulfur-containing organic compounds, derivatives of dithiocarbamic acids and are promising objects for both fundamental and applied research in chemical science.

In the Laboratory of Chemistry of Physiologically Active Substances of the A.B. Bekturov Institute of Chemical Sciences has been intensively conducting research for several years on the synthesis of polyfunctional heterocyclic, acyclic and aromatic dithiocarbamates and their derivatives: thioacetylene alcohols and ethers, thioanhydrides, thioesters and complexes with transition metals and natural polysaccharides, as well as on the search and creation of active substances with wide spectrum of biological activity based on them.

As a result of our research, we synthesized dithiocarbamates and their alkyl thioesters, thioanhydrides, thioacetylene derivatives and complexes with transition metals based on 1H-1,2,4-triazole, 1H-benzo[d][1,2,3]triazole, indole, indoline, pyrrolidine, morpholine, N-methyl-, N-diphenylmethyl-, N-ethylpiperazine, N-benzylmethanamine, diphenylamine, dibenzylamine, N-(4-methoxyphenyl)acetamide, bis(2-hydroxypropyl)amine, bis(3-aminopropyl)amine, hexane-1,6-diamine, N-methyl-1-phenylmethanamine.

Studies of the biological activity of synthesized dithiocarbamine derivatives have made it possible to identify substances with growth-stimulating, root-forming, fungicidal, herbicidal and antibacterial activity, which can subsequently find application in agriculture.

Among the synthesized dithiocarbamine derivatives, we discovered substances with flotation activity that can be used as foaming agents and collectors.

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# STUDY OF THE PHASE COMPLEX OF THE $\text{Na,K||SO}_4,\text{CO}_3,\text{HCO}_3,\text{F-H}_2\text{O}$ SYSTEM AT 25°C IN THE REGION OF VILLOMITE CRYSTALLIZATION

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The process of recycling liquid waste from industrial aluminum production<sup>1</sup> is determined by the regularities patterns of phase equilibria in the six-component water-salt system  $\text{Na,K||SO}_4,\text{CO}_3,\text{HCO}_3,\text{F-H}_2\text{O}$ , and therefore, it is of interest to determine the possibilities of joint crystallization of the salts that make up this composition.

Villomite (NaF) is the equilibrium phase in 6 of the 14 four-component systems that make up the six-component system under study and the phase equilibria in which were studied earlier by the translation method<sup>2</sup>.

It was found that villomite particle pates in the formation of 18 divariant fields, 22 monovariant curves and 9 nonvariant points. Based on the data obtained, a closed phase diagram (phase complex) of the studied system was constructed at 25°C in the crystallization region of villomite (NaF), which is fragmented by divariant fields<sup>3</sup>.

The obtained data can be used in the regeneration of liquid waste from industrial aluminum production containing sulfates, carbonates, bicarbonates and fluorides of sodium and potassium fluorides.

An analysis of the constructed fragment of the phase equilibrium diagram of the studied system at 25°C, at the level of five and six-component contents shows the participation of villomite (NaF) in the formation the following number of geometric images: nonvariant points - 13 and 9; monovariant curves – 18 and 22; divariant fields – 7 and 18.

## **Literature**

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# THERMODYNAMICAL PROPERTIES OF AMMONIUM HALIDES SOLUTIONS IN MIXED SOLVENTS N-METHYLPYRROLIDONE–WATER AT 298.15 K

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In this work, the heat capacities  $C_p$  and densities  $\rho$  of solutions of ammonium halides in a mixed solvent MP-water were measured with high accuracy over the entire range of compositions at 298.15 K. Heat capacity measurements were performed on the LKB 8700 calorimetric unit with an error of  $2 \cdot 10^{-3}$  J/g·K, density – on the Anton Paar DMA 4500 density meter with an error of  $5 \cdot 10^{-5}$  g/cm<sup>3</sup>.

On the basis of the data obtained, the apparent molar values of  $\Phi_c$  and  $\Phi_v$  were calculated, extrapolating the concentration dependences of which to the state of infinite dilution the standard partial molar heat capacities and volumes of ammonium halides in the mixed solvent MP-water at 298.15 K were determined. The values of  $\bar{C}_{p_2}^0$  and  $\bar{V}_2^0$  are shown in the table.

$\bar{C}_{p_2}^0 / \bar{V}_2^0$	$X_{\text{МП}}$						
	0,00	0,10	0,33	0,50	0,75	0,90	1,00
NH <sub>4</sub> Br	-67/42,9	-73/44,8	10/42,9	54/39,5	105/35,0	115/33,0	98/32,9
NH <sub>4</sub> I	-69/54,4	-76/57,1	12/55,5	58/51,0	110/45,7	121/42,9	104/42,3

**Table.** Standard partial molar heat capacities  $\bar{C}_{p_2}^0$  J/mole·K and volumes  $\bar{V}_2^0$  cm<sup>3</sup>/mole of ammonium halides in the mixed solvent MP-water at 298.15

The dependences on the composition of the mixed solvent for ammonium halides and the previously studied alkali metal halides have significant differences, which indicates the complex nature of intermolecular interactions in the studied solutions, which is influenced not only by the properties of the MP-water binary system, but also by the structural behavior of the ammonium ion.

*The research was carried out with the financial support of the Ministry of Science and Higher Education of the Russian Federation within the framework of the scientific project of the laboratory "Laboratory of Ion Materials" (LIM), project no. FSSM-2024-0006.*



# THE EFFECT OF SPECIFIC INTERACTIONS OF AMMONIUM ION WITH COMPONENTS OF THE N-METHYLPYRROLIDONE-WATER SOLVENT MIXTURE ON THE HEAT CAPACITY AND VOLUMETRIC PROPERTIES OF SOLUTIONS

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Based on calorimetric and densimetric measurements, we obtained standard values of the heat capacity  $\overline{C}_{p,i}^0$  and volume  $\overline{V}_i^0$  of alkali metal and ammonium ions in mixtures of N-methylpyrrolidone (MP)-water. The values  $\overline{C}_{p,i}^0$  and  $\overline{V}_i^0$  are usually represented as the sum of several contributions, taking into account different types of ion-solvent interactions. Theoretical methods currently exist to calculate some of them, but there are no such methods to assess the contribution of specific interactions. Given the same charge and almost equal sizes of  $\text{NH}_4^+$  and  $\text{Rb}^+$  ions, which means that the values of the other components are close, the difference in values  $\overline{C}_{p,i}^0$  and  $\overline{V}_i^0$  makes it possible to determine the contribution  $\Delta_{\text{sp.int.}} C_{p,i}^0$  and  $\Delta_{\text{sp.int.}} V_i^0$  of the ammonium ion for all compositions of the MP-water mixture.

	$X_{\text{МП}}$						
	0,00	0,10	0,33	0,50	0,75	0,90	1,00
$\Delta_{\text{sp.int.}} C_{p,i}^0 \pm 10 \text{ J/mole} \cdot \text{K}$	30	2	-7	-5	-8	-9	-28
$\Delta_{\text{sp.int.}} V_i^0 \pm 1,0 \text{ cm}^3/\text{mole}$	4,1	3,5	0,2	0,2	-0,7	-0,2	2,9

**Table.** The contribution to the values of  $\overline{C}_{p,i}^0$  and  $\overline{V}_i^0$  caused by the specific interactions of the ammonium ion with the components of the mixed solvent MP-water

As follows from the data in the table, the contribution of specific  $\text{NH}_4^+$  - solvent interactions is insignificant and noticeable only in two ranges of mixture compositions, where the values  $\Delta_{\text{sp.int.}} C_{p,i}^0$  and  $\Delta_{\text{sp.int.}} V_i^0$  exceed the error of their determination. In almost the entire range of  $0,1 < X_{\text{МП}} < 0,9$  compositions, where the formation of MP associates with water occurs due to the heterocomponent hydrogen bond, there are no specific interactions between the ammonium ion and the solvent.

*The research was carried out with the financial support of the Ministry of Science and Higher Education of the Russian Federation within the framework of the scientific project of the laboratory "Laboratory of Ion Materials" (LIM), project no. FSSM-2024-0006.*

# CONCENTRATION PARAMETERS OF THE FORMATION OF EQUILIBRIUM SOLID PHASES OF THE SYSTEM



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The study of multicomponent systems that are waste products of aluminum production in Tajikistan and the prediction of possible phase equilibria for water-salt chemical systems facilitates the solution of the problem of environmental protection and is economically and environmentally useful.

This paper presents the results of determining the concentration parameters of the formation of equilibrium solid phases in a five-component system of  $\text{Na}^+, \text{Ca}^{2+}, \text{Al}^{3+} // \text{SO}_4^{2-}, \text{HCO}_3^- - \text{H}_2\text{O}$  and its constituent four-component systems at 273 K, which for the first time we constructed the construction of their closed phase diagrams by the translation method<sup>1</sup>. Full information about the translation method can be seen in works<sup>2</sup>.

The five-component mutual system  $\text{Na}^+, \text{Ca}^{2+}, \text{Al}^{3+} // \text{SO}_4^{2-}, \text{HCO}_3^- - \text{H}_2\text{O}$  at 273 K includes the following four-component systems with equilibrium solid phases at non-invariant points:

- 1)  $\text{NaHCO}_3, \text{Ca}(\text{HCO}_3)_2, \text{Al}(\text{HCO}_3)_3, \text{H}_2\text{O}$ :  $E_1^4 = \text{Nh} + \text{CaH} + \text{AlH}$ .
- 2)  $\text{Na}_2\text{SO}_4, \text{CaSO}_4, \text{Al}_2(\text{SO}_4)_3, \text{H}_2\text{O}$ :  $E_2^4 = \text{Mib} + \text{Gp} + \text{Al} \cdot 18$ .
- 3)  $\text{Ca}^{2+}, \text{Al}^{3+} // \text{SO}_4^{2-}, \text{HCO}_3^- - \text{H}_2\text{O}$ :  $E_3^4 = \text{Gp} + \text{CaH} + \text{AlH}$ ;  $E_4^4 = \text{Gp} + \text{AlH} + \text{Al} \cdot 18$ .
- 4)  $\text{Na}^+, \text{Al}^{3+} // \text{SO}_4^{2-}, \text{HCO}_3^- - \text{H}_2\text{O}$ :  $E_5^4 = \text{Nh} + \text{AlH} + \text{Mib}$ ;  $E_6^4 = \text{Mib} + \text{AlH} + \text{Al} \cdot 18$ .
- 5)  $\text{Na}^+, \text{Ca}^{2+} // \text{SO}_4^{2-}, \text{HCO}_3^- - \text{H}_2\text{O}$ :  $E_7^4 = \text{Mib} + \text{Nh} + \text{Gp}$ ;  $E_8^4 = \text{Nh} + \text{CaH} + \text{Gp}$ .

As a result of the translation of the above four non-invariant points, five non-invariant points are formed at the level of the five-component composition.

Thus, it was found that the system under study at a given temperature is characterized by the presence of 12 - divariant fields, 10 - monovariant curves and 3 - nonvariant points.

The results of this work can be used as auxiliary information for cleaning the environment from saturated waste and pollutants containing salts that are part of the system under study, and are also used for the disposal of such waste.

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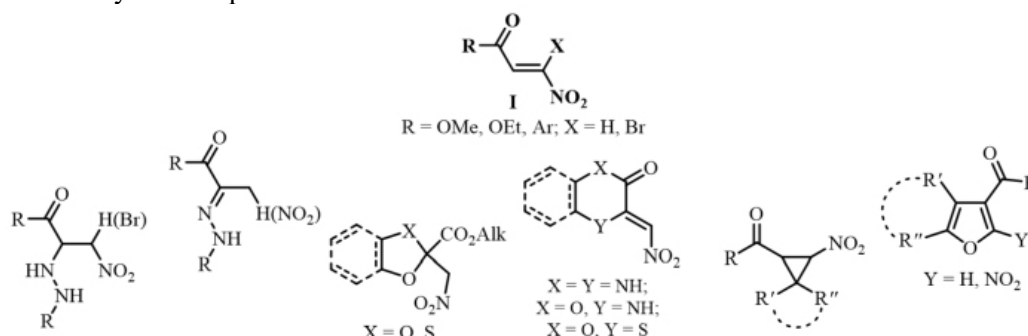
# β-CARBONYL CONTAINING NITRO- AND GEM-BROMONITROETHENES – HIGHLY ACTIVE SUBSTRATES FOR OBTAINING A WIDE RANGE OF ORGANIC SUBSTANCES

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β-Carbonyl containing nitro- and *gem*-bromonitroethenes are highly reactive compounds that combine several electrophilic centers in their structure. They are interesting objects of theoretical organic chemistry, as well as convenient reagents for the synthesis of polyfunctional acyclic nitro compounds, as well as carbo- and heterocyclic structures.

We have studied the behavior of alkoxy-carbonyl(aryl)-nitro- and *gem*-bromonitroethenes **I** in reactions with CH-acids and binucleophilic reagents, which opened up wide possibilities for the synthesis on their basis of a variety of acyclic, carbo- and heterocyclic compounds.



It has been shown that the primary attack of nucleophilic processes is carried out at the β-carbon atom of the nitroethene system (relative to the NO<sub>2</sub> group) and ends with the formation of Michael adducts or is accompanied by their further intramolecular transformation, determined by the structural features of the substrates:

- elimination of HNO<sub>2</sub> or HBr and isomerization of the resulting C=C bond;
- elimination of HBr and heterocyclization via the A<sub>D</sub><sub>N</sub> or S<sub>N</sub> pathway;
- carbo- or heterocyclization via C- or O-alkylation with the participation of a bromonitromethyl group.

The resulting polyfunctional compounds are of interest as promising objects for pharmacological research.

*The research was supported by an internal grant of The Herzen State Pedagogical University of Russia (project № 3VG).*

# NEW PROMISING PHOSPHORUS-CONTAINING AMINO ACIDS AND THEIR ANALOGUES BASED ON ORGANOSILICON METHODOLOGY

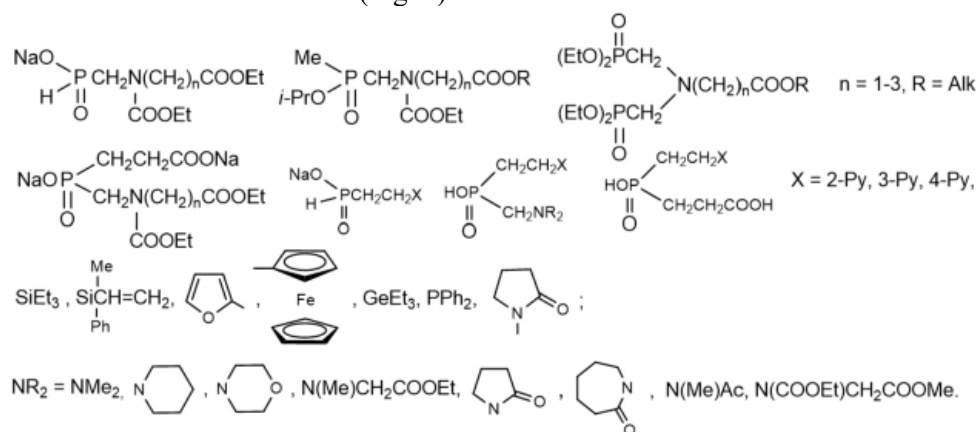
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Phosphorus-containing amino acids, including P-C bonds resistant to hydrolysis, have antibacterial, antiviral, herbicidal and antitumor properties, and are also effective extractants and polydentate ligands. Among them are the well-known plant growth regulators glyphosate, glufosinate and phosphinothricin - environmentally friendly substances that are easily broken down by soil bacteria to form only biogenic products - phosphoric acid and amino acids<sup>1</sup>. New types of phosphorus-containing amino acids and their analogues, capable of exhibiting inhibitory properties against a number of bacteria and viruses, were obtained by us on the basis of easily accessible synthons - trimethylsilyl esters of trivalent phosphorus acids under mild conditions<sup>2</sup> (Fig. 1).



**Figure 1.** Functionalized phosphorus-containing amino acids and their analogues

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# APPLYING A MODEL OF POLYMOLECULAR PROTEIN ADSORPTION TO DESCRIBE THE BEHAVIOR OF MODIFIED HUMIC ACIDS SALTS AT THE AIR-LIQUID INTERFACE

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In this work the expressions of a theoretical model of polymolecular adsorption, developed to characterize the adsorption properties of protein solutions as natural polyelectrolytes, were used for a semiempirical description of experimental results obtained for humic acids salts solutions<sup>1</sup>. The model considers the possibility of the macromolecules existence in  $n$  states and their ability to aggregate in adsorption layers during polymolecular adsorption,  $nA$  – aggregation number of macromolecules in the surface layer,  $\Gamma_c$  – adsorption value,  $\overline{M}$  – average molecular weight of HA salts. The calculated values of the adsorption model parameters for sodium humate salts (SH, also samples obtained by mechanochemistry through reaction of initial humic acids with PEG-6000, cyanoguanidine (CG) and simultaneously with PEG-6000 and CG) are given in the table. Model parameters for HA salts were calculated in the program «Protein G»<sup>2</sup>.

Sample	CMC $\times 10^{-4}$ , M	$\Gamma_c \times 10^{-7}$ , mol/m <sup>2</sup>	$n$	$nA$	$\overline{M}$
1. SH	2,6	5,8	26	7	14000
2. SH <sub>HA + PEG-6000</sub>	2,2	4,3	13	23	15500
3. SH <sub>HA + CG</sub>	0,9	3,0	9	5	14200
4. SH <sub>HA + PEG-6000 + CG</sub>	0,6	3,6	60	10	26000

**Table 1.** Parameters of the thermodynamic polymolecular adsorption model for HA salts

In the sample SH<sub>HA + PEG-6000</sub> due to a charge decrease during the interaction of –COOH groups with ethoxy groups of PEG, the  $n$  value decreases and the parameter increases. In the sample SH<sub>HA + CG</sub> both parameters decrease due to an increase in the total charge of the macromolecule (–COOH and –NH<sub>2</sub> groups). In the sample SH<sub>HA + PEG-6000 + CG</sub> due to the larger molecular weight the  $n$  value increases significantly, and the  $nA$  parameter stands between samples 2 and 3.

The applied adsorption model allows to obtain information about the adsorption behavior of natural polyelectrolytes such as HA salts.

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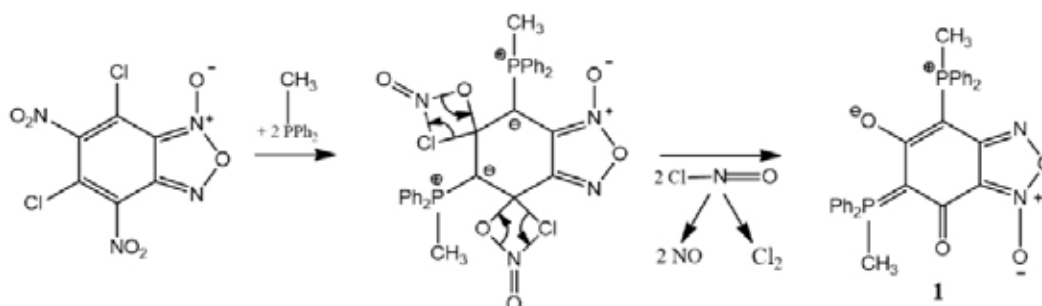


# SYNTHESIS AND BIOLOGICAL ACTIVITY OF PHOSPHORYLATED DERIVATIVES OF 5,7-DICHLORO-4,6-DINITROBENZOFUROXANE

**Romanov S.R., Bakhtiyarov D.I., Usupova L.M., Galkina I.V., Bakhtiyarova Y.V.**

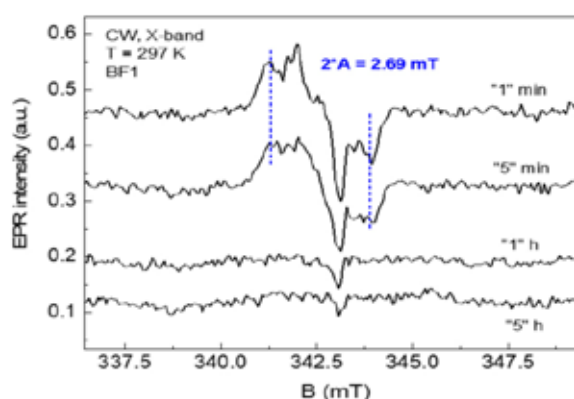
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Reactions of tertiary phosphines: methyldiphenylphosphine, 1,2-bis(diphenylphosphino)ethane and 1,3-bis(diphenylphosphino)propane with 5,7-dichloro-4,6-dinitrobenzofuroxane proceed by nucleophilic aromatic substitution of chlorine atoms and nitro groups in the six-membered ring of the latter heterocycle. The structure of phosphorylation products has been proved by EPR, IR, NMR<sup>31</sup>P spectroscopy, elemental analysis (Scheme 1).



**Scheme 1.**

To confirm the proposed schemes, it was important to record the formation of nitric oxide in these reactions by physical methods. In the process of kinetic studies by the EPR method, the formation of the NO radical from unstable nitrosyl chloride in the processes of phosphorylation of dichlorodinitrobenzofuroxane by various phosphines: methyldiphenyl phosphine, diphosphines: 1,2-bis (diphenylphosphino) was established ethane and 1,3-bis(diphenylphosphino)propane, as shown in Figure 1.



**Figure 1.** EPR spectral studies of reaction mixture of product 1 for 5 hours, bound NO radical and its parameters (Bruker Elexys E 580)

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# COMPLEX COMPOUND OF PRASEODYMIUM(III) PERCHLORATE WITH 4-AMINOANTIPYRINE: SYNTHESIS AND PROPERTIES

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The need to reduce toxic side effects and expand the spectrum of action of platinum-based drugs has led to consideration of the anticancer potential for complex compounds of transition metals with bioactive ligands, since these complexes are of special interest as promising anticancer drugs of a new generation<sup>1,2</sup>. The present work is devoted to synthesis and consideration of structure and properties for a complex compound  $[\text{Pr}(\text{AAP})_6](\text{ClO}_4)_3$  (**1**) (AAP is 4-aminoantipyrine) in comparison with a preliminary studied  $[\text{Pr}(\text{AP})_6](\text{ClO}_4)_3$  (**2**) (AP – antipyrine). The complex compound (**1**) was prepared from  $\text{Pr}(\text{ClO}_4)_3 \cdot 6\text{H}_2\text{O}$  and a ligand taken in a molar ratio of 1:3 in an acetonitrile-acetone mixture (1:1 in vol.). It was identified by the powder-, single crystal XRD methods, and by the IR-, ESI-spectroscopy data. The compound (**1**) crystallizes in a trigonal system (sp. gr.  $R\bar{3}$ .  $a = b = 13.9327(4)$ ,  $c = 33.1320$  Å,  $\alpha = \beta = 90$ ,  $\gamma = 120^\circ$ ,  $V = 5569.9(3)$  Å<sup>3</sup>) and is isostructural with the compound (**2**)<sup>3</sup>, but the latter is characterized by a lower unit cell volume. The cytotoxic activities of (**1**) and (**2**) with respect to different cell lines were determined and compared with those of ligands and  $\text{Pr}(\text{ClO}_4)_3 \cdot 6\text{H}_2\text{O}$ . Elucidation of the cytotoxicity – composition – structure regularities for the mentioned compounds (**1**) and (**2**) are in progress<sup>4</sup>.

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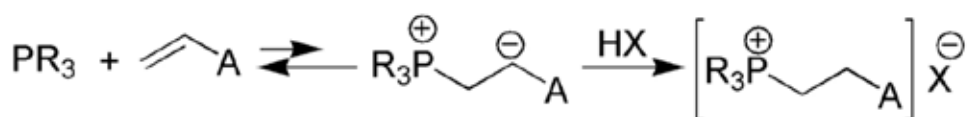
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# PHOSPHONIUM ENOLATES: KINETICS OF THEIR FORMATION AND APPLICATION IN ORGANOCATALYSIS

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Phosphonium enolates are key intermediates of phosphine-catalyzed reactions.<sup>1</sup> The kinetics of phosphonium enolates formation in the reaction of tertiary phosphines with unsaturated electrophilic compounds was studied. The reactions are acid-dependent, and due to the short lifetime of phosphonium enolate protonation step is the rate-determining. The rate law has general third order: first order in phosphine, alkene and proton source HX.



A = electron-withdrawing group, HX = proton source

Tertiary phosphines were found to catalyze the Pudovik reaction through generation of phosphonium enolate intermediate. Tertiary phosphines altered the regioselectivity of the addition of hydrophosphoryl compounds to activated alkynes from  $\beta$ -conjugated to  $\alpha$ -umpolung addition.

For the activated alkenes with locked *s-cis* geometry, the effect of anchimeric assistance was determined.<sup>2</sup> This effect originates from stabilization of the arising intermediate through intramolecular interaction between phosphonium and enolate centers. Based on this effect, methods for phosphine-catalyzed chemo- and stereoselective functionalization of sesquiterpene  $\alpha$ -methylene- $\gamma$ -butyrolactones with phosphorus-, nitrogen-, and carbon-centered pronucleophiles were developed. The synthesized adducts showed selective cytotoxic effects against cancer cell lines.

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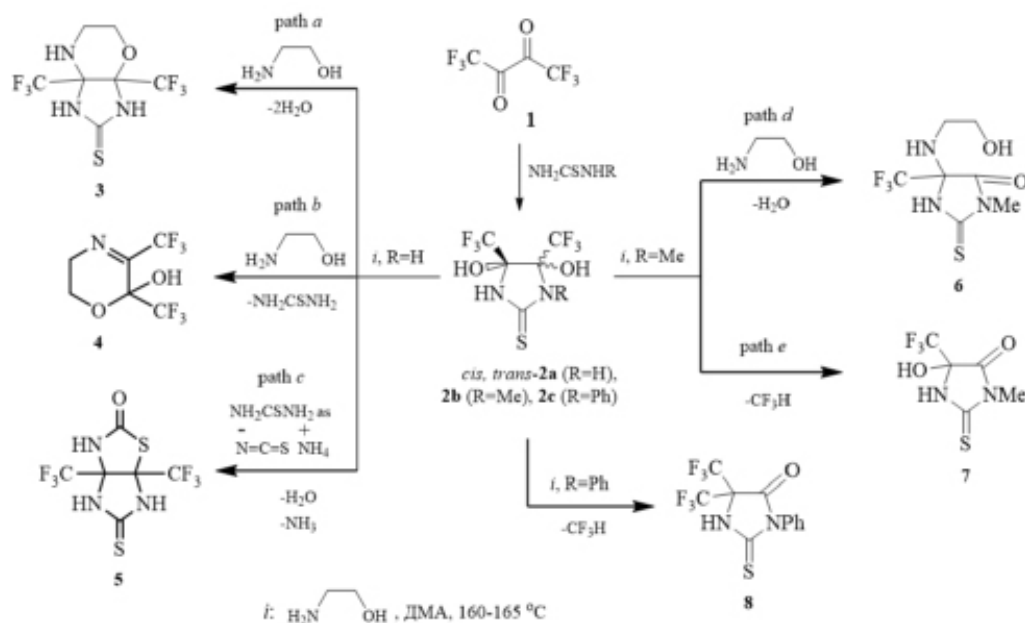
# FEATURES OF THE INTERACTION OF 4,5-BIS(TRIFLUOROMETHYL)IMIDAZOLIDIN-2-THIONES WITH 2-AMINOETHANOL

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The reaction of perfluorobiacetyl **1** with thiourea (TU) and substituted TU produced imidazolidine-2-thiones **2a-c** (scheme 1). Unlike non-fluorinated analogues, compound **2a**, when interacting with 2-aminoethanol (2-AE), gives only a small amount of the condensation product, imidazooxazine **3** (scheme 1, pathway *a*). The main product of the reaction is compound **5** (pathway *c*). When imidazolidine **2b** interacts with 2-AE, unexpected products are obtained: thioxohydantoin **6** (pathway *d*) and **7** (pathway *e*). A similar reaction of imidazolidine **2c** yields thioxo-*N*-phenylhydantoin **8** as a result of intramolecular rearrangement. The obtained compounds are of interest for the search for new biologically active substances.



The work was carried out with the financial support of the Ministry of Education and Science of Russia within the framework of the State task (topic State reg. № 124020200072-0).

# REACTIVITY OF HYDROGEN-BOUND COMPLEXES OF WATER, ALCOHOLS, AMINES AND PHENOLS

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Hydrogen-bonded complexes form a wide range of compounds. Considering their role in chemistry, first of all, they focus on their structuring role. Hydrogen bonds determine the secondary, tertiary structure of both natural and synthetic high molecular weight compounds. Chemical transformations, where reagents can form complexes with hydrogen bonds, are usually considered as simple reactions involving monomers. However, there are many reactions when complexes with hydrogen bonds themselves can act as reagents in transformations. To date, there are isolated works that take into account the possibility of interactions along such a path. At the same time, the reasons leading to differences in the reactivity of monomers and their associates are not considered at all. In this regard, the question arises whether there are premises that allow us to assume different reactivity of monomers and their associates in chemical transformations?

Adiabatic ionization potentials, electron affinities, proton affinities, gas-phase basicities, enthalpies and free energies of dissociation of monomers and homoassociates of water, methanol, phenol, methylamine, as well as mixed hydrogen-bonded complexes of phenol with methanol, methylamine with methanol were calculated by B3LYP/6-311++(df,p) density functional method. As a result of calculations, it was found that hydrogen-bonded complexes, in comparison with their monomeric forms, have increased donor-acceptor and acid-base properties. It has been established in a number of examples that this phenomenon leads to an increased reactivity of hydrogen-bonded complexes with compared to their monomers. Hydrogen-bonded complexes can act as effective acid-base catalysts. Accounting for the participation of hydrogen-bonded associates in reactions where they can form is absolutely necessary for the correct consideration of the kinetic and thermodynamic regularities of chemical reactions.



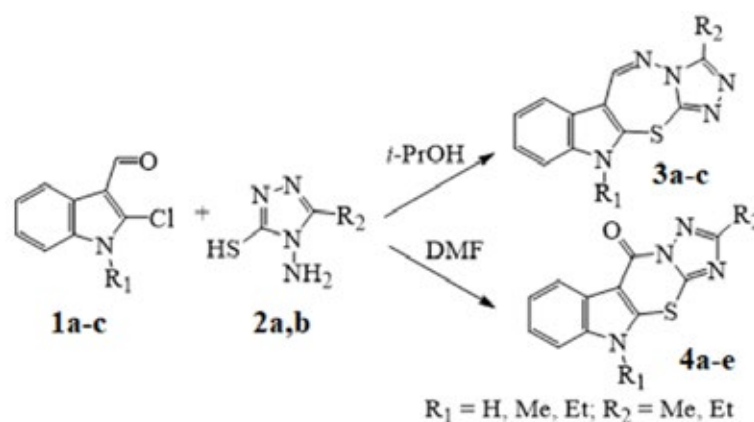
# REACTION OF CHLORINDOLOCARBALDEHYDES WITH AMINOALK-LTRIAZOLTHIOLS

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The indole system plays a key role in vital compounds such as hormones, alkaloids and proteins. Indole derivatives are widely used in medicine as antiviral, anti-inflammatory, antiemetic, antitumor agents, etc.<sup>1,2</sup>

To expand the range of such fused heterocyclic compounds with possible biological activity, the reactions of 2-chloroindole-3-carbaldehydes with aminoalkyltriazolethiols were studied. When carrying out the reaction in isopropanol, triazolothiadiazepinoindoles **3** were obtained, and in DMF, triazolothiazinoindolones **4** were obtained (Scheme 1)<sup>1,2</sup>.



**Scheme 1**

The structures of the obtained compounds were confirmed by NMR and IR spectroscopy, and X-ray structural analysis was performed for compounds **3a** and **4b**<sup>1,2</sup>.

Previously, heterocyclic systems of triazolothiadiazepinoindole and triazolothiazinoindolone have not been described in the literature.

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2. Vikrishchuk, N. I., Tkachev, V. V., Borodkin, G. S., Gazieva, G. A., Shilov, G. V. *Tetrahedron letters*, 2020, **61(45)**, 152490.

# ADSORPTION OF FLOCCULANTS ON NATURAL SORBENT

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Flocculation of pollutants present in wastewater occurs in two stages: adsorption of flocculant on particles and formation of particle aggregates<sup>1</sup>. The process of adsorption of cationic type flocculant on natural minerals of the Astrakhan region was studied and the influence of sorption on the treatment of oily wastewater by flocculation was evaluated. As a result of experimental studies the isotherms of flocculant sorption processes on clays<sup>2</sup> were obtained, the equilibrium sorption capacity of clay in relation to flocculant is 0.12 g/g.

It was found that the Freundlich model is most preferable for describing adsorption in the system of cationic flocculant clay.

Type of isotherm	The parameters of the isotherms		R <sup>2</sup>
	Intensity	Efficiency	
Freundlich	$n = 2,61$	$K_F = 12,8$	0,9866
Langmuir	$K_L = 2,46 \text{ дм}^3/\text{г}$	$Q_e = 0,12 \text{ г/г}$	0,9729
Temkin	$K_T = 73,7$	$\infty = 51,8$	0,9256

**Table 1.** Flocculant adsorption intensity and efficiency parameters obtained in the Langmuir, Freundlich and Temkin models.

The results obtained indicate that this process improves flocculation. The higher value of the intensity parameter in the Freundlich equation<sup>3</sup>, confirms the greater influence of sorption on the flocculation effect, which is associated with the formation of strong high-viscosity cross-linked structures on the surface of the solid phase.

Experiments on water purification from oil by test flocculation method were also made and the degree of purification efficiency was calculated, which amounted to 81.3% at the minimum addition of flocculant in the volume of 1 cm<sup>3</sup> per 100 cm<sup>3</sup> of model solution. Thus adsorption affects both flocculation processes and flocculation effect. Taking all the above into account, this study can provide a chemical basis for solving environmental safety problems.

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# CHELATION OF NICKEL(II) CATIONS WITH COMPLEXONES IN THE PRESENCE OF POLYAMINES

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In multicomponent solutions containing several complexing reagents, it is possible to implement heteroligand complexation processes with an increase in the functional activity of both the complexing agent and the ligands due to the formation of unusual structural forms. Competitive filling of the coordination sphere of a metal center in multicomponent systems usually occurs with discrimination of the electron-donating properties of some ligands and preferential binding of others. Moreover, the competitive nature of complexation is determined by a significant set of factors, the contribution of which is also very variable<sup>1-2</sup>.

Complexation in ternary systems containing nickel(II) cations, polyaminopolycarboxylate ligands (ethylenediaminetetraacetic Edta and diethylenetriaminepentaacetic Dtpa acids) and polyamines (diethylenetriamine Dien and triethylenetetramine Trien) was studied. It was established that in solutions of highly dentate Edta and Dtpa the chelating properties of polyamines were blocked. However in ternary systems with Dtpa and Dien (or Trien) a shift in the pH range of complexation to the alkaline region compared to systems without polyamines was observed. Apparently, in acidic solutions, electrostatic interaction of protonated amine cations and Dtpa anions occurred with the formation of ion pairs which complicated the process of intraspherical ligand exchange of water molecules for anions of the Dtpa complexone in the nickel(II) aqua complex. Therefore, the thermodynamic stability of protonated Dtpa nickel(II) chelates in aqueous solutions decreased, while the stability of the deprotonated nickel(II) chelate in neutral and alkaline media was maintained in the presence of a polyamine.

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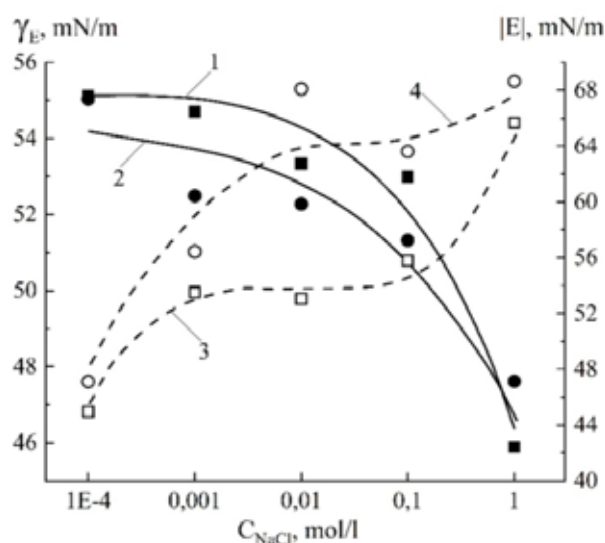
# INFLUENCE OF NaCl CONCENTRATIONS ON THE SURFACE PROPERTIES OF ETHOXYAMINOHUMIC ACID SALTS AT THE AIR BOUNDARY

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Studies of the interaction patterns between ionic surfactants and electrolytes are important in the optimisation of technological processes involving water-salt solutions. In this work, the effect of NaCl concentration on the surface-active properties (equal-weight surface tension,  $\gamma_E$  and dilatational viscoelastic modulus,  $|E|$ ) of solutions of sodium salts of ethoxyaminohumic acids (surfactants) obtained by mechanochemical synthesis through the interaction of humic acid with polyethylene glycol (PEG-6000) and urea or cyanguanidine was studied.

The addition of NaCl to the surfactant solution (figure) leads to a decrease in the value of  $\gamma_E$  and an increase in the parameter  $|E|$ . The reason for this is a decrease in the value of the electrostatic component of the adsorption barrier at the interface<sup>1</sup>. It is shown that salts of ethoxyaminogumic acids, possessing the functions of an anionic, cationic and non-ionic surfactants, increase surface activity at NaCl concentrations up to 1.0 mol/l.



**Figure.** Effect of NaCl concentration on  $\gamma_E$  (1, 2) and  $|E|$  (3, 4) parameters of sodium ethoxy aminogumate solutions at the air interface,  $SH_{HA+PEG-6000+urea}$  (1, 3) and  $SH_{HA+PEG-6000+cyanguanidine}$  (2, 4).

## References

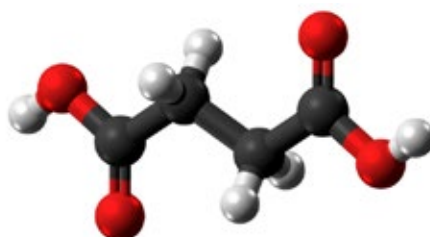
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# OBTAINING NEW PHYSICOCHEMICAL PROPERTIES OF WATER-ALCOHOL MIXTURES WHEN USING SUCCINIC ACID AS A BIOLOGICALLY ACTIVE ADDITIVE

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Succinic acid is known as a versatile intermediate metabolite that can reduce the negative effects of ethanol on the human body.



**Figure 1.** Chemical formula of succinic acid

The effect of succinic acid on the physicochemical properties of water-alcohol mixtures was studied. The results are in Table 1.

Образец	Contents of toxic impurities in solutions				
	acetaldehyde, mg/L	ethylacetate, mg/L	methanol, %	2-propanol, mg/L	methylacetate, mg/L
Water-Alcohol mixtures 40%	0,3536	0,4464	0,00132	0,4255	0,3573
Succinic acid 0,002%	0,2990	0,4538	0,00132	0,3850	-
Succinic acid 0,02%	0,5655	0,5332	0,00134	0,4094	0,2921
Succinic acid 0,2%	1,9466	1,1402	0,00138	0,4933	0,3216

**Table 1.** Results of gas chromatographic analysis

During the analysis of the obtained data it was found that alcohol solution with a mass fraction of 0.002% succinic acid can reduce the content of acetaldehyde, 2-propanol, methyl acetate.



# NEW BIOLOGICALLY ACTIVE 5-SUBSTITUTED 2-THIOXODIHYDROPYRIMIDINE-4,6(1H,5H)-DIONES

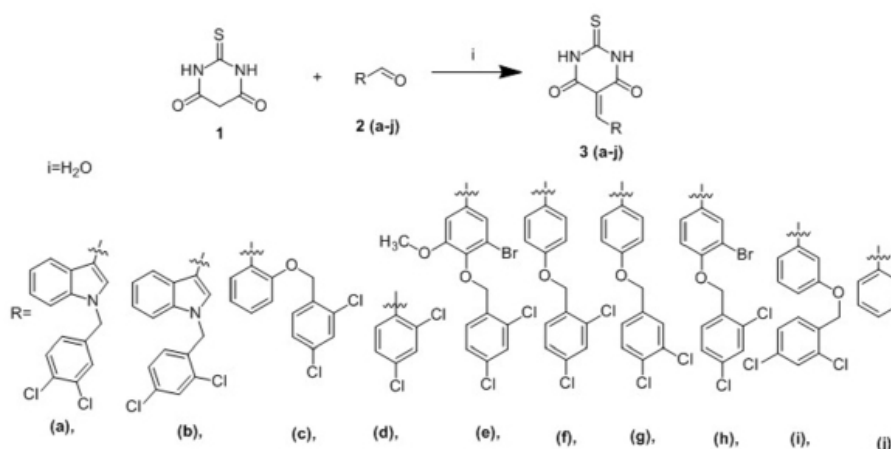
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Thiobarbituric acid derivatives are widely used as active pharmaceutical ingredients of drugs. We have obtained new 5-substituted 2-thioxodihydropyrimidine-4,6(1H,5H)-diones **3 (a-j)** by reacting thiobarbituric acid **1** with the corresponding substituted benzaldehydes **2 (a-j)** by boiling in water. For the obtained compounds, their biological activity was studied, presented in Table 1.



Compound	Staphylococcus aureus ATCC6538	Candida utilis LIA-01	Pseudomonas aeruginosa 0387	Influenza virus A/Puerto Rico/8/34 (H1N1)		
				CC50, µg/mL	IC50, µg/mL	SI
3a	—*	—	—	>300	12	25
3e	—	—	—	10,2	0,6	17
3f	—	—	—	4,9	0,5	10
3h	—	—	—	11,4	1	11

**Table 1.** Results of in vitro studies of the biological activity of the leading compounds

\*— no biological activity detected

This work was supported by the Russian Science Foundation (RSF), Project No. 23-13-00224.

# SYNTHESIS OF HETEROFUNCTIONAL DISUBSTITUTED DERIVATIVES OF THE *CLOSO*-DECABORATE ANION

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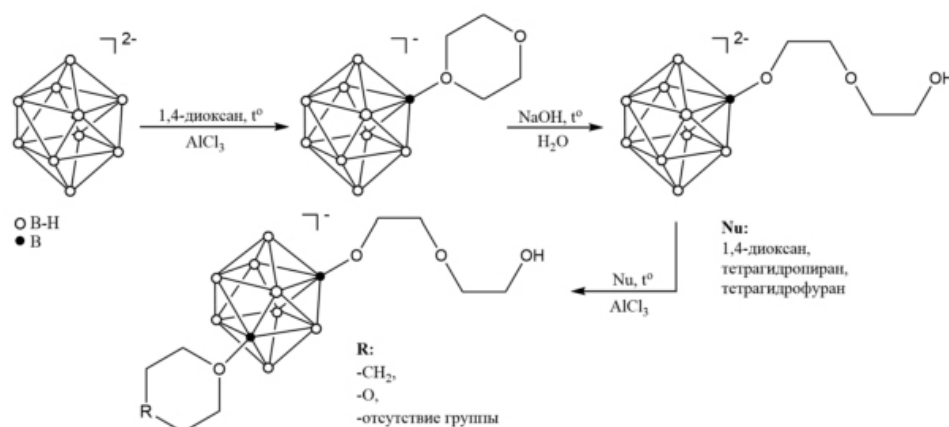
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The introduction of various functional groups into the cluster anions of boron  $[B_nH_n]^{2-}$  ( $n = 10, 12$ ) is an important step in the design of compounds promising for  $^{10}B$ -NCT. The use of electrophilically induced nucleophilic substitution (EINS) reactions makes it possible to use molecules of simple cyclic esters as substituents, convenient from the point of view of their subsequent modification.

In this study, a sequential modification of the *closo*-decaborate anion was carried out, including the introduction of an oxonium-type substituent, its nucleophilic disclosure and the introduction of a second substituent with the formation of 2,7(8)-derivatives:



**Fig. 1.** Scheme of synthesis of heterofunctional disubstituted derivatives of anion  $[B_{10}H_{10}]^{2-}$ .

The attached oxonium substituent in the final derivatives can also be introduced in reaction with nucleophiles to form *closo*-decaborates containing two pendant functional groups. The use of various cyclic esters makes it possible to regulate the structure and properties of synthesized compounds.

The obtained *closo*-decaborates are promising for use as polydentate ligands for the extraction of rare earth metals, as well as for the production of boron-containing functional materials.

# SYNTHESIS OF 5-[4-(ARYLSULFANYL)PHENYL]-2,2'-BIPYRIDINES USING ARYNE INTERMEDIATES

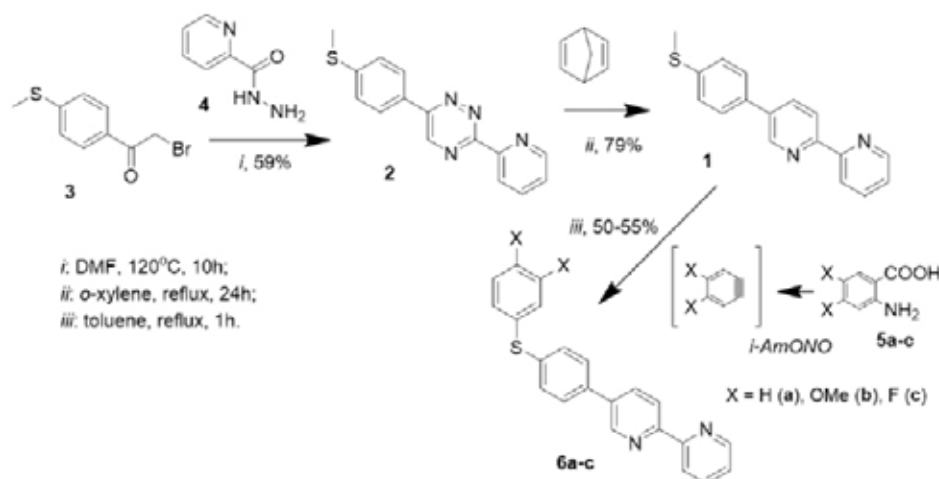
**Starnovskaya E.S.<sup>1</sup>, Krinochkin A.P.<sup>1,2</sup>, Rybakova S.S.<sup>1</sup>, Muzyka A.L.<sup>1</sup>, Slepukhin P. A.<sup>1,2</sup>, Kopchuk D.S.<sup>1,2</sup>, Zyryanov G.V.<sup>1,2</sup>, Chupakhin O.N.<sup>1,2</sup>**

<sup>1</sup> Ural Federal University

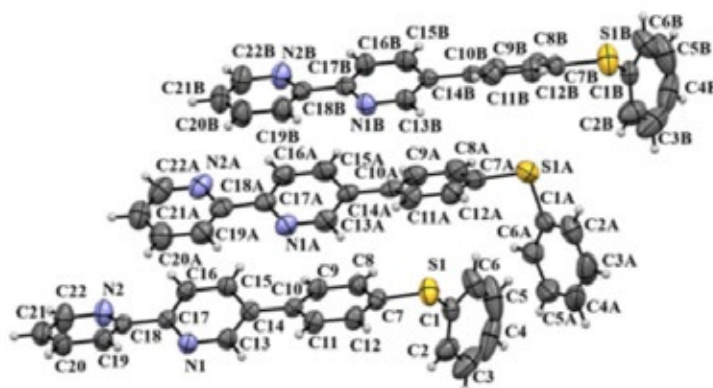
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A convenient method for the preparation of 5-aryl-2,2'-bipyridines with para-arylsulfanyl group in an aromatic substituent was proposed. The synthesis was performed using in situ generated aryne intermediates without the use of complex experimental procedures and expensive reagents/catalysts. The structure of one product was confirmed by XRD data. This approach is a new variant for the preparation of 5-aryl-2,2'-bipyridines with an extended conjugation system.



The structure of the target products was confirmed by <sup>1</sup>H, <sup>19</sup>F, and <sup>13</sup>C NMR spectroscopy, mass spectrometry, and elemental analysis. In addition, the structure of product 6a was additionally confirmed by X-ray diffraction data.



**Fig. 1.** General view of molecule of compound **6a** in crystal.

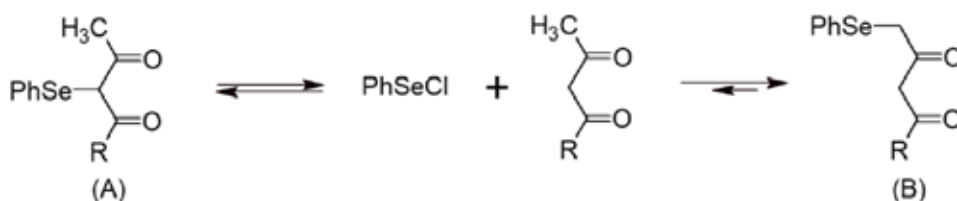
The study was carried out with the financial support of the grant No. 075-15-2022-118

# INVESTIGATION OF THE REACTION BETWEEN SELENIL CHLORIDES AND DYKETONES

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The reaction of PhSeCl with diketones having two reaction centers (at the central carbon atom and in the side substituent) occurs in both directions, with the first direction being predominantly realized. In the presence of releasing hydrogen chloride, the reaction is reversible and a dynamic equilibrium is established in the reaction mixture, in which the PhSe group passes from the substituted diketone to the unsubstituted diketone. However, for the isomer containing the PhSe group in the substituent (B), the equilibrium is shifted towards the products more than for the isomer containing the substituent at the central carbon atom (A). Such a ratio leads to a gradual accumulation of the isomer containing a PhSe group in the substituent (B) in the reaction mixture:



The necessity of the presence of hydrogen chloride indicates that the first stage of the reaction involves protonation of the substrate, followed by the formation of the PhSe<sup>+</sup> cation. Additionally, it was found that even a single carbonyl group significantly polarizes the Se-C bond, giving the selenium atom electrophilic properties. For diketones containing a sulfur-organic substituent (isomer A) under similar conditions, isomerization to B does not occur.

A similar isomerization process was previously described for the bromination of acetoacetic ether.<sup>1</sup>

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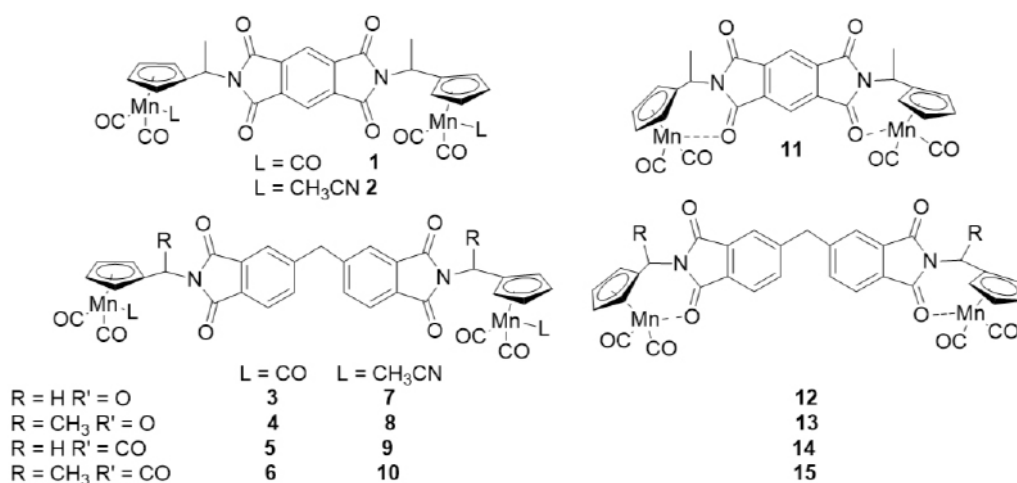
# CYMANTHRENYLAKYL DIIMIDES – MOLECULES WITH CHANGEABLE AND CONTROLLABLE PROPERTIES

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To create molecular devices, it is necessary to develop new multiparametric materials. Diimide derivatives are compounds with unique optical and electrochemical properties. The introduction of phthalimides as copolymers makes it possible to obtain semiconductor materials with specified electronic properties.<sup>1</sup> We have shown that exchanging the organic substituent on the nitrogen atom with a photo- and electroactive organometallic cymantrenylalkyl fragment opens the way to the creation of a new class of acceptor materials.<sup>2</sup>

In order to create materials with changeable and controllable properties, a series of compounds **1-15** (Figure 1), containing two linked imide fragments with a cymantrenealkyl group at each nitrogen, were prepared, and the influence of the nature of the linker, as well as photo- and thermally induced ligand exchange at manganese, on the optical and electrochemical properties of **1-15** was studied.



**Figure 1.** Complexes based on cymantrenealkyl diimides.

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*The work was carried out with financial support from the Russian Science Foundation (grant 23-23-00192).*



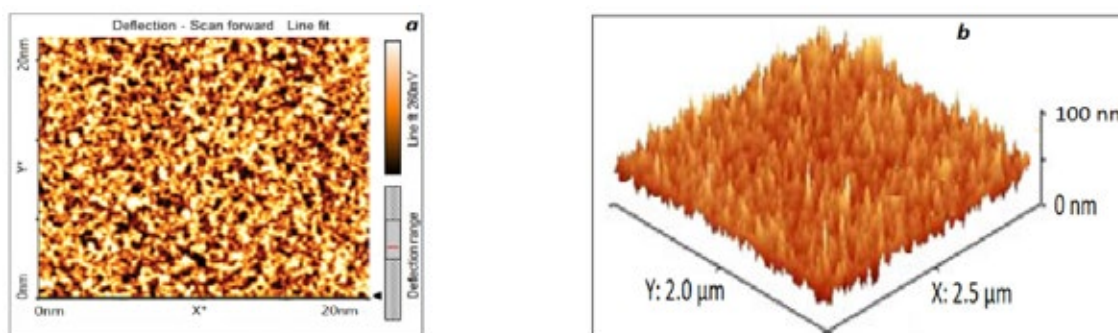
# SYNTHESIS OF THIN ZnO FILMS USING SAPONINS AS SURFACTANTS

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When synthesizing thin mesoporous ZnO films, recrystallized  $\text{Zn}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$  was used, and ethanol in the presence of HCl was used as a solvent. Saponin isolated from the plant root was used as a surfactant. The ratio of  $\text{C}_2\text{H}_5\text{OH}:\text{H}_2\text{O}:\text{HCl}:\text{saponins}$  was 1:20:10:0.15:0.05. The resulting solution was applied to the surface of a glass substrate by spraying at a speed of 10 cm/min.

The surface topography of a thin ZnO film was studied using an atomic force microscope (Fig. 1).



**Fig.1.** An atomic force microscope image of a ZnO film and its 3D view

The image shows that the ZnO film consists of numerous nanostructures, which are distributed evenly over the entire surface. The structures appear as columns or peaks, which is characteristic of nano-sized crystalline formations. ZnO has a potentially high surface area, which is a desirable property for photocatalytic applications.

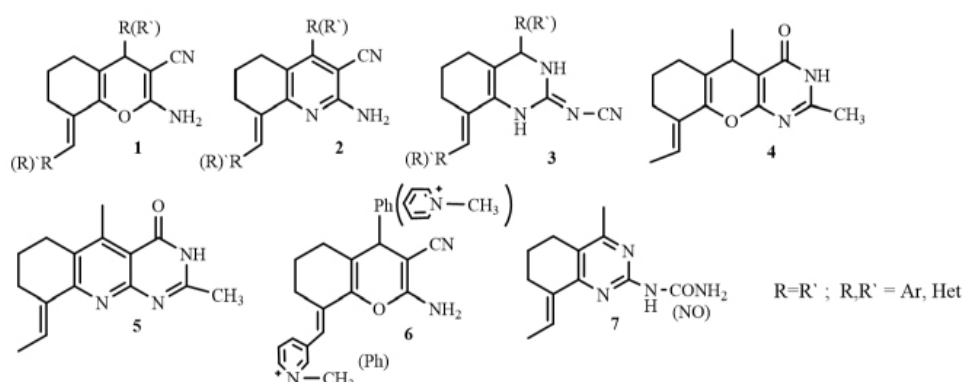
# METHODOLOGY OF “GREEN” CHEMISTRY IN THE SYNTHESIS OF FUNCTIONALLY SUBSTITUTED N,O-HETEROCYCLES OF THE CHROMENE, QUINOLINE, QUINAZOLINE SERIES WITH PHARMACOPHORE FRAGMENTS AND GROUPS

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The “green chemistry” methodology is widely used in the design of hybrid “drug-like” systems, including key nitrogen- and oxygen-containing heterocycles.

Based on the principles of this methodology, we have synthesized a series of new substituted aminochromene carbonitriles **1**, their functional quinoline analogues **2**, quinazolines **3** and the products of their transformations in reactions of heteroannellation **4,5**, quaternization **6**, oxidative dehydrogenation **7**, etc.



Synthetic approaches to compounds **1-3** are based on the condensation (two-, three-component) of available carbonyl compounds with C- and N-nucleophiles with a variety of approaches (ultrasound, thermal activation, electrolysis, homo-, heterogeneous catalysis).

The most effective in “green” syntheses are the electrochemical chromene **1** and the formation of heterosystems **4,5** using a recycled nanocatalyst - graphene oxide.

By modifying pyridyl-substituted chromenes, water-soluble iodomethylates **6** were obtained. Conditions for the spontaneous partial cleavage of racemates **3** with a predominance of the dextrorotatory antipode (CD spectra) were found.

Computer prediction and experimental evaluation (IBPRM RAS) made it possible to identify compounds with antibacterial and cytotoxic effects approaching those of the reference drugs.

# LUMINESCENT MULTI – LIGAND EUROPIUM(III) CARBOXYLATES

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Owing to working out of functional optical polymeric materials for optoelectronics, laser technics, sensorics, the search of new luminescent lanthanide complex compounds becomes topical<sup>1</sup>.

Some new intensive luminescent europium(III) complex compounds with cinnamic, methoxycinnamic and toluic acids as well as nitrogen- and phosphorus – containing neutral ligands of island and dimeric structure were prepared. The composition and structure of coordination compounds of europium(III) have been determined by methods of chemical elemental, X-ray phase analysis, X-ray electron and IR spectroscopy.

Spectral-luminescent characteristics of multi-ligand complex compounds have been studied. The data on the correlation between the geometric and electron structure, thermal, luminescent, triboluminescent and photochemical properties of the lanthanide complex compounds were also obtained and systematized. Complex compounds of europium(III) with maximum luminescence intensity in the studied series of compounds have been identified.

The factors promoting amplification of the antenna effect and intensification of luminescence in the mixed - ligand europium(III) carboxylates with nitrogen- and phosphorus – containing neutral ligands were revealed.

The correlation dependence between the luminescent characters and the charge state of the central europium(III) ion for the homologous series of europium(III) mixed - ligand complex compounds with carboxylic acids was established.

Luminescent polymer compositions based on complex carboxylates of europium(III), high-pressure polyethylene and polymethylmethacrylate were obtained. The kinetics of photo-decomposition of compositions has been studied.

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# NEW LIQUID-CRYSTAL POLYMER MATERIALS

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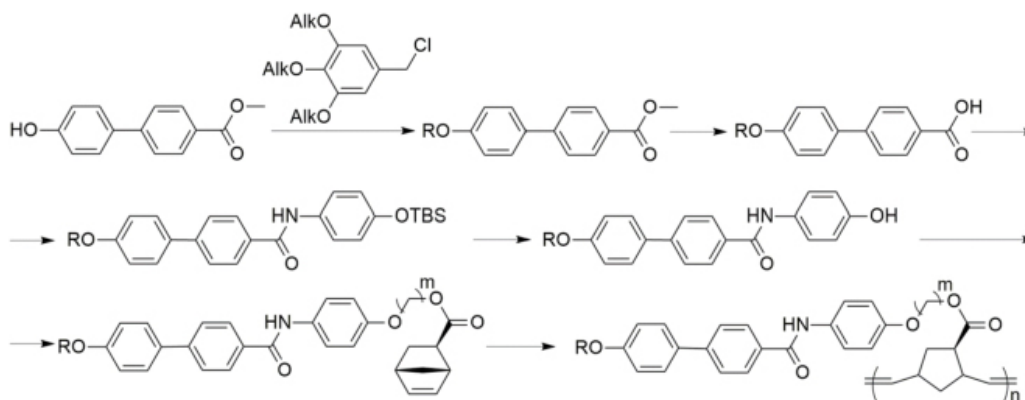
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Our research group is actively developing catalysts for the production of biodegradable polymers<sup>1-2</sup>, as well as functionalized polymers<sup>3</sup> for gas separation membranes used in fields, related with increasing environmental protection requirements.

As one of the key base material for gas separation, liquid-crystal polymer membranes can exhibit high permeability with high thermally controlled selectivity.

This work proposes methods for the synthesis of monomers to create materials based on functionalized norbornene derivatives.



The synthesized *exo*-substituted norbornenes, the structure of which was confirmed by <sup>1</sup>H and <sup>13</sup>C NMR spectroscopy, showed high activity in metathesis polymerization, and the resulting polymer materials contain a liquid-crystalline phase.

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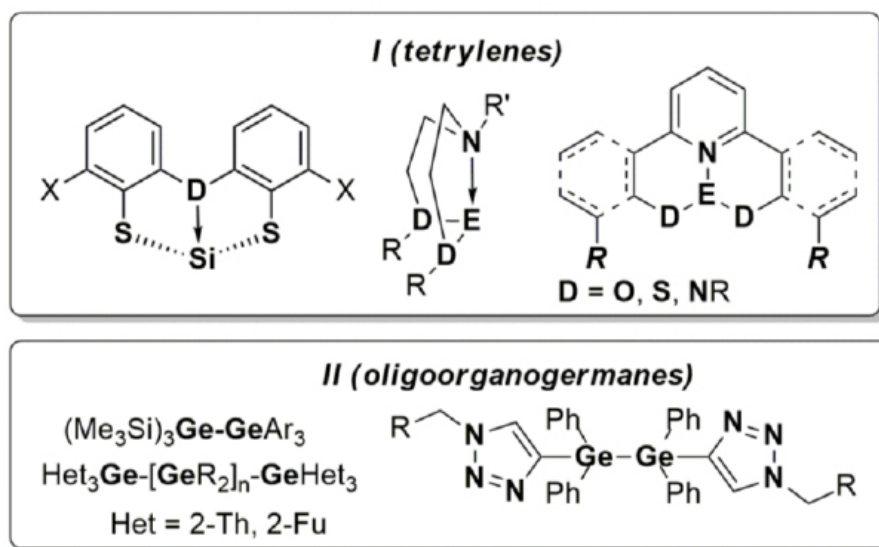
# TETRYLENES AND OLIGOORGANOTETRELANES: UNIQUE DERIVATIVES OF GROUP 14 ELEMENTS

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Nowadays, derivatives of Group 14 elements ( $E = \text{Si, Ge, Sn}$ ),<sup>1</sup> intensively investigated worldwide, which is caused by both fundamental interest (possibility of synthesis) and their applications due to unique properties (catalytic, coordination, optical, semiconductor, synthetic, biological).

The report summarizes the research of our scientific group in recent years on tetrylenes (**I**, heavy analogues of carbenes)<sup>2-5</sup> and oligoorganotetrelanes (**II**, compounds with E-E bonds).<sup>6-8</sup>



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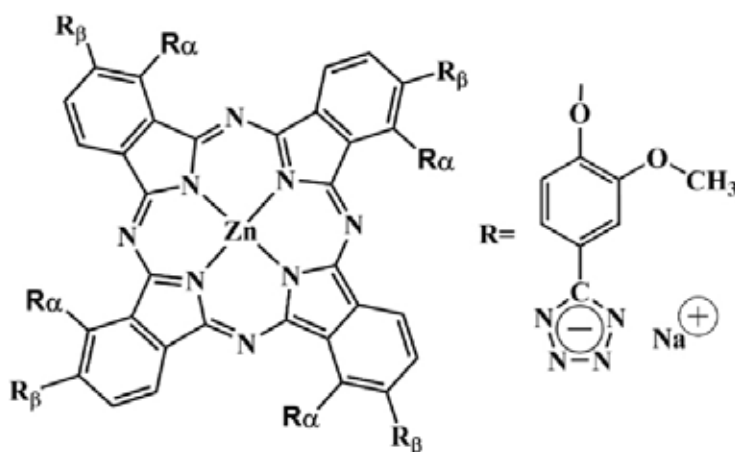


# SYNTHESIS AND STUDY OF WATER-SOLUBLE ZINC PHTHALOCYANINES BEARING TETRAZOLE HETEROCYCLES

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Metal phthalocyanines are potential photosensitizers for photodynamic therapy of cancer (PDT).<sup>1</sup> A limitation to the use of such macroheterocycles is their insolubility in water. A solution to this problem is the introduction of hydrophilic groups such as sulfo-, carboxy- or quaternary amino groups.<sup>2</sup> Tetrazoles, unique pharmacophoric heterocycles with high acidity, can act as a bioisosteric analogue of the carboxyl group.<sup>3</sup> In this work, novel anionic water-soluble peripherally and non-peripherally substituted zinc phthalocyanines with tetrazole fragments have been obtained for the first time.




Compounds	$\lambda_{\max}$ (log $\epsilon$ ) (DMSO)	$\lambda_{\max}$ (log $\epsilon$ ) (H <sub>2</sub> O)	$\Phi_{\Delta}$ (DMSO)	$\Phi_{\Delta}$ (H <sub>2</sub> O)	PD, % (DMSO)	PD, % (H <sub>2</sub> O)
$\alpha$ -ZnPcR <sub>4</sub>	702 (5.09)	697 (4.98)	64.07	76.74	8.02	5.07
$\beta$ -ZnPcR <sub>4</sub>	684 (4.99)	683 (5.04)	58.51	74.93	6.49	25.68

**Table 1.** Photophysical and photochemical properties of photosensitizers

The photophysical and photochemical characteristics of synthesized phthalocyanines have been studied in DMSO and water. It was shown that, due to intense absorption in the red region of the spectrum ( $\lambda_{\max}$ ), high quantum yields of singlet oxygen generation ( $\Phi_{\Delta}$ ) and a low percentage of photodestruction (PD), the synthesized compounds can be promising photosensitizers for PDT.

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Section 2

# CHEMISTRY AND TECHNOLOGY OF MATERIALS

# INVESTIGATION OF THE INFLUENCE OF THEIR STRUCTURE FACTOR ON THE PROTECTION ABILITY OF SOME FUNCTIONAL DERIVATIVES OF AMINOCARBON ACIDS DURING CORROSION OF C<sub>T-10</sub> BRAND STEEL IN THE ENVIRONMENT OF 0, 1 N HCL SOLUTION

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Despite numerous initiatives so far, it has not been possible for obvious reasons to create a unified theory of inhibition that can be applied in all conditions. Therefore, research in this area is of high relevance in modern times.

Based on our previous studies on some derivatives of phenol, we came to the conclusion that due to several adsorbed functional groups and heterogeneous atom-retaining compounds in the molecule at the same time, corrosion inhibitors of relatively high efficiency can be obtained.

With the help of gravimetric, electrochemical impedance spectroscopy and polarization curve drawing methods, the presented work is used to determine some derivatives of amino carbonic acids (specifically, I. Aliphatic mono amino mono carbonic acids (AL-MAMMK); for example, glycine  $H_2N-CH_2-COOH$ , alanine  $CH_3-CH(NH_2)-COOH$ , leucine  $CH_3-CH(CH_3)-CH_2-(NH_2)-COOH$ . II. Aliphatic monoamine dicarbonic acids (AL-MADKK); for example, aspartic and glutamic acids  $HOOC-CH_2-CH(NH_2)-COOH$ ,  $HOOC-(CH_2)_2-CH(NH_2)-COOH$ . III. Aliphatic diamine mono carbonic acids (AL-DAMKK); for example, arginine  $H_2N-C(=NH)-NH-(CH_2)_3-CH(NH_2)-COOH$ ) was devoted to the study of the inhibitory effect of against the corrosion of C<sub>T-10</sub> steel in the medium of 0.1 N HCl solution.

Analysis of the obtained results showed that some of the studied compounds have an inhibitory effect on corrosion of C<sub>T-10</sub> steel in the mentioned aggressive system. Due to the influence of some of these substances, the price of  $E_{cor}$  slides into the negative.  $b_a$ ,  $R_p$ ,  $R_c$  prices increase to a certain extent. It has been shown that the found inhibitors belong to the class of mixed inhibitors. It was determined that the studied compounds are located in the following order according to their effectiveness:

Arginine > leucine > glutamic acid ≥ aspartic acid > alanine ≥ glycine



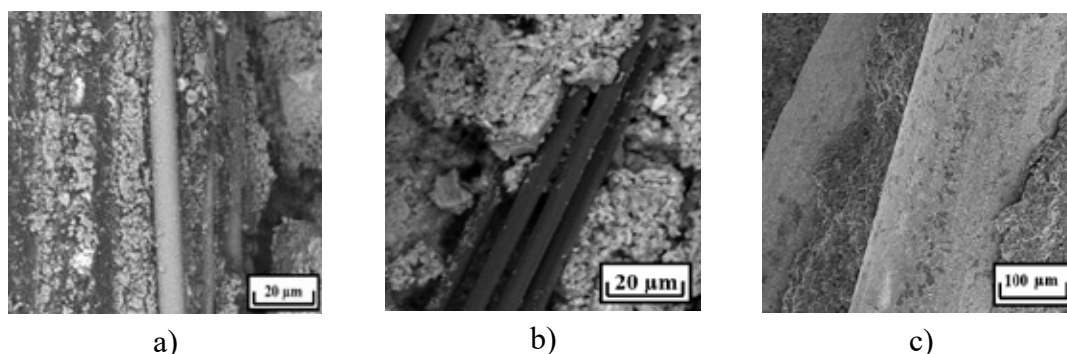
# ELECTRON MICROSCOPIC INVESTIGATION OF “CEMENT MATRIX – FIBER” INTERFACE IN 3D-PRINTABLE COMPOSITE STRUCTURE

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3D-build printing is developing innovative technology. The deficiency in reinforcement methods of structures adapted to this technology is the main problem that impedes development 3D-build printing technology.

The reinforcement effectiveness of 3D-printed structures is determined by the “cement matrix – reinforcing fiber” bond strength which depends on the adhesive mechanism of their interfacial transition zone interaction. The goal of this study was micro-structural investigation of fiber–matrix contact zone with scanning electron microscopy (SEM). The reinforcing fibers are differed in chemical composition, diameter and surface morphology.



**Figure 1.** SEM images of fiber–matrix contact zone: a) silicate fiber with adhesive coating; b) carbon fiber; c) steel wire

According to SEM data (fig.) obtained for the “fiber– cement matrix” contact zone the mechanism of bond strength formation for all fibers types was determined by the mechanical entanglement between the fiber surface and the components of the cement matrix. The covering of silicate fiber surface with the synthetic rubber coating influences the interaction of the cement matrix with fiber in the contact zone. Also, adhesion could be the result of the interaction of the cement hydration products and fiber due to intermolecular interaction forces.

*This research was supported by the Russian Science Foundation, No. 22-19-00280, <https://rscf.ru/en/project/22-19-00280/>*

# TECHNOLOGY FOR UTILIZATION OF ELEMENTAL SULPHUR AND OTHER TECHNOGENIC INDUSTRIAL WASTES

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According to official data, only about 2% of raw materials extracted from the bowels turn into the final product, the remaining 98% is waste. Therefore, recycling is an urgent problem of any chemical production.

The possibility of using chemical water treatment sludge, which is a by-product of heat and electric energy generation at a thermal power plant (TPP) as a filler in construction materials, has been experimentally proven. Based on the obtained results, the technological scheme of processing slurries of TPP and sulfur-containing waste into building materials is proposed. The developed process line is universal.

During the research work, samples based on sulfur and other man-made waste were obtained. The samples were tested for strength, density, water absorption, and the optimal technological parameters of the production process were determined.

The use of industrial waste expands the raw material base, reduces the cost of finished products, helps to solve the environmental problem of the region and reduce the volume of sludge during its storage.

In the obtained materials, sulfur played the role of binder, a by-product of the Tatarstan Oil Refining Complex of Taneko JSC was used [1]. As a filler, in addition to chemical water treatment sludge, ash and slag waste was used, coke - the waste of the coke-chemical enterprise Altai-Koks JSC in various ratios with quartz sand and siliceous rocks of various deposits.

The resulting material can be used in those areas where high-strength structures or coatings are needed that quickly gain strength, for example, prefabricated concrete structures such as curbs, foundation slabs, sleepers, power transmission poles, etc.

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# TEMPERATURE STABILITY OF FULLERENE C<sub>28</sub>

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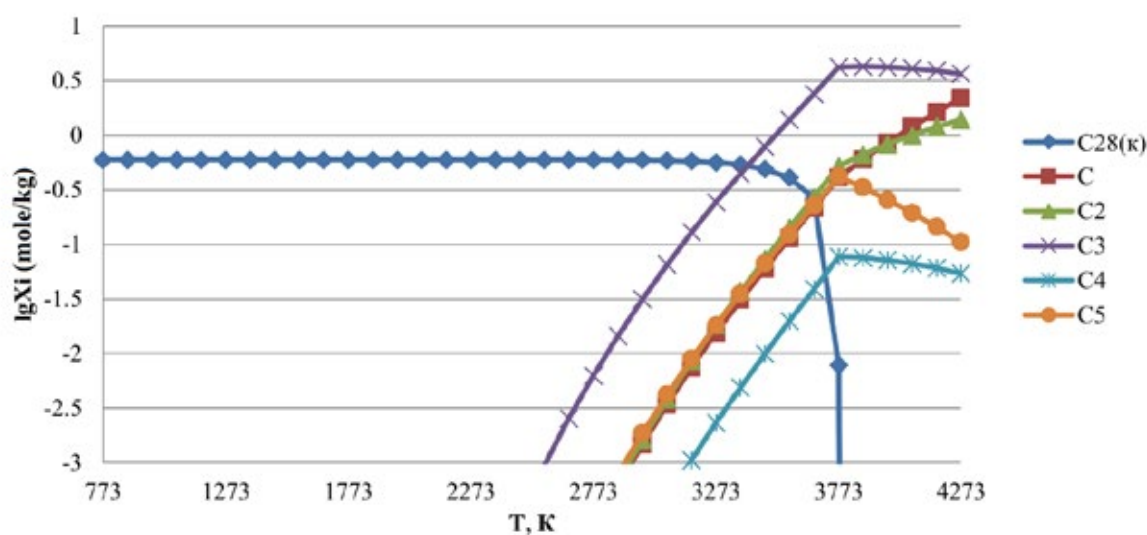
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The temperature of the onset of thermal decomposition of fullerene is an important characteristic of a carbon nanoparticle [1].

To determine it, thermodynamic modeling of the behavior of fullerene C<sub>28</sub> when heated in an argon atmosphere using the TEPPA program was carried out [2, 3]. The simulation results are shown in Figure 1.



**Figure 1.** Distribution of carbon nanoparticles in the system C<sub>28</sub>-Ar

It can be seen from the figure that the reduction of condensed C<sub>28</sub> begins at 3373 K.

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# ADHESIVE ORGANOMETALLIC LAYER ON THE SURFACE OF THE CONDUCTIVE PATTERN OF THE INNER LAYERS OF MULTILAYER PRINTED CIRCUIT BOARDS

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The standard process (GOST 23661-79) of creating a rough adhesion layer on the copper surface of the conductive pattern before pressing the inner layers of multilayer printed circuit boards (MPCBs) consists of forming an oxide layer on the copper surface. The bonding strength in this case is provided by mechanical “bonding” of the treated surface to the prepreg. However, this method is unsuitable for use in modern production of MPCBs (with high density of installation) because of the following disadvantages: insufficiently high strength of adhesion of the metal surface with prepreg, defect in the form of “pink” rings and low temperature resistance (reduction of adhesion by 30 - 60% at a thermal shock of 260 °C, 10 s)<sup>1,2</sup>.

To ensure the required adhesion of inner layers at modern MPCBs production facilities, a rough adhesive layer with a thin (200-300 Å) surface metal-organic layer is formed on the copper surface, which provides adhesion of layers not only by increasing the contact surface area, but also by chemical bonds with prepreg molecules<sup>3</sup>.

A technological process for copper surface modification in a solution containing (g/l): H<sub>2</sub>SO<sub>4</sub> 91, H<sub>2</sub>O<sub>2</sub> 14, Cl<sup>-</sup> 8-10 mg/l, PEG (1500) 3-7, corrosion inhibitor from the class of nitrogen-containing heterocyclic hydrocarbons 8, which allows at t 35 °C, τ 75 s to form an adhesive metal-organic layer that is not inferior to the foreign analog in terms of parameters of roughness (Ra = 0.60 μm, Ra (analog) = 0.50 μm) and strength of adhesion of inner layers.

By means of transmission electron microscopy of the sample, after prior sample preparation by the focused ion beam method, it was found that the thickness of the thinnest surface metal-organic layer formed in the developed solution is about 250 Å, and includes the following elements: N, C, Cu in its composition.

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# THE INFLUENCE OF METHODS OF PROCESSING COAL TAR ON THE COMPOSITION AND PROPERTIES OF COKE BASED ON IT

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Coal tar is a by-product of coal coking at a temperature of 900-1000 °C, obtained from steam-gas products of pyrolysis after their distillation and separation of target fractions, such as benzene and its homologues, naphthalene, phenanthrene, anthracene and absorptive fractions, indene, cumarone, which are in demand by the chemical industry. Depending on the composition of the coal charge and coking conditions, the fractions obtained during distillation vary slightly in quantity (yield). The yield of tar from dry coal charge is about 3.5%, and its properties and chemical composition depend on the technological conditions of coking<sup>1,2</sup>.

Coal tar is most often processed into coal tar pitch - a binder for the production of artificial carbon materials used in mechanical engineering, metallurgy, power and chemical industry. Several foreign companies have technologies for producing needle coke from coal tar. Technologies for processing coal tar allow for the production of materials with various properties. Pitches, differing in softening temperature and composition, are obtained by thermopolycondensation and thermo-oxidation. Thermal dissolution and extraction with filtration are also used. To obtain cokes with different structures and self-bonded mesophase carbon, methods allowing variation of the hydrocarbon composition of the tar are applied: thermal dissolution, hydrogenation, mechanochemical treatment, and others<sup>3</sup>.

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# METHOD FOR OBTAINING AVAILABLE NITROGEN-CONTAINING QUATERNARY SALTS IN THE ABSENCE OF SOLVENT

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Quaternary N-alkyl-substituted compounds (QAC) of ammonium, pyridinium, quinolinium and other tertiary amines are widely known as effective modifiers of the surface properties of various materials, antistatic agents, antibacterial agents, phase-transfer catalysts, and ionic liquids (ILs). The generally accepted method for their preparation is the interaction of alkylating reagents with tertiary amines (quaternization reaction) during prolonged heating in solvents such as acetone, ethanol, benzene and other flammable and toxic liquids.

In order to obtain available QAC, we have developed and tested a more economical and safe method of solvent-free quaternization of amines produced by domestic industry (pyridine, quinoline, piperidine, morpholine, trialkylamines, 2-dimethylaminoethanol), which made it possible to simplify the technology, increase efficiency and reduce the fire hazard of the chemical process. Alkylating agents were benzyl chloride, alkyl halides (from  $C_1$  to  $C_{16}$ ), 1-bromoadamantane, as well as methyl and ethyl esters of para-toluenesulfonic acid. It has been established that carrying out quaternization in a magnetic field of 300-400 Oe, even at room temperature, accelerates the reaction several times.<sup>1</sup>

As a result, several tens of QAC of various structures were obtained in high yields.<sup>2</sup> For one of the quaternary derivatives of 2-dimethylaminoethanol esters, technical specifications were developed (TU 6-06-32-465-83, All-Union Scientific Research Institute of Synthetic Fibers with an experimental plant, Tver), pilot batches were obtained and industrial tests were carried out as a textile auxiliary substance. Most of the synthesized quaternary salts are thermally stable at temperatures up to 180-200°C and higher, are highly soluble in water, have high surface activity and are effective antistatic agents for synthetic polymer materials.

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# ELECTRODEPOSITION OF ALLOYS FROM AQUEOUS SOLUTIONS OF HETERONUCLEAR COMPLEXES

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The aim of the work is to obtain data on the role of heteronuclear complexes and their electrochemical behavior in the production of alloys and corresponding coatings.

The processes of complexation in the following systems have been studied: zinc (II)-chromium (III)-nickel(II)-glycine-water. Heteronuclear complexes have been established  $\text{CrNiZn(HGly)}_4\text{Gl}_4^{3+}$  ( $\lg K = 1.01 \pm 0.32$ ), the constants of formation and the proportion of their accumulation depending on the pH.

The processes of complexation in the following systems have been studied: zinc (II)-chromium(III)-Co(II)-glycine-water. The compositions of heteronuclear compounds, the proportions of their accumulation and the constants of formation have been established:  $\text{CrCoZn(HGly)}_5\text{Gly}_3^{4+}$  ( $\lg K = 2.31 \pm 0.01$ );  $\text{CrCoZn(HGly)}_3\text{Gly}_5^{2+}$  ( $\lg K = -1.36 \pm 0.05$ ) и  $\text{CrCoZn(HGly)}_2\text{Gly}_6^{+}$  ( $\lg K = -4.23 \pm 0.09$ ).

By the method of removing polarization curves, the possibility of convergence of the potentials of the joint electrochemical reduction of metal ions in a heteronuclear compound is shown. As a theoretical justification for the convergence of electrode recovery potentials, some considerations are expressed, which are currently being confirmed. Thus, when filling molecular orbitals with electrons in a heteronuclear molecule, the orbital of a more electronegative atom makes a greater contribution to the binding orbital, and the orbital of a less negative atom makes a greater contribution to the loosening orbital, which reduces the overvoltage of the reduction of a more electronegative metal. In addition, an increase in the effective radius of complex heteronuclear ions in comparison with mononuclear compounds reduces the activation energy of their reduction. The elemental composition of the studied alloy sediments was determined by X-ray fluorescence analysis. It is shown that the alloy contains zinc, chromium, nickel, iron and manganese, while the other contains zinc, chromium, cobalt, iron and manganese with different ratios. Electrochemical measurements and determination of the mass index indicate a higher corrosion resistance of the coatings obtained in comparison with zinc coatings.



# CALS-TECHNOLOGY OF SCIENTIFIC RESEARCH FOR THE DEVELOPMENT OF ANTI-ICING REAGENTS AND ROAD IMPREGNATING COMPOSITIONS

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The solution to the problem of traffic safety on highways is associated with a complex of tasks, which includes the fight against winter slippery conditions with the use of anti-icing materials (AiM)<sup>1</sup> and maintaining road and sidewalks in optimal condition with special road impregnations (RI)<sup>2</sup> and hydrophobizing (HPI)<sup>3</sup> impregnations. The Computer-aided quality management systems (CQM)<sup>1</sup> are being developed to automate the procedure of analytical and environmental monitoring of road chemistry products.

With the help of CQM-system AiM analytical monitoring is carried out in the following information sections: chemical composition; quality indicators; methods of analysis; analytical instruments. The main quality indicators are grouped into 4 clusters: organoleptic, physico-chemical, technological and environmental<sup>1</sup>.

The use of AiM leads to negative environmental consequences. To address these problems, a CQM-system of environmental monitoring of AiM<sup>1</sup> was developed. Monitoring was conducted on the following objects: snow cover and water bodies; soil cover; green areas; atmospheric air.

Information CQM-systems have been developed for RI and HPI. For each type of impregnations the main subcategories are allocated, according to which impregnations of corresponding chemical compositions characterized by a set of quality indicators are grouped. The systematization of quality indicators by the proposed information clusters is carried out. The most promising methods of analysis and analytical equipment were added to the system architecture for each indicator.

The results obtained on the materials of road chemistry were included in the RFBR contracts № 16-07-00823 and № 18-29-24185mk, as well as in the reports on scientific contracts with the Department of Nature Management and Environmental Protection of Moscow.

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# THE CHEMISTRY AND TECHNOLOGY OF THE PHARMACOPOEIAL ASSORTMENT OF CHEMICAL REAGENTS AND HIGH PURITY SUBSTANCES

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The substances of reactive qualification and high purity<sup>1</sup> are widely used in the pharmaceutical industry. One of the main producers of these products is JSC «EKOS-1». The expansion of the range of reagents produced by the company is associated with the growth of pharmaceutical requirements for product quality, as well as with the tasks of import substitution. To solve these problems, a computer quality management system (CQM-system)<sup>2</sup> has been developed.

During the analytical monitoring, 3 groups of reagents produced by JSC «EKOS-1» were considered in the CQM-system: organic solvents, inorganic acids, custom reagents (more than 400 brands). The analysis is carried out for the 3 most promising Western firms (PanReac; Merck; Carl Roth). The analysis considers 5 pharmacopoeias: USP, DAB, JP, BP, Ph. Eur (USA, Germany, Japan, Britain, Europe).

The search algorithm is based on the fact that for each imported reagent for pharmacology, the same product is analyzed from the JSC «EKOS-1» assortment database available in the CQM-system. The search criterion is the maximum coincidence of quality indicators by name and numerical characteristics. In case of coincidence or exceeding of the quality indicators, the possibility (recommendation) of import substitution of the product without correction of the technological process is noted. In the case of differences in quality indicators between an imported reagent and its domestic counterpart, the directions of refining technology and analysis methods are noted (technical specifications projects, changes to existing technical specifications, appropriate analysis methods, etc. are being developed). The refinement is carried out at a pilot plant, which includes hardware modules for rectification purification, chemical treatment, adsorption purification and microfiltration.

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# FEATURES OF CHEMICAL APPLICATION OF Zn-, Cd-, Sn-CONTAINING FILMS FOR PHOTOVOLTAIC HETEROSTRUCTURES

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In photovoltaic thin-film heterostructures CdTe, complex chalcogenides, SnS are considered the most promising materials for the absorbing narrow-gap layer. Chalcogenides CdS and ZnS, as well as oxides ZnO, TiO<sub>2</sub>, SnO<sub>2</sub> and other semiconductors are being actively studied as wide-gap layers.

Our work presents the results of a study of wide-gap semiconductor films using the example of CdS and ZnO, as well as light-absorbing films using the example of SnS, obtained from solutions by chemical deposition (CBD), chemical layering (SILD) or electrochemical deposition (ECD), respectively.

The results of studying the resulting films showed that the wide-gap ZnO layers had a higher thickness of about 200 nm and a lower transmittance in the visible range (no more than 60%). Thinner CdS films (about 100 nm) were characterized by higher optical transmittance of about 70%. Light-absorbing SnS films with a thickness of 400-500 nm were characterized by a high absorption coefficient of the order of  $1.5 \cdot 10^4 \text{ cm}^{-1}$  and a band gap of 1.4 eV.

Sample designation	Preparation method	Film thickness, nm	Optical transmittance, %	Band gap, eV	Deposition rate, nm/min
ZnO	SILD	203	61	3,3	4,6
CdS	CBD	77	71	2,5	15,4
SnS	ECD	459	<	1,4	11,5

Thus, studies have shown that to obtain optically transparent homogeneous wide-gap films using CdS as an example, the chemical deposition method is preferable. For the deposition of thicker light-absorbing SnS films, the preferred method is pulsed electrochemical deposition, which allows the deposition of films close to the stoichiometric composition at a rate of more than 10 nm/min.

# THE INFLUENCE OF SHORT PULSE LASER TREATMENT ON THE FUNCTIONAL PROPERTIES OF COPPER ALLOYS

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The functional properties of copper and copper alloys determine their widespread use, including in the electrical field<sup>1,2</sup>. Factors of high humidity and aggressive production environments significantly reduce the corrosion resistance of products. A promising method is high-energy laser exposure to the surface, during which the composition and structure of the surface layer changes<sup>3,4</sup>. An essential characteristic remains the resistivity value.

**Table 1.** Parameters of samples in the initial state and after laser treatment

Material		Copper	Brass
Anodic dissolution currents I in the passive state area, $\mu\text{A}/\text{cm}^2$	before treatment	23,331	33,032
	after treatment	14,345	27,676
Contact resistance, $\text{ohm}/\text{cm}^2$	before treatment	0,092	0,054
	after treatment	0,037	0,024

The method of short-pulse laser processing makes it possible to obtain a nanolayer on the surface of copper and copper alloys, which provides increased corrosion resistance while maintaining an acceptable value of specific contact resistance.

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# SYNTHESIS AND STUDY OF PHYSICOCHEMICAL CHARACTERIZATION OF A NEW HETEROCYCLIC AZOPROISODIDE BASED ON 2,3,5,6-TETRAOXO-4-NITROPYRIDINATE AMMONIUM

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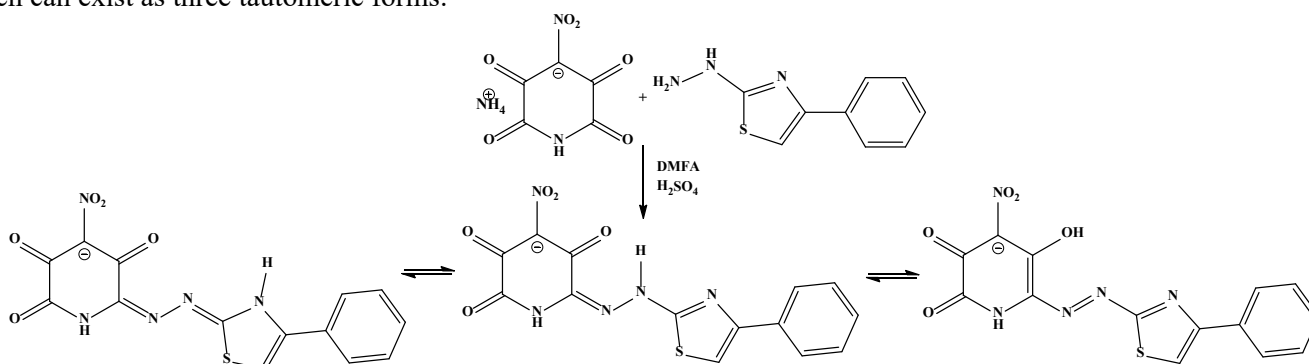
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Condensation of 2,3,5,6-tetraoxo-4-nitropyridinate ammonium with 2-hydrazino-4-phenylthiazole yielded a heterocyclic azo compound, (E)-4-nitro-2,3,5,5-trioxo-6-(2-(4-phenylthiazole)-2-yl)hydrozinyldene)piperidin-4-ide (HL), which can exist as three tautomeric forms:



According to elemental analysis and chromatography-mass spectrometry data, compound HL is individual and contains molecular ion  $M^+ = 358$ , which corresponds to the gross formula  $C_{14}H_8N_5O_5S$ .

In the IR spectrum of compound HL in the polycrystalline state in the region of  $3060\text{ cm}^{-1}$ , a broad band related to the valence vibrations of the hydrogen bonded N-H group is observed. The presence of absorption bands in the range of  $1654\text{--}1550\text{ cm}^{-1}$  indicate the valence vibrations of C=O and C=N groups of compound HL. In the  $^1\text{H}$  NMR spectra of compound HL in  $\text{CDCl}_3$ , the 6H signals of aromatic protons lie in the range of 7.2–8.5 m.d. The presence of a band at 11.8 m.d. corresponds to the position of the N-H bond of the hydrazogroup [1], and the peak at 9.8 m.d. can be attributed to the N-H bond of the tetraoxo-4-nitropyridine fragment. The data obtained indicate the existence of HL in the crystal-line state and in solution in the form of hydrazotautomer.

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# SORPTION OF CHLOROCOMPLEXES OF PLATINUM METALS BY CHEMICALLY MODIFIED SILICAS. SEPARATION THE RHODIUM-IRIDIUM PAIR

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At present, there is no doubt that sorption is the most promising method for the selective isolation of platinum metal (PM) ions from technological solutions of complex composition. In this regard, chemically modified silicas (CMS) become of particular importance as sorbents.

The presented report summarizes the data obtained by the authors on the sorption of PM ions from acidic chloride and sulfate-chloride solutions by silicas (Davisil Grade 62 (W.R. Grace Co., USA), fraction 0.07–0.2 mm). The silicas were modified with various polyethylenimines (PEI) [1]. The process was studied in statics and dynamics depending on the most significant factors: the ionic state and concentration of the metals in the solutions, acid concentration, H<sup>+</sup>, Cl<sup>–</sup>. The anion exchange mechanism of sorption of platinum metal complexes is substantiated. Reagents that provide quantitative elution of sorbed ions and methods for their isolation from eluates are proposed. It is shown that the proposed sorbents provide selective separation of Pt(IV), Rh(III) and Ir(IV) from the above media in their joint presence and against the background of non-ferrous metal ions.

It was found that the sorption properties of silicas modified with polyethylenimine, PEI (–CH<sub>2</sub>NHCH<sub>2</sub>CH<sub>2</sub>NHCH<sub>2</sub>–) and with polyethylenimine quaternized by methyl iodide, PEI-mn (–CH<sub>2</sub>N<sup>+</sup>(CH<sub>3</sub>)<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>N<sup>+</sup>(CH<sub>3</sub>)RCH<sub>2</sub>–) are similar to each other and with respect to [RhCl<sub>6</sub>]<sup>3–</sup> and [IrCl<sub>6</sub>]<sup>2–</sup> ions. The separation of this pair is possible only under dynamic conditions. Hexachloroiridate(IV) ion has a greater affinity for these sorbents, and therefore it is sorbed at the top of the chromatographic column. As the initial solution passes through, the Rh(III) zone is displaced, and the entire sorbent layer is gradually saturated with Ir(IV) ions. Complete separation can be achieved in a system of several columns connected in series depending on the content of valuable components in the solution.

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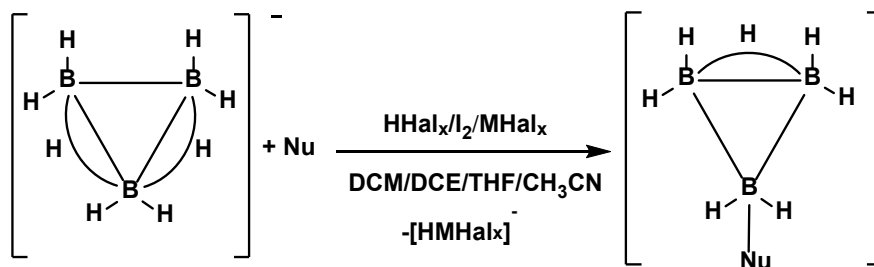
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# FEATURES OF SUBSTITUTION REACTIONS IN $[B_3H_8]^-$ ANION

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The aromatic structure of the  $[B_3H_8]^-$  anion allows it to enter into nucleophilic substitution reactions<sup>1</sup> along with the well-studied  $[B_{10}H_{10}]^{2-}$  and  $[B_{12}H_{12}]^{2-}$  anions. Such reactions occur in the presence of an electrophilic inductor capable of eliminating hydride hydrogen (iodine, bromine, Bronsted acids, metal halides) and proceed according to the well-known EINS mechanism.



In the course of this work, it was found that the highest yields of the substituted product result from the use of Ti(IV), Hf(IV), Zr(IV) chlorides in the case of O-, S-nucleophiles and nitriles. This reaction produced a series of substituted derivatives  $[B_3H_7Nu]$ , Nu = THF, dioxane,  $CS(NH_2)_2$ ,  $CS(N(CH_3)_2)_2$ , R-CN. However, in the case of using amines as a nucleophile, the formation of their strong complexes with metals occurs, which greatly reduces the yield of the product. In this case, the use of their hydrochlorides was found to minimize the formation of by-products. In this way, substituted derivatives  $[B_3H_7NH_2R]$ ,  $[B_3H_7NHR_2]$ ,  $[B_3H_7NR_3]$ , R = Et, Me, Ph,  $C_9H_{19}$ ,  $C_{16}H_{34}$  were obtained. Iodine and bromine are also effective inducers of substitution reactions in octahydrotriborate, but their use is hampered by the presence of reaction by-products, as well as a limited number of nucleophiles.

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*This work was supported by IGIC RAS state assignment*

# SYNERGISTIC COMPOSITIONS FOR INHIBITION OF STYRENE THERMAL POLYMERIZATION

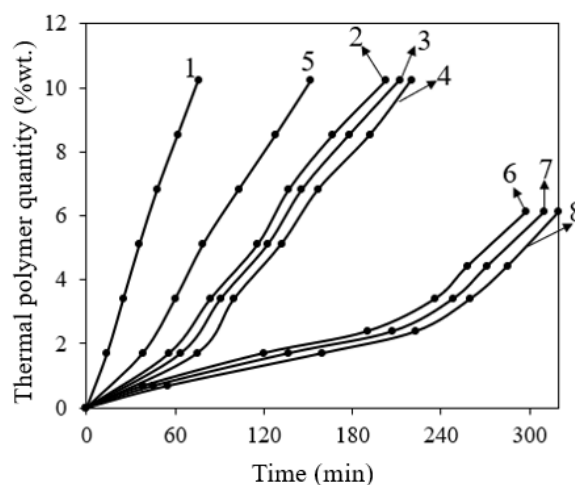
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Substituted phenols are used to inhibit polymerization during the isolation of monomers for polymer production. Their efficiency is not always sufficient. The aim of the present work was to study the effectiveness of a co-inhibitor for the process of inhibition of styrene polymerization. A compound with the property of an effective color stabilizer was used as a co-inhibitor.

2,6-di-tertbutyl-4-dimethylaminomethylphenol (OM) was used as the main polymerization inhibitor at an amount of  $10^{-3}$ - $10^{-1}$  %wt. Copper chelate was tested as a synergist at a concentration of  $10^{-9}$  %wt.

The dilatometric method was used to monitor the progress of styrene thermal polymerization. The efficiency of inhibition of styrene thermal polymerization was determined by the duration of the induction period before the appearance of 2 %wt. polystyrene in the system according to the method<sup>1</sup>. The experiments were carried out at a temperature of 120 °C in a nitrogen atmosphere. It was found that the induction period increased more than 2-fold when the co-inhibitor HM was introduced into the sample containing OM (Fig. 1.).



**Figure 1.** Effect of OM inhibitor ( $10^{-3}$  to  $10^{-1}$  %wt.) and co-inhibitor HM ( $10^{-9}$  %wt.) on the quantity polystyrene formed ( $T = 120^{\circ}\text{C}$ ): 1 - without inhibitor; 2 - OM ( $1 \cdot 10^{-1}$  %wt.); 3 - OM ( $1 \cdot 10^{-2}$  %wt.); 4 - OM ( $1 \cdot 10^{-3}$  %wt.); 5 - HM; 6- composition OM ( $1 \cdot 10^{-3}$  %wt.) + HM; 7 - composition OM ( $1 \cdot 10^{-2}$  %wt.) + HM; 8 - composition OM ( $1 \cdot 10^{-1}$  %wt.) + HM

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# EFFECTS OF NATURAL MODIFIED POLYMERS ON THE SWELLING CAPACITY OF VULCANIZATES

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Influence of partially carboxylated lignocellulose from rice straw (CMC-Rice) (composition:  $\alpha$ -cellulose – 89 %, lignin 6,7 %), chitosan (HTS) in comparison with sodium carboxymethylcellulose (Na-CMC) (degree of substitution 0,9) on the swelling ability of rubber in aqueous media of different mineralization and on its basic physical and mechanical properties was studied. Nitrile butadiene rubber is used as elastomeric matrix. The base rubber compound without swelling filler was prepared according to the standard rubber formulation for nitrile butadiene rubber. The amount of swelling polymer was 150 parts per 100 of rubber.

It was found that in mineralized model formation water the degree of swelling of rubber filled with CMC-Rice is comparable to the degree of swelling of rubber filled with Na-CMC; the tensile strength of the rubber increases. At partial replacement of Na-CMC by chitosan both in aqueous media of high mineralization and in aqueous media with low mineralization, the degree of rubber swelling decreases, but the strength characteristics increase (Tables 1, 2).

Table 1 – Degree of rubber swelling in model aqueous media

Ion content (g/dm <sup>3</sup> ) in model aqueous solution; density of aqueous solution	Composition of swelling filler		
	Na-CMC	Na-CMC: HTS (4:1)	CMC-Rice
	Swelling degree, % (25 days)		
Cl <sup>-</sup> (176), Na <sup>+</sup> (94), Ca <sup>+2</sup> (16), $\rho=1160$ g/dm <sup>3</sup>	53,7	43,9	55,1
Cl <sup>-</sup> (110), Na <sup>+</sup> (59), Ca <sup>+2</sup> (11), $\rho=1100$ g/dm <sup>3</sup>	66,9	50,6	68,2
Cl <sup>-</sup> (139), Na <sup>+</sup> (70), Ca <sup>+2</sup> (11), Mg <sup>+2</sup> (3), $\rho=1157$ g/dm <sup>3</sup>	70,5	54,7	74,6
Deionized water, $\rho=1000$ g/dm <sup>3</sup>	588,2	285,9	591,3

Table 2 – Physical and mechanical properties of rubbers

Properties	Composition of swelling filler		
	Na-CMC	Na-CMC: HTS (4:1)	CMC-Rice
Tensile strength, MPa	3,3	4,1	4,9
Elongation at beak, %	450	320	270

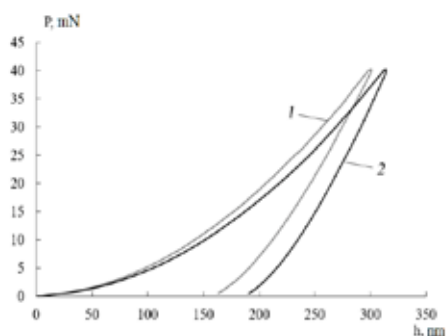
# HARDNESS ESTIMATION OF ZIRCONIUM CARBIDE CERAMICS

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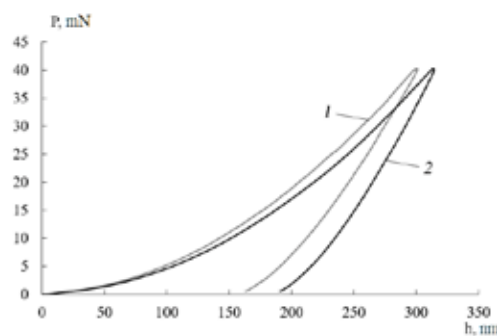
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Zirconium carbide is characterized by its refractory properties, low electrical resistance, hardness, and wear resistance.<sup>1</sup> The industrial methods of obtaining such materials are based on powder sintering, the complexity of which determines the high cost of the products. The technology optimization is achieved by using an oxidative constructing approach that allows the production of complex shape workpieces with the lowest energy consumption.<sup>2</sup>

Ceramics based on stoichiometric zirconium carbide were synthesized by direct carburization of zirconium rolled ribbon in an atmosphere of a mixture of ethylene and argon. The metal was heated at a constant rate to 2100 °C and held at this temperature for 180 minutes. The mechanical properties of obtained carbides were studied by nanoindentation measurement.



**Figure 1.** SEM images illustrating the morphology of a transverse fracture surface of zirconium carbide



**Figure 2.** P-h diagrams constructed by indenting the transverse cleavage of a zirconium carbide sample at a distance from the surface of 10 microns (1) and 110 microns (2).

The process of carburization appears to be a two-stage process of carbide formation due to the differences in nano-hardness in the surface layer and in the bulk of the samples. The hardness levels in the surface layer correlates with the hardness values of gas phase coatings, while the bulk hardness is comparable to the value for ceramics obtained by sintering powders.

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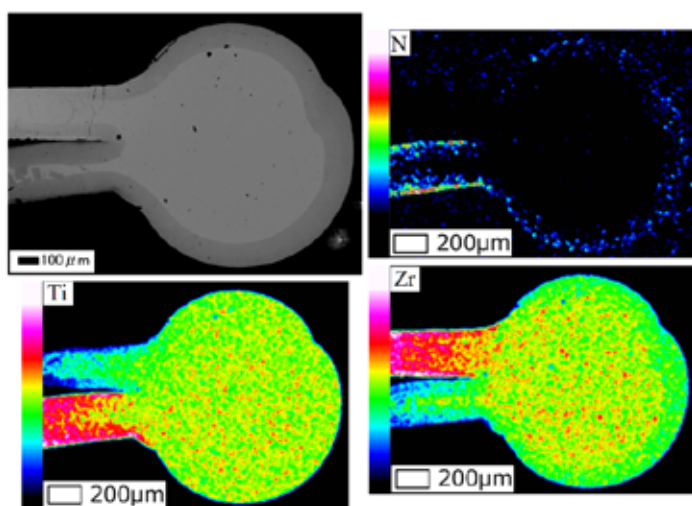
# FEATURES OF NITRIDIZATION OF SOLID SOLUTIONS BASED ON METALS OF THE Ti AND V SUBGROUPS

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The synthesis of thermoelectric converters based on binary nitrides of titanium and vanadium subgroups<sup>1</sup> by oxidative construction<sup>2</sup> and the study of their thermoelectric characteristics is of considerable interest and is a promising direction.

Nitridization of metals of the Ti and V subgroups proceeds through the formation of three and two-layer gradient structures followed by the formation of ceramics of stoichiometric composition. The nitridization process of a bimetallic solid solution in the junction region is determined by the chemical affinity of metals to nitrogen. The reaction of titanium with nitrogen leads to the decomposition of the Ti-Zr solid solution and the separation of zirconium metal at the grain boundaries. The nitriding of zirconium begins in the process of reducing the amount of titanium in a solid solution.



**Figure 1.** Optical image of the surface of the transverse nitridization strip of the alloy,  $T=1900^{\circ}\text{C}$ , 50 minutes and a map of the distribution of element concentrations over the surface of the sample.

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# ON THE IDENTIFICATION OF FERRITES BY MOSSBAUER ISOMER SHIFTS

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*Materials based on iron oxides play an important role in modern electronics. These materials can be created from binary oxides such as  $\text{Fe}_2\text{O}_3$  and  $\text{Fe}_3\text{O}_4$  or from sophisticated oxides (ferrites) such as  $\text{BaFe}_{12}\text{O}_{19}$ . Ferrites have various structures and properties that make them suitable for different applications.*

Mossbauer spectroscopy is a valuable technique for studying ferrites. This technique allows researchers to perform phase analysis and investigate the magnetic and other properties of the materials. Within the crystal lattices of ferrites, iron may occupy several crystallographic sites. A correct interpretation of the components of a Mossbauer spectrum is essential for understanding the processes occurring in a material.

An important parameter of the Mossbauer spectrum is the isomer shift. It has been established that the dependence of the isomer shift on the average Fe-O interatomic distance in iron oxocompounds (oxides, silicates, phosphates, etc. salts, as well as organic compounds) is well approximated by straight lines with a slope of approximately  $0.04 \text{ mm}\cdot\text{s}^{-1}\cdot\text{pm}^{-1}$ . A quantitative assessment of the isomer shift by the average Fe-O interatomic distance and vice versa provides good practical results, as it is noticeably easier than known approaches and has predictive capability.

The accuracy of the isomer shift estimation can be improved by considering the effect of polarization of oxygen ions forming the iron coordination polyhedron. The effect can be qualitatively assessed based on the structure of the substance using a simple electrostatic approach.

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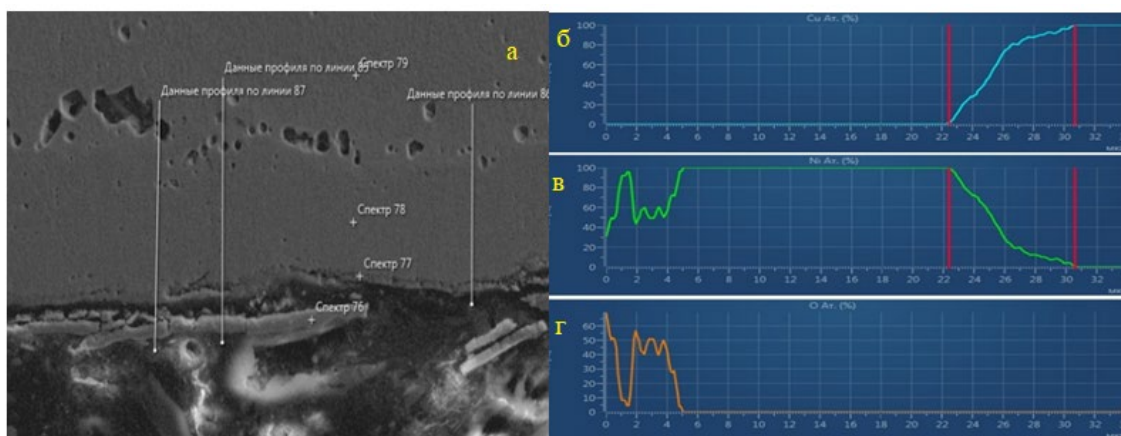
*The study was supported by the Russian Science Foundation, project no. 24-13-00268, <https://rscf.ru/en/project/24-13-00268/>.*

# GALVANIC PRECIPITATION OF NICKEL UNDER HIGH TEMPERATURE OPERATION CONDITIONS

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A nickel coating obtained from a cold nickel plating colloid electrolyte of optimal composition was studied for the purpose of applying it to industrial copper products, as an effective way to combat the oxidation of the external surface of products under conditions of superheated steam at high temperatures<sup>1,2</sup>. The studies were carried out on a dual-beam scanning electron microscope SEM Crossbeam 340.



**Figure 1.** Electronic image of the cross section of a sample with a nickel coating obtained from an electrolyte of optimal composition - a; diagram of element concentration along the depth of the sample: b – copper; c – nickel; g – oxygen

The conducted studies showed that the studied galvanic nickel deposit fulfilled its task of protecting against oxidation and resistance to copper diffusion under high-temperature operating conditions.

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# FORMATION OF A NEW CALCINITE PHASE IN A CONCRETE MATRIX BY BIOMINERALIZATION

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Modern concrete structures suffer from a disadvantage associated with shrinkage and fatigue, such as the formation of microcracks during their operation. This may compromise their technical and functional suitability due to a possible decrease in durability, which may lead to a decrease in the bearing capacity of the structure. In recent years, experimental studies on biomineralization have shown the potential to solve this problem.

Biomineralization is a process in which microorganisms induce the production of calcium carbonate, which can improve the ability to heal itself by filling microcracks and pores in structures, similar to traditional materials.

The most common method of biomineralization is the hydrolysis of urea, which is caused by the enzyme urease secreted by ureolytic bacteria. Despite numerous laboratory studies that have yielded positive results, a number of limitations still prevent the widespread introduction of this technology into practical use.

The purpose of this work is to show the possibility of forming a new phase of calcinite in cement matrices using biomineralization.

The calcinite phase was formed using a number of isolated strains of bacteria *Sp. pasteurii*, *B. Sphaericus*, *B. Pseudofirmus*. Bacterial strains were previously immobilized by encapsulation using various agents. The improvement of concrete properties due to the inclusion of bioadditives was associated with calcite deposition and the presence of bacterial biomass in the pores of the concrete matrix. Microstructural studies have also shown that concretes made using bacteria have a greater calcite formation compared to the additive-free matrix. An assessment of formations with the use of RFA was also carried out. The results of the study showed that the use of pure cultures of microorganisms can be used to improve the properties of cement matrices, reduce the formation of cracks and improve the properties of concrete, which will be used for the construction of various infrastructure facilities.

# LOW TEMPERATURE OXIDATION OF BENZYL ALCOHOL IN THE PRESENCE OF MESOPOROUS MOLYBDATE- SUBSTITUTED HYDROXYAPATITE

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**Leonov A.V.**<sup>b</sup> **Konovalov A.A.**<sup>a</sup> **Akopyan A.V.**<sup>b</sup> **Barinov S.M.**<sup>a</sup> **Komlev V.S.**<sup>a</sup>

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Hydroxyapatite (HA) is a stoichiometric calcium phosphate with the chemical formula  $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$ . Due to its mesoporous structure, it is able to show high efficiency as a heterogeneous catalyst in various reductive and oxidative reactions, including in the presence of hydrogen peroxide. Molybdenum peroxo-complexes are effective liquid-phase catalysts for oxidation reactions, including epoxidation of olefins<sup>1</sup>, oxidation of sulfides and alcohols.

Powders containing 0; 1.0; 2.5; 5.0; 10 mol%  $\text{MoO}_4$  were prepared by co-precipitation from solutions. The obtained materials were investigated by XRD, IR spectroscopy, BET and TEM and their catalytic activity was also investigated.

The obtained materials were both single phase materials and composites based on HA and  $\text{CaMoO}_4$ . As the concentration of molybdate ion increased, the particle size increased and the shape changed from rounded to elongated rod-shaped.

The SSA of the powders increased from 87.8 to 121.1  $\text{m}^2/\text{g}$ , and the shape of the hysteresis loop corresponded to type IV, indicating a predominant mesoporous structure.

In the study of catalytic activity, the best performance was obtained by the material containing 2.5mol%  $\text{MoO}_4$ . The conversion reached 59%, and the activity of the catalyst was maintained during 3 cycles of reuse, indicating the stability of the powder.

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# HYDRATION OF POLYMERIC SYNTHETIC SORBENTS AS A CONTROL PARAMETER OF THEIR SELECTIVITY

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The problem of selectivity is crucial when choosing industrial sorbents for solving the practical problems of isolation, separation, concentration of components. The existing theories of selectivity are based on a thermodynamic approach and have a formalized nature, which does not make it possible to clearly establish the chemical nature of the bonds between the sorbent and the sorbate.

The paper attempts to establish a relationship between the selectivity of sorbents used in aqueous media and the characteristics of their hydration. The assessment of the effect of changes in sorbent hydration during the transition from the initial to the working form on selectivity was carried out using two approaches. The thermodynamic characteristics of the complete swelling of the ionic forms of sorbents and the quantitative characteristics of the distribution of energetically inhomogeneous water in ion exchangers are determined. As a result, the dependence between the selectivity constants and the energy characteristics of the sorbent hydration was obtained. Ion exchangers with various functional groups and known ranges of selectivity to transition metal ions established by traditional methods were used as objects of research.

In general, it is known that the value of the selectivity of the ion exchanger to the extracted ion is a function of the average amount of water per active group. The paper establishes the relationship between the selectivity of polar sorbents and the characteristics of their hydration in various forms, determines the equilibrium characteristics of hydration, including Gibbs energy and enthalpy of hydration, ion-exchange resins and fibers in various ionic forms, establishes the amounts of kinetically inhomogeneous water and identifies the controlling symbiotic parameters of the two processes. The exchange of cations on polyampholites in sodium form is accompanied by a restructuring of the first hydrate shell of the functional groups of the ion exchangers, small values of the Gibbs energy of interphase water transfer, a decrease in the total amount of hydrated water and an increase in the hydration energy of polyampholites during the transition to the form of the extracted cation. The results obtained will further predict the effectiveness of the sorbent and facilitate the task of selecting a material for the isolation or separation of target components.

# ALKALINE ION ACTIVATOR FOR THE CHEMICAL COPPER PLATING PROCESS IN PRINTED CIRCUIT BOARD PRODUCTION

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The most important process of the metallized transition stage in printed circuit board (PCB) manufacturing is chemical copper plating, which is necessary to create an electrically conductive copper sublayer 0.3- 1.0  $\mu\text{m}^1$  thick on the dielectric surface of PCB holes prior to subsequent electroplating.

Before the electroless deposition of copper, the dielectric surface is activated with acidic (colloidal) or alkaline (ionic) palladium-containing activators after cleaning and conditioning. As a result of the treatment in the activation solution, catalytically active centers of metallic palladium are created on the dielectric surface. The advantages of the alkaline activator are high wettability of the dielectric, which facilitates penetration of the solution into small holes of the PCB, as well as homogeneity and uniformity of the palladium layers formed and, consequently, lower consumption of the precious metal.

Ionic activation systems are alkaline solutions containing complex compounds of divalent palladium with an organic ligand.

At MUCTR, an ionic alkaline activator is being developed, which contains:  $\text{PdCl}_2$  – 0,001-0,002 mol/l,  $\text{HCl}$  – 0,06-0,08 mol/l,  $\text{H}_3\text{BO}_3$  – 0,02-0,03 mol/l, heterocyclic nitrogen-containing compound as an organic ligand – 0,002-0,003 mol/L, as well as  $\text{KOH}$  – to bring the pH to 10-11.

The developed activator makes it possible to form continuous electroless copper coatings on the walls of printed circuit board holes, the continuity of which is assessed with the maximum score according to the international backlight test<sup>2</sup> scale.

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# SYNTHESIS OF COMPLEX COMPOUND $\text{Fe}^{2+}$ WITH QUERCETIN AND STUDYING ITS STABILITY

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This article is devoted to the synthesis of the complex compound  $\text{Fe}^{2+}$  with quercetin and the study of its stability.

The synthesis was carried out at room temperature by mixing a solution of 0.120 g of quercetin ( $\text{C}_{15}\text{H}_{10}\text{O}_7$ ) in 25 ml of methanol and 0.055 g of  $\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$  in 10 ml of methanol. The mixture was continuously stirred in a reflux water bath at  $60^\circ\text{C}$  for 2 hours and then cooled.

The resulting dark brown precipitate was washed with water, then with methanol to remove unreacted  $\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$  and quercetin and dried.

To study the stability of the  $\text{Fe}^{2+}$  complex compound with quercetin using an isomolar series, a series of experiments were carried out by varying the ratio between the metal ion and the ligand at a constant total concentration.

Based on the data obtained, the stability constants of the complex compound ( $\beta$ ) were calculated (see table).

Table  $\beta$ -stability constants of the  $\text{Fe}(\text{II})$  complex in various media

№	pH	273 nm	402 nm
1	2,0	0,00210	0,00208
2	4,0	0,00314	0,00261
3	6,0	0,00224	0,00227
4	7,0	0,00194	0,00204
5	9,0	0,00207	0,00277

Based on the data in the table, it can be noted that the influence of the solution environment on the stability of the complexes is insignificant, and the bonds in the resulting complexes are predominantly covalent and non-covalent, that is, supramolecular systems.

# USE OF CARBON NANOTUBES IN POWDER LABELLING

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The highly developed surface structure of carbon nanotubes allows them to be used in marking gunpowder and establishing an operational type of ammunition. Previously, a method for marking gunpowder with carbon nanotubes (CNT) was developed<sup>1</sup>. Atomic force microscopy analysis of traces of gunpowder combustion products and ugleode nanotube material revealed a variety of ag-lomerates on the surface of carbon nanotubes<sup>2,3</sup>.

The main parameters of the mechanism of sorption of aluminum, lead and antimony on the surface of CNT with various edge modifies were determined<sup>4</sup>. In this work, using the methods of a computer model, the interaction of metals (tin, iron, copper, magnesium), which are part of the products of a shot with an arm-chair molecular cell-ster (6.6), was investigated. The main parameters of the mechanism of adsorption of these metals on the outer surface of the CNT were studied, and the process of filling the tubulene cavity was also studied. The analysis of energy curves, the interaction of metals with CNT found that in all cases there is an adsorption of metals on the surface of nanotubulene and the inner cavity of the tube is filled with metal data.

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# DEVELOPMENT OF THE HEAD-END STAGES FOR REPROCESSING OF NEW TYPES OF FUEL AS APPLIED TO RT-1 PLANT TECHNOLOGY AND THEIR TESTING AT THE OPERATING FACILITY

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The RT-1 plant is one of the few operating plants worldwide dealing with reprocessing of spent nuclear fuels. Until the end of the 20<sup>th</sup> century, it reprocessed spent fuel assemblies from VVER-440, BN-350, BN-600 and research reactors in the form of aluminum-clad uranium dioxide, as well as several types of propulsion reactor spent fuel. However, since the beginning of the 21<sup>st</sup> century, the need has become obvious to reprocess the stored SNF from many other reactors varying in fuel compositions and auxiliary materials used in the manufacture. To involve such kind of fuels in reprocessing, it was necessary to adapt the basic technology of the RT-1 plant.

The RT-1 process includes the following stages: fuel cutting, fuel dissolution in nitric acid, solution clarification and PUREX process extraction. After dissolution, target actinides (U and Pu) are in the same chemical form regardless of the initial SNF type. In this regard, optimization of the extraction stage is not necessary, with rare exceptions. Thus, to involve a new type of fuel in the reprocessing, it is sufficient to optimize the parameters of its cutting and dissolution.

In this connection, a set of experimental and analytical works was carried out to determine safe conditions for new fuel cutting and dissolution. Uranium-beryllium, nitride, magnesium- and zirconium-containing fuels, uranium metal fuel, as well as such material as chips of unirradiated uranium metal were involved in reprocessing. Features of the reactions of these materials with nitric acid have been determined, methods for elimination of negative aspects of the process have been proposed.

In all cases, the adapted processes of material cutting and dissolution ran routinely, without deviations. As a result, the work has proposed a generalized algorithm for solving problems related to the adaptation of the RT-1 plant technology to the reprocessing of other prospective types of spent fuel.

The implementation of the program represents an important milestone of the strategic objective of creating a universal fuel recovery facility on the basis of the RT-1 plant.



# ON APPLICABILITY OF THE MATERIALS USED FOR 3D PRINTING IN AGRICULTURE

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Agriculture is the most important area of human production activity. Due to the seasonal nature of the work, continuity in the production cycle is critical. One of the most powerful methods of production and manufacturing in the last decade has been 3D printing (or additive manufacturing). Thanks to the ability to create rapid prototypes, additive technologies are showing great promise for use in agriculture to produce parts to replace failed equipment. 3D printing allows new equipment to be developed and existing equipment to be adapted to local conditions (climate, terrain, soil type). In addition, the use of additive technologies contributes to the transition to precision agriculture by enabling timely processing on a specific site. Finally, 3D printing technologies provide the link between precision and digital agriculture, as well as the concept of the Internet of Things.<sup>1</sup>

Currently, one of the most common 3D printing methods is Fused Deposition Modelling (FDM), due to the wide range of materials used and the low initial cost of printers. In this work, the applicability of materials used in FDM 3D printing for agricultural needs and strategies to improve print quality were analyzed.<sup>2,3</sup>

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# OBTAINING MICROPOWDERS OF TUNGSTEN PSEUDO-ALLOYS WITH SPHERICAL SHAPE OF PARTICLES FROM NANO-SIZED COMPONENTS

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Currently, an urgent task is to develop approaches to the formation of nanocrystalline or submicron internal structures in tungsten pseudo-alloy materials. One of them is the additive manufacturing technologies of metal products, in particular, those using composite micro powders with spherical particle shapes as materials. A.A. Baikov Institute of Metallurgy and Materials Science RAS (IMET RAS) is one of the leading organizations in the Russian Federation, where active research and development of design and technological schemes of plasma processes, as well as equipment for the production of nano-sized, spherical powders of various materials in thermal plasma, is carried out<sup>1</sup>.

The paper presents the results of experimental studies of the processes of obtaining micro powders of tungsten pseudo-alloys of the W-Ni-Fe and W-Cu systems with spherical particle shape in an installation for plasma spheroidization of metal powders. Nanopowder microgranules of the W-7wt.%Ni-3wt.%Fe and W-20wt.%Cu systems of the «-50 μm» and «+50-125 μm» fractions, obtained by granulating the nanopowder product of the plasma-chemical synthesis process, were used as precursors. The possibility of obtaining a product with high technological properties has been shown (W-Ni-Fe: fluidity 6÷10s/50g, bulk density 8÷9.4 g/cm<sup>3</sup>; W-Cu: fluidity 10÷15s/50g, bulk density 4÷7 g /cm<sup>3</sup>), with a high degree of particle spheroidization up to 98%, with a dense, pore-free submicron internal structure.

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# BIOMEDICAL MATERIALS BASED ON CALCIUM PHOSPHATES PREPARED USING 3D-PRINTING

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Ceramics made of tricalcium phosphate (TCP,  $\text{Ca}_3(\text{PO}_4)_2$ ) is used in medicine to repair damaged bone tissue. The ceramics osteoconductive properties are determined by the presence of macropores connected system (at least 100 microns in size) necessary for the circulation of body fluids, as well as for the osseointegration of the implant with the surrounding bone tissue. To create ceramics with a porous structure, the stereolithography method is used to produce ceramic samples with a given architecture.

TCP was synthesized by precipitation method followed by heat treatment at 900 °C. The resulting TCP powder was mixed with an acrylic photopolymer composition optimized for 405nm radiation in a ratio of 60:40 by weight. 3D printing of the material was carried out using an LCD printer on a fluoroplastic tape.

To remove the polymer and sinter the ceramics, firing was carried out at temperatures of 1100 and 1200 °C.

To determine the biocompatibility of the obtained materials, in vitro studies were conducted on a stem cells cultured from tooth pulp. The materials was found to be biocompatible.

Thus, the resulting ceramics are promising for use in medicine to repair damaged bone tissues.

*The synthesis of TCP and the characterization of the obtained samples were performed within the framework of State Task No. 075-00320-24-00*

*Stereolithographic 3D printing was carried out within the state assignment of NRC «Kurchatov Institute».*

*In vitro tests were performed according to State Task No.075-01025-23-01.*

# SYNTHESIS OF $\text{CoFe}_2\text{O}_4$ BASED ON SAPONINS AND THEIR TEXTURE CHARACTERISTICS

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The magnetic properties of  $\text{CoFe}_2\text{O}_4$  nanoparticles can be used for selective destruction of cancer cells and targeted drug delivery.

The synthesis of  $\text{CoFe}_2\text{O}_4$  was carried out using Zol-Gel technology using solutions of  $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ ,  $\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$  in ethanol, and saponins as surfactants.

The surface morphology of the magnetic material was studied using an atomic force microscope (Fig. 1).

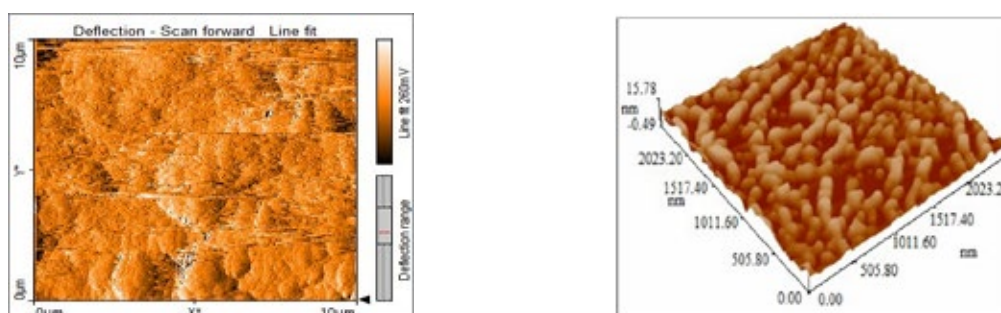


Fig.1. 2D and 3D view of the surface of the magnetic material  $\text{CoFe}_2\text{O}_4$  in AFM

From Fig. 1 it is clear that the surface of magnetic materials is inhomogeneous and porous, and the particles on the surface are monodisperse and of the same size.

The specific surface area, pore size, average pore diameter, monolayer capacity and adsorption capacity values were calculated using the BET equation.

An increase in temperature led to an increase in the average pore diameter and a decrease in the specific surface area. It was found that 8.57% of benzene vapors are adsorbed on the monolayer at 50°C, and 6.67% at 90°C.

# CERAMICS AND COATINGS ON TITANIUM IMPLANTS MADE OF CATION-SUBSTITUTED TRICALCIUM PHOSPHATES

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To increase biocompatibility and to improve osseointegration of metal implants the formation of calcium phosphate coatings on their surface is used. The antibacterial ions ( $\text{Mn}^{2+}$ ,  $\text{Cr}^{3+}$ ,  $\text{Cr}^{2+}$ ) into the structure of tricalcium phosphate (TCP,  $\text{Ca}_3(\text{PO}_4)_2$ ) can give coatings antibacterial activity and increase their bioresorbability in the body.

The purpose of this work is to synthesize and study the physical and chemical properties of double substituted TCP doped with  $\text{Sr}^{2+}$  and  $\text{Mn}^{2+}$  or  $\text{Gd}^{3+}$  ions, to make targets and to obtain coatings from this targets on titanium substrates and to study the phase composition, microstructure and biocompatibility of coatings *in vitro*.

TCP and double substituted TCP were synthesized by the solid-phase method at 1200°C and by precipitation from an aqueous solution followed by heat treatment were used as targets. Ceramic targets with a diameter of 20 mm were pressed and sintered in a chamber furnace with silite heaters at 1200°C for 2 hours. The phase composition of sintered targets is represented by a single phase – whitlockite. According to the results of SEM and EDX, it was found that dopants are distributed evenly in the samples.

*In vitro* biological studies have shown that ceramics made of double substituted TCP doped with gadolinium and strontium ions, as well as manganese and strontium, are biocompatible: when studying the biocompatibility of samples on NCTC clone L929 cells. It was shown that they did not have an inhibitory effect on cells. So, these materials can be used in medicine.

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



# PECULIARITIES OF PHASE FORMATION IN HYDROTHERMAL SYNTHESIS OF TUNGSTATE- CONTAINING HYDROXYAPATITE, PROMISING FOR APPLICATIONS IN CATALYSIS

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Hydroxyapatite (HA), one of the least water-soluble calcium phosphates widely used in biomedicine for the replacement of bone tissue defects<sup>1</sup>, has recently been considered as a promising catalyst for various processes, including oxidation reactions<sup>2</sup>. This is due to the presence in the structure of HA of both alkaline and acidic centers that are important for the oxidation reaction, which can be further modified by cationic and anionic substitutions in the HA structure. The high thermomechanical stability of HA, the ability to ion-exchange and adsorption behavior, and the exposure of oxygen and hydroxyl groups of the lattice<sup>3,4</sup> should be noted. A promising field of application necessitates research on the introduction of anionic substituents that are unusual among those studied for biomedicine, such as molybdate, tungstate and several others.

In the present work the data on hydroxyapatites obtained under hydrothermal conditions containing tungstate anions in the amount of up to 5 mol.% are presented. The peculiarities of phase formation, microstructure, textural characteristics depending on the modes of hydrothermal treatment are considered.

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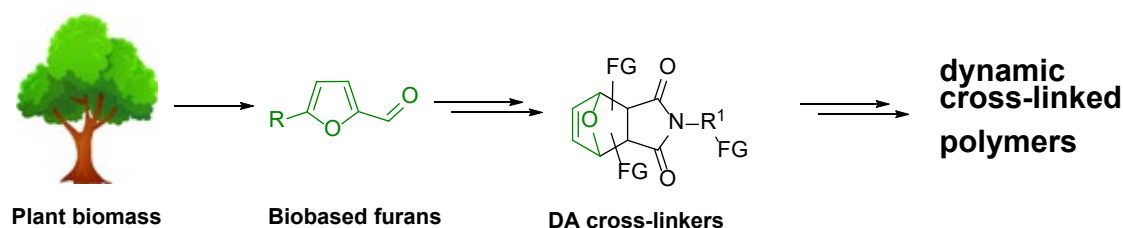
# NEW THERMALLY RESPONSIVE CROSS-LINKED POLYMERS BASED ON RENEWABLE FURANS

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It is believed that a new technological level is currently being actively formed, which is characterized by active automation and digitalization of many spheres of life. Various unmanned technologies and autonomous systems are being introduced that require virtually no human intervention. The creation of automated systems often requires polymers that themselves have a high degree of autonomy. These are so-called “smart” polymers, capable of self-organization, self-healing, have shape memory and other practically useful properties. Several types of such polymers can be produced using renewable plant feedstocks, including those based on the reversible Diels-Alder reaction of renewable furans with maleimides. [1,2] Following this concept, we have developed a new approach to obtain smart materials from bio-based feedstocks using previously undescribed “cross-linkers” derived from renewable furans.



As a result, dynamic cross-linked thermosets were obtained, which under the influence of temperature can “unfold” into a linear thermoplastic. Due to their high fluidity when heated, such polymers can be used to produce various thermally responsive materials, such as films, adhesives, sealants, hydrogels, etc.

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## SYNTHESIS OF IDOMETHANE

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Dimethyl disulfide (DMDS) is widely used as a sulfidating agent for catalysts of hydrogenation processes and an inhibitor of coke formation of pyrolysis in the production of lower olefines<sup>2</sup> and in scientific experimental practice.

The synthesis of DMDS is based on the oxidation reaction of methyl mercaptan, which is formed by the interaction of methyl halides with hydrosulfides of alkaline earth metals.

One of the key reagents is methyl halide, which is most often used as iodomethane.

The production of iodomethane is based on the acid-catalyzed reaction of methanol and potassium iodide.

A concentrated solution of sulfuric acid was gradually introduced into an aqueous solution of potassium iodide with constant stirring and a temperature not exceeding the boiling point of methanol. After that, the resulting solution was gradually heated from 90 to 120 degrees for 4 hours. Iodomethane was decanted from the resulting mixture, dried, and its yield was determined.

With an increase in the amount of methanol introduced into the reaction mass, the yield of the target reaction product increases, reaching a maximum with a molar ratio of methanol : potassium iodide equal to 6.

However, the yields of iodomethane are low due to the side reaction of the formation of molecular iodine, which volatilizes from the reaction mass. To prevent iodine loss from the reaction mass, a special technique was used, consisting in the introduction of iodine-binding additives. A number of compounds of various natures were used, the most active of which was a mixture of the cubic residue of benzene rectification (KORB) with polystyrene dissolved in benzene. Introduction of 10% by weight. this addition to the reaction mass of iodomethane synthesis allowed to increase the yield of the target product from 30 to 61.4%.

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# SELECTION OF STRUCTURING AGENTS FOR MODIFICATION OF SILICATE BINDER ZINX SILICATE ANTI-CORROSIVE COATING

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Zinc-rich anti-corrosion coatings are a two-component system consisting of a solid phase of fine zinc powder and a high-modulus silicate binder. These coatings have proven themselves in the oil and gas industry, where they are successfully used to protect pipelines from underground corrosion in various coating systems as a primer layer [1]. Indirectly, the physical and chemical properties of the coating (higher silicate modulus, reduced drying time and interlayer drying, wear resistance, heat resistance) are largely determined by the structure of the final coating. To control such a structure, it was of some interest to try various organic structure formers.

Structure formers based on phthalic acid dibutyl ester (DBP) and adipic acid esters (DEAC) were chosen as the object of study.

As a result, it was found that with the introduction of DBP starting from 0.1% by weight, a noticeable (visually) gelation process began.

When up to 0.5% by weight DEAC was introduced into the silicate system, no destructive effect on silicate was observed, the density remained at the level of 1.8 kg/m<sup>3</sup>, and the viscosity did not exceed 20 s according to GOST 9070-75.

Thus, we can conclude that it is impossible to use DBP as a structure-forming agent in two-component zinc-filled systems, in contrast to the silicate binder composition we previously developed, with a structure-forming component based on adipic acid esters ((DEAC) [2].

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# MECHANISM OF FORMATION OF THE $\text{Cr}_2\text{Ta}$ PHASE BY METALTHERMAL SYNTHESIS

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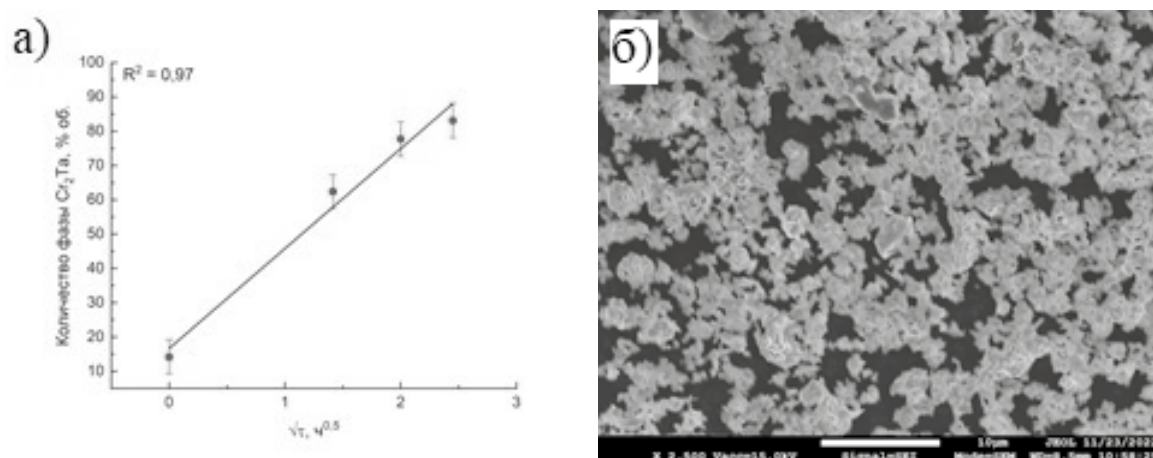
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The purpose of this work was to determine the mechanism of formation of the intermetallic compound  $\text{Cr}_2\text{Ta}$  (Laves phase) during the hydride-calcium reduction of the oxides  $\text{Cr}_2\text{O}_3$  and  $\text{Ta}_2\text{O}_5$ .

It is known that if the increase in the amount of phase is directly proportional to the square root of the interaction time, then this is a diffusion process<sup>1</sup>.

The diffusion nature of the synthesis of the  $\text{Cr}_2\text{Ta}$  phase is illustrated in Fig. 1a. This means that the formation of the  $\text{Cr}_2\text{Ta}$  phase is controlled by solid-phase diffusion. With this morphology, the resulting  $\text{Cr}_2\text{Ta}$  particles inherit the form of reduced Ta particles, which has a spongy structure<sup>2</sup>.

The activation energy of phase formation, calculated using method<sup>3</sup>,  $E_a = 291 \pm 69$  kJ/mol, in a number of sizes corresponds to the activation energy of heterodiffusion in various Laves phases and especially close to the  $\text{Cr}_2\text{Nb}$  compound ( $E_a = 291$  kJ/mol).



**Figure 1.** Dependence of the increase for  $\text{Cr}_2\text{Ta}$  phase on the square root of calcium hydride synthesis over time (a) and the morphology of the synthesized  $\text{Cr}_2\text{Ta}$  powder (b)

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# OBTAINING WEAR-RESISTANT SUPERHYDROPHOBIC COATINGS ON THE SURFACE OF THE AMg6 ALLOY

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One of the ways to protect metal surfaces from a corrosive environment that recently gained popularity is the creation of continuous surface films that feature water-repellent properties and the self-cleaning ability (the so-called superhydrophobic films).

A known drawback of chemically produced superhydrophobic coatings (SHCs) is their low wear resistance. In this study, we examined the possibility of enhancing the wear resistance of SHC by preliminary anodic oxidation of aluminum and its alloys<sup>1</sup>.

An electrolyte for anodic oxidation of the surface of an AMg6 aluminum alloy containing 15 wt.%  $H_2SO_4$  and 15 wt.%  $H_3PO_4$  was developed. It was found that anodizing in the electrolyte based on sulfuric and phosphoric acids results in the formation of anodic oxide films with the required well-developed microstructured relief<sup>2</sup>. The surface of anodized aluminum mainly contains pores with a diameter of 17.7–30.9 nm and a specific area of 0.15 m<sup>2</sup>/g.

It has been found that the preliminary anodizing of the aluminum surface leads to an increase in the adhesion strength with the next SHC and, consequently, to an increase in its wear resistance.

It was found that an increase in the concentration of stearic acid in the hydrophobizing solution to 4 g/L led to a significant increase in the contact angle of the surface up to 170°.

Corrosion tests in a salt fog chamber showed that the developed coating withstands 830 hours in salt fog (5% NaCl) before the first centers of corrosion of the substrate appear, while the untreated aluminum alloy begins to corrode after 22 hours of exposure.

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# OBTAINING NICKEL NANOPARTICLES ON THE REDUCED GRAPHENE OXIDE SURFACE

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Reduced graphene oxide (RGO) is a nanomaterial obtained by chemical or thermal reduction of graphene oxide, which is increasingly attracting the attention of scientists due to its unique properties and application prospects. RGO contains functional surface groups, most often located at the edges of flakes and carbon layer defects, which can act as active centers for the nanoparticles deposition on the RGO surface during composites synthesis. Nanocomposites based on nickel nanoparticles are actively used in various practical applications<sup>1</sup>. Therefore, maintaining their dispersity and homogeneity during the deposition onto the reduced graphene oxide substrate surface is of crucial importance.

The present study demonstrates a new method for obtaining a composite based on nickel nanoparticles on the reduced graphene oxide surface using supercritical isopropanol. The reduction of graphene oxide in a supercritical media is an accessible, scalable, inexpensive and environmentally friendly technique. It has been shown, that when a graphene oxide with previously incorporated  $\text{Ni}^{2+}$  salt is treated by the isopropanol at the supercritical conditions, nickel organic salt is reduced to  $\text{Ni}^0$ , with simultaneous deoxygenation of the graphene oxide substrate.

The resulting composite is a solid film or powder exhibiting magnetic properties. XRD, FTIR-, Raman spectroscopy, and TEM HR methods were used to study all obtained materials. It was shown that nickel nanoparticles on the surface of the reduced graphene oxide had an average diameter of 27 nm and were gradually distributed on the surface of reduced graphene oxide sheets.

Thus, the reduction method in supercritical alcohols opens the route to obtain highly dispersed crystalline nickel nanoparticles located on the surface of RGO both in the form of a powder material and in the form of an extended film with magnetic and conductive properties.

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# GLOSSARY OF ABBREVIATIONS AND LETTER DESIGNATIONS IN THE FIELD OF ORGANIC LIGHT-EMITTING DIODES BASED ON TRANSITION METAL COMPLEXES

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The formation of terminological (so-called “thesaurus”) competence, which presupposes not only knowledge and understanding of the special concepts of the subject area and the relationships between them, but also the fluent reading of special abbreviations, letter designations, etc., is a necessary condition for the formation of a competent specialist. The growth of interdisciplinary research in recent years has become one of the dominant trends in the development of science. This “new reality” requires the researcher to be able to quickly master the terminology of often unrelated fields of knowledge. A large number of unfamiliar abbreviations when reading scientific literature complicates understanding and reduces the speed of immersion in the material.

When analyzing the incoming flow of scientific and technical literature for the formation of the thematic fragment Chemistry of the VINITI RAS polythematic database, we identified the topic of organic light-emitting diodes (OLEDs) based on luminescent complexes of transition metals as one of the “growth points”. In their development, chemical means (strategic molecular design of complex compounds, including theoretical quantum mechanical studies) are used to achieve a physical goal (effective light emission). For the production of high-performance OLEDs, the creation of optimal materials and the improvement of technological processes are also important.

Studying this subject area, we came across a significant number of abbreviations and designations from various fields of knowledge that are unfamiliar to chemists. The formation of a glossary of abbreviations and letter designations (more than 160 items) has become an independent part of our information research. The compiled glossary can be useful for chemists, engineers, physicists, and all researchers working at the intersection of sciences.

*The work was carried out within the State Assignment of VINITI RAS (FFFU-2022-0004)*

# COMPARATIVE CHARACTERISTICS OF THERMAL STABILITY OF METALLATE IONIC LIQUIDS BASED ON QUATERNARY AMMONIUM AND PYRIDINIUM SALTS

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Ionic liquids (IL's) are organic compounds consisting of an organic cation and an organic or inorganic anion with a melting point below 100 °C. It is known that metallate IL's can act as a substitute for classical catalysts - Lewis acids. The temperature range in which ionic liquids can be used depends on the thermal stability of ionic liquids. The aim of the work was to obtain iron-containing ionic liquids based on quaternary ammonium and pyridinium salts and to study their thermal stability in air.

The structure of all the obtained IL's is confirmed by IR spectroscopy and UV-Vis spectroscopy. Thermal stability in air, in the temperature range of 25-500 °C, has been studied. It has been established that pyridinium trichlorobromferrates have greater thermal stability in air compared with ammonium trichlorobromferrates. It is shown that among the studied IL's trichlorobromoferrates of N-butylpyridinium and triethylbutylammonium have the highest thermal stability.

**Table 1.** Data of thermal analysis in air.

R	T <sub>decomp</sub> , °C <sup>a</sup>	T <sub>50</sub> , °C <sup>b</sup>	Mass loss, %					Residue, %
			100 °C	200 °C	300 °C	400 °C	500 °C	
<div><math>\left[ \text{C}_6\text{H}_5\text{N}^+\text{R} \right] \text{FeCl}_3 \text{Br}^-</math></div>								
C <sub>4</sub> H <sub>9</sub>	357	442	3.14	3.12	2.73	27.81	62.01	20.63
C <sub>8</sub> H <sub>17</sub>	326	407	0.13	1.61	3.21	46.7	68.33	17.28
C <sub>10</sub> H <sub>21</sub>	324	407	1.93	2.61	3.97	47.05	67.16	16.77
C <sub>12</sub> H <sub>25</sub>	328	405	1.82	3.93	9.88	47.96	67.33	16.97
C <sub>16</sub> H <sub>33</sub>	332	399	1.35	3.17	6.34	50.44	71.92	17.57
<div><math>\left[ (\text{H}_5\text{C}_2)_3\text{N}^+\text{R} \right] \text{FeCl}_3 \text{Br}^-</math></div>								
C <sub>4</sub> H <sub>9</sub>	354	433	2.36	1.93	2.22	34.07	62.6	20
C <sub>8</sub> H <sub>17</sub>	307	425	2.38	3.61	8.37	40.19	61.23	27.21
C <sub>10</sub> H <sub>21</sub>	315	398	8.32	11.37	14.40	51.11	72.42	16.86
C <sub>12</sub> H <sub>25</sub>	311	401	3.97	6.08	11.45	49.37	71.43	15.15

<sup>a</sup> T<sub>decomp</sub> – the temperature of the beginning of thermal decomposition.

<sup>b</sup> T<sub>50</sub> – the temperature corresponding to a 50% mass loss.

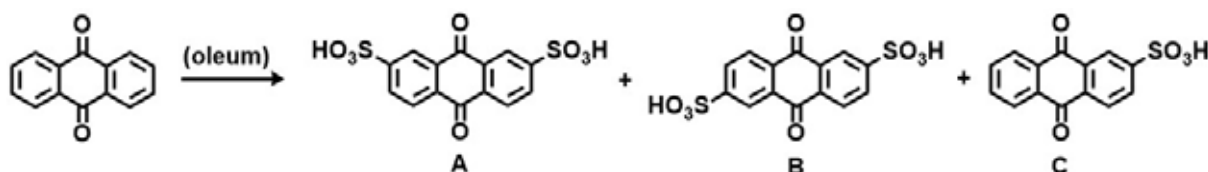
# SYNTHESIS AND STUDY OF MIXTURES OF ANTHRAQUINONE SULPHO DERIVATIVES AS NEGOLYTES IN FLOW CURRENT SOURCES

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Sulfo derivatives of anthraquinone are electroactive materials. They are the most promising and accessible among organic compounds in the field of developing highly efficient flow current sources<sup>1-3</sup>.



The synthesis was carried out and the electroactivity of mixtures of anthraquinone sulfonate derivatives with different contents of 2-anthraquinone sulfonic acid, 2,6-anthraquinone disulfonic acid and 2,7-anthraquinone disulfonic acid was investigated (Table 1).

**Table 1.** The synthesis of mixtures of electroactive anthraquinone sulfonic acids.

№	Mixture of sulfonic acids	Yield A, B, C, %	Ratio A/B/C, %
1	MIX 1	45	20/20/60
2	MIX 2	60	10/10/80
3	MIX 3	95	50/50/0

The MIX 3 sulfonic acid mixture, which did not contain 2-anthraquinone sulfonic acid, was found to exhibit the highest energy efficiency and electrochemical stability.

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*The work was carried out with the financial support of the Russian Science Foundation, project 21-73-30029.*



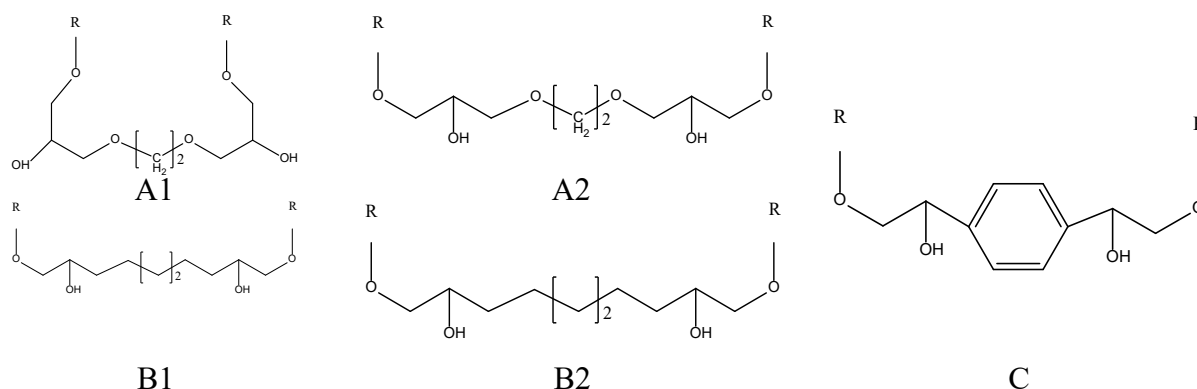
# CONFORMATIONAL FEATURES OF GEMINI SURFACTANTS AT INTERFACES: FLEXIBLE VS. RIGID BRIDGES

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Dimeric nonionic surfactants with flexible bridges including ethylene oxide fragment and a fatty hydrocarbon chain (compounds A and B correspondingly, where R is the hydrocarbon chain  $C_nH_{2n+2}$ ,  $n=8-17$ ), as well as with rigid bridge containing an aromatic ring (compound C) are the objects of the study. Calculations of the thermodynamic parameters of surfactant formation were performed within the Mopac 2000 software package using the quantum chemical semiempirical PM3 method.



It is possible to build the conformers of a “compact” (A1 and B1) and “stretched” (A2 and B2) structure for surfactants with flexible bridge. The formation of gemini-surfactant monomers with a “compact” bridge structure is more energetically advantageous due to the emerging intramolecular  $CH\cdots HC$  interactions. On the other hand, the possibility of aggregation of two alkane molecules between two hydrophobic “tails” of gemini-surfactants of a “stretched” conformation allows us to consider their joint clusterization at the interface of water/alkane vapor and compare the thermodynamic parameters of clusterization with those for film formation at the air/water interface.

*The work is supported by the Ministry of Science and Higher Education of the Russian Federation, the budget topic “Carbon nanoparticles with a given morphology: synthesis, structure and physico-chemical properties, FRES-2023-0006”*

# HEAT CAPACITY AND ELECTROPHYSICAL CHARACTERISTICS OF THE NEW NANOSTRUCTURED $\text{LaBaCuZnMnO}_6$ MANGANITE

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A large class of complex oxide compounds, which include substituted manganites of rare earth and alkaline earth metals, form the basis of many materials with a combination of electric, magnetic, etc. properties [1].

In [2], we obtained nanoscale  $\text{LaBaCuZnMnO}_6$  particles by the interaction of  $\text{La(III)}$ ,  $\text{Cu(II)}$ ,  $\text{Zn(II)}$ ,  $\text{Mn(III)}$  and  $\text{BaCO}_3$  oxides in the range of 800-1200 °C and further grinding on a «Retsch» vibrating mill (Germany).

The study of the heat capacity of  $\text{LaBaCuZnMnO}_6$  was carried out in the range of 298.15-673 K on the calorimeter IT-S-400.

It has been established that an abnormal jump in the heat capacity at 548 K is observed on the curve of the dependence of  $C_p \sim f(T)$ , probably associated with a phase transition of the II -kind. Taking into account the temperature of the phase transition, the equations of dependence of  $C_p \sim f(T)$  are derived, which are described by the following polynomials:

$$C_p = (52 \pm 3) + (576,8 \pm 28,4) \cdot 10^{-3}T + (4,76 \pm 0,23) \cdot 10^5 T^{-2}, \quad (298,15-548 \text{ K}), \quad (1)$$

$$C_p = (908 \pm 45) - (983,4 \pm 48,4) \cdot 10^{-3}T, \quad (548-623\text{K}), \quad (2)$$

$$C_p = -(531 \pm 26) + (1326,7 \pm 65,3) \cdot 10^{-3}T, \quad (623-673\text{K}). \quad (3)$$

The temperature dependences of electrical resistance and permittivity were measured at the LCR installation (manufactured in Taiwan) in the range of 293-483 K. The semiconductor character of the conductivity is established, the band gap width (0.43 eV) and the activation energy of the conductivity (18.73 kJ/mol) are calculated.

It has been revealed that this compound has high values of dielectric constant.

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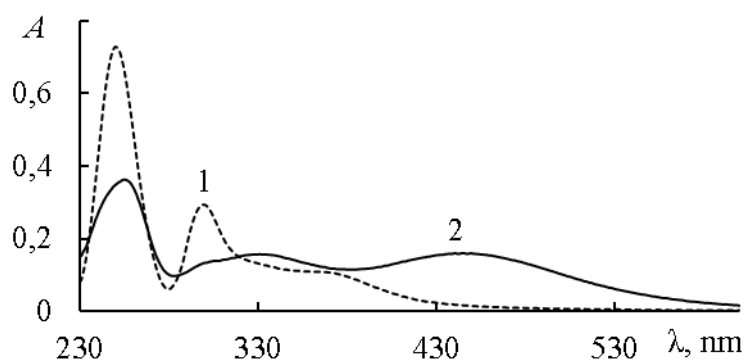
# NITROSATION OF KRAFT LIGNIN UNDER CONDITIONS OF SOLID-PHASE CATALYSIS

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Nitrosation reactions of aromatic compounds belong to  $S_E$  reactions. Various classes of compounds are prepared using nitrous acid and its derivatives due to their high chemical activity and mild reaction conditions.<sup>1-3</sup> Kraft lignin (KL) is a type of technical lignins. KL is poorly soluble in water and aqueous acid solutions, which makes its nitrosation difficult, since the reaction takes place under heterogeneous conditions.

We have developed a method for nitrosation of KL under homogeneous conditions. The method consists in the fact that the reaction was carried out in water-dioxane or water-DMSO medium, and cation-exchange resin in H-form was used as an acid catalyst. In these conditions precipitation of KL did not occur, and cations were removed from the reaction medium, i.e. there was no need to purify nitrosated KL from mineral impurities. The optimal amount of reagents was determined. A new absorption band with a maximum at 443 nm appeared on the electronic spectrum of nitrosated KL (Figure 1). The study of nitrosation kinetics by electron spectroscopy showed that the reaction is completed in 30-50 min.



**Figure 1.** Electronic spectra of the initial (1) and nitrosated (2) KL

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# POLYFUNCTIONAL DERIVATIVES OF ALIZARIN CONTAINING THE TRIFLUOROMETHYL FRAGMENT

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One of the ways to search for new effective biologically active substances is the targeted construction of polyfunctional molecules from pharmacophore structural fragments, among which the basic structures are natural compounds and their chemically modified derivatives. 9,10-anthraquinone derivatives, diverse in structure, are convenient synthons for introducing new polyfunctional substituents into their structure and have shown themselves to be compounds with diverse biological activities [1,2]. Moreover, the presence of polyfunctional substituents in the molecule can serve as an additional factor in structure-specific and hydrophobic effects on biological targets. The main objective of the study is the targeted synthesis of new derivatives of 1,2-dihydroxyanthraquinone (alizarin) by varying the nature of the substituent on the oxygen atom of the hydroxyl group and introducing additional pharmacophore fragments into the molecules. The primary chemical modification at the  $\beta$ -hydroxyl group introduced a bromophenacyl substituent, which is confirmed in the IR spectrum by the presence of an additional band of stretching vibrations of the carbonyl group of the introduced substituent, and in the PMR spectrum by the absence of a signal from the  $\beta$ -OH proton and the identification of aromatic protons of the phenacyl substituent at 7.77 and 7.92 ppm and protons  $-\text{CH}_2-$  at 5.84 ppm. Further, various trifluoromethyl benzoates were obtained from  $\alpha$ -OH. The resulting compounds are crystalline substances. Identification of compounds was carried out using spectral analysis data.

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*The work was carried out under the PCF program: “Innovative methods of synthesis and technologies for obtaining functional inorganic and organic substances and materials from natural and technogenic raw materials” IRN BR18574042.*

# ASSESSMENT OF THE INFLUENCE OF PHYSICOCHEMICAL MODIFICATION OF BIOCHARS ON THEIR SORPTION CHARACTERISTICS

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To obtain biochars from wood waste of pine sawdust and birch sawdust no larger than 1 mm in size were used. Carbonization was carried out in a closed reactor at a temperature of 500°C. The yield of pine biochar is 29%, birch biochar – 36%. Modification of carbonate with alkali and ultrasonic treatment leads to a decrease in the size of biochar particles in general and a decrease in the particle size of the predominant fraction. For activated birch biochar, the maximum particle size decreased from 160 µm to 100 µm, and the size of the predominant particle fraction decreased from 20-80 µm to 20-60 µm. For pine biochar, after activation, the maximum particle size changed from 350 to 250 µm, the size of the main fraction - from 50-250 to 50-150 µm. The carbon basis of biochars was established using the energy dispersive analysis method. After activation of birch biochar, the carbon content increases slightly from 76.46 to 79.04 at.%, while the oxygen content decreases slightly from 23.22 to 20.37 at.%. The same trend is observed for pine biochar: the C content before and after activation is 76.38 and 79.84 at.%, the O content is 23.17 and 19.48 at.%, respectively. The IR method confirms the multifunctional nature of the biochar surface (main groups -OH, -CH<sub>2</sub>, C=O, C=C and -CH<sub>3</sub>).

The adsorption of Cu<sup>2+</sup> ions on birch biochar is mainly due to complex formation between metal ions and surface oxygen-containing functional groups, as well as electrostatic interaction between the metal ion and the negatively charged surface of the coal. The degree of Cu<sup>2+</sup> extraction is 33% on the original and 50% on the activated birch charcoal samples. Unmodified pine and birch biochars absorb 67 and 71% of the methylene blue dye, activated - up to 96 and 98%, respectively, and activation largely increases the sorption capacity of pine biochar.

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



# QUANTUM CHEMICAL STUDY OF 1,3,5-TRIS-( $\beta$ -OXYETHYL) HEXAHYDRO-S-TRIAZINE COMPLEX WITH $\text{Ni}^{2+}$ IONS

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Using the DFT/B3LYP/6-31/G\*\*(p,d) method, the structural stability of complexes of  $\text{Ni}^{2+}$  cations with 1,3,5-tris-(beta-oxyethyl)hexahydro-s-triazine, charge transfer effects, and the position of reaction centers of the molecule, distance between atoms and other quantities.

The figure shows a graph of the frontier orbitals of the complex, calculated by the DFT/B3LYP/6-31G\*\*(p,d). As can be seen from the figure, the highest occupied molecular orbital in the complex indicates the possibility of the formation of a coordination bond. It was determined that in the complex the HOMO energy  $E = -1.819$  eV and the LUMO energy  $E = -1.415$  eV, the difference between them is 3.404 eV.

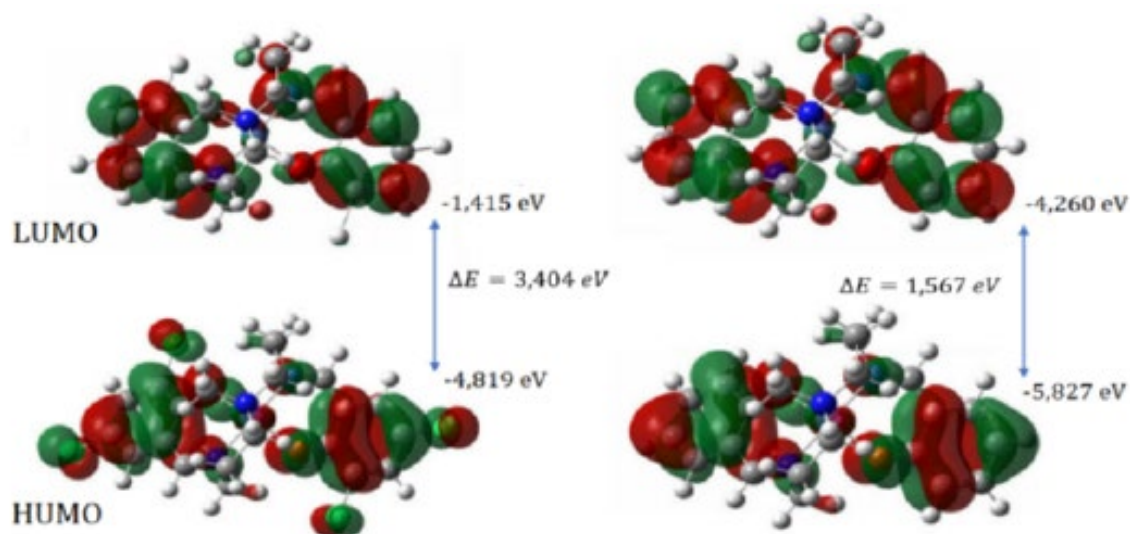


Fig. Energies of the HUMO and LUMO orbitals of the complex

The dipole moment ( $D$ ), chemical potential ( $\mu$ ), electrophilic index ( $\omega$ ), and total energy ( $E$ ) of the molecule were calculated.

Method	$D$ , debay	$\mu$ , eV	$\omega$	$E$ , a.u.
DFT	5,77±0,54	-3,725±0,08	4,213±0,05	- 614,37
PM3	2,31±0,65	-6,420±0,04	5,096±0,05	-284,12
Ab I	5,56±0,18	-3,525±0,03	4,173±0,07	-210,29

# SYNTHESIS OF HIGH-TEMPERATURE CERAMICS BASED ON HAFNIUM CARBIDE

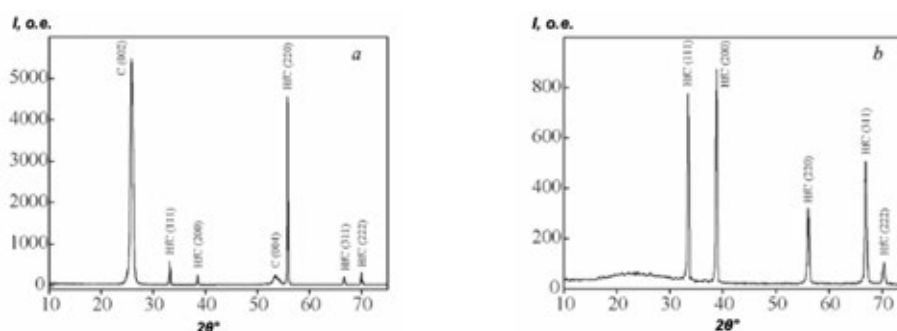
**Kochanov G.P., Rogova A.N., Kovalev I.A., Chernyavskii A.S., Solntsev K.A.**

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Materials based on hafnium carbide are characterized by high melting point, hardness, chemical and wear resistance.<sup>1</sup> Such ceramics are obtained by sintering powders, which complicates the process of its production and obtaining articles of complex shape. An alternative to traditional powder technologies is an oxidative constructing approach based on a one-stage process of metal oxidation in an atmosphere of controlled composition.<sup>2</sup>

The carburization of hafnium was carried with controlled heating of a metal billet by electric current in an atmosphere of a mixture of ethylene and argon.

The sample was heated to the temperature of up to 1850°C for 1 h at a constant rate. Then, the reactor was purged with argon until the hydrocarbons were completely removed, the temperature was raised to 2400°C, and the sample was held for 45 min.



**Figure 1.** X-ray diffraction pattern of hafnium carbide: (a) sample surface; (b) matrix.

The study of the near-surface layer and the powder test sample of the obtained ceramics show the presence of the main phase of hafnium carbide of equiatomic composition HfC and the absence of other carbide phases, which indicates the completeness of the considered process.

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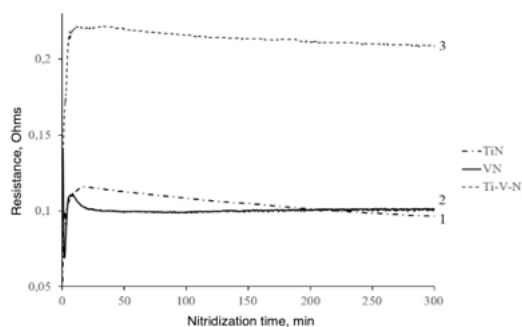
# THERMOELECTRIC CERAMIC CONVERTERS BASED ON TITANIUM AND VANADIUM NITRIDES

**Kovalev I.A., Kochanov G.P., Rogova A.N., Chernyavskii A.S., Solntsev K.A.**

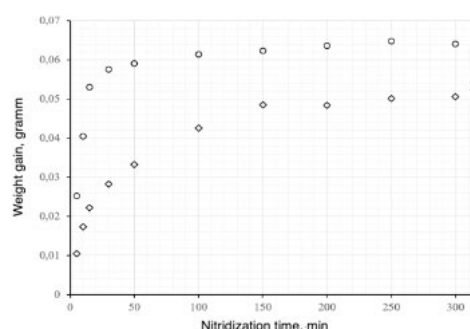
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Titanium and vanadium nitrides have high electrical conductivity, which determines their use as thermoelectric converters. Such materials are produced by powder sintering, however, obtaining dense ceramic products of complex shape is difficult. The usage of the oxidative constructing approach makes it possible to obtain ceramic nitrides of various geometries for their entire depth.<sup>1</sup>

The nitridization of vanadium and titanium was carried out by resistive heating of metallic tapes soldered one side in a nitrogen atmosphere with rapid heating up to 1900 °C. The samples were held at a set temperature in the range from 10 to 300 minutes. During the experiment, the changes in the voltage characteristics of the samples, the nitridization temperature of the junction, vanadium and titanium were monitored.



**Figure 1.** The current-voltage characteristics of the nitridization process of individual metals and metal pairs



**Figure 2.** The dependences of the weight gain of absorbed nitrogen for vanadium (1) and titanium (2) on time during nitridization

It was found that the duration of the nitriding process of a metal pair is determined by the nitridization of the junction area. The nature of the dependence of the thermal EMF of nitrides is defined by the composition and structure of ceramics. For all nitrided pairs, a monotonous enhancement in the Seebeck coefficient was observed over the entire temperature range.

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*The work was supported by Russian Science Foundation, the project no. 23-13-00324.*

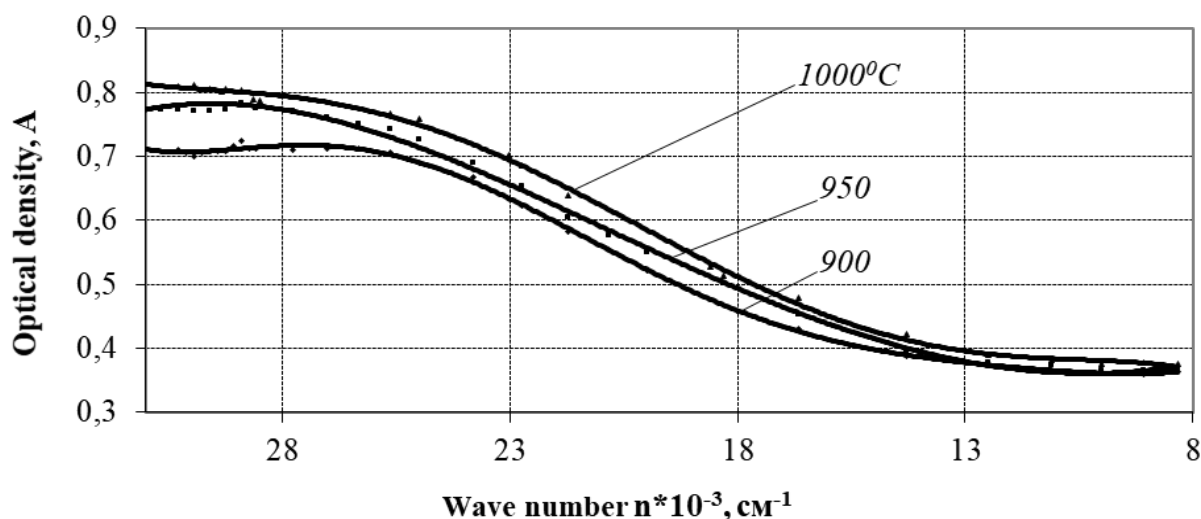
# DISSOLUTION MECHANISM OF GASEOUS CHLORINE IN MOLTEN ALKALI METAL CHLORIDES

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Electronic absorption spectra of gaseous chlorine and its saturated solutions in molten NaCl, NaCl – KCl, KCl, CsCl were obtained at various temperatures. In all studied melts, a long-wavelength edge of the absorption band was recorded, which shifts to the long-wavelength region with increasing temperature<sup>1</sup>. The coincidence of the absorption band maximum in salts with the absorption maximum of gaseous chlorine, as well as a small shift of the maximum and an increase in solubility with temperature, allow us to conclude about the inert gas mechanism of chlorine dissolution. On the other hand, from the analysis of our results and data on the chlorine spectra in other solvents (water, organic solvents), we can conclude that Cl<sup>3-</sup> groups are formed. Thus, both physical dissolution and chemical interaction with the formation of particles of the Cl<sup>3-</sup> type take place.



**Figure 1.** Electronic absorption spectra of Cl<sub>2</sub> saturated solutions of in molten NaCl. In the range of 26÷28 thousand cm<sup>-1</sup> a wide maximum is observed

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# ABOUT THE PHASE TRANSITION QUARTZ GLASS – HIGH-TEMPERATURE CRISTOBALITE

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For the manufacture of refractory quartz ceramics, JSC DINUR uses opaque quartz glass of its own production. The crystallization of quartz ceramic products is due to the high-temperature transition quartz glass (QG)→high-temperature cristobalite (H-T C). Data from different authors are shown in Table 1.

**Table 1.** Temperature and volume change during the phase transition quartz glass-high-temperature cristobalite

Transformation	T, °C	Volume change $\Delta V$ , %	Authors
QG→ H-T C	900	+0,9	Gasic M.I.
QG → H-T C	>1150	0	Allencshtein I.
QG → H-T C	1000	-0,9	Budnicov P.P., Cucolev G.V.
QG → H-T C	1200	-0,4	Moroz I.I.
QG→H-T C (a fast-moving transformation)	1728	-0,9	Strelov C.C., Mamycin P.S., Cachsheev I.D.

With increasing temperature and duration of isothermal exposure, the amount of cristobalite increases (table 2)<sup>1</sup>.

**Table 2.** The amount of cristobalite (% , volume) depending on the firing time of quartz glass samples.

Firing time Temperature, °C	1 h	2 h	5 h
1200	0,0 %	0,7 %	1,1 %
1300	1,0 %	2,0 %	5,0 %
1400	6,0 %	8,0 %	23,0 %

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Kolobov A.Yu. Features of crystallization and characteristics of quartz glass obtained on JSC DINUR plasma torches from the quartz sand of the Ramenskii deposit / Kolobov A.Y., Sycheva G.A. // Glass Physics and Chemistry. – 2020. – V. 46, N 3. – P. 249-255.



# GALVANIC REPLACEMENT AS APPROACH TO OBTAINING HIGH ENTROPY ALLOY PRECURSORS

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High-entropy alloys (HEA) are multicomponent metal systems that differ from traditional ones by high entropy due to the uniform distribution of element atoms in the crystalline lattice. One of the possible approaches to obtaining HEA is galvanic replacement. In this process, metal ions in solution are reduced to the oxidation state (0) and deposited on the surface of a template (for example, aluminum), the atoms of which are oxidized to form the corresponding ions. Based on fundamental principles, this method provides a simple and universal way to obtain a wide range of different structures with a controlled elemental composition [1].

The process occurs spontaneously due to heating as a result of exothermic dissolution of aluminum. The short-circuit mode, intensive local heating of particles and the reaction medium allow for a short time to change the potential of the suspension electrode over a wide range. It is possible to precipitate elemental metals with significantly different values of electrochemical potentials (Pt, Fe, Mo, W, etc.), while forming multi-element systems, for example, Fe-Ni-Co-Cu, Fe-Ni-Co-Cu-In, Fe-Ni-Co-Cu-Sn-In, Fe-Ni-Co-Cu-Sn-In-Pt, etc.

The dispersed objects obtained in this way are precursors of bulk materials. It has been established by spectral and electron microscopic methods that the elements isolated on the surface of the aluminum matrix are relatively evenly distributed and are in equimolar ratio. The particles are spherical micro-sized skeletal structures (~75  $\mu\text{m}$ ) with a large number of filamentous nuclei 50-60 nm in size. To consolidate dispersed precursors, high-temperature sintering in combination with pressing is used. The detected phase transitions make it possible to control the processes of obtaining HEA with given composition.

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*This work was supported by the Ministry of Science and Higher Education of the Russian Federation within the framework of the state assignment № 075-01508-23-00, 29.12.2022.*

# LUMINESCENT PLATINUM COMPLEXES AS ADVANCED MATERIALS FOR ORGANIC LIGHT EMITTING DIODES

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In the process of analytical and synthetic processing of the incoming scientific and technical literature to form the thematic fragment “Chemistry” of the VINITI RAS polythematic database we came to conclusion that the subject area of organic light-emitting diodes (OLEDs) based on luminescent transition metal complexes is actively developing and is in serious demand.

In 2022, on the scientometric platforms Web of Science and Scopus we analyzed the scientific and technical literature on the topic of luminescent platinum complexes and their use as the OLEDs emitting basis for the period 2018-early 2022. We studied the dynamics of scientific publications on the topic, its distribution by subject areas, rating of journals and collections, publication activities of scientists from different countries, etc. The study of the collection of the most cited articles made it possible to identify the key trends and perspective directions in the field of creating highly efficient emitters based on platinum coordination compounds.

Currently the design and creation of such devices are associated with serious research both in the field of classical chemistry, namely, the strategic molecular design of metal complexes with various organic ligands, and in the field of materials science – the creation of new materials for increasingly advanced OLEDs, as well as technology. Researchers are studying the influence of structural factors on the quantum yield and color luminescence characteristics in order to create new highly efficient emitters with predetermined photophysical properties. Scientists are paying close attention to theoretical quantum mechanical research, allowing one to predict the luminescent characteristics of not-yet-synthesized complexes.

In our research, we studied the approaches and results of mononuclear platinum (II) complexes molecular design to create efficient organic light-emitting diodes for the red area of the optical range and infrared region of the spectrum (Red-NIR OLEDs).

*The work was carried out within the VINITI RAS State assignment (FFFU-2022-0004).*

# OPTIMIZATION OF TECHNOLOGY FOR PRODUCING QUARTZ CERAMIC PRODUCTS FOR THE AVIATION AND SPACE INDUSTRY USING ELECTROPHORESIS

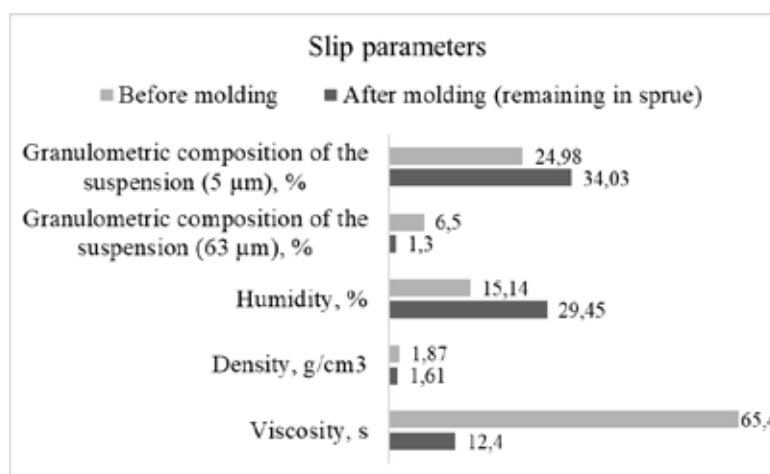
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Electrophoretic casting is an alternative method to slip casting for producing thick-walled quartz ceramic workpieces<sup>1</sup>. Solid slip particles are deposited onto a copper forming electrode (anode) under the influence of an electric field. A cathode with holes for leakage of slip from the gating area is placed on top.

Forming time is reduced by 24 times when the workpiece thickness increases to more than 50 mm. The distribution of density and strength of individual fragments of workpieces is uniform, within the range of 1.96–1.99 g/cm<sup>3</sup> and 62.8–69.7 (±1.2) MPa. There is no loss of slip in the sprue, associated with the movement of solids towards the anode, and water in the opposite direction. The results indicate a high content of solid particles in the workpiece, which has a positive effect on the uniform distribution of physical and mechanical properties throughout the volume of the product and on the quality of the resulting samples (Picture 1).



**Picture 1.** Slip parameters before and after electrophoretic spinning

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# KINETIC STUDY OF THE DIELS-ALDER REACTIONS OF ANTHRACENE DERIVATIVES WITH TETRACYANOETHYLENE AND N-PHENYLMALEINIMIDE IN THE SOLID STATE

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Solid-state reactions that occur in high yields are among the most successful examples of green chemistry. Solid-state reactions open up the possibility of carrying out quantitative transformations without solvents or catalysts. There are several known examples of successful Diels-Alder reactions without a solvent, when solid and liquid reagents are mixed. Reactions between solid reagents proceed successfully when a small amount of solvent (5-10% by weight) is added to them<sup>1-5</sup>. However, in these examples, successful reaction is often associated with a high concentration of both reactants in the liquid phase.

We have studied the kinetics of Diels-Alder reactions of anthracene and 9,10-dimethylantracene with tetracyanoethylene and N-phenylmaleimide in the solid state without the addition of a solvent. The rate of these reactions in the solid phase is compared with the rate of these reactions in solution. The rate constant for the reaction of anthracene with tetracyanoethylene in 1,2-dichloroethane is 125 times higher than the rate constant for the reaction of 9,10-dimethylantracene with N-phenylmaleimide<sup>6</sup>. And in the solid state, the rates of these reactions differ by only 4 times. For reactions of tetracyanoethylene with anthracene and 9,10-dimethylantracene in 1,2-dichloroethane, the ratio of rate constants is  $3 \cdot 10^4$ , and in the solid phase the ratio of rates does not exceed 2. Since the rate of reactions in the solid phase is mainly determined by the energy of the crystal lattice, then we can assume that the ratio of the activities of the reagents in the solid phase may not coincide and even be inverted compared to reactions in solution.

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*The work was carried out within the framework of the state assignment of the Ministry of Science and Higher Education of the Russian Federation (scientific code FZWU-2023-0002) and with the support of the Scientific and Educational Center of the Republic of Bashkortostan (Contract No. TsPD-ML-4/RF-23).*

# SURFACE AND VOLUME HYDROPHOBIZATION OF BUILDING MATERIALS WITH EMULSIONS BASED ON OLIGOALKYLHYDRIDESILOXANES AND TITANIA

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Methods of creating hydrophobic photocatalytically active coatings based on organosilicon compounds and doped titania by applying water emulsions of oligoalkylhydridesiloxanes (OAGS) and  $\text{TiO}_2/\text{Ce}$ ,  $\text{TiO}_2/\text{Dy}$ ,  $\text{TiO}_2/\text{Hf}$ ,  $\text{TiO}_2/\text{Zr}$ , to various surfaces have been studied. As a result of thermal fixation of the coating, a water-repellent layer is formed, decomposing organic pollutants. The synthesized compositions have also been studied for volumetric hydrophobization of gypsum mixtures.

The characteristics of the obtained hydrophobic films are determined - the wetting angle ( $\theta$ ), drop-off time, water absorption, photocatalytic activity (PKA) and their effect on the properties of the obtained materials. It was revealed that the marginal angles on the studied surfaces are 120-140 degrees, the optimal concentration of OAGS for wood is 4.5-7.5% with a content of GMTS of 5%. For refractory, red bricks and foam silicate blocks, surface modification leads to an increase in the edge angle to 143 degrees at a concentration of 4.5-7.5% OAGS, 1% GMTS. In this case, the concentration of the alloying additive should be 2-6%. It was revealed that the edge angle on the studied surfaces is greater on those samples that were treated with compositions containing doped  $\text{TiO}_2$ .

Gypsum samples containing synthesized hydrophobic compounds have high values of the marginal angle – 120-130 degrees with a content of OAGS of 10-15%,  $\text{TiO}_2/\text{Me}$  -1-5%. The proposed modifiers make it possible to obtain materials with high PKA. On gypsum samples, the organic dye rhodamine decomposes under the influence of sunlight within 5-10 hours. The developed compositions operating in the visible range of electromagnetic radiation can significantly reduce energy costs and solve environmental problems of using such materials.

*The study was carried out with the support of the Ministry of Science and Higher Education of the Russian Federation as part of the execution of state task No. FSSM-2024-0006 (Laboratory of Ion Materials).*



# STRUCTURE AND PROPERTIES OF NANOMATERIALS BASED ON TITANIA DOPED WITH HAFNIUM AND CERIUM

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In this work, titania nanoparticles were obtained by hydrolysis of titanium tetrachloride in an ultrasonic field and methods for its alloying with Hf(IV), Ce(III) compounds were developed to achieve PCA in the visible spectral region. To characterize the obtained materials, the methods of XRD, DTGA, IR spectroscopy, laser diffraction, and SEM were used. The temperatures of the anatase-rutile phase transitions of synthesized doped particles are determined: at 4500C, the  $\text{TiO}_2$  crystal lattice acquires the anatase structure, and in the range 670-900°C, titania is rutilized.  $\text{TiO}_2$  heat-treated at 450 °C, has a high PKA (rhodamine D varies from 1.5 to 0.25), in samples treated at 600-900°C, PKA is weak (D varies from 1.5 to 1.35). An increase in the processing temperature (more than 450°C) leads to dehydration, formation and enlargement of crystals, and the transition of anatase to rutile, which negatively affects PKA. Doping with Hf(IV), Ce(III) compounds leads to an increase in the temperature of rutilization

The particle sizes of the initial  $\text{TiO}_2$  are 0.08-0.14  $\mu\text{m}$ , the average size of the doped particles decreases slightly and the fraction 0.05-0.07  $\mu\text{m}$  prevails, the specific surface area of the particles is 15-25  $\text{m}^2/\text{g}$ . It was found that with a decrease in the particle size and an increase in the specific surface area of titanium dioxide, its PCA increases. A fraction of  $\text{TiO}_2$  with a size of 0.08-0.14  $\mu\text{m}$  changes the optical density of the dye from 1.5 to 0.15, a fraction of 0.05-0.07  $\mu\text{m}$  – from 1.5 to 0.02 within 2-5 hours.

It is noted that the particles of the obtained materials tend to aggregate, forming agglomerates. this reduces their catalytic activity tenfold. Individual particles of unmodified conglomerates have sizes of about 200  $\mu\text{m}$ , and doped ones - 70  $\mu\text{m}$ , the agglomeration of doped samples is less than that of the original  $\text{TiO}_2$ . It was revealed that the values of the PKA  $\text{TiO}_2/\text{Ce}$  and  $\text{TiO}_2/\text{Hf}$  are comparable. The phase composition, morphology, size, and specific surface area of synthesized titanium dioxide have a significant effect on its PHA.

*The study was financially supported by Ministry of Science and Higher Education of the Russian Federation, Laboratory of ionic materials (LIM), project number FSSM-2024-0006.*

# GAS-SENSITIVE PROPERTIES OF NANOPOWDERS BASED ON $\text{LaFeO}_3$

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The formation of nanopowders is an important step in the manufacture of functional materials (for example, materials with gas-sensitive properties). Gas sensors are promising in the manufacture of gas-sensitive devices that are able to detect many gases. Semiconductor thin films are used as a gas-sensitive element. The principle of operation of such sensors is based on the fact that reversible chemisorption of active gases on their surface is accompanied by reversible changes in conductivity. Such sensors are highly sensitive to the content of toxic and explosive gases in the atmosphere. Such materials are also attractive because of the ability to control surface processes and processes in the semiconductor volume.<sup>1</sup>

Nanopowders of lanthanum orthoferrite with a perovskite structure can be considered as the basis of thin films for gas-sensitive elements. They are characterized by unique physical and chemical properties.<sup>2</sup>

In this work, sol-gel technology was used as a method for producing nanopowders. The choice is due to the simplicity and speed of implementation, cheapness and use of available equipment.<sup>3</sup>

In this work, the gas sensitivity of powders  $\text{LaFeO}_3$  was investigated. The values of the specific surface resistance of these samples in air and in the presence of a reducing agent gas -  $\text{NH}_3$  (50ppm) were obtained. Based on the data obtained, it can be concluded that the specific surface resistance decreases sharply for all samples in the presence of  $\text{NH}_3$  with increasing temperature. As a result of near-surface processes, the concentration of charge carriers changes, which leads to a sharp decrease in resistance. This indicates n-type conductivity.

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# SYNTHESIS AND ADSORPTION PROPERTIES OF FERROSILICATE NANOCOMPOSITE BASED ON SBA-15 TYPE MESOPOROUS SILICA MATRIX WITH MONOMODAL AND BIMODAL PORE SIZE DISTRIBUTION

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By hydrolysis of a mixture of tetraethoxysilane and nonionic surfactant Synperonic F108, combined polymodal iron silicate mesophases of the Fe@M41S and Fe@SBA-15 Type with different molar ratios of Fe(II)/Si, possessing a supermicro-mesoporous structure, were synthesized. Unlike MCM-41, obtained on a cetylpyridinium template, silicas of the SBA-15 Type have not only monodisperse cylindrical mesopores with a diameter in the range of 5–30 nm, but also supermicropores and ultramesopores inside the walls of hexagonally packed SiO<sub>2</sub> channels with nanoscale wall thickness.

Using an integrated approach by means of XRD, FT-IR, XRF, SEM, N<sub>2</sub> adsorption-desorption methods, synthesized submicron spherical supermicro-mesoporous SiO<sub>2</sub> particles with a specific surface area A<sub>BET</sub> 451–841 m<sup>2</sup>/g, A<sub>DFT</sub> 569–1033 m<sup>2</sup>/g, A<sub>ext</sub> 346–647 m<sup>2</sup>/g and A<sub>micro</sub> 105–200 m<sup>2</sup>/g were studied. It has been proven that the particles consist of close-packed SiO<sub>2</sub> capillaries, similar to materials of the MCM-41 Type, and have two porous subsystems: monodisperse cylindrical mesopores with a controlled variable average diameter of more than ≈ 10 nm and supermicropores located inside the walls of SiO<sub>2</sub> channels, with a diameter of less than ≈ 5 nm.

The material is characterized as a heterogeneous Fenton-like catalyst in the decomposition reaction of methylene blue.

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# BOOSTING THE EFFICIENT RESOURCE-USE OF THE EXTRACTION PROCESS IN THE LIQUID-LIQUID SYSTEMS

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The extraction processes in liquid-liquid processes are widely applied in chemical, refining, petrochemical and other industries. They are efficiently used to extract pure various products of organic and petrochemical synthesis, to recover and to separate rear and dispersed elements, waste water treatment and etc.<sup>1</sup>

The liquid extraction represents selective extraction of components(s) from the liquid mixture using a liquid solvent<sup>2</sup>.

Enhancement of efficient resource use and energy efficiency of the extraction mass transfer process can be reached through one of the following techniques or using their combination: first – via enhanced process deployment, selection of more efficient solvents or via the second method – with use of design modifications in process hardware and equipment.

The specific equipment item shall be selected out of all available extraction contact vessels only after technical-and-economic analysis completion.

Based on results of the operations analysis of liquid extractors available in industry, patent studies, research study activities, there has been developed a new column-type liquid extractor<sup>3</sup>. The developed vessel, in comparison with the existing vessel fleet, has the following advantages: simple design and manufacturing process, low solvent consumption for the processes, easy process maintaining and maintenance.

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# STUDY OF THE PROMISING SOLID ELECTROLYTE $\text{Li}_{1.5}\text{Al}_{0.5}\text{Ge}_{1.5}(\text{PO}_4)_3$ : FROM PRECURSOR TO HIGHLY CONDUCTIVE CERAMICS

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The goal of the study was to develop an effective method for producing lithium-conducting ceramics with the composition  $\text{Li}_{1.5}\text{Al}_{0.5}\text{Ge}_{1.5}(\text{PO}_4)_3$  (LAGP) at low temperatures and a comprehensive study of physicochemical, electrochemical and mechanical characteristics.

The developed method<sup>1</sup> is characterized by lower energy consumption compared to known methods for producing LAGP by melting refractory oxides, followed by hardening of the melt and crystallization of glass<sup>2</sup>.

Analysis has been performed using the Rietveld method for single-phase LAGP powder after sintering at 650°C. Using the method of full-profile analysis of XRD patterns, the lattice parameters of rhombohedral LAGP with space group  $R\bar{3}c$  ( $a = b = 8.26522 \text{ \AA}$ ;  $c = 20.6266 \text{ \AA}$  and  $\alpha = \beta = 90.0^\circ$ ,  $\gamma = 120.0^\circ$ ) have been calculated. The values of the WPPF parameters ( $R_p = 3.54\%$ ,  $R_{wp} = 4.63\%$  and  $\chi^2 = 1.1168$ ) confirm the good quality of the results obtained. The presence of a single phase in the synthesized LAGP can be explained by the advantage of homogeneous mixing of the components of the precursor solution at the molecular level<sup>3</sup>.

The microstructure of LAGP has been studied and chemical analysis has been carried out using energy-dispersive X-ray spectroscopy (EDS). The correspondence of the observed and theoretical values of element content according to EDS data has been determined. Distribution maps show a uniform distribution of the elements Ge, P, O and Al in the microstructure of the particles, but there are grains with increased Al content.

The temperature dependence has been studied and the activation energy of LAGP conductivity has been determined in the stepwise heating mode in the range of 25-120°C. The conduction activation energy ( $E_a$ ), calculated from the slope of the graph in Arrhenius coordinates, is 0.28 eV.

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# INVESTIGATION OF THE EFFECT OF GRAIN SIZE ON THE STRENGTH PROPERTIES OF HOT-PRESSED 08X18H10T STEEL PIPES

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Austenitic stainless titanium-stabilized steel 08X18H10T has found wide application due to its good technological and operational properties, as well as resistance to intercrystalline corrosion.

At the moment, acceptance tests of hot-pressed pipes reveal a discrepancy between the temporary resistance at room temperature and the yield strength at elevated +350 °C. With the temperature requirements of TU 14-3P-197 and GOST 9940 for 10% of batches. One of the main parameters affecting mechanical properties is the grain size.

The aim of the study was to assess the effect of the metal grain size of hot-pressed 08X18H10T steel pipes on strength properties.

The object of the study was longitudinal samples, including the entire wall thickness of pipes, cut from hot-pressed pipes measuring Ø219×11.0 mm, heat-treated (austenitized) at a temperature of 1020-1070 °C.

The microstructure of the samples was revealed by electrolytic etching of polished samples in a 10% aqueous solution of oxalic acid and examined with a LeicaDMi8 optical microscope at a magnification of 100 times.

It was determined that the microstructure is an austenitic matrix with inclusions of titanium nitrides and carbonitrides (located along grain boundaries and in the form of lines) and a small amount of δ-ferrite.

In samples from pipes with higher strength properties, the proportion of “small” austenite grains (up to 40 microns in size) is 17.2% higher, and the proportion of “large” grains (over 40 microns) is 15.9% less than in samples from pipes with reduced strength properties.

When processing the results, it was determined that the difference has statistical significance, that is, the grain size is one of the factors explaining the difference in the strength properties of the metal of the hot-pressed pipes.



# SYNTHESIS OF CALCIUM-SODIUM PHOSPHATES, GERMANATE-PHOSPHATES AND SILICOPHOSPHATES BY SOL-GEL METHOD

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Tricalcium phosphate (TCP) and sodium rhenanite are promising for the production of bioimplants due to their high resorption rate. Further complication of the composition by inclusion of silicon and germanium involved in bone metabolism is the next step to obtaining osteostimulating materials. The osteoconductivity of the implant implies the presence of macropores and, as a consequence, the use of stereolithographic 3D-printing method, which imposes certain requirements on the size of the initial particles. The sol-gel method is suitable for obtaining such powders.

The synthesis of  $\text{CaNaPO}_4$ ,  $\text{Ca}_3(\text{PO}_4)_2$ ,  $\text{Ca}_{2+n}\text{Na}_n(\text{PO}_4)_n\text{GeO}_4$  and  $\text{Ca}_{2+n}\text{Na}_n(\text{PO}_4)_n\text{SiO}_4$  compositions was carried out according to the Pecchini method using tetraethoxysilane (TEOS) as a silicon source, while the phosphorus source was orthophosphoric acid, sodium trimetaphosphate, ethylenediaminetramethylene phosphonic acid (EDTMPA) and a number of other compounds.

In the case of TCP, the formation of the crystalline phase is observed above  $600^\circ\text{C}$ , while in the case of rhenanite the samples are well crystallized already at  $500\text{--}600^\circ\text{C}$ . The use of trimetaphosphate allows to obtain final compounds without violation of stoichiometry. In the case of EDTMPA, the compositions calculated for TCP and rhenanite contain an admixture of apatite, which indicates the removal of phosphorus during the firing process. For complex compositions (phosphate silicates and phosphate germanates) a series of samples were prepared corresponding to phase equilibria in the systems  $\text{CaNaPO}_4 - \text{Ca}_2\text{SiO}_4$  and  $\text{CaNaPO}_4 - \text{Ca}_2\text{GeO}_4$ . According to XRD data, the samples of phosphate germanates after firing at  $1000^\circ\text{C}$  are represented by the glaserite phase. In the case of silicophosphates, the firing products are represented by a low-temperature phase.

In this work, a number of phosphorus-containing precursors were used for the synthesis of a wide range of complex phosphates by sol-gel method for the first time.

*This work was supported by the Russian Science Foundation, project no. 22-19-00219.*

# INTERACTION OF ALCOHOL-MODIFIED OLIGOMERS WITH ACTIVE GROUPS OF COLLAGEN

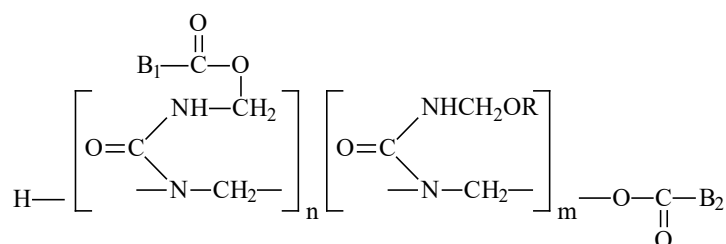
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Urea formaldehyde oligomers modified with aliphatic alcohols: isopropyl alcohol and 1,1,3-trihydroxytetrafluoropropanol were synthesized in the research. This type of compounds are used in the leather and fur industry as filling and additional structure formation reagents.

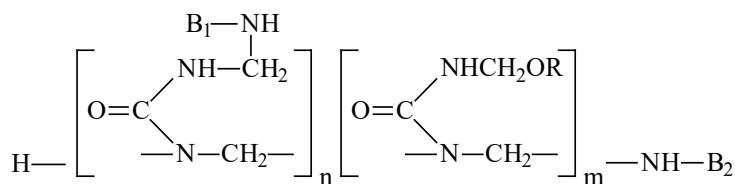
Additional structure formation – retanning, suggests chemical reaction. Collagen has amino, hydroxyl and carboxyl functional groups in its side chain. The reaction mechanism of  $\text{—CH}_2\text{OH}$  groups of alcohol-modified oligomers with the collagen carboxyl group proceeds under acid catalysis conditions with the esters formation<sup>1</sup>.

The reaction result of the synthesized oligomers with the carboxyl group of collagen is represented as follows:



$\text{R—CH(CH}_3)_2$  either  $\text{CH}_2(\text{CF}_2\text{—CF}_2)\text{H}$ ;  $\text{B}_1, \text{B}_2$  – collagen polypeptide chains.

It is also possible to react the methyl groups of the synthesized oligomers with the hide protein amino groups in the side chain by condensation:



$\text{R—CH(CH}_3)_2$  either  $\text{CH}_2(\text{CF}_2\text{—CCF}_2)\text{H}$ ;  $\text{B}_1, \text{B}_2$  – collagen polypeptide chains.

In this way, a reaction model of methyl groups of alcohol-modified oligomers with collagen functional groups is shown.

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# SYNTHESIS OF TELLURIDES OF LEAD, TIN, ANTIMONY AND BISMUTH AND THEIR ALLOYS FOR THERMOELECTRIC APPLICATIONS.

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Metal tellurides of groups 4-6 and their alloys are most often used in various devices due to their relatively high thermoelectric properties. The latter are structurally sensitive and their thermal efficiency can be increased by alloying, reducing grain sizes, and adding nano-sized particles.

Solid-phase synthesis methods are promising, allowing the introduction of alloying additives, inert nanoparticles already at the synthesis stage, ensuring uniformity of their distribution in the volume of the material. Using tellurium emulsions in acetate solutions to create thermoelectric modules using an inkjet printer or similar devices. In this regard, the processes of thermolysis of Pb, Sn, Bi, and Sb acetates in the presence of elementary tellurium powder have been studied. The influence of tellurium on the process of thermal decomposition of acetates, the mechanism and chemistry of the process of formation of tellurides in a hydrogen current were studied using thermogravimetry and differential thermal analysis. Solid-phase synthesis methods are promising, allowing the introduction of alloying additives, inert nanoparticles already at the synthesis stage, ensuring uniformity of their distribution in the volume of the material. Using tellurium emulsions in acetate solutions to create thermoelectric modules using an inkjet printer or similar devices. In this regard, the processes of thermolysis of Pb, Sn, Bi, and Sb acetates in the presence of elementary tellurium powder have been studied.

Electron microscopy and X-ray phase analysis of the obtained powders confirm the formation of tellurides during the thermal decomposition of acetates in the presence of tellurium in a hydrogen current at relatively low temperatures.



Figure 1. Micrographs of antimony telluride.

## ON THE ISSUE OF MODELING STRUCTURE AND PROPERTIES

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The authors propose a method for predicting the "parameter-property" dependencies of reagents and reagent compositions in process fluids as a system for interpreting experimental data.

According to this approach, the authors understand the initial state as the values of the structural parameters of compounds calculated by the UB3LYP/6-311++G(d,p) method. Under the final state of the object are the properties of the studied substances obtained as a result of a laboratory experiment (antioxidant, antimicrobial). There are various ways between the initial and final states by which these properties can be described. The authors use the theory of a planned experiment, which allows, with a minimum number of experiments, to obtain a mathematical model of the process and determine the optimal ways of its course. The type of response function  $y=F(x_1, x_2, \dots, x_n)$  is unknown in advance, where  $x_1$  (% wt.end), electrophilicity  $x_2$ ,  $x_3$  are the bond lengths of  $R_{OH}$ , for example, and other variables that affect the property under study [1-2]. To find this unknown function, the idea is proposed to consider not the function itself, but its decomposition into a Taylor series. The decomposition coefficients are found based on the results of experiments, and the optimization criterion is the coefficient of determination, which can reach 100%.

The authors managed to obtain adequate equations that allow us to visually demonstrate the effectiveness of the use of the studied substances and further apply them to certain classes of compounds

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# SYNTHESIS OF BINARY HYDROSOL OF GADOLINIUM HYDROXIDE AND SILICA AND ITS SOME PROPERTIES

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Currently, the application of binary core-shell particles is widespread. The use of such systems makes it possible to improve the performance characteristics of materials and expand the scope of their application. One of the methods for obtaining such systems is heterocoagulation<sup>1</sup>.

Binary systems were obtained from synthesized gadolinium hydroxide hydrosol<sup>2</sup> and commercial silica sol LUDOX TM-40. The heterocoagulation process was carried out as follows: the same volume of gadolinium hydroxide hydrosol was added dropwise to the silica hydrosol with stirring. Diluted sols with pH 7.5-8.0 units in a ratio of 8:1, respectively, were used. The range of aggregative stability of the binary hydrosol was in the pH interval from 6.9 to 8.0.

For the gadolinium hydroxide sol, it was previously established<sup>2</sup> that in the pH range under study the particles are positively charged, and the charge value of the particles was 40 mV. In the case of silica hydrosol, the particles of the dispersed phase are negatively charged, the value of the  $\zeta$ -potential was about -17 mV. Electrokinetic studies of the mixed system were also carried out, as a result of which it was shown that the  $\zeta$ -potential of the particles is negative and averages -19 mV. This suggests that negatively charged silica particles are adsorbed on the surface of positively charged gadolinium hydroxide particles.

The results obtained are consistent with transmission electron microscopy data indicating that smaller spherical particles of silica form a shell on the surface of larger spherical particles of gadolinium hydroxide.

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# REGULATION OF SURFACE COMPOSITION AND PROPERTIES OF CARBON FIBER MATERIALS

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Chemical methods of surface modification are becoming increasingly widespread in inorganic materials science, making it possible to influence in the desired direction the reactivity and final properties of solid-phase materials. Among the variety of known methods of forming the chemical composition and structure of the surface of a solid (impregnation, deposition from a liquid or gas phase, coprecipitation, mixing, sol-gel processes, etc.) its precision (accuracy of specifying the composition and structure at the atomic-molecular level) The molecular layering method is distinguished by the high conformity of surface nanolayers.

The work examines the targeted chemical modification of the surface of precursor fibers and the carbon fiber materials themselves using the molecular layering method to control the processes of thermal transformations and the target properties of both the carbon fibers themselves and composites based on them.

Using the functional groups present on the surface of the precursor fibers, as well as purposefully creating them, the synthesis of surface mono-multicomponent oxide nanostructures was carried out on the surface of the carbon fiber using the technology of molecular layering. The resulting initial modified materials and the products of their subsequent thermal transformations were characterized using modern physicochemical methods of analysis.

The activating effect of modifying oxide nanolayers on the processes of carbonization and subsequent graphitization, which contribute to improving the structure of the resulting carbon fibers and accordingly improving their physical and mechanical characteristics compared to unmodified predecessors, has been established.

As a result of the developed approaches to the creation of surface element oxide nanostructures selected from a number of titanium, chromium, vanadium, phosphorus, silicon, aluminum, and zirconium oxide by the method of molecular layering, the regulation of the adhesive, electrical and thermal-oxidative properties of CFM has been demonstrated.



# SYNTHESIS OF THE PRACTICALLY IMPORTANT ZEOLITE CLINOPTILOLITE AND CALCULATION OF ITS STRUCTURAL CHARACTERISTICS

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Considering the above, that is, the practical significance of clinoptilolite zeolite, we set the goal of its synthesis based on the mineral resources of Nakhchivan under more moderate conditions, in the presence of fewer chemical reagents, so that the process of hydrothermal crystallization becomes more accessible and economical.

Hydrothermal synthesis of clinoptilolite-type zeolite was studied in the temperature range 100-250°C, the weight ratio of the initial components of halloysite (H) and obsidian (O) H:O = 1:1, 1:2, 1:3, 2:1, 3:1. For the synthesis, thermal solutions of NaOH were used, the concentration of which was varied in the range of 10-30 wt. %, the duration of the process was 10-50 hours. The synthesis of clinoptilolite zeolite was carried out in the presence of a structure-forming agent - tetramethylammonium hydroxide (TMAOH). It has been established that the optimal conditions for the synthesis of clinoptilolite with 100% crystallinity and phase purity is as follows: temperature 150±2°C, concentration of thermal solution of NaOH of 15-20%, quantitative ratio of the initial components of H:O, equal to 1:2, processing time – 20 hours.

When considering the physicochemical properties of zeolites, a phenomenological description is often sufficient, but these phenomena can only be truly understood by studying the crystal structure of zeolites in detail. The connectivity between cavities and channels, size, shape, arrangement of cavities and free pore volume, describes the type of framework, which plays an important role in determining the specific properties of a particular zeolite.

According to elemental analysis, the structural characteristics of the synthesized clinoptilolite were calculated. Structural characteristics include properties such as pore volume, free pore volume (without water and cations), density of the zeolite framework (without water and cations), density of hydrated zeolite, density of dehydrated zeolite, number of tetrahedra in 1 cm<sup>3</sup> of zeolite, concentration of exchangeable cations, concentration oxygen ions, activation energy of water self-diffusion.

The calculated values of the above characteristics suggest that the clinoptilolite we synthesized is a good adsorbent.

# THE EFFECT OF $\text{SnF}_2$ AND $\text{PbF}_2$ ON THE PROPERTIES OF $\text{Er}^{3+}$ -DOPED FLUOROZIRCONATE PHOSPHATE GLASSES AND GLASS CERAMICS

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Great attention to glasses and glass ceramics activated rare-earth element (REE) ions is related to their potential applications in solid-state lasers, optical amplifiers, and telecommunication systems. In order to search for new REE-activated materials, the influence of  $\text{SnF}_2$  /  $\text{PbF}_2$  on the thermal and luminescent properties of  $\text{Er}^{3+}$ -doped glasses and glass ceramics of the composition  $55\text{ZrF}_4-(34.5-x)\text{BaF}_2-10\text{NaPO}_3-x\text{SnF}_2(\text{PbF}_2)-0.5\text{ErF}_3$  ( $x=0-20$  mol.%) was investigated.

The introduction of tin/lead difluorides decreases the glass transition and crystallization temperatures of the samples by about  $65^\circ\text{C}$  and  $30^\circ\text{C}$  for  $\text{SnF}_2$  and  $\text{PbF}_2$ , respectively. The addition of  $\text{SnF}_2$  expands the optical transmittance range compared to the original glass.  $\text{PbF}_2$  /  $\text{SnF}_2$  fluorides reduce the luminescence intensity of the  $^2\text{H}_{11/2} \rightarrow ^4\text{I}_{15/2}$ ,  $^4\text{S}_{3/2} \rightarrow ^4\text{I}_{15/2}$  and  $^4\text{F}_{9/2} \rightarrow ^4\text{I}_{15/2}$   $\text{Er}^{3+}$  transitions. However, when 20 mol%  $\text{SnF}_2$  is introduced, an increase in the  $\text{Er}^{3+}$  luminescence intensity by about 1.6 times is observed.

After heat treatment of the samples in the  $T_g$ - $T_x$  range, the luminescence intensity decreases, which is characteristic of  $\text{ZrF}_4$ -based glass-ceramics<sup>1,2</sup>. But for samples containing 20 mol %  $\text{PbF}_2$  after annealing (1 h) at temperatures near  $T_g$ , an increase in luminescence intensity (by 30%) is observed. The microstructure of the samples after 1 h of heat treatment consists of nanoparticles of 5-20 nm in size, but in tin-containing samples, aggregates of 180-250 nm are additionally present. The growth of particle size contributes to the increase of erbium ion concentration inside them, which can cause concentration quenching and, as a consequence, decrease of luminescence intensity.

Transparent glass ceramics in fluorozirconate phosphate systems doped with fluorides  $\text{SnF}_2$  and  $\text{PbF}_2$  were obtained, the most optimal compositions are those containing 5-10 mol. %  $\text{SnF}_2$  and 10-15 mol. %  $\text{PbF}_2$ .

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# OBTAINING MAGNESIUM AND TERBIUM DOPED LITHIUM NIOBATE CHARGE FOR OPTICAL GROWTH HOMOGENEOUS SINGLE CRYSTALS $\text{LiNbO}_3\text{:Mg:Tb}$

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Much attention is being paid to the development of new materials resistant to optical damage based on ferroelectric single crystals of lithium niobate ( $\text{LiNbO}_3$ ) of different stoichiometry and with various dopants (Mg, Zn, In, Gd, Sc, etc.) at present. Double doped crystals are of particular interest. The possibilities for significantly improving the optical quality and physical characteristics of  $\text{LiNbO}_3$  crystals lie in the features of its deeply defective oxygen-octahedral structure as a non-stoichiometric phase of variable composition with a wide homogeneity region in the phase diagram<sup>1</sup>.

The goal of this study was to develop a method for the synthesis of a single-phase lithium niobate charge, doped simultaneously with both Mg and Tb in given concentrations with a chemically uniformly distributed dopant. To then use it to grow  $\text{LiNbO}_3\text{:Mg:Tb}$  crystals using the Czochralski method.

A technological scheme for the synthesis of the  $\text{LiNbO}_3\text{:Mg:Tb}$  charge with the preliminary preparation of the  $\text{Nb}_2\text{O}_5\text{:Mg:Tb}$  precursor has been proposed. Optimal conditions at each stage of the process have been determined. It has been established that when the temperature is 1100°C, a monophasic charge of congruent composition with concentrations of dopants corresponding to the specified  $[\text{Mg}] = 4 \text{ mol\%}$  and  $[\text{Tb}] = 1 \text{ wt\%}$  is synthesized from the precursor and  $\text{Li}_2\text{CO}_3$ . Comparative studies of the quality of the charge obtained by various methods have been carried out<sup>2</sup>. It is shown that the proposed method helps to obtain a charge more homogeneous in composition than the charge that is synthesized by the solid-phase method from  $\text{LiNbO}_3$  with the addition of  $\text{MgO}$  and  $\text{Tb}_4\text{O}_7$  oxides.

The results are important for the development of industrial technology for the production of new functional materials based on lithium niobate.

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## FINISH COATINGS FOR PRINTED CIRCUIT BOARDS (PCBs)

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Due to the rise of the PCB density layout in the production of printed circuit boards (PCB) the finishing coatings are essential to provide both good solderability and surface coplanarity for the installation and soldering of highly integrated components, including BGAs. The technique of finishing coatings also known as ENIG (Electroless Nickel / Immersion Gold) takes a leading position in terms of prevalence among the products for critical use. Nowadays the extremely important issue is the development of immersion gold solution for the internal application.

The main problems of immersion gold plating are insufficient capacity and low stability of solutions. In order to solve these problems various chelating agents with effective complexing properties are added in plating solutions<sup>1</sup>.

Based on a literature data the following solution was chosen as the study object. The study solution contains small quantities of organic acid salts as the chelating agents, potassium dicyanoaurate as a source of gold ions, as well as a reducing agent and buffering components. A solid thin layer can be formed from the study solution. The thickness of 0.05-0.15  $\mu\text{m}$  is gained in 10 minutes at a bath temperature of 85 °C. Furthermore, a good adhesion to the base can be obtained which is in compliance with the standard of the immersion gold plating process<sup>2</sup>.

The investigation shown that the capacity of the solution provides cycle amount of 8 MTO (metal turns), while the treated surface area is 25  $\text{m}^2/\text{l}$ , if the solution adjustment is given periodically. The coating thickness is no possible to obtain according to standard when process is carried out further.

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# WEAR-RESISTANT PHOSPHATE COATINGS ON STEEL

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Phosphate coatings are widely used in modern industry. Good anti-friction properties, corrosion resistance, and protective ability, as well as ease of application and relatively low cost, allow these coatings to be used to prevent seizing during break-in, as well as wear of rubbing surfaces during the running-in process in engineering. Currently, the development of a process for depositing phosphate coatings with high wear resistance, formed at a lower temperature compared to existing ones, is relevant.

The object of the study was a solution for applying manganese-phosphate coatings to steel. The solution, in addition to the main layer-forming ions, contained nitrate ions as an accelerator and  $\text{Ni}^{2+}$  to increase corrosion resistance and fine crystal layers<sup>1</sup>. The quality of wear resistance of the coating on steel can be determined by testing on an orbital shaker in a solid dispersed medium<sup>2</sup>. Fine sand consisting mainly of silicon dioxide<sup>3</sup> is suitable for this.

The effect of the addition of ultrafine diamond suspension to the phosphating solution in the following concentrations (g/l): 10, 20, 50, 100, 200 on the characteristics of deposited coatings has been studied. It was found that the optimal concentration of the suspension is 100 g/l. The coatings formed from the test solution have an increased hardness (180 HV) compared to those obtained in the absence of an additive (155 HV), while the specific wear of the coating after 3 hours of orbital shaker tests decreases from 0.57 g/m<sup>2</sup> to 0.38 g/m<sup>2</sup>. The introduction of the suspension into the phosphating solution has a slight effect on the change in the specific mass of the phosphate layer, which is 5.4 g/m<sup>2</sup> and 5.2 g/m<sup>2</sup>, respectively.

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# PREPARATION OF THIN FILM FUNCTIONAL MATERIALS FROM PEROXIDE SYSTEMS

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The preparation of the functional materials from peroxide systems relies on several distinctive properties of hydrogen peroxide. Firstly, it exhibits acidic properties. Secondly, it is a weak ligand and does not form coordination compounds in the presence of coordinating solvents. In basic media,  $\text{H}_2\text{O}_2$  deprotonates and forms peroxo and hydroperoxo complexes.<sup>1</sup> Additionally, hydrogen peroxide forms strong hydrogen bonds. The  $\text{H}_2\text{O}_2$  molecule always participates in the formation of two H-bonds as a proton donor. These bonds are higher in energy than those of water molecules in isostructural hydrates due to the acidic properties of hydrogen peroxide.<sup>2</sup>

Addition of hydrogen peroxide to the solution of hydroxo compounds of p-block elements results in competing reactions of polycondensation and coordination of peroxo ligands. This can lead to the formation and stabilization of sol particles with high surface activity to the substrate material. The presence of terminal hydroperoxo groups capable of forming strong hydrogen bonds provides this activity. Sol particles are a building block for obtaining composites with different morphologies. Sol deposition allows to obtain 2D composite materials in which oxide nanoparticles of the corresponding element form continuous thin films.<sup>3</sup>

The presence of peroxo groups in sol particles enables simple modification of films through interaction with various oxidizing and reducing agents. For instance, treating the film of nanoparticles of peroxocomplexes of tin, antimony, zinc, and other elements with hydrogen sulfide followed by heat treatment results in the thin film of corresponding sulfides.<sup>3</sup>

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# METHOD OF PRODUCING LIGHT-ABSORBING NICKEL-CONTAINING COATING

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Black nickel coatings have certain disadvantages such as low corrosion resistance, low ductility and poor adhesion to the base metal, especially when applied to steel<sup>1</sup>.

Despite the fact that in the scientific literature there are some data about the influence of the concentration of initial components and organic additives in the solution on the composition and properties of the obtained coatings, the mechanism of deposition of “black” nickel has not yet been investigated in detail.

In the present work, the possibility of deposition of “black” nickel-containing coatings from a solution with the addition of organic additives - saccharin and glycine - in steady-state and step current deposition modes was investigated. The optimum concentration of additives for the solution was selected - 0.2 g/l saccharin and 1.5 g/l glycine.

It was found that both the steady-state and the step electrodeposition mode produce uniformly deposited.

It is shown that “black” nickel coatings deposited by this method contain mainly zinc (59 %), nickel (28 %) and sulfur (13 %).

It was found that the composition of the coating deposited under these conditions includes metallic nickel as well as nickel and zinc sulfides.

It is found that corrosion resistance, colour characteristics and abrasion resistance of black nickel-containing coatings deposited by this method are slightly higher than those of black chrome coatings and nickel-containing coatings that were deposited from solutions without the addition of organic additives. At the same time, the deposited coatings have a more homogeneous distribution and fewer visible defects.

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# PRODUCTION OF METALLISED BASALT FIBRES

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This study is devoted to the production of metallized basalt fibers for further use in radio engineering and radio electronics as microconductors and other fields of technology.

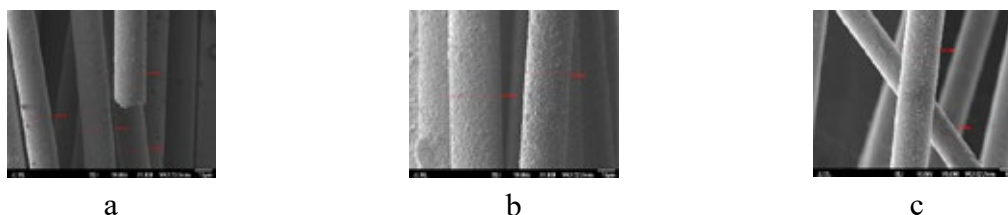
To obtain a metal coating, a chemical metallization method was used, followed by electrochemical deposition of metals.

The process of preparing complex textile structures from hydrocarbon fibers before chemical metallization consists of a number of mandatory stages, including surface degreasing, etching, sensitization, activation<sup>1</sup>.

The optimal conditions for the application of copper and nickel coatings were identified. Current density at copper flow of 5 A/dm<sup>2</sup>, at nickel plating of 3 A/dm<sup>2</sup>, coating thickness varied from 5 to 40 μm.

As a result, metallized basalt fiber is obtained. The nickel or copper content of the 40 μm coated basalt fiber reaches the maximum content over the entire surface area.

Using raster electron microscopy and auger-electron spectroscopy, it was found that of the two nickel and copper coatings obtained, copper has better morphology. It differs in continuity, that is, the metal layer repeats the configuration of each individual filament of the basalt bundle.



**Figure 1.** Micrographs of samples coated with: a - copper by chemical method; b - electrodeposited copper; c - electrodeposited nickel

Measurement of the electrical resistance of the samples showed that as the coating thickness increases, the electrical conductivity increases.

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# NEW ORGANIC DERIVATIVES OF POLYOXOTUNGSTEN METALLATES: SYNTHESIS, STRUCTURE, PROPERTIES

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Polyoxotungsten metallates are actively used by researchers in various fields of science and technology: catalysis, materials science, energy, and medicine. They are promising materials for the production of catalysts for oxidation reactions of organic compounds, photo- and electrocatalytic processes of water decomposition and carbon dioxide absorption, the synthesis of carbon nanomaterials, composite electrochemical sensors, etc.<sup>1</sup>. This work presents the results of the synthesis of new tungstenphosphates and tungstensilicates with organic cations in the outer sphere of the complexes  $\text{Cat}_n[\text{P}(\text{Si})\text{W}_{12}\text{O}_{40}] \cdot x\text{H}_2\text{O}$ ,  $\text{Cat}=(\text{CH}_3)_4\text{N}^+$ ,  $(\text{C}_2\text{H}_5)_4\text{N}^+$ ,  $[\text{Fe}(\text{C}_5\text{H}_5)_2]^+$ , tungstenphosphate- and tungstensilicametal-lates  $\text{Cat}_m[\text{P}(\text{Si})\text{W}_{11}\text{O}_{39}\text{Z}(\text{H}_2\text{O})] \cdot y\text{H}_2\text{O}$ ,  $\text{Cat}=(\text{CH}_3)_4\text{N}^+$ ,  $(\text{C}_2\text{H}_5)_4\text{N}^+$ ,  $\text{Z}=\text{Fe}^{3+}$ ,  $\text{Co}^{2+}$ ,  $\text{Ni}^{2+}$ , as well as tungsten phosphatemetallates with hexamethylenetetramine in the coordination sphere of the complexes,  $\text{Cat}=\text{Na}^+$ ,  $\text{NH}_4^+$ ,  $\text{Z}=\text{Co}^{2+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Zn}^{2+}$ . The compounds were identified by electron and IR spectroscopy, and the zinc complexes were additionally identified by  $^1\text{H}$  and  $^{13}\text{C}$  NMR in  $\text{D}_2\text{O}$  solution. The IR spectra of the synthesized compounds have a shape similar to known compounds with the Keggin anion structure. The thermal transformations of the resulting compounds in air and in an inert atmosphere were studied. According to X-ray phase analysis and electron microscopy, the products of their thermolysis at  $600^\circ\text{C}$  are fine powders with the structure of tungsten bronze. Their catalytic activity in the reaction of microwave synthesis of carbon nanomaterials was studied<sup>2</sup>.

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# PREPARATION OF BARIUM AND STRONTIUM HEXAFERRITES USING THE ELECTROCHEMICAL METHOD

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Hexagonal barium and strontium ferrites occupy a special place among magnetic materials; they exhibit high values of electrical resistivity, coercive force, saturation magnetization and are widely used in electrical engineering, radio electronics, and computer technology. The properties of ferrite-based materials are largely determined by the technological methods of their manufacture<sup>1</sup>.

Traditional ceramic technology for producing ferrites has a number of disadvantages: insufficient activity of powders after grinding, laboriousness, duration of individual stages, high consumption of reagents, high temperatures. At the same time, there is a significant amount of relatively homogeneous technogenic raw-stuff, including waste from the metalworking industry, in particular, scrap and shavings of carbon steel and technical iron.

To utilize this waste and improve the technology for producing barium and strontium hexaferrites, the authors<sup>2</sup> propose to use an electrochemical method, which involves the anodic dissolution of carbon steel in an aqueous solution containing barium and/or strontium nitrate and chloride, at a current density of 0.1-0.2 A/cm<sup>2</sup>. The precipitate obtained during electrolysis process was kept in a matrix solution, filtered and dried. This approach makes it possible to obtain a highly dispersed product, which is a precursor of the target material. After thermal treatment of the dried precipitate, ferrites are formed that have electromagnetic characteristics superior to those of barium and strontium hexaferrites obtained using chemical methods.

In addition, during the synthesis of precursors, it is possible to dope the products with ions of elements that increase some of the electrical and magnetic properties of the synthesized ferrites.

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# SCALING THE METHOD FOR PRODUCING METAL-CONTAINING LIQUID ORGANIC SCINTILLATORS

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A new method has been developed for producing a liquid organic scintillator containing gadolinium, intended for use in detectors of elementary particles, in particular, neutrinos. Functional material provides the ability to remotely monitor the operation of nuclear reactors, for example, the IDREAM detector at the Kalinin NPP. A gadolinium-containing scintillator in a volume of more than 10 tons was manufactured using technology developed at KKH SRC KI1.

In contrast to known methods based on the extraction of gadolinium compounds from an aqueous medium, the developed method makes it possible to obtain water-free scintillation compositions that are stable for a long time<sup>2-5</sup>. For this purpose, an intermediate low-boiling solvent, tetrahydrofuran, was used. A production line has been created that allows for the entire range of technological processes, starting from the production of gadolinium chloride from high-purity oxide to the production of a finished scintillation composition based on linear alkylbenzene containing a gadolinium carboxylate complex, as well as a primary and secondary fluorophore.

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# SYNTHESIS AND STUDY OF MAGNETIC PHOTOCATALYSTS BASED ON NICKEL FERRITE AND ZINC OXIDE

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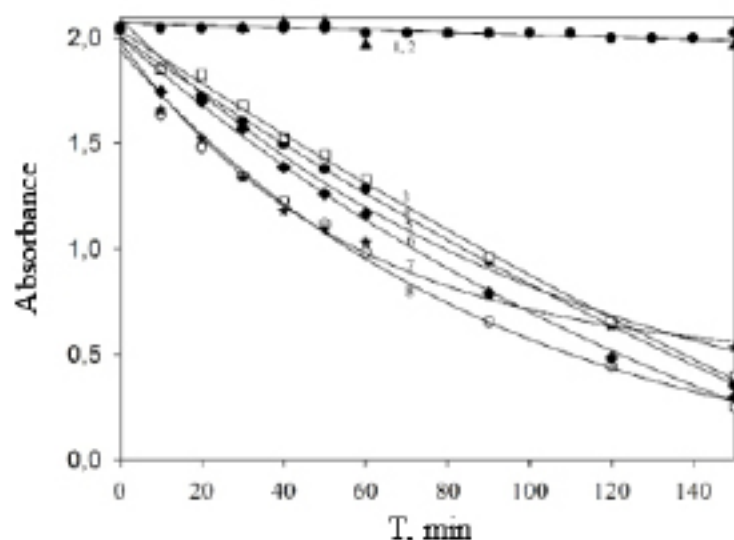
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Recent studies have shown that nonferrous metal ferrites are promising magnetic photocatalysts that, after use, can be easily separated from purified water using a magnetic field. Ferrites are characterized by a fast electron-hole relaxation time, which reduces their activity in photoreactions; however, this problem can be solved by obtaining hybrid nanostructures based on ferrites. In this work, magnetic composite materials  $\text{NiFe}_2\text{O}_4/\text{ZnO}$  were obtained. It was shown that they can be used as an easily separated magnetic photocatalyst for the decomposition of crystal violet (CV) dye.

**Table 1. Composition and parameters of the composite cell**

	$\text{NiFe}_2\text{O}_4$	K1	K2	K3	K4	K5
$a(\text{NiFe}_2\text{O}_4)$ , Å	8.3570	8.3773	8.3916	8.3925	8.3917	8.3883
$\omega(\text{Zn}_x\text{Ni}_{1-x}\text{Fe}_2\text{O}_4)$	-	91.4	93.1	72.5	50.4	37.7
$\omega(\text{ZnO})$	-	5.3	1.8	23.6	46.8	61.1
$\omega(\text{Fe}_2\text{O}_3)$	-	3.3	5.1	3.9	2.7	1.2



1 –  $\text{NiFe}_2\text{O}_4$ , 2 –  $\text{ZnFe}_2\text{O}_4$ , 3 – K4, 4 – K3, 5 – K2, 6 – K5, 7 – K1

**Figure 1. Change in the absorbance of the CV solution depending on the duration of the photocatalytic decomposition process**

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# INVESTIGATION OF THE EFFECT OF $\text{Sr}^{2+}$ IONS ON THE GAS-SENSITIVE PROPERTIES OF $\text{GdCrO}_3$

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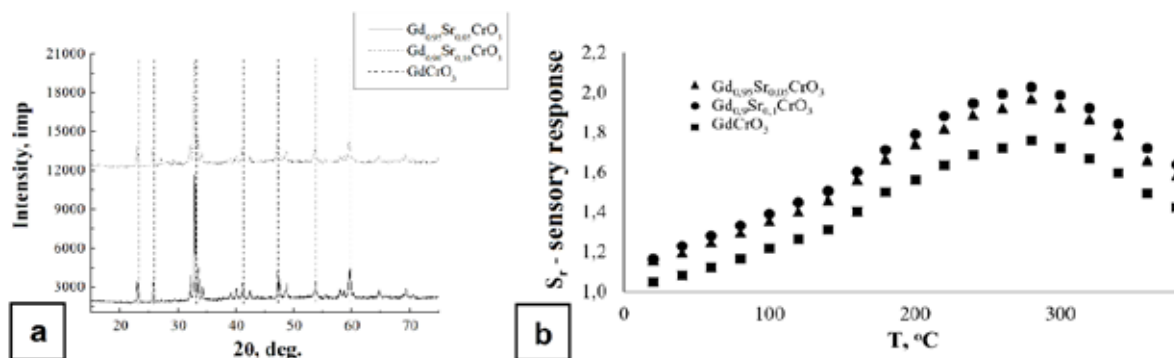
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The study of the gas-sensitive properties of chromites of rare earth metals led to the fact that in order to improve the sensory response of the obtained compounds, it was decided to dope them with  $\text{Sr}^{2+}$  ions.

Starting materials for the synthesis of  $\text{Gd}_{1-x}\text{Sr}_x\text{CrO}_3$  systems (where  $x = 0.05$  and  $0.10$ ): nitrates of the corresponding metals, citric acid, aqueous ammonia. The synthesis was carried out according to the Pechini method<sup>1</sup>, followed by annealing of the precipitate in a muffle furnace at a temperature of  $900^\circ\text{C}$  for 4 hours.

The study of the phase composition by the XRF<sup>2</sup> method of the obtained series of  $\text{Gd}_{1-x}\text{Sr}_x\text{CrO}_3$  nanopowders (where  $x = 0.05$  and  $0.10$ ) showed the presence of only the target phase (Fig. 1.a).

The dependence of the sensory response of the samples on temperature was investigated by determining the resistivity by the four-probe Van der Pau method<sup>3</sup>. The results obtained shown in Fig.1.b.



**Figure 1. a)** Comparison of X-ray diffractograms of a series of  $\text{Gd}_{1-x}\text{Sr}_x\text{CrO}_3$  nanopowders (where  $x = 0.05$  and  $0.10$ ) with pure  $\text{GdCrO}_3$ ;

**b)** Comparison of the sensory response to ammonia vapor (concentration 50 ppm) of  $\text{Gd}_{1-x}\text{Sr}_x\text{CrO}_3$  films (where  $x = 0.05$  and  $0.10$ ) with pure  $\text{GdCrO}_3$ .

## Literature

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# MONO- AND HETEROMETALLIC OXIDE PHASES OF III-V GROUPS OF THE PERIODIC SYSTEM: DIRECTED SYNTHESIS, COMPOSITION, STRUCTURES, PROPERTIES

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Complex oxides of zirconium, hafnium, niobium and tantalum, used either in the form of individual compounds or as components of solid solutions, have a clear prospect of practical use. The methods being developed for the synthesis of these important oxide materials should ensure the maximum possible reduction in the process temperature, the possibility of using precursors of different chemical natures, a high degree of phase and chemical homogeneity, and the reproducibility of a set of properties.

The goal of the work was to develop methods for producing simple and complex oxide phases of d-elements (zirconium, hafnium, niobium and tantalum) with controlled composition and high phase homogeneity using their mono- and bimetallic hydroxo- and alkoxo compounds as precursors.

As a result of the research^

- new methods have been developed for the preparation of simple and complex oxides of d- and f-elements of the Periodic Table, in which low-hydrated hydroxides and alkoxocompounds are used as precursors;

- for the first time, using the developed methods, a number of complex oxides were obtained, the crystal structure of which was studied;

- the effectiveness of using the Supercritical AntiSolvent method in the processes of obtaining individual oxides  $\text{L-Ta}_2\text{O}_5$ ,  $\text{T-Nb}_2\text{O}_5$  and their solid solutions  $(\text{Nb}_x\text{Ta}_{1-x})_2\text{O}_5$  was demonstrated for the first time, and the synthesis of amorphous mono- and bimetallic oxides of zirconium and/or hafnium was carried out for the first time using zirconium acetylacetonate, zirconium propoxide, and hafnium butoxide as precursors;

- A new method has been developed for the synthesis of bimetallic niobium and tantalum carbides at relatively low temperatures ( $\leq 1400^\circ\text{C}$ ), based on the interaction of a polymer composite material based on a phenol-formaldehyde binder and highly dispersed bimetallic low-hydrated niobium-tantalum hydroxide.

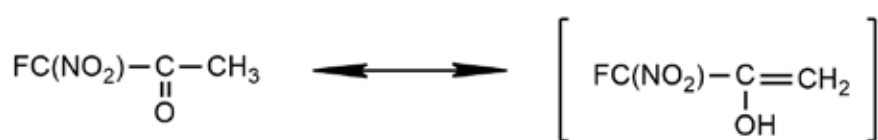
# SYNTHESIS, STRUCTURE AND CHEMICAL PROPERTIES OF FLUORODINITROALKANOLS

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Fluorodinitroalkanols represent an interesting class of specialty organic chemistry. Based on them, complex ethers have been obtained, which plasticize nitrocellulose.

We have studied the Henri reaction of fluorodinitromethane addition to aliphatic aldehyde series.<sup>1</sup>



Further, the synthesized fluorodinitroalkanols were oxidized into ketones. Potassium and ammonium dichromates were used as oxidants in concentrated sulfuric acid.

The syntheses showed that the yields of fluorodinitroketones using potassium dichromate as the oxidant are 20-30% higher than when using ammonium dichromate.

The oxidation product of 1-fluoro-1,1-dinitropropanol-2, distilled under vacuum and identified by IR and <sup>1</sup>H NMR spectra, turned out to be a mixture of isomers: ketone form and enol form in a ratio of 45:55%.



<sup>1</sup>H NMR: 1.3s (CH<sub>3</sub>), 6.2 and 6.6s (CH), and 12s (OH - enolic).

The isolated tautomers were chemically proven: the ketone form yielded the corresponding 2,4-dinitrophenylhydrazones, and the enol form yielded the enol acetate. It was established that in non-polar solvent (CCl<sub>4</sub>) only the ketone form is present, while in polar solvents (CHCl<sub>3</sub>, CH<sub>2</sub>Cl<sub>2</sub>) both ketone and enol exist.

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# OBTAINING LIQUID ORGANOMINERAL FERTILIZERS BASED ON NATURAL RAW MATERIALS OF KAZAKHSTAN

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It has been established that for the normal development of plants, along with the main nutrients (nitrogen, phosphorus, potassium, calcium, magnesium and sulfur), biologically active substances and microelements are also necessary<sup>1,2</sup>. The presence of humic substances and microelements in liquid organomineral fertilizers (LOMF) allows one to more fully balance the mineral nutrition of plants and thereby increase crop yields by an average of 20-30%. In addition, the use of such fertilizers helps to significantly increase the efficiency and reduce the costs of using mineral fertilizers.

In connection with the above, the processes of LOMF synthesis have been studied through the interaction of sodium humate with ammonium heptamolybdate. The experiments have been carried out for 10-120 minutes at a temperature of 20-80°C and a S:L ratio of 0.3÷0.7:100 with a sodium humate concentration of 1.0%. In the synthesized samples have been determined the yield of humic acids (HA<sup>daf</sup>), the content of molybdenum and nitrogen, and the number of acidic functional groups.

It has been established that for all values of the S:L ratio, an increase in the time and temperature of the process leads to an increase in the yield of HA<sup>daf</sup>, N and Mo content, which at S:L = 0.3:100 reaches 37.17, 6.05 and 0.36%, respectively. From the analysis of the results obtained, it follows that during the interaction of sodium humate and ammonium heptamolybdate, a change in their ratios in the system has different effects on the composition of LOMF. It was revealed that with an increase in S:L, the yield of HA<sup>daf</sup> decreases to 36.97%, and the N content increases to 6.0% and Mo - to 0.37%. It has been shown that an increase in the content of COOH and OH<sub>phen</sub> groups enhances the biological activity of the synthesized LOMF samples.

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# SILICON ELECTRODEPOSITION FROM $\text{LiCl-KCl-CsCl-K}_2\text{SiF}_6$ MELT BY REVERSE ELECTROLYSIS

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Silicon materials are among the most in demand in energy, microelectronics, metallurgy and other fields. Promising methods are the electrolytic production of silicon from molten salts, which have recently been increasingly used for the synthesis of pure substances and alloys.

Reverse electrolysis involves cycling of the cathode and anode current, and the magnitude of the cathode current is greater than that of the anode, in order to prevent complete dissolution of the silicon deposit.

The sample in Figure 1 was obtained under the following conditions: the cathode current density is  $28.6 \text{ mA/cm}^2$ , the anode current density is  $4.8 \text{ mA/cm}^2$ . The time of each pulse is 30 seconds, the total duration of electrolysis is 1 hour. The temperature is  $550^\circ\text{C}$ .



**Figure 1.** SEM-image of electrodeposited silicon

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# ANOMALOUS OXIDATION STATE OF EUROPIUM IN DOPED PHOSPHATES $Me_3(PO_4)_2$ ( $Me = Sr, Ba$ )

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The report presents data on the self-reduction of europium in the palmierite-like matrix  $Me_3(PO_4)_2$  ( $Me = Sr, Ba$ ).  $Ba_{3-x}Eu_{2x/3}(PO_4)_2$  ( $x = 0.01, 0.02$ ) and  $Sr_{2.98}Eu_{0.01}M_{0.01}(PO_4)_2$  ( $M = Li^+, Na^+, K^+$ ) solid solutions were obtained by solid-phase synthesis in air at temperature of 1233 K (40 h) and 1423 K (48 h), respectively. The synthesized phosphates are isostructural with the palmierite mineral  $K_2Pb(SO_4)_2$ . Photoluminescence spectra upon excitation at a wavelength of 395 nm consist of intense luminescence bands at 585 nm and 610 nm, characteristic of  $Eu^{3+}$  cations. When excited at a wavelength of 330 nm, a broad band centered at 425 nm, characteristic of  $Eu^{2+}$  cations, is observed in the luminescence spectra. The luminescence of phosphates has been studied in a wide temperature range of 5–350 K (Sr) and 80–500 K (Ba). In  $Ba_{3-x}Eu_{2x/3}(PO_4)_2$  solid solutions, the luminescence intensity of  $Eu^{3+}$  cations significantly depends on temperature and decreases with increasing temperature, while the  $Eu^{2+}$  luminescence practically remains stable in the range of 150–500 K. In  $Sr_{2.98}Eu_{0.01}M_{0.01}(PO_4)_2$  solid solutions  $Eu^{2+}$  luminescence dominates at room temperature, while  $Eu^{3+}$  luminescence is higher at low temperature ( $T < 50$  K). Alkali metal ions noticeably affect the luminescence intensity of  $Eu^{3+}$  and  $Eu^{2+}$ . Phosphate  $Sr_{2.98}Eu_{0.01}Li_{0.01}(PO_4)_2$  shows the highest luminescence intensity. Analysis of the luminescence spectra in the region of the  $^5D_0 \rightarrow ^7F_0$  transition shows that  $Eu^{3+}$  cations occupy two different crystallographic positions in the structure of  $Ba_3(PO_4)_2$  and one in  $Sr_3(PO_4)_2$ . Partial self-reduction of  $Eu^{3+} \rightarrow Eu^{2+}$  in  $Me_3(PO_4)_2$  ( $Me = Sr, Ba$ ) matrices is apparently realized due to the transfer of electrons from the matrix to europium cations. The results of studies of  $Ba_{3-x}Eu_{2x/3}(PO_4)_2$  ( $x = 0.01, 0.02$ ) and  $Sr_{2.98}Eu_{0.01}M_{0.01}(PO_4)_2$  ( $M = Li^+, Na^+, K^+$ ) solid solutions show that the synthesized phosphates are orange-red phosphors and can find application as materials for solid-state lighting. The synthesized phosphates can also be used as temperature measuring materials.



# POLYMER CHEMOSENSORY MATERIALS BASED ON Eu (III) COMPLEXES

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Intensive research is currently underway in the field of the development of multifunctional materials with optical chemosensory properties. Of particular interest is the development of promising sensor materials designed for the rapid and effective detection of ammonia and volatile organic amines in the environment, as well as for rapid analysis of food quality and biomedical purposes.

The luminescent chemosensory properties of Eu(III) carboxylate bis-dibenzoylmethanates with carboxylic acids ((Eu(Dbм)<sub>2</sub>Acid·nH<sub>2</sub>O, where Acid is the carboxylic acid anion, n=0-2) [1] when interacting with ammonia and amine vapors. Quantitative measurements of the optical response showed that with an increase in the analyte concentration in the range of 3-330 ppm, an increase in the luminescence intensity of europium(III) is observed. The reversibility of the luminescent response has been established: after removal of analyte vapors, the initial luminescence of Eu(III) is restored. The high stability of the luminescent response over time in the studied polymer compositions has been established.

The mechanism of the optical effect was revealed by methods of stationary, time-resolved spectroscopy and quantum chemical modeling: the interaction of the analyte with the sensor leads to a change in the type of coordination of carboxylate ions from tridentate-bridged cyclic to bidentate-bridged and an increase in the efficiency of ligand-metal energy transfer.

The resulting chemosensory compositions with the effect of “turning on” luminescence when exposed to analyte are promising for environmental monitoring, food quality analysis, and personalized medicine

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# METHOD FOR PRODUCING SUPERHYDROPHOBIC PROTECTIVE COATINGS ON THE SURFACE OF ALUMINUM ALLOYS

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One of the recently popular ways of protecting metal surfaces from an aggressive environment is the formation of continuous films with water-repellent properties and the self-cleaning ability on their surface, which give the material the property of superhydrophobicity and also protect them from abrasion<sup>1</sup>.

This work proposes a method for increasing the wear resistance of superhydrophobic coatings (SHC) through the preliminary application of an adhesive Ti-Zr-containing sublayer with the required microstructural roughness<sup>2</sup>.

It has been established that this method of forming coatings makes it possible to deposit layers with the highest contact angle (168°) and the highest protective ability (68 s).

It has been shown that preliminary application of a Ti-Zr-containing adhesive sublayer onto an aluminum surface leads to an increase in adhesive strength with subsequently applied SHC and to an increase in the wear resistance of the coating.

It has been established that the application of a Ti,Zr-containing adhesive sublayer improves abrasion resistance: 800 cycles instead of the previous 200, and an increase in corrosion resistance when exposed to a salt fog chamber from 140 to 430 hours.

Taking into account the results obtained, the developed technology can be used to produce superhydrophobic coatings on the surface of aluminum alloys of the AMg6 type. These coating have moisture resistance and anti-icing properties, and thus can be used for protection against the deposition of ice and frost and as a result of that can be also used for the protection against the associated corrosion of building structures (building frames, trusses, window frames, stairs, etc.) and energy, transport, including air transport structures, etc.

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# BRITTLE FRACTURE RESISTANCE OF CERAMIC OXIDE COMPOSITES REINFORCED WITH DISPERSION PHASE

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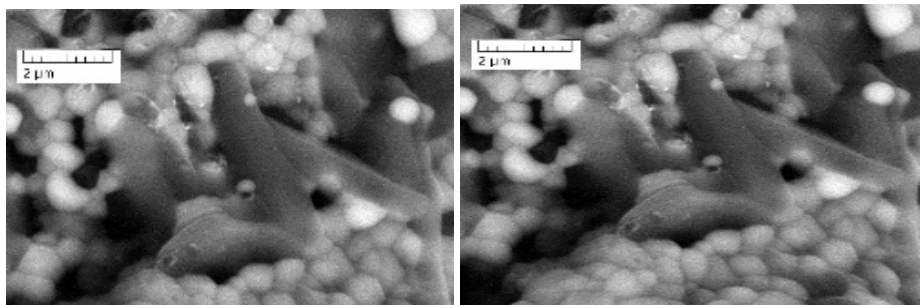
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Oxide-based ceramics as technical materials have a significant drawback: low resistance to brittle fracture. The leveling of this parameter is determined by the development of oxide composites, which include phases that exhibit the effects of transformation and dispersion strengthening.

The purpose of the work is to establish the dependence of the resistance to brittle fracture of ceramic composites of the corundum - tetragonal zirconium dioxide system on the content of the dispersion phase and the type of matrix.

The composites were obtained on the basis of initial powders of the following compositions (mol %) 20-65Al<sub>2</sub>O<sub>3</sub> - 80-35[ZrCe]O<sub>2</sub> (1), 20-65Al<sub>2</sub>O<sub>3</sub> - 80-35[ZrYb]O<sub>2</sub> (2), modified with Ca and Sr cations.<sup>1,2</sup>

It has been shown that the formation of hexaaluminates (Ca,Sr) occurs "in situ" during the sintering of the initial charge. The figure shows SEM images of the fracture of the composites, showing the presence in the microstructure of grains of long-prismatic habit, corresponding to hexaaluminates, which perform the function of dispersion strengthening.



It has been established that in composites of composition 1 complex hexaaluminates (Ca<sub>0.8</sub> Ce<sub>0.2</sub>) Al<sub>12</sub>O<sub>19</sub> are formed, and in composites of compositions Al<sub>2</sub>O<sub>3</sub> - SrO - [ZrYb]O<sub>2</sub> or [ZrCe]O<sub>2</sub> is formed SrAl<sub>12</sub>O<sub>19</sub>. Hexaaluminates have a positive effect on the resistance to brittle fracture of composites, increasing the crack resistance coefficient to 11 MPa·m<sup>1/2</sup>.

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*The work was carried out according to state order No. 075-00320-24*

# OBTAINING EUROPIUM AND GADOLINIUM HAFNATES WITH PYROCHLORE STRUCTURE: INFLUENCE OF MICROWAVE RADIATION ON THEIR PHASE COMPOSITION

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Rare earth element (REE) hafnates with an ordered pyrochlore structure are widely in demand in the field of protective coatings and high-temperature ceramics due to their high melting point, low thermal conductivity, and phase stability<sup>1</sup>.

Europium and gadolinium hafnates with a pyrochlore structure were obtained using a method based on the interaction of hafnium hydroxide and acetates of rare earth elements, followed by microwave treatment of the reaction mixture at different durations and heat treatment.

In the diffraction patterns of samples thermally treated at 1200°C and with insufficient or excessive microwave treatment time, there are reflections characteristic of rare earth hafnates with a disordered structure such as fluorite and oxides of parent metals; the average time of microwave treatment led to the formation of single-phase products with a fluorite structure. Single-phase samples were additionally processed at temperatures of 1350°C and 1450°C. Diffraction patterns showed the presence of reflections corresponding to hafnates with an ordered pyrochlore structure: (111); (311); (331); (511): in samples thermally treated at a temperature of 1450°C, they were more intense. Calculation of the cell parameters for these samples confirms the production of hafnates with an ordered structure already at a temperature of 1350°C: the cell volume of  $\text{Eu}_2\text{Hf}_2\text{O}_7$  is 10.455 Å, and that of  $\text{Gd}_2\text{Hf}_2\text{O}_7$  is 10.454 Å (for the pyrochlore structure, the cell parameters are 10–10.5 Å)<sup>2</sup>.

Thus, microwave treatment makes it possible to obtain rare-earth hafnates with an ordered structure and at a lower temperature.

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# STUDY OF THE MECHANISM OF FORMATION OF SUBSTANCES ON ROTORS OF GAS-BLOWING MACHINES OF COKE AND BY-PRODUCT PLANTS

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A number of coke plants are facing problems of formation of substances on rotors of gas-blowing machines of coke by-product plants. The forming deposits are negatively affecting operation of gas-blowing machines, which are providing specified vacuum in coke ovens of coke oven batteries as well as supply of coke oven gas for heating of coke oven batteries and to other consumers.

Earlier in the paper<sup>1</sup> the review of publications concerning the formation of deposits on valves, gas pipe-lines and gas-blowing machines of coke oven gas has been given. However, in former investigations compositions and reasons of sedimentation of substances on the rotors of gas-blowing machines were not defined.

With the aim of determination of properties of the forming on rotors of gas-blowing machines of coke by-product plant deposits the studies of solubility of the same in water, ethanol and coal tar wash oil have been made<sup>2</sup>. For determination of composition of substances complex of various investigations of sediments from rotors of gas-blowing machines and direct coke oven gas lines was performed<sup>3</sup>.

As a result of investigation implemented mechanism of formation of deposits was determined and found that the formation of deposits in coke oven gas lines is effected by process conditions (cooling and treatment) of coke oven gas. With the aim of excluding overheating and subsequent drying of coke oven gas to prevent the formation of deposits electric tar precipitators are reasonably to be installed downstream (after) gas-blowing machines.

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# STRUCTURE OF THERMOELECTRIC CONVERTERS BASED ON TITANIUM AND ZIRCONIUM NITRIDES

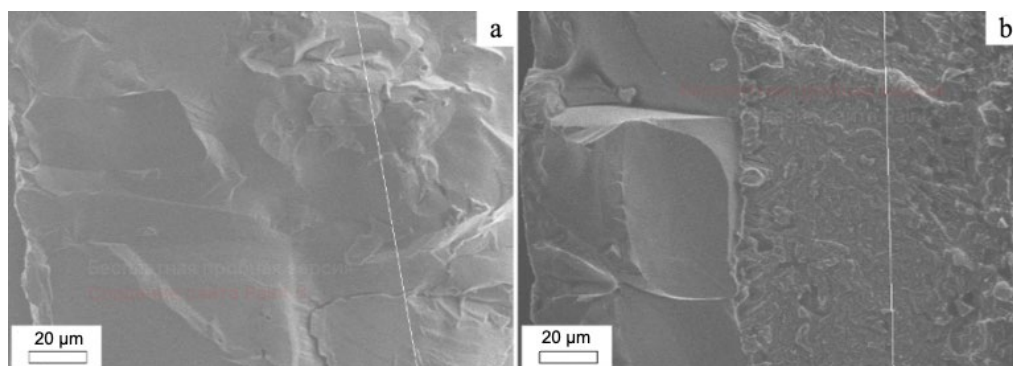
**Kovalev I.A., Rogova A.N., Kochanov G.P.,  
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The high electrical conductivity of titanium and zirconium nitrides makes it possible to use materials based on them as thermoelectric converters. In industry, they are obtained by powder compaction, which, due to the complexity of the nitride sintering process, does not allow to obtain products of complex form. The previously presented approach of oxidative constructing allows to solve this problem and obtain composite materials of various stoichiometries.<sup>1</sup>

Ceramic nitride samples of a given composition and shape were synthesized by controlled nitridization of Ti-Zr metal pairs. The morphology of the transverse chips was studied using a scanning electron microscope.

Studies have shown the three-layer gradient structure of ceramics persists for up to 50 minutes from the beginning of nitridization. The surface layer of the titanium composite presents to be  $\text{TiN}_{0.76}$ , the bulk of the sample has the composition of  $\text{TiN}_{0.5}$  and a thickness of  $\sim 20\text{ }\mu\text{m}$ , in the central area of solid nitrogen solution in titanium of the composition  $\text{TiN}_{0.3}$  was observed. Ceramics based on  $\text{ZrN}$  also have a layered structure, the surface layer of  $\text{ZrN}$  has a thickness of up to  $10\text{ }\mu\text{m}$ , the bulk of  $\text{Zr}_2\text{N}$  is  $70\text{--}80\text{ }\mu\text{m}$  and in the center is a solid solution of nitrogen in zirconium.



**Figure 1.** SEM images illustrating the structure of the transverse chips of Ti-V pair synthesized up to 50 min:  $\text{TiN}_x$  (a),  $\text{TiN}_x$  (b).

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*This work was supported by Russian Science Foundation, the project no. 23-13-00324.*



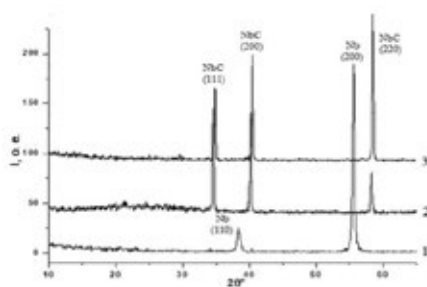
# FEATURES OF THE PROCESS OF OBTAINING CERAMICS BY DIRECT NIOBIUM CARBURIZATION

**Kochanov G.P., Rogova A.N., Kovalev I.A., Chernyavskii A.S., Solntsev K.A.**

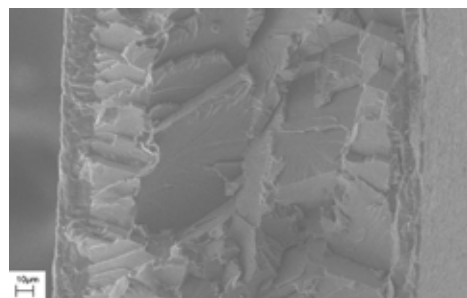
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Ceramics based on niobium carbide are notable for its refractoriness, chemical resistance, hardness, and wear resistance.<sup>1</sup> Conventional approaches to the fabrication of ceramic articles mostly rely on sintering powders.<sup>2</sup> The application of the oxidative constructing allows to obtain ceramics by direct carburization of metallic workpieces of particular shape.<sup>3</sup>

Niobium carbide was synthesized via Joule heating of niobium foil. The metal was carburized in an atmosphere of ethylene and high-purity argon at temperatures of up to 2100 °C. The ethylene was introduced into the reactor during heating of a sample to a preset temperature, after which the carburized sample was held in an argon atmosphere. The temperature control of the sample was monitored with the help of an optical pyrometer.



**Figure 1.** X-ray diffraction patterns of the samples studied: (1) parent niobium, (2) niobium carbide powder sample, (3) niobium carbide surface.



**Figure 2.** SEM images illustrating the morphology of niobium carbide.

The studies have shown the process of niobium carburization comprises two steps. In the first step, carbon is formed on the metal surface, reacts with the metal, and diffuses into the bulk of the material. The second step is the formation of niobium carbide.

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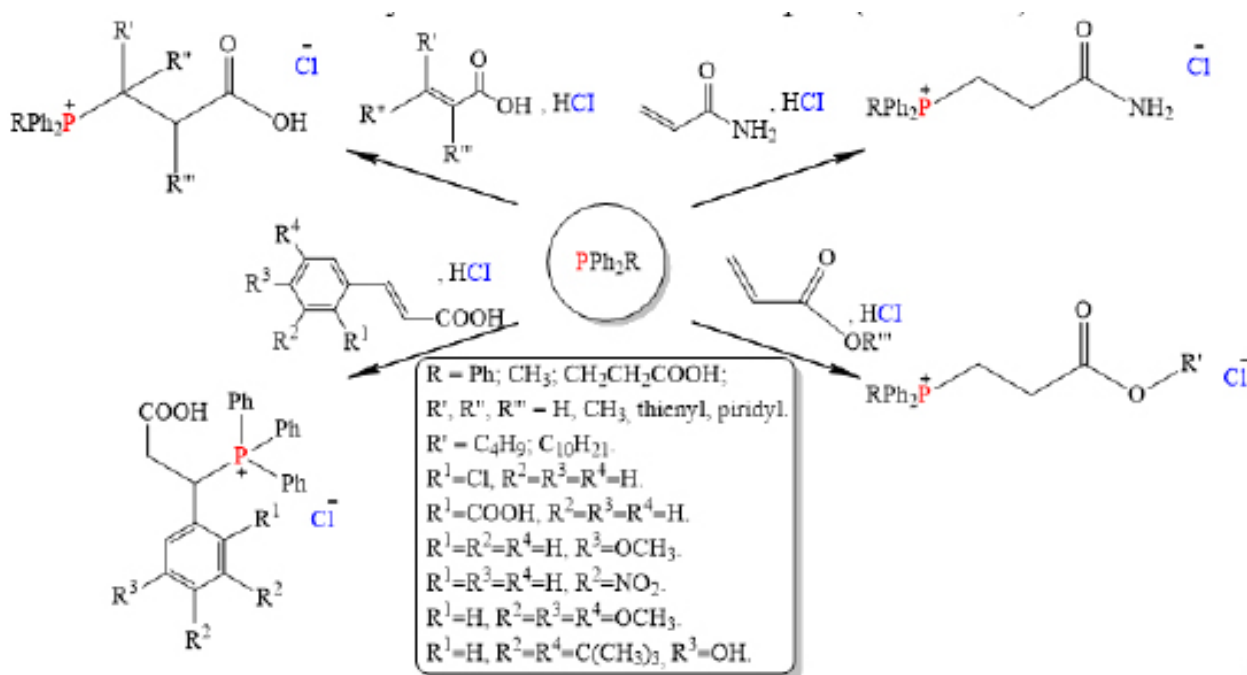
# NEW APPROACHES TO THE SYNTHESIS OF QUATERNARY PHOSPHONIUM SALTS BASED ON ONE-POT REACTIONS

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Quaternary phosphonium salts are of interest to researchers due to their wide biological activity. Arylphosphonium compounds have also recently been actively used as drug delivery systems<sup>1</sup>. In this regard, the development of new methods for the synthesis of such compounds is an urgent task<sup>1</sup>.

The convenient and effective approach to the synthesis of quaternary phosphonium salts based on tertiary phosphines and unsaturated electrophilic compounds: substituted acrylic, cinnamic acids, as well as on the basis of amides and esters of acrylic acid has been developed (Scheme 1).



Scheme 1.

This method makes it possible to obtain wide ranges of phosphonium salts with antimicrobial activity under identical conditions.

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# NEW STRUCTURAL COMPOSITES WITH MATRIXES BASED ON AMORPHOUS AND CRYSTALLINE PHASES

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Many effects achieved by the use of nanomaterials in compositions with traditional binders can form the basis for the creation of modern unique technologies for the production and effective use of nanoelectronic devices based on composite nanomaterials.

Studies on the effects of absorption of microwave EMR in composites based on epoxy polymer matrices containing nano- and microparticles of ferromagnetic alloys, transition element oxides, and carbon nanotubes have shown that the effects of ferromagnetic resonance and antiresonance observed in such composites depend on the distribution and orientation of magnetic particles, which form nano- or microregions<sup>1</sup>. In epoxy polymer matrices, the effects of significant changes in electrical, mechanical, and thermophysical properties have also been noted with the introduction of oxide and carbon nanoparticles<sup>2</sup>. New opportunities for a special structural organization of nanocomposites arise when the ratios of allotropic states of sulfur are stabilized during the curing of its compositions with nanoparticles in the presence of modifiers—polymer sulfur stabilizers.

A comparative analysis of the processes of structure formation of matrices of various compositions (using the example of epoxy resins, sulfur) was carried out in order to identify the potential capabilities of binders for the formation of nanocomposite materials with specified properties.

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# OBTAINING AND STUDYING THE PROPERTIES OF COMPOSITE BUILDING MATERIALS BASED ON WASTE PETROCHEMICAL AND THERMAL POWER COMPLEXES

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As is known, one of the current trends in building materials science is the creation of new types of composite building materials, capable long-term time be exploited in various aggressive environments and climatic conditions. In particular, such a building material is sulfur concrete, consisting of inert fillers (with varying degrees strength and dispersion), acting as an internal frame, and sulfur itself, the melt of which acts as a binder for the entire composition with the addition of various modifiers. Using the “hot” technology method, fifty compositions of sulfur concrete were obtained and their physical and mechanical properties were studied: strength, density, water absorption and biostability. It has been established that in order to obtain sulfur concrete with optimal characteristics, the compositions must contain sulfur (waste from the oil refining complex) and two fillers with varying degrees of dispersion: quartz sand and ash and slag waste from the thermal power complex. The optimal sulfur content in sulfur concrete compositions, necessary to obtain concrete with maximum physical and mechanical characteristics, should make up 40% or 45% (by mass). Installed basic patterns changes in the physical and mechanical characteristics of sulfur concrete depending on variations in the composition of the compositions. The process of biodamage to sulfur concrete compositions was modeled in model media of carboxylic acids corresponding in composition to cultural liquids produced by mold fungi of the genera *Aspergillus niger* and *Aspergillus fumigatus*. It has been established that the biostability of sulfur compositions is comparable with similar values for Portland cement concrete.

It has been established that the sodium silicate modifier affects the physical and mechanical characteristics and biostability of sulfur concrete in various ways. A conclusion is drawn about the influence of the composition on the properties of sulfur concrete and the possibility of their practical use.

# INCREASING THE CORROSION RESISTANCE OF TITANIUM ALLOYS BY ELECTROCHEMICAL SURFACE ALLOYING WITH NOBLE METALS

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To increase the corrosion resistance of titanium alloys, various surface treatment techniques are used. This study presents a method for electrochemical surface alloying of a titanium alloy with noble metals (in particular, palladium) and justifies the choice of the mode of electrochemical deposition of local nano-sized coatings.

The electrode polarization mode of VT1-0 titanium alloy has a significant effect on the number of nuclei on the surface and the thickness of the layer of elemental palladium. Scanning electron microscopy and Auger electron spectroscopy were used to study the morphology, elemental composition of the surface and near-surface layers, and the distribution of elements over the thickness. The size of elemental palladium nuclei on the surface of a sample of titanium alloy, kept without polarization in a solution containing 1% Pd(II), is approximately 3 nm. The thickness of the elemental palladium layer on a titanium alloy sample, polarized by a direct current with a density of 2  $\mu\text{A}/\text{cm}^2$  in the solution under study, reaches 6 nm. A sample of a titanium alloy, polarized by a weak alternating current of infra-low frequency in a solution containing 1% Pd(II), has on the surface a layer of elemental palladium 40-600 nm thick, unevenly distributed throughout its depth. Using the Auger spectroscopy method, the elemental composition of titanium alloy samples with a modified surface was established: in order of the content of elements along the thickness of the surface layer, they are arranged as follows - Pd, O, Ti.

Samples of a titanium alloy with a surface modified with palladium using alternating and direct current in the test solution were subjected to corrosion tests in hydrochloric acid with a concentration of 5.0 M. Tests showed that the most corrosion-resistant is a sample with a surface alloyed using alternating current .

# DEPOSITION OF ZINC SULPHIDE FILMS FROM SOLUTIONS OF COMPLEX COMPOUNDS $[\text{Zn}(\text{N}_2\text{H}_4\text{CS})_2\text{Br}_2]$ IN THE PRESENCE OF MANGANESE IONS

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By spray pyrolysis method from complex compounds  $[\text{Zn}(\text{N}_2\text{H}_4\text{CS})_2\text{Br}_2]$  at a temperature of 450 °C were synthesized the ZnS films doped by manganese ions with concentration  $10^{-7}$ – $10^{-3}$  at. %. Manganese bromide (II) was used as an activating dopant. The samples were investigated by optical spectrophotometry and photoluminescence spectroscopy.

The study of the absorption spectra of deposited samples in the region of the edge of fundamental absorption showed that the optical band gap  $E_g$  for undoped zinc sulfide is 3,55 eV, and for  $\text{ZnS:Mn}^{2+}$  films increases from 3,58 eV to 3,70 eV with an increase in the concentration of manganese ions (Table 1).

This change of  $E_g$  may be due to disordering in the cationic sublattice of the sulfide and a change in the band structure of ZnS upon the introduction of an activating impurity of manganese.

**Table 1.**

Concentration of manganese ions, at. %	0	$10^{-7}$	$10^{-6}$	$10^{-5}$	$10^{-4}$	$10^{-3}$
Optical band gap, eV	3,55	3,58	3,59	3,61	3,63	3,70

The photoluminescence spectra of ZnS films are broad complex bands consisting of several elementary bands with maxima in the wavelength ranges 470–490 nm, 510–520 nm, 570–600 nm, and 710–750 nm. The introduction of an impurity of manganese ions practically does not change the position of the elementary bands and leads to an increase in the intensity of the glow up to 2,5 times. The maximum photoluminescence intensity is observed at an activator concentration of  $10^{-3}$  at. %.

The detected luminescence bands are caused by luminescence centers based on intrinsic and impurity defects: bromine and oxygen, occupying the places of sulfur; zinc vacancies, free and occupied by manganese ions.



# PREPARATION OF IRON-, COBALT- AND NICKEL-CONTAINING NANOSCALE COMPOSITES BY THERMAL DECOMPOSITION OF THEIR SATURATED CARBOXYLATE SALTS

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Nanoscale particles serve as the basis for many unique materials and are widely used in energy conversion and storage, catalysis, measuring instruments, imaging, magnetic media with high density recording information based on them, biomedicine and many others<sup>1</sup>.

Thermolysis of carboxylates provides virtually unlimited possibilities for the creation of various types of nanocomposites and is the simplest and most common method that allows up to 90 wt.% to be introduced into a polymer composition of colloidal metal particles<sup>2</sup>.

In this work, iron, cobalt, and nickel-containing nanocomposites in which nanoparticles are distributed in an amorphous carbon matrix are obtained by thermal decomposition of saturated carboxylates. The obtained products were characterized using the methods of elemental analysis, IR spectroscopy and XRD. TEM and SEM images of metal-containing nanocomposites were obtained, as well as magnetic studies were carried out. There is conclusion about possible applications of the obtained composites.

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# INFLUENCE OF THE CONDITIONS OF ZIRCONIUM DIOXIDE SYNTHESIS ON TEXTURAL AND STRUCTURAL PROPERTIES

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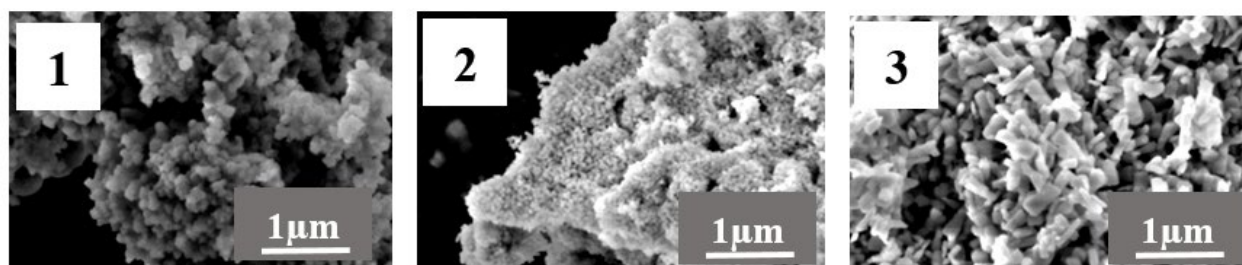
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Zirconium dioxide is currently widely used to produce various materials. Interest in it is due to its properties – high melting point, low thermal conductivity, resistance to chemical reagents<sup>1,2</sup>.

Zirconium dioxide was obtained in the process of sol-gel synthesis in three ways (table 1). Zirconium (VI) butylate 80% in 1-butanol was used as a precursor.

**Table 1.** Textural and structural properties of zirconium dioxide samples obtained by various methods

№	Conditions of receipt	Spec. surface area, m <sup>2</sup> /g	Pore volume, cm <sup>3</sup> /g	Pore size, nm	The detected phase	Crystallite size, nm
1	NH <sub>4</sub> OH precipitation followed by drying and calcination	147	0,24	7,7	t-ZrO <sub>2</sub> + m-ZrO <sub>2</sub>	8,22
2	Hydrothermal exposure in the presence of surfactants (CTAB)	48	0,14	7,1	m-ZrO <sub>2</sub> + c-ZrO <sub>2</sub>	8,81
3	Deposition of NaOH under conditions of hydrothermal exposure and ultrasonic exposure	27	0,08	10,7	m-ZrO <sub>2</sub>	38,39



**Figure 1.** SEM images of synthesized samples.

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# SYNTHESIS AND STUDY OF GAS-SENSITIVE PROPERTIES OF THIN FILMS $\text{Cd}_x\text{Pb}_{1-x}\text{S}$

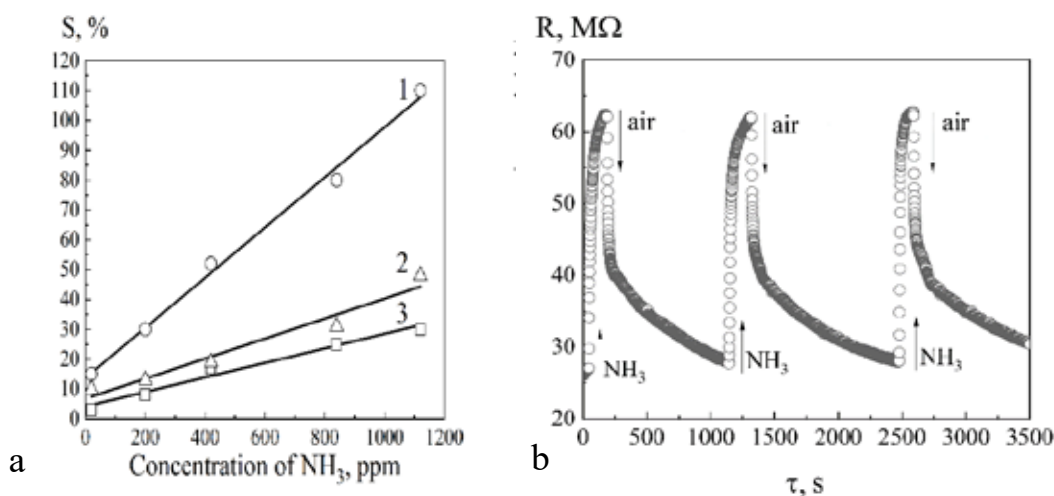
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The most common materials for resistive gas sensors are mixed metal oxides. However, such sensors require heating to high operating temperatures of 423–1173 K, which complicates their design and increases production costs. An alternative to these materials can be thin films of solid solutions in the CdS–PbS system, obtained by a simple and economical method of chemical deposition. Moreover, these compounds have a developed surface due to the formation of various defects associated with lattice distortion. It makes it possible to create sensors based on them that are sensitive to toxic gases and operate at room temperature (20–25° C).

This work demonstrates the possibility of using sensor elements based on chemically deposited thin films of  $\text{Cd}_x\text{Pb}_{1-x}\text{S}$  solid solutions to determine the  $\text{NH}_3$  content in air at room temperature. Fig. 1a shows the dependence of the response value ( $S$ ) of the  $\text{Cd}_{0.068}\text{Pb}_{0.932}\text{S}$ ,  $\text{Cd}_{0.056}\text{Pb}_{0.944}\text{S}$  and  $\text{Cd}_{0.040}\text{Pb}_{0.960}\text{S}$  films obtained in the presence of 0.06, 0.08 and 0.10 mol/l  $\text{CdCl}_2$  on the ammonia concentration (14.3–800  $\text{mg}/\text{m}^3$ ) in the air environment under study, as well as the resistance change of the  $\text{Cd}_{0.068}\text{Pb}_{0.932}\text{S}$  film (b) under cyclic injection of ammonia (1120 ppm) followed by relaxation in air.



**Figure 1.** Dependence of the response value ( $S$ ) (a) of  $\text{Cd}_{0.068}\text{Pb}_{0.932}\text{S}$  (1),  $\text{Cd}_{0.056}\text{Pb}_{0.944}\text{S}$  (2) and  $\text{Cd}_{0.040}\text{Pb}_{0.960}\text{S}$  (3) films. The resistance changes of the  $\text{Cd}_{0.068}\text{Pb}_{0.932}\text{S}$  film (b) to the cyclic  $\text{NH}_3$  gas injection (1120 ppm). Temperature – 25° C.

# CHEMICAL PROTECTIVE COMPOSITE MEMBRANE ON THE BASIS OF POLYAMIDE IMIDE

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New tasks brought forward by current requirements to living standards can only be solved on the basis of fundamentally new technologies and new materials. Polymer membrane materials, widely used in many industries, hold a special place among them<sup>1</sup>.

The use of polymer membrane materials for the manufacture of protective clothing (protection from toxic and hazardous chemicals) is a brand new direction in domestic membrane science and technology. The creation of modern protective clothing requires, along with high protective properties from the gas and liquid phases of a toxic chemical product, high physiological and hygienic characteristics.

Research has been carried out to develop a permeation-selective polymer composite membrane with the required set of properties, namely, to provide the required protection from toxic chemicals with satisfactory physiological and hygienic characteristics of the material.

In the present paper, a polymer composite membrane was obtained, which is a filled polymer film based on the basis of polyamide imide. The use of a high-molecular polyvinylpyrrolidone additive, characterized by hydrophilicity and compatible with the matrix polymer of the film, that made it possible to develop a composition that possess high protective characteristics for the vapor and liquid phase of the toxic chemical and the physiological and hygienic properties necessary for the exploitation of the material (in terms of vapor permeability). The properties of the resulting membrane are comparable to foreign-made samples, it is ready for use without the use of an additional sorbing layer, retains its protective characteristics at 100% moisturization, and has also light weight and shallow thickness.

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1. Plate N.A. Membrane technologies are an avant-garde direction in the development of science and technology of the 21st century. Membranes. 2002, 1, pp. 2-12.

# CHEMICAL PROTECTIVE COMPOSITE MEMBRANE ON THE BASIS OF POLYAMIDE IMIDE

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# SYNTHESIS AND PROPERTIES OF NANOCOMPOSITES BASED ON COBALT ACETATE

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Materials containing nanoparticles (NPs) are widely used in various fields of chemistry, physics, and biology, which stimulates further research into a number of theoretical and practically significant problems [1]. Thermal transformations of metal-containing monomers are a modern and effective method for producing nanocomposites, allowing to combine the formation of highly dispersed metal NPs with a polymer matrix that stabilizes them [2]. In the presented work, the electrical properties of nanocomposites obtained as a result of the thermal decomposition of cobalt acetate were studied [3]. Using an extruder, 1 mm thick plates were obtained, which were a dispersion of a cobalt-containing nanocomposite in high-density polyethylene (LDPE). The composite content was 0, 10, 25, 35, 50 wt. %. The dependences of  $\epsilon$  and  $\text{tg}\delta$  of the samples on frequency, as well as the resistance of the samples on the exposure time at different voltages (10...500 V), were obtained. It has been established that the resulting material is a dielectric with values of  $\epsilon$  2.3...3.5,  $\text{tg}\delta$  0.003...0.07 at frequencies of  $10^3$ ... $10^6$  Hz and with a specific volume resistance comparable to the values for unfilled LDPE.

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# HIGH-TEMPERATURE OXIDATION OF THE COBALT-NICKEL DISPERSION-HARDENED ALLOYS ALLOYED WITH NIOBIUM AND TANTALUM AND SURFACE SATURATED WITH CHROMIUM

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The oxidation resistance of cobalt alloys in air is significantly lower than that of nickel alloys. To improve oxidation resistance, one way is to modify the surface composition of materials to reduce the oxidation reaction rate.

In this study, the surface of the dispersion-hardened cobalt-nickel alloys<sup>1,2</sup> alloyed with niobium and tantalum was saturated with chromium vapour in a vacuum at 1375 K for 48 hours (Figure 1a).

The study analysed the oxidation of these alloys in air at 1200 K and found that the oxidation rate decreases as a result of the formation of a  $\text{Cr}_2\text{O}_3$  layer on the surface of the alloys (Figure 1b).

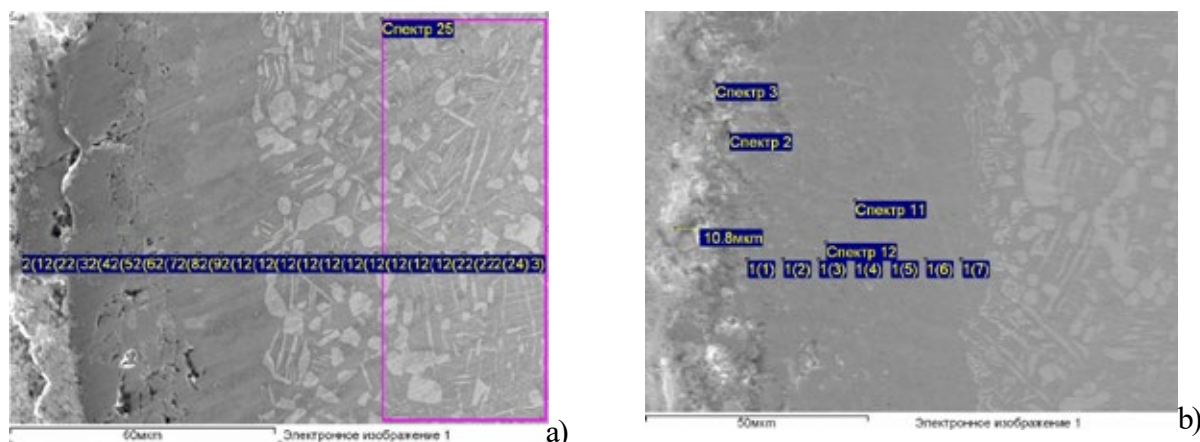


Figure 1. Microstructure of the alloy (Co54.4Ni38.3Ta7.3, at. %) saturated with chromium:  
a) before oxidation; b) after oxidation in air at 1200 K for 100 hours.

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# PHASE EQUILIBRIA IN THE TERNARY SYSTEMS OF COBALT WITH NIOBIUM, TANTALUM, MOLYBDENUM AND TUNGSTEN AT 1200 AND 1375 K

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The optimisation of compositions of the modern superalloys requires the construction of isothermal cross sections at the temperatures of homogenisation (1375 K) and dispersion solidification (1200 K). Cobalt and heat-resistant metals from 5-6 groups of the Periodic System are the most important components of these superalloys.

Table 1 presents the phase equilibria established for cobalt systems with niobium, tantalum, molybdenum, and tungsten at 1375 K and 1200 K.

Five phases are in equilibrium with the  $\gamma_{Co}$ -solid solution (the Cu-type of the crystal structure) in the ternary Co-Me<sub>1</sub>-Me<sub>2</sub> (Me = Nb, Ta, Mo and W) systems: the  $\alpha'$  phase (the MgCd<sub>3</sub>-type of the crystal structure) at 1200 and 1375 K, the  $\alpha''$  phase (the BaPb<sub>3</sub>-type of the crystal structure) at 1200 and 1375 K, the  $\epsilon_{Co}$  phase (the Mg-type of the crystal structure) only at 1375 K, the  $\lambda$  phase (it is polytype: the MgCu<sub>2</sub>-type of the crystal structure and the MgZn<sub>2</sub>-type of the crystal structure) only at 1375 K and the  $\lambda'$  phase (the MgNi<sub>2</sub>-type of the crystal structure) only at 1375 K.

Only the  $\alpha'$  and  $\alpha''$  phases can be used for hardening cobalt alloys. These phases form equilibria with the  $\gamma_{Co}$ -solid solution at both 1375 and 1200 K.

**Table 1.** Three-phase equilibria in ternary systems of Co with Nb, Ta, Mo and W.

Ternary system	Heat treatment conditions	
	1375 K, 1000 h	1200 K, 1500 h
Co-Nb-Ta	$(\gamma_{Co}+\lambda+\lambda'_{Nb}), (\gamma_{Co}+\lambda+\lambda'_{Ta}), (\beta+\mu+CoTa_2)$	$(\alpha'+\alpha''+\gamma_{Co}), (\alpha'+\alpha''+\lambda), (\beta+\mu+CoTa_2)$
Co-Nb-Mo	$(\gamma_{Co}+\epsilon_{Co}+\lambda), (\gamma_{Co}+\lambda+\lambda'), (\epsilon_{Co}+\lambda+\mu)$	$(\alpha'+\lambda+\mu)$
Co-Nb-W	$(\alpha'+\gamma_{Co}+\lambda), (\alpha'_W+\gamma_{Co}+\lambda), (\alpha'+\lambda+\mu), (\gamma_{Co}+\lambda+\lambda'_{Nb})$	$(\alpha'+\lambda+\mu)$
Co-Ta-Mo	$(\alpha'+\gamma_{Co}+\lambda), (\gamma_{Co}+\epsilon_{Co}+\lambda), (\gamma_{Co}+\lambda+\lambda'), (\epsilon_{Co}+\lambda+\mu), (\beta+\mu+CoTa_2)$	$(\alpha'+\alpha''+\gamma_{Co}), (\alpha'+\alpha''+\lambda), (\alpha'+\lambda+\mu), (\beta+\mu+CoTa_2)$
Co-Ta-W	$(\alpha'+\alpha''+\gamma_{Co}), (\alpha'+\alpha''+\lambda), (\alpha'+\lambda+\mu), (\alpha''+\gamma_{Co}+\lambda), (\gamma_{Co}+\lambda+\lambda'_{Ta}), (\beta+\mu+CoTa_2)$	$(\alpha'+\alpha''+\gamma_{Co}), (\alpha'+\alpha''+\lambda), (\alpha'+\lambda+\mu), (\beta+\mu+CoTa_2)$
Co-Mo-W	$(\alpha'+\gamma_{Co}+\epsilon_{Co}), (\alpha'+\epsilon_{Co}+\mu)$	-

# SYNTHESIS, STRUCTURE AND PROPERTIES OF A COPPER(II) BINUCLEAR COMPLEX BASED ON TRIFLUOROMETHYL CONTAINING BIS(PYRAZOLYL) HYDRAZONE

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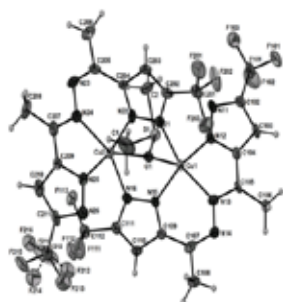
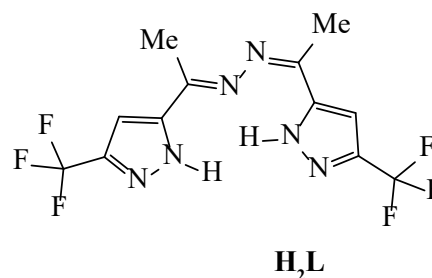
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A complex of copper(II) with methyl-5-(trifluoromethyl) pyrazole-3-yl-ketazine ( $H_2L$ ) of the composition  $[Cu_2L_2] \cdot C_2H_5OH$  (**1**) has been synthesized and studied. Upon recrystallization of **1** from DMSO, a single crystal of the complex  $[Cu_2L_2((CH_3)_2SO)]$  (**2**) suitable for X-Ray structure determination has been obtained, (Fig. 1).



**Figure 1.** Molecular structure of complex **2**

In **2**, copper(II) ions replace both protons in the  $H_2L$  ligand; the resulting  $L^{2-}$  anion acts as a tetradentate ligand, coordinating to two Cu(II) ions by nitrogen atoms. DMSO oxygen is coordinated to both Cu(II) ions.

The  $\chi_p(T)$  dependence measured for complex **1** within the temperature range of 1.77–300 K at magnetic fields  $H = 0$ –10 kOe points to the predominance of antiferromagnetic interactions between copper(II) ions.

A study of cytotoxic properties on human tumor cell lines HepG2, MCF7, Hep2 has shown that complex **1** has a strong dose-dependent cytotoxic effect on cells with LC50 values from  $0.79 \pm 0.01$  to  $2.53 \pm 0.03 \mu M$ , which significantly exceeds the activity of comparison drugs (cisplatin and carboplatin) under similar experimental conditions. A study performed on non-tumor fibroblasts of human lung MRC5 has revealed the selectivity of the activity of **1** towards tumor cells (selectivity index > 2.5).

# SOLUTION OF CHEMICAL COPPER PLATING OF HOLES OF MULTILAYER PRINTED CIRCUIT BOARDS

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One of the main stages of the printed circuit board (PCB) production technology is the process of chemical metallization, as a result of which a thin conductive layer with a thickness of 0.3–1.0  $\mu\text{m}$  is formed, which ensures good adhesion of the metal to the dielectric<sup>1</sup>.

One of the necessary components of a chemical copper plating solution is an organic ligand, which as a rule uses ethylenediaminetetraacetic acid (EDTA) or its salts, for example trilon B, as well as tartaric acid salts, in particular, potassium-sodium tartrate.

The addition of potassium-sodium tartrate into the solution of chemical copper plating as a chelating agent for copper ions and trilon B as a stabilizing component, presumably, will increase the stability of the solution while maintaining the quality of the copper coating and facilitate wastewater treatment.

A previously developed solution of chemical copper plating of PCB holes YM-X5C<sup>2</sup> was chosen as base. The addition of trilon B to the solution in the amount of 1.62–4.86 g/l makes it possible to precipitate copper coatings with a thickness of 0.87–1.70  $\mu\text{m}$  in 15 minutes at the temperature of 35°C.

It was found that the increase of the concentration of EDTA in a chemical copper plating solution significantly accelerates the deposition process. The addition of 3.24 g/l of trilon B to the base solution significantly increases the surface roughness: the arithmetic mean parameter increases from 0.59 to 0.79. The continuity of the copper coating in the holes of the test coupons is estimated by points D7–D10 according to the rating scale using the “backlight test” method<sup>3</sup>. The stability of the base solution in the presence of trilon B increases approximately 5 times.

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# INVESTIGATION OF THE INTERACTION OF TITANIUM(IV) COMPOUNDS WITH PALLADIUM(II) AMINO COMPLEXES

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Titanium dioxide powders with immobilized noble metal particles are of interest, in particular, as catalysts in which titanium dioxide acts as a carrier. The process of obtaining such materials is quite laborious and includes the stages of obtaining a carrier (titanium dioxide), followed by its impregnation with a metal salt solution and calcination. The aim of the work was to obtain palladium-containing titanium dioxide by combining the hydrolysis process of titanium-containing products with simultaneous sorption of palladium(II) cationic complexes with subsequent heat treatment of the product.

The hydrolysis of titanium compounds was carried out by the interaction of an ammonia solution containing  $[\text{Pd}(\text{NH}_3)_4]^{2+}$  ions with titanium-containing compounds: isopropoxide or titanium(IV) tetrachloride. In both cases, the instantaneous formation of white precipitation was observed. Presumably, palladium complexes are sorbed by freshly deposited hydrated titanium oxide during hydrolysis. At the same time, palladium is quantitatively extracted from the solution obtained by interaction with titanium isopropoxide (EPd > 99.5%); with titanium tetrachloride under the same experimental conditions by about 60%. The study of the thermal stability of the dried samples showed that the decomposition of the products proceeds in a number of difficult-to-separate stages, the end of decomposition in the case of the initial compound of titanium tetrachloride occurs at 750 °C; in the case of titanium isopropoxide, in the temperature range of 480-750 °C, the mass of the decomposition product is stable, which significantly reduces the temperature of subsequent heat treatment.

The phase composition of thermal degradation products at 1000 °C is represented by palladium metal (Fm3 m) and TiO<sub>2</sub> in the form of rutile, however, the final product obtained using titanium isopropoxide additionally contains an anatase phase. Isothermal exposure at a temperature of 500 °C from a substance obtained using titanium isopropoxide, it was possible to obtain a product in which titanium dioxide is represented only by a modification of anatase, which is more preferable as a carrier for the catalytic purpose of the material.

*“The work was performed using the equipment of the RTU MIREA Central Research Center with the support of the Ministry of Education and Science of the Russian Federation under Agreement No. 075-15-2021-689 dated 09/01/2021” within the framework of the initiative theme 194-ITHT*



# OBTAINING OF ALUMINUM ALLOY – TITAN POWDER COMPOSITE MATERIALS

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Metal matrix composite materials (MMCM) show promise for industrial application due to their unique properties<sup>1</sup>. Powder metallurgy is often used to produce ligatures including Al-Ti<sup>2,3</sup>. The MMCM were obtained in the research institute using powdered Ti (table.1).

**Table 1.** Micro-hardnes of original and new materials

Original alloy, micro-hardness, HV, GPa.		Composite alloy	After centrifuge	
			Ti content, mass%	Micro-herdness, HV, GPa.
1421	1.33	1421-Ti	3.2	1.71
1570	1.03	1570-Ti	6.4	2.60
A99	0.39	Al-Ti	14.8	2.10

Prolonged interaction of Ti with molten Al creates particles of intermetallic compound (IMC) –  $Al_3Ti$ , that increase the melt's viscosity to a paste-lake condition that prevents obtaining of the MMCM. The authors suggest injection of powdered Ti into Al melt with inert gas followed by centrifugalization as the optimal method to obtain the MMCM. On the surface of the Ti powder the IMC film with increased density ( $Al - 2.7$ ,  $Al_3Ti - 3.5$ ,  $Ti - 4.5$  g/sm<sup>3</sup>) is formed, allowing to concentrate Ti with centrifugal force. The MMCM are created on the bottom of the crucible with its properties depending on the amount of introduced Ti and the rotation rate of the centrifuge.

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*The work was carried out in accordance with the state task and plans of scientific research work of the ISSC UB RAS (№ AAAA-A19-119031890028-0).*

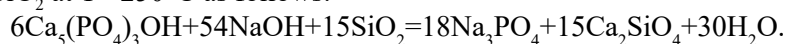


# ALKALINE METHODS OF PHOSPHORUS EXTRACTION

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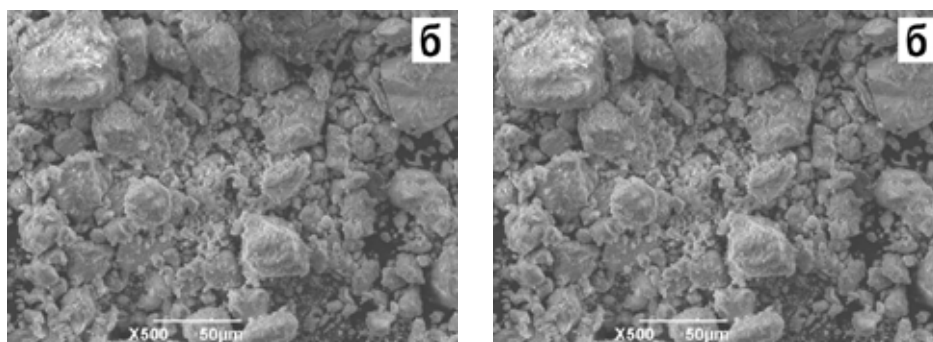
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Modern technology of phosphorus extraction and processing raw minerals into phosphoric acid utilizes two approaches: 1) sulfuric extraction; 2) thermal reduction methods with consequential capturing of phosphorus fumes. These technologies have significant drawbacks: industrial wastes and possible unsanctioned emissions of harmful materials into environment. Non-waste technology of apatite processing could be achieved with utilization of alkaline technologies aimed at obtaining water solutions of alkali metal phosphates to use as fertilizers and insoluble calcium silicates for chemical and construction industries. The research had shown apatite to break in NaOH solution in presence of SiO<sub>2</sub> at T >250°C as follows:



Leaching was conducted in Parr 4560 autoclave (USA) for 3 hours, phosphorus extraction into solution >90%. Insoluble residue (pic.1 a) consisted of acerous calcium silicates.

Obtaining calcium phosphates requires higher temperatures. Apatite was sintered in muffle furnace with SiO<sub>2</sub> and KOH at the temperature of 400°C for 4 hours followed by hot-water leaching. >80% of phosphorus went into solution, insoluble residue consisted (pic.1 b) of the mixture of calcium silicates.



**Fig. 1.** Micrographs of the formed calcium silicates: a – using autoclave method of leaching in NaOH solution; b – using the KOH sintering technology with water leaching

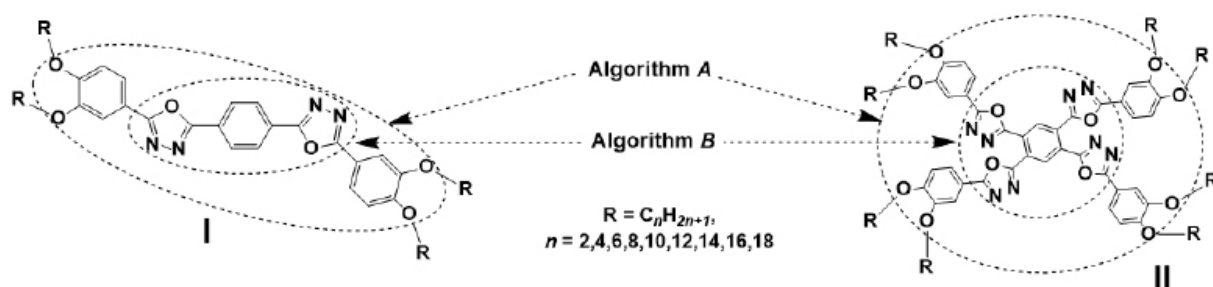
*The work was carried out in accordance with the state task and plans of scientific research work of the ISSC UB RAS (№ AAAA-A19-119031890028-0).*

# DERIVATIVES OF TEREPHTHALIC AND PYROMELLITIC ACIDS WITH OXADIAZOLE SYNTHONS AND PREDICTION OF COLUMNAR MESOMORPHISM

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Terephthalic and pyromellitic acids can be used in both polymer production and synthesis of new compounds with liquid crystalline, luminescent and gel-forming properties. These compounds are in demand in nanoelectronics, sensors, and other instrument technologies<sup>1,2</sup>. Expanding the number of such materials is a crucial task. In this work, we have conducted molecular design, modeling, and prediction of columnar (Col) mesomorphism of terephthalic and pyromellitic acid derivatives **I** and **II** (Fig. 1), which contain oxadiazole fragments. Such fragments contribute to the manifestation of fluorescent properties. To predict the possibility of Col mesophase formation, the molecular parameter method (MPM)<sup>3</sup> was used, according two algorithms.



**Figure 1.** Derivatives of terephthalic **I** and pyromellitic **II** acids and algorithms for dividing their structures into center and periphery for calculating molecular parameters used in predicting columnar mesomorphism by the MPM method

Calculations by the *algorithm A* showed that the formation of Col mesophases is most likely for the homologues **I** and **II** with  $n = 10-18$ . According to the *algorithm B*, a positive prediction was obtained for **I** ( $n = 8-14$ ) and **II** ( $n = 4-8$ ). The prediction is tested by synthesizing individual homologues.

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# GOLD PLATING OF THIN COPPER-NIOBIUM ALLOY WIRE

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The reflective fabric of modern folding transformable antennas is a flat textile material woven from metal threads (thin wires) with a gold coating 0.2-0.3 microns thick.<sup>1</sup> Such a product configuration is capable of ensuring the operability of the antenna in the Ka range, and the efficiency of reflecting the radio signal of the cloth is 97-99%. In addition, the reflector is very light, flexible and elastic, which ensures multiple folding and bringing the antenna into the unfolded state without reducing the performance characteristics of the product. Copper-niobium alloy wire with gold electroplating is suitable as a material for creating a grid.

Nanostructured micro-conductors made of copper-niobium alloy are very practical material for creating mesh walls from them. In comparison with copper, the temporary rupture resistance of which is 250-350 MPa, the copper-niobium nanocomposite alloy has a temporary rupture resistance on a par with steel, of the order of 1200-1500 MPa, and an electrical resistance of 55-75% IACS.<sup>2</sup>

The researchers were tasked with developing a continuous process for cleaning and metallizing thin copper-niobium alloy wire when rewinding from one coil to another. A necessary condition for metallization was the minimum linear velocity of the wire, which is at least 20 m/min.

Optimal gilding conditions have been established at a wire speed of 20 m/min: current density 12.5-15.0 A/dm<sup>2</sup>, electrolysis time 3 s, electrolyte temperature 20-25°C. Gilding electrolyte (g/l): 81 citric acid (pH was adjusted by KOH to 4.7 units), 35 potassium dicyanurate.

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# APPLICATION OF ELECTRONIC SPECTROSCOPY OF DIFFUSE REFLECTANCE FOR ZONE STRUCTURE ESTIMATION OF THE $\text{ZrO}_2$ NEAR-SURFACE LAYER

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The development of technologies for creation nanoscale structures and nano-coatings on the surface of a solids, allowing to change the properties of the initial matrix, requires the development of methods for analyzing the structure and state of the material surface. One of the promising materials of interest as a thermo- and chemically resistant matrix is zirconium dioxide. However, the structure of the  $\text{ZrO}_2$  surface and its activity in reactions that ensure the formation of surface nanostructures and nanolayers change due to the polymorphism of the dioxide, which requires the development of methods sensitive to differences in the structure of the material's surface. This work considers the application of electronic spectroscopy of diffuse reflectance (ESDR), which allows us to evaluate the coordination state of atoms in a thin ( $1.5\text{-}2\text{ nm}^1$ ) near-surface layer during the polymorphic transformation of zirconium dioxide.

Studies were carried out on  $\text{ZrO}_2$  powder obtained by ammonia precipitation from zirconium oxynitrate solution, subjected to annealing at  $300\text{-}1300^\circ\text{C}$  to remove from the surface all forms of sorbed water and to complete crystallization of amorphous component of dioxide. The phase composition of the samples was controlled by XRD. The ESDR spectra obtained on a Specord M40 (Carl Zeiss, Germany) spectrophotometer with a photometric sphere, in the region of the fundamental absorption boundary the bands described by the Fermi-Dirac<sup>2</sup> distribution, corresponding to interzone transitions in the near-surface region of  $\text{ZrO}_2$ , were identified.

The selected spectral transitions corresponding to the coordination state of Zr atoms in the monoclinic ( $\sim 5.05\text{ eV}$ ) and tetragonal ( $\sim 4.65\text{ eV}$ ) modifications of  $\text{ZrO}_2$ . The formation of  $\text{ZrO}_2$  levels in the forbidden zone corresponding to the formation of oxygen vacancies has been established, and schemes of the zone structure of two polymorphic forms of  $\text{ZrO}_2$  have been proposed.

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# PHASE RELATIONSHIPS IN THE P–As SYSTEM

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Recently, due to the enormous interest in layered structures, in particular in the orthorhombic modification of phosphorus (black phosphorus), new results have appeared in the study of both pnictogens themselves and the systems formed by them<sup>1,2</sup>. In an attempt to obtain orthorhombic modifications of phosphorus and arsenic<sup>2</sup>, the mutual influence of the components on the possibility of forming various allotropic forms was shown. This fact leads to disagreements in the interpretation of the nature of phase equilibria in the P – As binary system. The generally accepted version is that the system contains an intermediate berthollide phase that melts according to the peritectic scheme<sup>3</sup>. At the same time, a version of diagram is presented<sup>4</sup>, according to which in the P – As system there are limited solid solutions based on the components, but the peculiarity of the experiment was that the alloys were obtained in the presence of metallic mercury, which already at normal pressure catalyzes the formation of black phosphorus with an orthorhombic structure.

In this work, a mixture of amorphous red phosphorus and gray, rhombohedral arsenic, taken in a 1:2 ratio, was studied by X-ray phase analysis. It was shown that already after 50 hours of annealing at a temperature of 773 K, the presence of an orthorhombic phase based on the structure of black phosphorus is detected in the samples. In samples with an arsenic content of 85 mol. % obtained by cooling from the melt, in addition to this phase there is an arsenic-based solid solution with a rhombohedral structure ( $\beta$ -phase) with a phosphorus concentration of no more than 3 mol. %. In samples with phosphorus content of 36 and 60 mol. % this phase is missing. It has been established that arsenic promotes the crystallization of phosphorus, with the formation of a monoclinic structure of violet phosphorus (Hittorf phosphorus), which can serve as an intermediate stage of the transition to the orthorhombic modification of the phase of arsenic solid solution in black phosphorus ( $\gamma$ ). The temperature of the phase transformation involving the orthorhombic phase, corresponding to the invariant peritectic process  $L + \beta \leftrightarrow \gamma$ , was established by differential thermal analysis to be 960 K.

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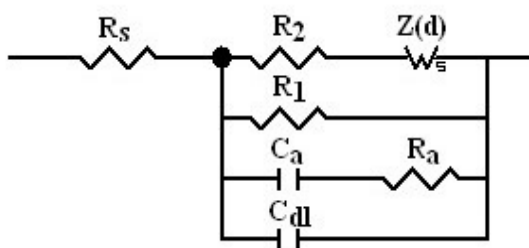
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# INFLUENCE OF THE MIXED INHIBITOR ON THE HYDROGEN SULFIDE |CORROSION RATE OF ST3 IN THE NACE MEDIUM

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In the gas industry the most common method of protecting equipment against the hydrogen sulfide corrosion is an inhibitor's applying. In this work the influence of the inhibitor of the imidazoline series, including thioalcohols and substituted amines of the C6-C10 hydrocarbon series, on the corrosion rate of St3 in the NACE medium (NaCl - 5 g/l; CH<sub>3</sub>COOH - 0.25 g/l) in the presence of 400 mg/l H<sub>2</sub>S has been studied by impedance spectroscopy in the frequency range 10 kHz - 0.05 Hz with an alternating voltage amplitude of 10 mV (electrochemical measuring complex from Solartron (UK), consisting of an SI 1255 impedance analyzer and SI 1287 potentiostat; Pt - auxiliary electrode, reference electrode silver chloride). Analysis of the impedance hodographs on the steel electrode was carried out using the equivalent scheme (Figure 1).



**Figure 1.**  $R_s$  – solution resistance,  $C_{dl}$  – capacitance of the electrical double layer,  $R_1$  – charge transfer resistance in the anodic process,  $C_a$ ,  $R_a$  – capacitance and adsorption resistance of intermediate compounds of the anodic reaction. The cathodic process corresponds to the series connection of the charge transfer resistance  $R_2$  and the diffusion impedance  $Z_D$ .

The inhibitor's protective effectiveness  $Z$  was calculated by the equation:

$$Z, \% = 100[(R_{1, \text{inh}} - R_{1, \text{NACE}}) / R_{1, \text{inh}}],$$

where  $R_{1, \text{NACE}}$  and  $R_{1, \text{inh}}$  are the charge transfer resistance in the anodic reaction in the NACE medium and in the inhibited solution, respectively.

It has been shown that the capacity of the electrical double layer decreases with the inhibitor concentration increasing, which is probably due to the adsorption of its components. At inhibitor concentrations ( $C_{\text{inh}}$ ) of 25 to 200 mg/l,  $Z$  increases from 35 to 60%. In the presence of 400 mg/l H<sub>2</sub>S in the NACE medium at  $C_{\text{inh}} = 200$  mg/l, the charge transfer resistance in the anodic process increases significantly, and the inhibitor's  $Z$  increases respectively.



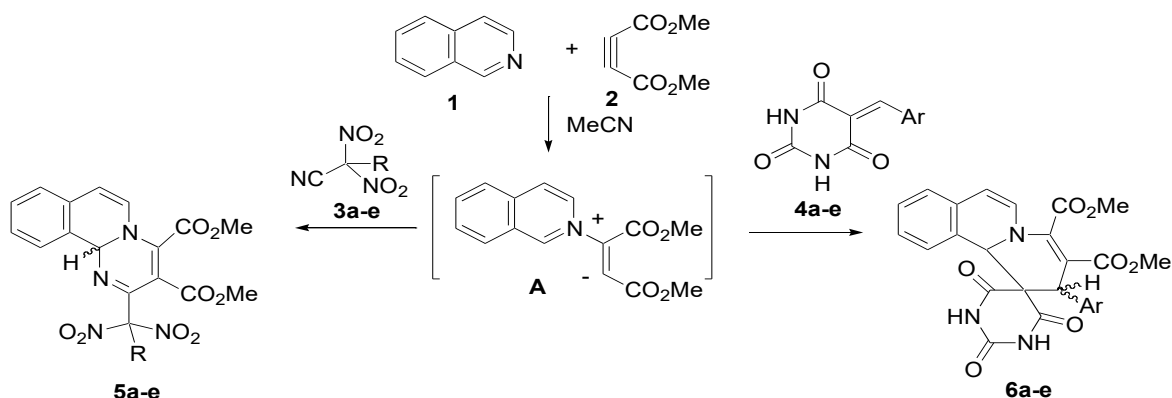
# 5-(ARYLMETHILDENE)-2,4,6-PYRIMIDINE(1H,3H,5H)-TRIONES AND DINITROACETONITRLES IN THE REACTION OF TECHCOMPONENT HETEROCYCLIZATION WITH ISOQUINOLINE IN THE PRESENCE OF DIMETHYL BUT-2-INDIOATE

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We have established that the interaction of dipolarophilic compounds **3** or **4** with 1,3-dipole **A**<sup>1</sup> generated from isoquinoline **1** in the presence of dimethylbut-2-indioate **2** ends with the formation of diastereoisomeric substituted dimethyl-2-dinitromethyl-11*b*H-pyrimido[2,1-*a*] isoquinoline-3,4-dicarboxylates **5 a-e** from compounds **3 a-e** or dimethyl-2-aryl-1,1*b*-dihydro-2*H*-spiro[pyrimidin-5,1'-pyrido[2,1-*a*]isoquinoline-2,4,6(1*H*,3*H*,5*H*)-trione]-3,4-dicarboxylates **6 a-e** from compounds **4 a-e** in 60-70% yield.



**3,5** R=NO<sub>2</sub> (**a**), CO<sub>2</sub>Et (**b**), CO<sub>2</sub>Me (**c**), Cl (**d**), F (**e**)

**4,6** Ar=Ph (**a**), 4-MeOC<sub>6</sub>H<sub>4</sub> (**b**), 4-ClC<sub>6</sub>H<sub>4</sub> (**c**), 3-NO<sub>2</sub>C<sub>6</sub>H<sub>4</sub> (**d**), 4-MeC<sub>6</sub>H<sub>4</sub> (**e**)

The structure of the target compounds **5 a-e** and **6 a-e** was established by IR, <sup>1</sup>H, <sup>13</sup>C spectroscopy, mass spectrometry, and the composition was determined by elemental analysis.

The obtained compounds can be considered as potential biologically active compounds exhibiting anti-tuberculosis and anti-leprosy activities<sup>2</sup>.

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# INFLUENCE OF THE TYPE OF POROUS SUPPORT ON THE TEXTURAL AND STRUCTURAL PROPERTIES OF ZINC OXIDE

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Zinc oxide is one of the key components in the rubber and tire industry<sup>1</sup>. Due to environmental restrictions, an urgent task is to reduce the content of zinc oxide in the composition of the rubber compound, while maintaining its function and effectiveness as an activator of the vulcanization process<sup>2</sup>. One of the possible ways to solve this issue is the use of nanodispersed zinc oxide particles deposited on the surface of a dispersed carrier. This approach will make it possible to reduce the dose of the metal oxide vulcanization activator in the mixture, while increasing the efficiency of its action due to a higher specific surface area, and also solve the problem of agglomeration of nanodispersed metal oxide particles.

This paper presents the results of a study of the influence of various types of porous supports on the textural and structural properties of zinc oxide, which was deposited on their surface in the form of nanodispersed particles.

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# HEAT-RESISTANT CERAMICS FROM NANOSTRUCTURED PRECURSORS

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ZrO<sub>2</sub> ceramics are used in mechanical engineering, space technology, refractories, jewelry and medicine. However, its cost is high, and polymorphism at temperature differences causes the destruction of products. This causes the ZrO<sub>2</sub> to be combined with other refractory compounds that would increase the properties of the ceramic and lower its price.

The purpose of the study was to make 3-component ceramics from nano-structural precursors (needle powders) of complex structure: Al<sub>2</sub>O<sub>3</sub>–ZrO<sub>2</sub>–MgO and the Al<sub>2</sub>O<sub>3</sub>–(ZrO<sub>2</sub>–Y<sub>2</sub>O<sub>3</sub>) with a variable ratio of components: from 98:1:0.5 to 85:10:2.5 (1-st system) and from 20:(80) to 80:(20) (2-nd system). Precursors were prepared by impregnating cellulose filaments in salt solutions, followed by removal of the polymer matrix according to a given temperature program.<sup>1</sup> The synthesized needle powders consisted of oxide crystallites of 7-10 nm in size. Agglomerates of particles were crushed, sieved into fractions, samples were formed at a pressure of 500 MPa and annealed at 1580-1600°C. Their crystal and microstructure were studied, physical-mechanical properties were determined. Al<sub>2</sub>O<sub>3</sub> during annealing blocked the growth of ZrO<sub>2</sub> crystallites, their size did not exceed 55-60 nm, which increased the density of ceramics to 98.5%. Above 1500°C, a small part of magnesium oxide reacted with Al<sub>2</sub>O<sub>3</sub>, forming spinel layers on the surface of the needle particles, which strengthened the bond at the phase boundary.

A tribological experiment showed that the wear of ceramics from nanopowders is 1.5-2 times lower than that of similar ceramics from micron industrial powders. They have high chemical resistance, when boiling ceramic samples for 1 hour in solutions of 20% HCl and 35% NaOH, the weight loss was 0.01-0.08%. Ceramic composites are heat resistant, they withstand 50 cycles of 900/10 ° C (water) without failure, which makes it possible to recommend them as filters, protective layers, catalyst carriers and machine components when operating in aggressive gaseous and liquid media at the high temperature.

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# PLASMA-ELECTROLYTIC SYNTHESIS OF PHOTOACTIVE FILM COMPOSITES BASED ON TRANSITION METAL TUNGSTATES

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Transition metal tungstates with the general formula  $MWO_4$  have attracted considerable attention due to their wide range of functional properties [1]. Such compounds are obtained mainly in the form of dispersed particles, while for solving many practical problems it is advisable to use film composites in which the active components are immobilized on solid surfaces, including metals. Certain possibilities for the synthesis of various oxide structures on the surface of metals are provided by the method of plasma electrolytic oxidation (PEO) [2].

We have studied the capabilities of the PEO method for the one-step formation of photoactive film composites  $Ti/TiO_2$ - $MWO_4$  (M-Mn(II), Co(II), Zn(II), Ni(II) or Cu(II)). Aqueous homogeneous electrolytes containing sodium tungstates and complexes M(II) with EDTA were used as electrolytes for PEO. In some cases, electrolytes contained sodium phosphate or tetraborate, as well as weak organic acids. The influence of PEO synthesis conditions on the characteristics of the formed composites and their photocatalytic activity in the degradation reaction of such organic pollutants as indigo carmine, methyl orange and rhodamine C was studied. The results obtained showed that some formed  $Ti/TiO_2$ - $MWO_4$  composites can be considered promising candidates for further practical application in photocatalytic wastewater treatment.

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# INFLUENCE OF DISPERSION PHASE NATURE ON FORMATION OF ELECTROCHEMICAL COMPOSITE COATINGS

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To create effective and functional electrochemical composite coatings (ECC), substances of dispersed phase (DPh) of micro- and nanometer order are used. The efficiency of using ECC is largely determined by the nature of the dispersed phase.

Recently, fine particles obtained using plasma chemistry, as well as by chemical reactions directly in the electrolyte or in solutions, components of electrolytes, have been used as the dispersed phase<sup>1,2</sup>.

Barium sulfate particles are a promising particulate material. Solutions of  $\text{BaCl}_2$  and  $\text{Na}_2\text{SO}_4$  were used as reagents for their preparation. The content of the obtained particles  $\text{BaSO}_4$  100-200 nm in size of about 50%. Fine particles of barium sulfate make it possible to obtain compact and uniform coatings<sup>3</sup>.

The conditions for producing zirconium oxide used as DF have been studied. Zirconium oxychloride-synthesized amorphous zirconium hydroxide was also used as DPh, but no coprecipitation with the nickel matrix was observed. Dehydration of zirconium hydroxide was carried out at 600 °C. As a result, a zirconium oxide powder consisting of two crystalline forms was obtained. X-ray diffraction analysis showed the presence of tetragonal and cubic phases, with the concentration of the first phase being 73.2% and the second phase 26.8%. X-ray phase analysis of the obtained ECC

showed that the zirconium oxide particles co-precipitate with the nickel matrix, their share in the coating is 2-3%, at a concentration of 30-50 g/dm<sup>3</sup> in the nickel plating electrolyte. The obtained coatings have increased corrosion resistance in 3% NaCl solution.

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# INVESTIGATION OF THE BONDING ZONE OF THE COMPOSITE MATERIAL Cu-Al OBTAINED BY EXPLOSION WELDING NEAR THE LOWER LIMIT OF WELDABILITY

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Explosion welding (EW) is a promising method that ensures the formation of a strong joint between two (or more) metals upon their collision under the action of the energy released during the detonation of an explosive charge.

The Cu+Al bimetal is intended for the production of contact pads and current-carrying elements of electrical equipment with an improved set of physico-mechanical characteristics. The use of this material enables the achievement of perfect electrical contact. However, the formation of crystalline intermetallic compounds between them is possible, so the aim of the study was to investigate the dependencies of the joint zone formation on the formation of intermetallic compounds.

EW was carried out near the lower boundary of weldability. Three samples welded at different energies  $W_2$  were obtained. Microgrinds and samples for layer separation tests were prepared. The microstructure, fracture surface, and chemical analysis of the melt zones in the joint area were investigated using the Versa 3D DualBeam scanning electron microscope (Fig. 1a-c).

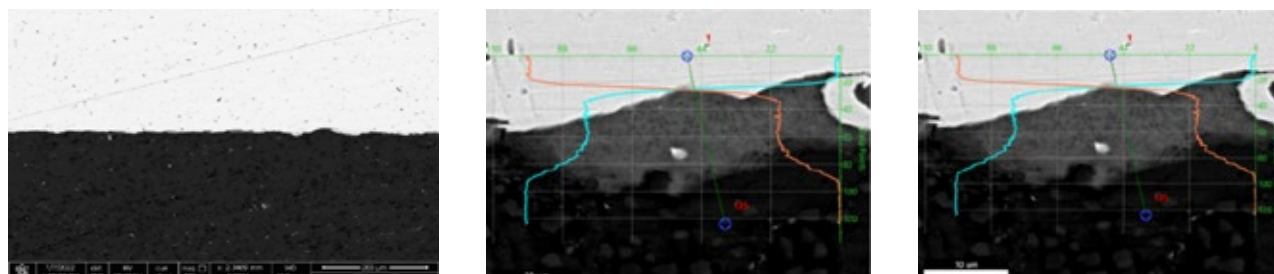


Fig. 1 - Microstructure (a), fracture surface (b), and chemical analysis of the melt zone (c) at the Cu-Al bimetal joint boundary.

It was found that with an increase in energy  $W_2$ , the amount of melt zones increases both linearly and in area. It was also observed that during the layer separation test of the sample welded at the highest energy, the separation occurred not along the melt zones, but along the aluminum. From this, it can be concluded that during welding near the lower boundary of weldability, the melt zones in the joint area do not negatively affect the strength of the joint. This is supported by the chemical analysis graph, which shows that they consist mainly of aluminum.



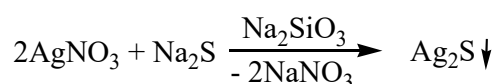
# SYNTHESIS OF COLLOIDAL SILVER SULFIDE SOLUTION

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Colloidal particles of silver sulfide have physical and chemical properties that determine its application in various industries, for example, in photovoltaic cells and photochemical cells,<sup>1-3</sup> in IR detectors,<sup>4</sup> in the catalysis of chemical reactions.<sup>5</sup> In connection with the possibility of application in medicine and biology,<sup>6</sup> works devoted to the development of methods for the synthesis of quantum dots based on silver sulfide are of considerable interest.<sup>7</sup>

The developed method of synthesis of colloidal silver sulfide solution is based on the reaction:



The sodium silicate used to stabilize the colloidal solution had a concentration of 1%. Concentrations of solutions:  $\text{AgNO}_3$  0.43...2.16 mg  $\text{Ag(I)}/\text{mL}$ ,  $\text{Na}_2\text{S}$  22 mg/mL. The synthesis was carried out at room temperature with stirring on a magnetic stirrer as follows: to a given volume of silver nitrate solution (5...25 mL) were added given volumes of sodium silicate (0...1 mL) and sodium sulfide solutions (0.25...1 mL). As a result, stable for a long time colored solutions of colloidal silver sulfide were formed. When the reaction was carried out without the addition of sodium silicate, precipitation occurred. Colloidal solutions of silver sulfide were characterized by electron spectroscopy. The electron spectrum of silver sulfide colloidal solution shows a significant increase in absorption in the region of 200...500 nm. The spectrum is well approximated using 6 Gaussians with absorption maxima at 476, 407, 345, 299, 256 and 200 nm. The accuracy of approximation is 3.4 %.

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# GAS-SENSITIVE PROPERTIES OF YTTRIUM AND LANTHANUM CHROMITES DOPED WITH STRONTIUM IONS

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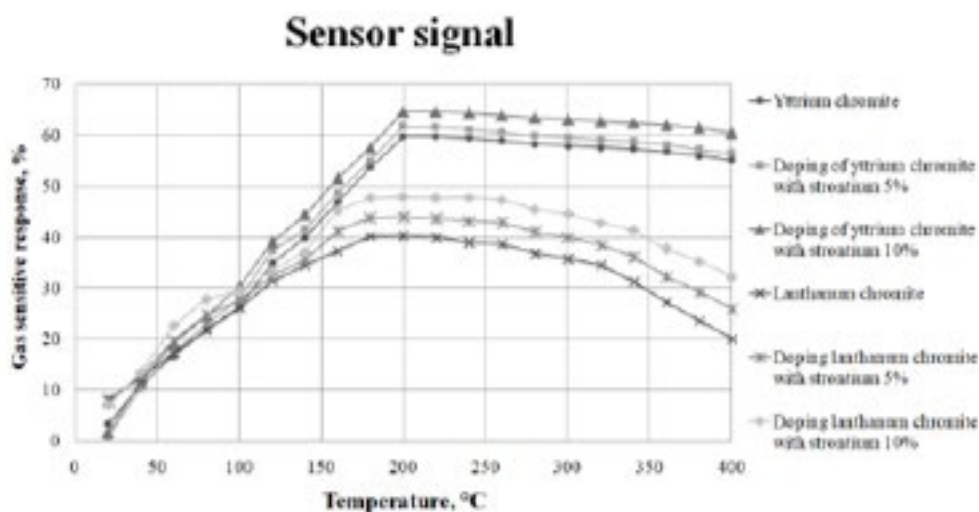
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The aim of this work was the synthesis of yttrium chromite by citrate method and lanthanum chromite by sol-gel method, doping of powders with strontium ions, determination of their phase composition and investigation of gas-sensitive properties.

The calculated amount of chromium and yttrium nitrate salts to obtain yttrium chromite was dissolved in water, heated, an ammonia solution was added, and then citric acid. Then they were boiled and evaporated until ash was formed. To obtain lanthanum chromite, sol was prepared by dissolving chromium nitrate and lanthanum salts in boiling water, cooled to room temperature, and ammonium hydroxide was added. The resulting precipitate was filtered and dried. The resulting powders were annealed in a muffle furnace. Doping with strontium ions was carried out by replacing salts of yttrium and lanthanum nitrates with a salt of strontium nitrate in a stoichiometric ratio.

The obtained powders were examined by X-ray phase analysis (XRD). It was found that all powders are single-phase and contain only yttrium chromite or lanthanum chromite.

To study the gas-sensitive properties, nanopowders of yttrium and lanthanum chromites were dispersed and deposited on a conductive element. The specific surface resistance of the obtained films was measured in air, and then in the presence of CO gas, the concentration of which was 50 ppm. Thus, in the studied temperature range, the gas-sensitive response of the obtained samples reaches a maximum of 60–65% for yttrium chromites and 40–47% for lanthanum chromites.



# TOXICITY STUDY OF A POTENTIAL DYE - 5-(2-(2Z, 5E)-2-(CYANOMETYLENE)-4-OXOTIAZOLIDIN-5-ILIDEN) HYDROXYENZIC ACID (HL)

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Metal complex dyes are the predominant dye class for dyeing wool, nylon and silk due to their excellent resistance to washing and light exposure compared to non-metallic dyes. To determine the coloristic properties, a test dyeing of samples of bleached hair from ethanol solutions with HL solution and with the addition of  $\text{Ni}^{2+}$ ,  $\text{Fe}^{2+}$  and  $\text{Zn}^{2+}$  metal salts to the stock HL solution at a neutral pH was performed (Fig. 1).



**Figure 1.** The results of a test study of the coloristic properties of HL and its metal complexes

Based on the GUSAR program, the toxicity of the compounds was calculated for intravenous and oral administration<sup>1</sup>. According to the calculated values, HL and metal complexes based on it belong to the group of non-toxic or low-toxic compounds. The results were confirmed *in vivo*.

The study of toxic and local irritant effects was carried out on mature mice (males) with a single intragastric administration of the studied substance in the maximum possible dose/volume, which is 1500, 2650 and 3500 mg/kg.

The results of toxicometry, observational data of experimental animals for 14 days after a single administration, and also necropsy data allow HL to be classified as class IV low-toxic substances.

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# OXIDATIVE DEPOLYMERIZATION PRODUCTS OF HYDROLYSIS LIGNIN WITH NITRIC ACID FOR THE SYNTHESIS OF SILVER NANOPARTICLES

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Nanosilver is widely studied due to its antimicrobial, optical, catalytic and other properties.<sup>1</sup> For its synthesis, a chemical method with stabilizers is often used to provide the desired size and shape of nanoparticles. Technical lignins such as lignosulfonates<sup>2</sup> and kraft lignin<sup>3</sup> have already been used as stabilizers for the synthesis of nanosilver. In this work, hydrolysis lignin (HL) was used for the same purpose.

Oxidative depolymerization was carried out by treating 0.1 g of HL with 1 mL of dimethylsulfoxide-nitric acid (DMSO-NA) mixture of different compositions (1:4, 1:1 or 4:1 by volume) at 100 °C for 10 min followed by cooling, alkalization with 3 mL of 14% ammonia solution and dilution to 25 mL with water. The resulting solution was filtered to separate the cellulosic residue and used to synthesize silver nanoparticles. For this purpose, 3 mL of glucose solution (18 g/L) and 1 mL of 0.1 M silver nitrate solution were added to 5 mL of the filtered solution, the resulting reaction mixture was heated at 100 °C for 10 min, then cooled and diluted to 25 mL with water.

HL when treated with DMSO-NA mixture dissolves due to oxidation and depolymerization. With other equal synthesis conditions, silver nanoparticles were formed using a 4:1 mixture of DMSO-NA, a characteristic absorption band with a maximum at 425 nm appeared on the UV-Vis spectrum of its solution. For the 1:1 DMSO-NA mixture the similar absorption band was 2 times less intense, and for the 1:4 DMSO-NA mixture such a band was almost not visible. Consequently, the mild depolymerization products of HL by small amounts of nitric acid are preferable for the synthesis of silver nanoparticles.

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# FORMATION OF CARBON NANOSTRUCTURES AT MICROWAVE PYROLYSIS OF PLASTIC MATERIALS

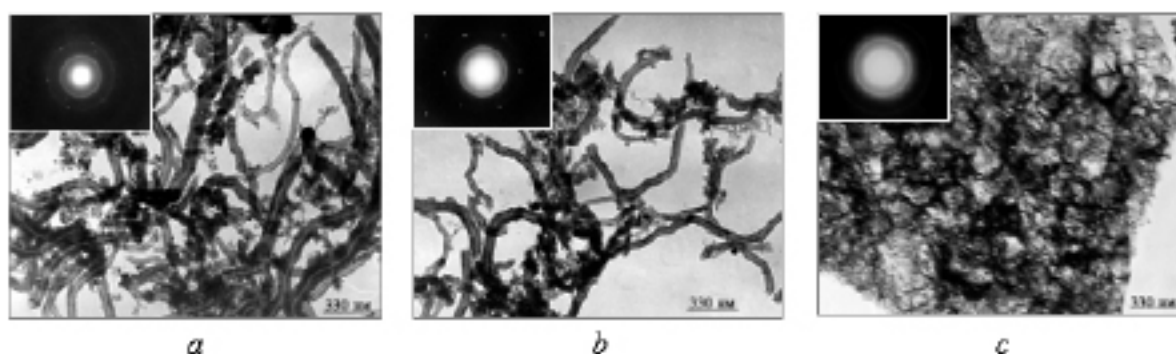
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Production of carbon nanostructures, hydrogen, gaseous and liquid fuels is one of the promising directions of utilization of plastic waste by their thermochemical transformation with the participation of ultrahigh-frequency electromagnetic field energy<sup>1</sup>.

The catalytic microwave process of synthesis of carbon nanotubes by pyrolysis of high-carbon polymeric materials (polystyrene, polyethylene terephthalate, polypropylene) in the presence of metal catalyst precursors from a number of iron, cobalt, nickel compounds and their mixtures has been studied.

The formed nanostructures, according to electron microscopy data, consist of multi-walled carbon nanotubes of different morphologies and low-layer packages of graphene planes (Fig. 1).



**Figure 1.** TEM micrographs of MW pyrolysis products: (a) polystyrene, (b) polyethylene terephthalate, (c) polypropylene

The structure of nanocarbon materials obtained by plastic recycling was confirmed by X-ray phase analysis.

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# SOLUTION FOR PASSIVATION OF ELECTROLYTIC ZINC-NICKEL ALLOY

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Zinc-nickel electrolytic coatings on the surface of steel products are superior to widely used zinc coatings in their protective ability and corrosion resistance, but inferior to cadmium coatings. In order to increase the corrosion resistance of products with a protective Zn-Ni alloy coating, they are additionally treated in passivation solutions. The main method of passivation of the surfaces of metals and alloys in the domestic industry is still the formation of conversion protective films in solutions based on hexavalent chromium.

We developed solutions for chromate-free passivation of galvanized surfaces based on salts of rare earth metals and hydrogen peroxide as the oxidizing agent<sup>1,2</sup>. In these solutions, passivating coatings are formed that are capable of self-healing defects and with a protective ability comparable to iridescent chromate coatings. The disadvantage of these technologies is the difficulty of adjusting and controlling the main components due to the rapidly changing ratio of the concentrations of  $\text{Ce}^{3+}$  and  $\text{Ce}^{4+}$  ions in the solution under the influence of hydrogen peroxide.

A cerium-containing solution has been developed for the passivation of an electrolytic zinc-nickel alloy, which does not contain oxidizing agents. The composition of the solution is based on water-soluble cerium (III) and (IV) salts. The total cerium content in the solution is 1.5 g/l (for metal), and the concentration ratio  $\text{Ce}^{3+}/\text{Ce}^{4+} = 2/1$ . The solution does not pose an environmental hazard, is cost-effective, and the protective ability of the resulting coatings is comparable to chromate coatings on the surface of the alloy.

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# SYNTHESIS AND PHYSICAL-CHEMICAL PROPERTIES OF PHOTOCATALYTIC CdS QUANTUM DOTS COATED WITH STABILIZERS WITH HYDROPHILIC GROUPS

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The work investigated the dependence of the optical and photocatalytic properties of cadmium sulfide quantum dots obtained by the colloidal method under the same conditions on the type of stabilizer used in the synthesis. The synthesis was carried out at elevated temperature for 30 minutes. For the study, 4 types of surfactants were selected that can be adsorbed on the surface of sulfide nanoparticles and have a hydrophilic group at the opposite end: mercaptoethanol, mercaptoacetic acid, mercaptopropionic acid, L-cysteine, the adsorption of which occurs along the thiol group. The synthesis of QDs was carried out in an aqueous medium by condensation from a supersaturated solution at alkaline pH values. All these stabilizers are of the thiol type, attached to chalcogenide nanoparticles with an –SH group.

Using the experimentally obtained polynomial, the sizes of nanoparticles were calculated. The optical and dimensional characteristics of QDs coated with various types of stabilizers are given in Table 1.

Table 1. Size and luminescence characteristics of the quantum dots under study.

Stabilizer	$\lambda_{\text{absorb}}$ , nm	$\lambda_{\text{lume}}$ , nm	D, nm
Mercaptoethanol	371	535	2,55
Mercaptoacetic acid	436	665	4,69
Mercaptopropionic acid	404	575	3,51
L-cysteine	386	545	2,95



Section 3

# PHYSICO-CHEMICAL BASES OF METALLURGICAL PROCESSES

# RESEARCH ON PYRO-HYDROMETALLURGICAL METHOD FOR PROCESSING HIGH-IRON NIOBIUM-RARE-EARTH ORES OF THE CHUKTUKON DEPOSIT

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The Chuktukon deposit (Krasnoyarsk region) is one of the richest russian sources of niobium and rare earth metals, the consumption of which is growing rapidly. However, due to high iron content and inability of Chuktukon ores to be processed by physical methods, standard processing technologies become ineffective<sup>1</sup>.

Taking into account all the features of the Chuktukon ores, IMET RAS is developing a new effective technology for the complex processing of raw materials, which includes both pyro- and hydrometallurgical processes. At the first stage, during reduction firing (1300-1400°C), up to 98% of iron and phosphorus in the form of cast iron are removed, and niobium along with manganese remains in the rare-earth metal slag<sup>2,3</sup>. At the second stage, during hydrochloric acid leaching of slag, rare earth metals and manganese go into solution, from where they are subsequently extracted in the form of selective concentrates by fractional precipitation with ammonium carbonate<sup>4</sup>. In this case, the hydrochloric acid leaching residue, in which niobium and titanium are concentrated, is treated with a dilute NaOH solution to convert amorphous silica into solution in the form of  $\text{Na}_2\text{SiO}_3$ . Then the manganese spinel (non-degradable slag phase) is separated by wet magnetic separation from the residue, which is subsequently a niobium-titanium concentrate. Thus, the developed method makes it possible to obtain concentrates of niobium, rare earth metals and manganese, suitable for further processing and obtaining finished products from them.

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*This work was carried out in the framework of state assignment no. 075-01176-23-00.*



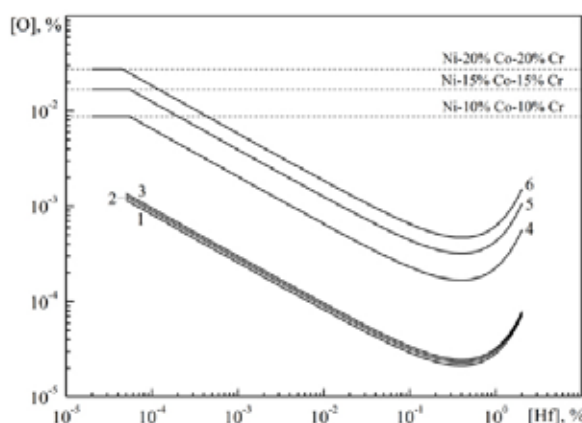
# EFFECT OF HAFNIUM ON THE OXYGEN SOLUBILITY IN THE Ni-Co-Cr MELTS

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The high-temperature alloys based on the Ni-Co-Cr system are widely used in modern technologies. The main areas of their application are power engineering, aviation, and marine transport. Oxygen is a harmful impurity in these alloys. It results in the deterioration of service properties of metal. Hafnium is used upon production of these alloys as an alloying element. This leads to the improvement of their service characteristics.

Thermodynamic analysis of oxygen solutions in the hafnium-containing Ni-Co-Cr melts was carried out. The oxygen solubilities in the Ni-Co-Cr melts at 1873 K depending on the hafnium content were calculated (Fig. 1).



**Figure 1.** Oxygen concentration depending on hafnium content in melts at 1873 K:  
Ni-10%Co (1); Ni-15%Co (2); Ni-20%Co (3); Ni-10%Co-10%Cr (4); Ni-15%Co-15%Cr (5);  
and Ni-20%Co-20%Cr (6)

At very low contents, hafnium does not affect the oxygen concentration. The further increase in the hafnium content higher than  $4,34 \cdot 10^{-5}$ – $5,42 \cdot 10^{-5}\%$ , depending on the alloy composition, results in a significant decrease in the oxygen concentration, and then, after passing the minima (0.397–0.407% Hf), to its rise. Hafnium is characterized by the high deoxidation ability in the Ni-Co-Cr melts but it is considerably lower than in the Ni-Co melts.

*This work was carried out according to State Assignment 075-00320-24-00.*

# OXYGEN SOLUBILITY IN THE CARBON-CONTAINING Fe-70% Ni MELT

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Modern instrumentation and mechanical engineering require alloys with diverse properties. Those include precision alloys based on the Fe-Ni system. For example, the production of magnetic-amplifier cores, rectifiers, pulse and broadband transformers necessitates alloys with high values of the permeability and induction increments upon pulse magnetization, i.e. magnetically soft alloys. In particular, the 68NM magnetically soft alloy with 67–69% Ni and 0.03% C is suitable for these intentions.

Oxygen solutions in the carbon-containing iron melts, Fe-70% Ni alloy, and pure nickel were thermodynamically studied. The equilibrium constants of carbon-oxygen interaction, the activity coefficients at infinite dilution, and the interaction parameters in these melts at 1873 K were determined. The oxygen solubility depending on the carbon concentration in the studied melts was calculated. The oxygen concentration in iron differs from that in nickel at the same carbon content by two orders of magnitude. As a result of carbon deoxidation, the reaction products are monoxide (CO) and dioxide (CO<sub>2</sub>). At the carbon concentration in these melts more than 0.05%, CO<sub>2</sub> content in the gas phase is low (less than 3.5%). A decrease in the pressure of gas phase ( $\Sigma p = p_{\text{CO}} + p_{\text{CO}_2}$ ) substantially increases the deoxidation ability of carbon. The oxygen concentrations in the alloys with the same composition reduce by an order of magnitude as a minimum if the gas-phase pressure is lowered by a factor of ten.

The deoxidation ability of carbon in the Fe-70% Ni melt was experimentally studied. The results obtained in argon and correlated with a certain pressure  $\Sigma p$  showed that, probably, an unmixable gas layer takes place above the melt surface, which contains CO and CO<sub>2</sub>. The amount of these oxides is determined by the carbon and oxygen concentrations in the melt.

*This work was carried out according to State Assignment 075-00320-24-00.*

# OBTAINING TiN PRODUCT BY REDUCTION NITRIDATION ROASTING OF QUARTZ-ILMENITE CONCENTRATE

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To increase the efficiency of complex processing of Pizhem sandstones, IMET RAS is conducting research on the development of processes aimed at additional extraction of valuable components from mud, with which titanium, rare earth and other valuable elements are lost. During magnetic separation of mud, a quartz-ilmenite concentrate containing 30-45%  $\text{TiO}_2$  and 20-25%  $\text{Fe}_2\text{O}_3$  is released into a magnetic product. Titanium is found in pseudorutile, a product of leucoxenization of ilmenite. Together with titanium-containing minerals, some of the finely dispersed quartz and clay minerals pass into the separation product. Due to the high dispersion of the material, its further processing using known methods is practically impossible.

A perspective solution to the problem of extracting titanium and other valuable components from mud may be the use of preliminary reduction nitridation roasting, which results in the formation of TiN. Titanium can then be extracted from TiN by low-temperature chlorination of the resulting product (200-500°C). In this case, there is no interaction of ore components with chlorine, which ensures selective extraction of titanium in the form of  $\text{TiCl}_4$  from low-quality raw materials.

In this work, the possibility of nitridation a quartz-ilmenite product by a carbothermic method in a nitrogen atmosphere was studied. As a result of the studies, it was found that the complete conversion of  $\text{TiO}_2$  to TiN is achieved at temperatures of 1300-1350°C with the addition of a reducing agent 1.5 times more than the stoichiometrically required amount for the reduction of  $\text{TiO}_2$  and  $\text{Fe}_2\text{O}_3$ . Under these conditions, in addition to TiN, the nitridation product contains quartz, an amorphous silicate phase, Fe and  $\text{Fe}_3\text{C}$ . Before chlorination of the nitridation roasting product, it will be necessary to remove iron from it by hydrochemical methods.

*The study was carried out according to the state order № 075-00320-24-00.*



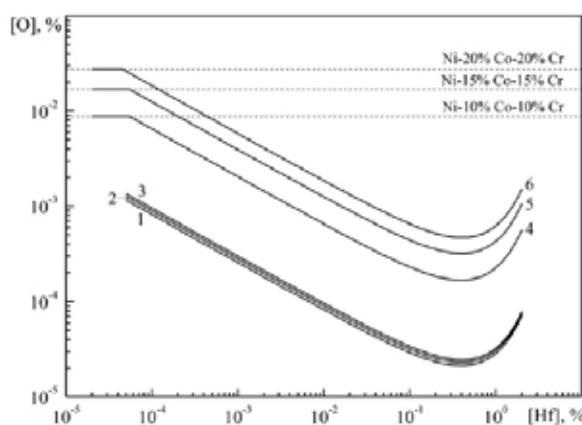
# EFFECT OF HAFNIUM ON THE OXYGEN SOLUBILITY IN THE Ni-Co-Cr MELTS

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The high-temperature alloys based on the Ni-Co-Cr system are widely used in modern technologies. The main areas of their application are power engineering, aviation, and marine transport. Oxygen is a harmful impurity in these alloys. It results in the deterioration of service properties of metal. Hafnium is used upon production of these alloys as an alloying element. This leads to the improvement of their service characteristics.

Thermodynamic analysis of oxygen solutions in the hafnium-containing Ni-Co-Cr melts was carried out. The oxygen solubilities in the Ni-Co-Cr melts at 1873 K depending on the hafnium content were calculated (Fig. 1).



**Figure 1.** Oxygen concentration depending on hafnium content in melts at 1873 K:  
Ni-10%Co (1); Ni-15%Co (2); Ni-20%Co (3); Ni-10%Co-10%Cr (4); Ni-15%Co-15%Cr (5);  
and Ni-20%Co-20%Cr (6)

At very low contents, hafnium does not affect the oxygen concentration. The further increase in the hafnium content higher than  $4,34 \cdot 10^{-5}$ – $5,42 \cdot 10^{-5}\%$ , depending on the alloy composition, results in a significant decrease in the oxygen concentration, and then, after passing the minima (0.397–0.407% Hf), to its rise. Hafnium is characterized by the high deoxidation ability in the Ni-Co-Cr melts but it is considerably lower than in the Ni-Co melts.

*This work was carried out according to State Assignment 075-00320-24-00.*

# STUDY OF WETTABILITY OF THE AL<sub>2</sub>O<sub>3</sub>-BASED REFRACTORY CERAMICS BY RAIL STEEL

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Refractory ceramics is the main material for the production of casting nozzles, purging plugs, and pouring spouts. Molten steel affects a refractory material, which results in the wear of lining, the formation of micro- and macroinclusions, and, therefore, in the degradation of steel quality. In recent decades, a great attention was paid to the influence of harmful impurities and nonmetallic inclusions on the quality of steels and alloys produced. This results in the increased requirements to the refractory materials, which depend on the assortment of steels produced and the specific production conditions. Therefore, studies of the interaction of refractory ceramics with a metal melt and the phenomena occurring at the melt-refractory interface continue to be relevant.

The wettability and interaction of the rail steel (0.79% C, 0.89% Si, 0.55% Cr, 0.93% Mn, 0.0021% O) with the material of purging plugs (91,77% Al<sub>2</sub>O<sub>3</sub>; 3,22% MgO; 2,67% Cr<sub>2</sub>O<sub>3</sub>; 0,8% CaO; 0,15% Fe<sub>2</sub>O<sub>3</sub>; 0,07% SiO<sub>2</sub>) depending on the gas-phase composition, temperature and time of contact were studied. It was shown that the greatest change in the contact angle ( $\theta$ ) was observed during isothermal holding after melting the specimen (from 145° to 125° for 30 min).

The further change in the temperature and the isothermal holdings at high temperatures do not affect significantly on the  $\theta$  values. Analysis of cross sections of metal and ceramics (before and after experiments) showed that, in comparison with the initial steel, it was observed a decrease in the carbon content (up to 0.4% mass.) and an increase in the chromium concentration (up to 1% mass.) for all samples.

Also, the metal contained to 0.2 % mass. Al after experiments. This indicates the interaction of carbon of the steel with the ceramics, the reduction of elements from the ceramic oxides and their transition to the melt. The two-fold increase in the oxygen concentration after the experiment indicates a possible increase in the quantity of nonmetallic inclusions as a result of interaction of the metal with the ceramics.

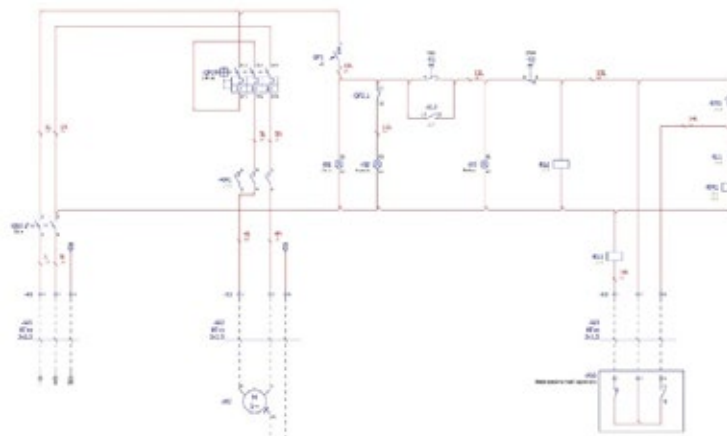
*This work was carried out according to State Assignment 075-00320-24-00.*

# VACUUM STATION CONTROL ORGANIZATION

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The vacuum station consists of electronic vacuum gauge DV2010f, vacuum rotary vane pump RS28 and vacuum chamber.



**Figure 1:** Schematic diagram

Vacuum infusion is a process that is widely used in metallurgy to improve the quality and properties of metallic materials. This method reduces the number of gas inclusions and other defects in the metal, resulting in improved strength, hardness and other characteristics. Let's take a closer look at how vacuum infusion works and the benefits it offers in the metallurgical industry. Vacuum infusion in metallurgy is based on the principle of removing gases from molten metal by creating a vacuum in a special chamber. The process begins with heating the molten metal to a certain temperature, at which the gases contained in it begin to be released. The metal is then placed in a vacuum chamber where a low pressure is created, allowing the gases to escape from the metal and be removed from the system.

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# DETERMINATION OF THERMAL CONDUCTIVITY OF OILY MILL SCALE

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The problem of recycling fine iron-containing waste generated at a metallurgical enterprise is mainly solved by using them as components of the sintering charge<sup>1,2</sup>. Difficulties are caused when recycling by this scheme the finest oily mill scale, containing up to 20-30 % (wt.) oil<sup>3</sup>. Existing processing methods (chemical treating, briquetting, pyrometallurgical methods) are currently unprofitable. It seems relevant to develop a method for recycling oily scale by direct loading into a blast furnace<sup>4</sup>. With this end additional studies of the physicochemical properties of oily scale were conducted.

The thermal conductivity of oily scale was determined by comparing the results of a difference solution of the thermal conductivity problem with experimental data on heating a container package with a volume of 280 ml, filled with 585 g of an oily scale, with logging of temperature along the axis of symmetry and in the peripheral layers of the container. Heating was carried out in a muffle furnace to a temperature of 200 °C. The heating rate was 4 °C/min. This technique made it possible to determine the thermal conductivity of the sample amounting to 9 W/m·°C.

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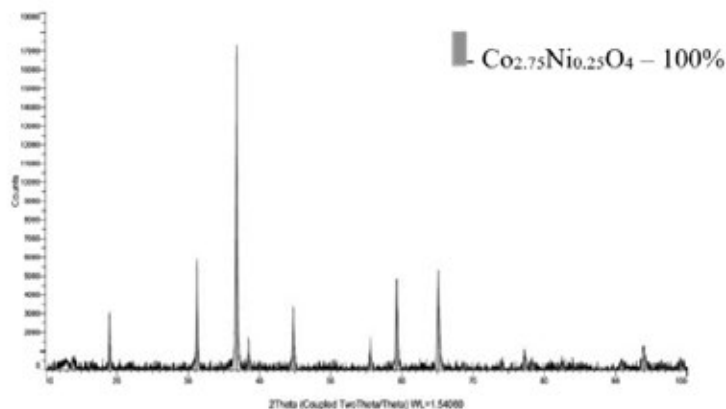
# COBALT EXTRACTION FROM LEACHING SOLUTIONS OF OXIDIZED NICKEL ORES

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The development of science and the transition to a low-carbon economy in recent decades has stimulated the growth of global cobalt consumption. Today cobalt deposits are practically exhausted. Cobalt is produced as an associated element in the extraction of nickel and copper from cuprous sandstone, copper-nickel-sulfide and oxide nickel ores.<sup>1,2</sup> A key production step that affects the profitability of ore processing is the separation of copper, nickel and cobalt.<sup>2</sup>

Precipitation of oxidized nickel ores (ONO) from Sulphuric acid leaching solution with 2-naphthol was applied as a method of selective cobalt extraction.<sup>3</sup> A 99% recovery of cobalt in the precipitate was achieved. After roasting at 750 °C, a cinder containing 90% of cobalt in terms of  $\text{Co}_3\text{O}_4$  was obtained.



**Figure 1.** Cobalt burnt stone

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# INFLUENCE OF ELECTROMAGNETIC STIRRING ON THE STRUCTURAL STATE OF CONTINUALLY CAST LOW CARBON STEEL BILLET

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In the production of continuous cast billets, a rather important parameter to be achieved is a defect-free internal structure formed during smelting. Disturbed macrostructure of a continuous cast ingot due to axial liquation of chemical elements, accumulation of various kinds of non-metallic particles are among the few defects that can persist throughout the processing and in the finished product.

This paper analyzes the effect of treatment in the secondary cooling zone (SCZ) by electromagnetic stirring (EMS) of mild steel 25GYU on the change of slab crystallization zones, as well as on the formation of non-metallic inclusions.

The scheme of the experiment was to compare quantitative and morphological parameters of non-metallic inclusions and macrostructure of the slab metal under study, poured at the continuous-casting plant at two flows, one of which included EMS equipment in the secondary cooling zone. The assessment was carried out on metallographic slabs throughout the slab thickness: macrostructure (dimensions of crystallization zones) using a Leica Sapo stereomicroscope with Thixomet software after etching with Stad's reagent; contamination with non-metallic particles using a Tescan Mira 3 scanning electron microscope with an OXFORD energy dispersive attachment with Aztec 5.0 software (ASTM E2142).

As a result of investigations revealed:

- the central zone of equiaxed crystals of the continuous cast ingot increased up to 80 %; in the zone of columnar crystals a decrease in the size of the 1st and 2nd order axes of the dendritic structure were noted;
- the total share of non-metallic inclusions decreased by one third, oxysulfide's - by 33 %, sulfides - by 17 %, oxides - by 30 %; the size of inclusions throughout the slab thickness increased by 16 %, in the central equiaxed zone - by 18 %;
- the structure of complex inclusions, such as oxysulfide's, has changed: the Al content in non-metallic inclusions decreased by 14 % throughout the slab thickness and by 26 % in the equiaxed zone.



# INVESTIGATION OF THE EFFECT OF CERIUM DIOXIDE GENESIS ON ITS ENERGY CONTENT

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Cerium dioxide is a component of solid oxide fuel cells, oxygen sensors, automotive catalysts, polyrites and others.

In this work, the influence of  $\text{CeO}_2$  genesis on its energy content ( $\Delta E_\Sigma$ ) is investigated using the energy state lattice characterization (ESCL)<sup>1</sup> method: ( $\Delta E_\Sigma$ ):  $\Delta E_\Sigma = \Delta E_d + \Delta E_s + \Delta E_e$ , where the energy contribution  $\Delta E_d$  is related to the deviation of the lattice parameters of synthesized  $\text{CeO}_2$  from the equilibrium lattice, and  $\Delta E_s$  and  $\Delta E_e$  are related to the size of the coherent scattering and microstrain regions, respectively (Table 1).

№	Precipitation				Sludge heat treatment t, °C/τ, h	ΔE <sub>d</sub>	ΔE <sub>s</sub>
	System	[Ce], M/ [environment]	Precipitant/ [P], M	Regimes		kJ/mol	
1 <sup>2</sup>	Ce(NO <sub>3</sub> ) <sub>3</sub> –H <sub>2</sub> O	0,08	NH <sub>4</sub> OH/ 3	Z= 20000 %	400/2	7,94	21,12
					600/2	3,97	11,37
					800/2	0,00	2,11
2 <sup>2</sup>	(NH <sub>4</sub> ) <sub>2</sub> Ce(NO <sub>3</sub> ) <sub>6</sub> – Ce(NO <sub>3</sub> ) <sub>3</sub> – изопропанол– H <sub>2</sub> O	0,08/1:1		Z= 20000% [Ce <sup>4+</sup> /Ce <sup>3+</sup> ]=0:1	60/2	63,68	49,29
				[Ce <sup>4+</sup> /Ce <sup>3+</sup> ]=1:3		75,66	50,99
				[Ce <sup>4+</sup> /Ce <sup>3+</sup> ]=1:1		87,66	50,99
				[Ce <sup>4+</sup> /Ce <sup>3+</sup> ]=3:1		99,67	52,81
				[Ce <sup>4+</sup> /Ce <sup>3+</sup> ]=1:0		107,68	52,81
3	Ce(NO <sub>3</sub> ) <sub>3</sub> –H <sub>2</sub> O	0,36	(NH <sub>4</sub> ) <sub>2</sub> CO <sub>3</sub> / 2,25	Z= 55 %	300/4+900/ 0,5	11,91	3,50

**Table 1.** Modes of  $\text{CeO}_2$  production and results of energy content calculation  
 Note to Table 1: [P] - concentration of precipitant; Z - mole excess of precipitant

Table 1 shows that  $\Delta E_\Sigma$  of  $\text{CeO}_2$  of series 2 is 3,9-76,1 time higher than in series 1 and 3. The peculiarity of  $\text{CeO}_2$  of series 1 is the predominance of  $\Delta E_s$  over  $\Delta E_d$ , and of series 3 is the maximum ratio  $\Delta E_d / \Delta E_s$  equal to 3.4.

Calculation of the energy content is necessary to evaluate the reactivity of  $\text{CeO}_2$  and to determine the areas of its prospective application.

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# THERMODYNAMIC OF SULFIDES EVAPORATION

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The availability of reliable data on the thermodynamics of evaporation of chemical compounds (including sulfides) that are part of the processed raw materials of complex genesis is a necessary component for the development of the physicochemical foundations of pyrometallurgical processes.

Our thermodynamic analysis of sulfide evaporation processes showed that many elements of D.I. Mendeleev form chemical compounds with sulfur in both condensed and vapor (gas) states. It was found that the molecular composition of the vapor-gas phase of many sulfides and their mixtures is much more complex and diverse than previously thought. In addition to monomer molecules, various gaseous molecules of these compounds were found in sulfides vapors<sup>1</sup>.

Experimental results on the thermodynamics of evaporation and dissociation of sulfides of practically all elements of the periodic system of D.I. Mendeleev are systematised for the first time. A wide range of data on vapour pressure, vapour composition, as well as thermodynamic characteristics of gaseous sulfides obtained from the study of evaporation processes are presented. Temperature dependences of vapour pressure over Me-S systems are established. Tables on enthalpies of atomisation and formation of gaseous sulphides and vapour composition over sulphides of chemical elements located by groups of the periodic system of D.I. Mendeleev are given.

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# THE INFLUENCE OF NON-METALLIC INCLUSIONS WITH A CORE-SHELL STRUCTURE OF OXIDES AND NITRIDE ON THE WEAR RESISTANCE OF A COMPOSITE BASED ON A Fe-Cr-Mn-Mo ALLOY

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Currently, metal-based materials are very promising, the surface layers of which, as a result of processing, are wear-resistant metal matrix composites<sup>1</sup>. However, parts made from such materials can be destroyed quite quickly during operation due to the small thickness of the functional layer. Manufacturing the part entirely from metal matrix composites will avoid this problem. In this regard, in this work, composites based on Fe-Cr-Mn-Mo alloy with different contents of non-metallic inclusions were prepared using the method of self-propagating high-temperature synthesis. Depending on the concentration of the non-metallic phase, these inclusions were individual inclusions with a core-shell structure or groups of them. In the central part of the inclusion with a core-shell structure, oxides of magnesium (mainly) and aluminum are concentrated, and aluminum nitride is located along the periphery. Comparative tests for abrasive wear of the resulting composites were carried out under conditions of dry friction of samples on the surface of a fixed abrasive – electrocorundum sandpaper P400 and P80 with abrasive particle sizes of 28 – 40  $\mu\text{m}$  and 200 – 250  $\mu\text{m}$ , respectively. As a result, it was shown that an increase in the content of inclusions with a core-shell structure from 1.09 to 1.73 wt. % helps to increase the wear resistance of composites when tested on all abrasives. However, with a subsequent increase in the concentration of inclusions in the composites up to 3.38 wt. % when using P80 sandpaper, wear resistance decreased, and when using P400 sandpaper, wear resistance increased. The revealed dependencies are explained taking into account the detected change in the structure of inclusions with an increase in the proportion of the non-metallic phase in the composites. In particular, taking into account the discovered tendency of inclusions with a core-shell structure to unite into large groups when the content in composites is more than 1.73 wt. % non-metallic phase.

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# THE INFLUENCE OF CARBON ON THE STRUCTURE AND PROPERTIES OF THE ALLOY OF THE Fe-Cr-Mo-N-C SYSTEM OBTAINED BY THE SHS METHOD

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One of the main ways to prevent and prevent pitting corrosion of metal parts is the rational choice of alloy for their manufacture. A preliminary assessment of the potential pitting corrosion resistance of an iron-based alloy can be made by calculating the *MARC* index <sup>1</sup>. This index is calculated based on the chemical composition of the alloy:

$$MARC = \%Cr + 3,3 \cdot \%Mo + 20 \cdot \%N + 20 \cdot \%C - 0,5 \cdot \%Mn - 0,25 \cdot \%Ni$$

where %Cr, %Mo, %N, %C, %Mn, %Ni – content of chemical elements in the alloy (wt %).

In the formula for the *MARC* index, carbon, nitrogen and molybdenum are considered to have a positive effect on corrosion resistance, while nickel and manganese are considered to have a negative effect. However, carbon can reduce corrosion resistance due to the formation of carbides. One of the most rational methods for producing a high-nitrogen alloy of the Fe-Cr-Mo-N-C system is self-propagating high-temperature synthesis (SHS) <sup>2</sup>. Thus, in this work, we investigated the effect of carbon concentration on the structure, hardness and resistance to pitting corrosion of alloys produced by the SHS method under nitrogen pressure. Chemical composition of alloys (wt. %): chromium 21.0 – 23.5; molybdenum 2.0 – 2.3; nitrogen 1.15 – 1.20 and carbon 0.09 – 0.30 with a *MARC* index value of more than 50. As a result of the work, it was found that in the cast state, alloys containing 0.09 and 0.30% carbon have a microstructure of a mixture of ferrite-nitride structure and austenite. After quenching from 1250 °C, the samples become completely austenitic. Moreover, their hardness is 22 – 24 *HRC* (0.09 % carbon) and 28 – 30 *HRC* (0.30 % carbon). Tests for resistance to pitting corrosion according to GOST 9.912-89 showed that samples containing both 0.09 and 0.30 % carbon are resistant to pitting corrosion.

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# PRODUCTION OF TRIMETALLIC PLATES WITH AN INTERMEDIATE LAYER BY EXPLOSION WELDING

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Homogeneous materials do not always fulfil the growing requirements of different industries. Therefore, multilayer materials combining the properties of the original materials are often used. One of the best ways to produce such materials is explosion welding. For example, explosion welding is used to produce a multilayer material based on aluminium alloy and steel. Due to the sharp difference in properties, such materials are produced using intermediate layers of different metals and alloys.

In this work three trimetallic samples with different intermediate layer were obtained by explosion welding from the following components: the base layer – AlMg6, intermediate layer – titanium/molybdenum/vanadium, and throwable layer – 12Cr18Ni10Ti. As an explosive used a mixture of ammonium nitrate with diesel oil. The gaps between the layers in all experiments were equal to 2 mm.

Metallographic studies of the samples allowed us to assess the continuity of the joint and determine the type of the obtained boundaries of the joint. In all three samples, the boundary between the intermediate and the base layer has a plane profile, and wavy – between the thrown and the intermediate layer. In the titanium and molybdenum samples, areas of dynamic recrystallisation were observed at the joint boundaries in the region of vortex zones and localised shear bands formed as a result of intense plastic deformation of the joint boundary. In the sample with vanadium interlayer, a mechanical mixture of vanadium particles in the matrix of AlMg6 with a thickness of 40 µm was found, which indicates a high degree of material mixing. Thus, the study confirms the prospect of using the selected intermediate layers to obtain trimetallic plates with strong bonding.

*This research was funded by Russian Science Foundation (RSF) No. 23-19-00446.*

# AC ELECTROCHEMICAL SYNTHESIS OF MICRODISPERSED TUNGSTEN(IV) OXIDE

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A comparative analysis of electrochemical methods for metal tungsten processing under the influence of direct and alternating sinusoidal current (industrial frequency - 50 Hz) in solutions of ammonium carbonate ( $0,5 \div 1,0$  M) has been carried out. The electrolytes used make it possible to obtain ammonium paratungstate by evaporation<sup>1</sup>. The current density was varied in the range from 0,3 to 2,0 A/cm<sup>2</sup>, the electrolyte temperature from 20 to 50°C. It has been shown that the use of direct current provides high-speed dissolution of tungsten ( $\sim 2300$  mg/cm<sup>2</sup>·h) with a current efficiency of  $\sim 100\%$ . When replacing direct current with alternating current, the tungsten dissolution rate decreases by 2 times, and the current efficiency drops to  $\sim 80\%$  (with comparable process parameters).

It has been established that the advantage of using alternating current in ammonium carbonate solutions is the possibility of electrochemical synthesis of microdispersed powder based on WO<sub>2</sub> from metal tungsten at a current density of more than 0,5 A/cm<sup>2</sup> and an electrolyte temperature of 20°C. The resulting powder has a developed surface structure with a predominant particle size of  $3 \div 10$  microns.

A regime has been identified for the electrochemical tungsten scrap recycling under the influence of alternating current, which makes it possible to achieve a degree of tungsten extraction into microdispersed powder of  $\sim 40\%$ . The powder can be subjected to additional milling in order to further obtain microdispersed powder of metal tungsten by hydrogen reduction<sup>2</sup>.

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# INFLUENCE OF TECHNOLOGY FOR MELTING HALF-PRODUCT IN EAF ON THE HYDROGEN CONTENT IN STEEL

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The influence of wet materials and air in contact with steel during the steelmaking process on the hydrogen content in the resulting metal has been known to metallurgists for a long time.<sup>1-3</sup> In this study, these factors are considered in conjunction with the impact of the technology features for smelting semi-products in a modern electric arc furnace.

Preliminary thermodynamic study of the formation of products of interaction of moisture with metal in a high-temperature zone near electric arcs showed the possibility of the formation of various molecular compounds, which should lead to an increased flow of hydrogen into the intermediate product.

Statistical analysis of industrial data from melts carried out in real metallurgical production showed that an increase in atmospheric humidity and the duration of operation of electric arcs in an EAF leads to an increase in the hydrogen content in steel at the tundish stage of a continuous casting machine.

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# PHYSICAL AND CHEMICAL PROPERTIES OF Al-Ni-Co-Cu-Zr HIGH-ENTROPY ALLOYS IN SOLID AND LIQUID STATES

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High-entropy alloys (HEA) have been actively investigated in recent years due to the possibility of obtaining materials with improved mechanical properties and corrosion resistance. In this work we investigated physical and chemical properties (density, electrical resistivity, magnetic susceptibility) and corrosion resistance of AlNiCoCuZr HEAs.

Density of the alloys was studied by gamma-absorption method, electrical resistivity by contact-less method in rotating magnetic field and magnetic susceptibility - by the Faraday method. All experiments were carried out in the temperature range 300 - 1800 K. The relative error of property measurements does not exceed 3%. Corrosion resistance was investigated after 1500 hours of exposure in 5% NaCl solution by measuring cyclic voltammetry dependences also.

It is found that AlNiCoCuZr HEA are characterized by unusual dependences of electromagnetic properties<sup>1</sup>, but have high values of corrosion resistance.

Experimental data on structural-sensitive and corrosion properties of AlNiCoCuZr alloys can be used for optimization technological processes.

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# PHYSICAL AND CHEMICAL PROPERTIES OF Al-TM-REM GLASS-FORMING MELTS

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 Son L.D.,<sup>b</sup> Perevyshin V.A.,<sup>a</sup> Ladyanov V.I.,<sup>c</sup> Beltyukov A.L.<sup>c</sup>**

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Aluminum alloys with transition (TM) and rare-earth metals (REM) have unique mechanical and anticorrosion properties in amorphous and nanocrystalline states. However, the main problem here is to obtain high-quality amorphous and especially nanocrystalline samples, and this is impossible without special preparation of melts for rapid quenching.

In the present work, samples of  $\text{Al}_{86}\text{Ni}_{8-x}\text{Co}_x\text{R}_6$  ( $x = 2-4$ ;  $\text{R} = \text{Ce}, \text{Sm}, \text{Tb}$ ) alloys were prepared. Their atomic structure (by X-ray diffraction), microstructure and surface morphology (by optical and electron microscopy) were determined. Characteristic temperatures (solidus, liquidus) and values of thermal reactions occurring during heating up to 1600 K and subsequent cooling were established. The temperature dependences of density, viscosity, electrical resistivity and magnetic susceptibility of these alloys were studied in heating and subsequent cooling regimes. Density and viscosity polytherms show hysteresis of properties (mismatch of heating and cooling curves) at temperatures below 1350 - 1300 K, whereas the temperature dependences of electrical resistivity and magnetic susceptibility obtained during heating and cooling coincide.

To obtain high-quality amorphous ribbons, some regimes of melts heat treatment before quenching were proposed. Amorphous alloys were obtained in the form of ribbons by planar flow method in protective argon atmosphere. It was found that aluminum nanoparticles appear at the first stage of crystallization of the studied amorphous ribbons, whereas the formation of intermetallics  $\text{Al}_{19}\text{Ni}(\text{Co})_5\text{R}_3$  и  $\text{Al}_{23}\text{Ni}(\text{Co})_6\text{R}_4$  takes place at the second stage. These compounds occur at the boundaries of aluminum nanoparticles and inhibit their further growth, which leads to the stabilization of the nanocrystalline state.

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# HISTORICAL ASPECTS OF CREATION OF PRODUCTION VANDI-UM IN RUSSIA AND ACTUAL DIRECTIONS ITS DEVELOPMENT

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The production of vanadium in Russia was organized during the years of industrialization of the USSR. The first work has begun at the Kerch Metal-lurgical Plant using V-poor phosphorous iron ores. In 1932, an experi-mental workshop was built, and in 1937, about 16 tons of V were produced.

At the same time, work was carried out on blast furnace smelting of ti-tanomagnetites to produce V-cast iron. Already in 1936, a ferrovanadium workshop began operating at ChMZ. Sylvinit technology was adopted for roasting slags. This made it possible to completely free the country from its imports. In 1939, blast furnace smelting of Kusa titanomagnetites was tested at ChMZ and then introduced into industry. V-cast iron was processed in Marten furnaces. In March 1941, industrial tests continued at the Yenakievo Metallurgical Plant in the Donbass. Cast iron was processed in the Bessemer workshop to produce V-slag and steel, which made it possible to refine the technology for the Bessemer workshop of ChMZ, which was being built at that time. In 1942, ChMZ began construction of a large blast furnace. By the beginning of 1945, the production of V-cast iron increased by 3 times com-pared to 1940. After the war, ChMZ continuously improved its V produc-tion technology. Since 1963, the plant began to receive titanium-magnetite concentrate from the Gusevogorsk deposit. The V content in the slag in-creased and the Si and Cr content decreased. In 1977, ChMZ switched to so-da technology for slag roasting. In 1960-1970 NTMK mastered the smelting of V-cast iron from concentrate from the Gusevogorsk deposit. In 1974, lime technology for extracting V from converter slag was implemented at the No-votulsky MP. As a result, the USSR became a major producer of V.

In 1997-2001 at IMET RAS, together with Vanadium-Tula, large-scale research was carried out to improve lime technology. As a result, the tech-nical and economic indicators of production were significantly improved. Currently, the Evraz Company in the Tula region is building a new plant for the production of V using lime technology.

At the IMET RAS research continues on actual direction in the extraction of V from various types of raw materials.

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# VOLATILITY OF COMPONENTS OF MOLTEN MCL<sub>4</sub>–MECL MIXTURES (M = U, Th, Hf, Zr, Ti; Me = Cs–Li)

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Based on experimental data obtained mainly by researchers of the Institute of High–Temperature Electrochemistry of the Ural Branch of the Russian Academy of Sciences (IHTE UB RAS), the regularities of changes in the composition of saturated vapors and the volatility of components of molten mixtures of uranium and some other metals tetrachlorides (ThCl<sub>4</sub>, HfCl<sub>4</sub>, ZrCl<sub>4</sub>, TiCl<sub>4</sub>) with alkali metal chlorides depending on the temperature, concentration and cationic composition of the melts are discussed<sup>1</sup>.

Tetravalent uranium, thorium, hafnium, zirconium and titanium in molten alkali metal chlorides act as powerful complexing agents; therefore, their dissolution is accompanied by significant rearrangements of particle bonds, leading to the formation of stable complex anions. The complex formation is manifested as a sharp decrease in the pressure of saturated vapors of the corresponding metal tetrachloride. The strength of complex chloride anions of polyvalent metals formed in the melts increases significantly with a decrease in their concentration, replacement of the solvent salt in the series from LiCl to CsCl, and decreasing temperature. As a result, the volatilities of UCl<sub>4</sub>, ThCl<sub>4</sub>, HfCl<sub>4</sub>, ZrCl<sub>4</sub>, and TiCl<sub>4</sub> and the compositions of vapors above the solutions in the ionic melts vary greatly. Hafnium, zirconium, and titanium tetrachlorides (especially TiCl<sub>4</sub>) are significantly more volatile in the individual state than UCl<sub>4</sub> and ThCl<sub>4</sub> and have higher volatilities and contents in the saturated vapors over the solutions in molten alkali metal chlorides.

The temperature, concentration, and composition dependences of the saturated vapor compositions and volatilities of the molten mixtures components can be used as reference materials to perform diverse pyrometallurgical and pyrochemical (e.g, electrolytic) processes based on salt melts, in particular, to produce pure metals and alloys, as well as to regenerate spent nuclear fuel and etc.

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# MATHEMATICAL MODELING OF STATE DIAGRAMS

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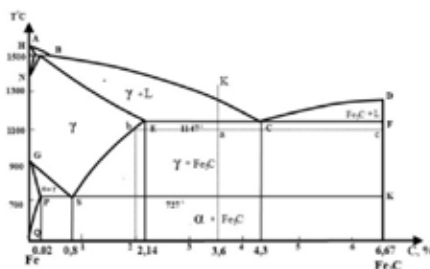
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The main method of constructing state diagrams is experimental<sup>1</sup>. However, calculations based on the study of the dependence of the free energy of the system on temperature, pressure, and the concentration of all components in all phases are also used<sup>2</sup>.

In this paper, another problem is posed and solved. It provides a mathematical description of existing state diagrams to find the type and number of phases formed.

The Fe-Fe<sub>3</sub>C diagram, graphically represented in the figure, is chosen as the object of research.



**Figure.** Diagram of the state of Fe the Fe-Fe<sub>3</sub>C

System on the basis of equations describing the liquidus and solidus lines in all regions of the c diagram c, a mathematical model and a computer program are developed for calculating the phase composition of metal in the Fe-Fe<sub>3</sub>C system. When you enter в компьютер the carbon content and temperature into the computer, the program automatically determines the area of metal location, calculates and displays the phase composition in mass percentages. This approach can also be used to develop mathematical models and programs for other systems. The method is tested using the well-known method of segments (lever) and gives more accurate values of the number of phases.

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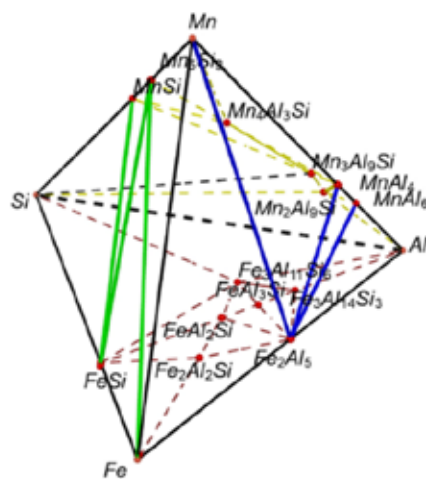


МИНИСТЕРСТВО ОБРАЗОВАНИЯ И НАУКИ  
РОССИЙСКОЙ ФЕДЕРАЦИИ ГОСУДАРСТВЕННОЕ  
ОБРАЗОВАТЕЛЬНОЕ УЧРЕЖДЕНИЕ ВЫСШЕГО  
ПРОФЕССИОНАЛЬНОГО ОБРАЗОВАНИЯ  
PHASE COMPOSITION DIAGRAM OF ALSIMN

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One of the ways to improve the quality of steels is to use complex alloys based on aluminum, silicon, manganese, chromium, etc. in their production.



**Figure 1.** Phase diagram of the Fe-Si-Al-Mn system

The composition of the AlSiMn alloy (Fe – 15-20%; Si – 40-50%; Al – 10-25%; Mn – 10-30%) is modeled by the FeSi-Fe<sub>3</sub>Al<sub>11</sub>Si<sub>6</sub>-Si-MnSi tetrahedron. AlSiMn with a high aluminum content includes the following phases (in %): FeSi = 1,755; Fe<sub>3</sub>Al<sub>11</sub>Si<sub>6</sub> = 53,175; Si = 29,92; MnSi = 15,15. The composition of AlSiMn with low aluminum content includes the phases (in %): FeSi = 21,59; Fe<sub>3</sub>Al<sub>11</sub>Si<sub>6</sub> = 21,27; Si = 11,69; MnSi = 45,45<sup>2,3</sup>.

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# THE EFFECT OF THE DEGREE OF DEFORMATION ON THE MICROSTRUCTURE AND MICRO-HARDNESS OF CORROSION-RESISTANT STEEL AUSTENITIC CLASS

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Pipe blanks made of austenitic corrosion-resistant steels are widely used in mechanical engineering, nuclear, oil refining and chemical industries. The production process of semi-finished products and finished products from these steels includes a stage of hot deformation by rolling and forging.

The aim of the study was to assess the effect of the degree of deformation on the microstructure and microhardness of austenite corrosion-resistant steel.

The object of the study were samples cut from a pipe billet obtained after forging and rolling from 08X18H10T steel. A continuously cast blank with a diameter of 184 mm was rolled to a diameter of 160 mm (sample No. 1,  $\varepsilon = 13\%$ ). Another blank with a diameter of 360 mm was forged to a diameter of 190 mm (sample No. 2,  $\varepsilon = 45\%$ ).

The microstructure of the cut-out samples was revealed by electrolytic etching of polished samples in a 10% aqueous solution of oxalic acid using an optical microscope LeicaDMi8, MIM-8 and Versa-3D at magnifications of 250 and 1000 times, respectively.

Microhardness was measured on a LOMO PMT – 3 microhardness meters with a load of 50 grams.

The microstructure of the samples is austenite and carbides. There is a tendency to reduce the size of the austenitic grain from the center to the surface of both the forged and hot-rolled billet, but there is a grain diversity in the forged billet.

The average microhardness index in the surface part of the forged plate is 255 HV, in the central 219 HV. In a hot-rolled furnace, there are 176 HV in the surface, 174 HV in the center.

Thus, the presence of different grains in the forged workpiece and higher microhardness values indirectly confirms the recrystallization that did not fully take place during forging.

# DEVELOPMENT OF COMBINED TECHNOLOGY SURFACE MODIFICATIONS CHROMIUM-NICKEL STEELS

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Electrochemical modification of the surface in combination with low-temperature plasma nitriding enhances the diffusion of nitrogen into the surface layer and is an effective way to increase wear resistance and corrosion resistance<sup>1</sup>. A change in the surface condition under the action of an applied alternating current leads to a change in the properties of the surface layer, which becomes more susceptible to plasma exposure. It is not just accelerates the process of nitrogen diffusion at low temperatures, but also allows you to increase the thickness of the diffusion coating with higher corrosion resistance<sup>2</sup>.

The study of the surface of a sample treated in a low-temperature plasma with the supply of a variable component of the current looks homogeneous. Ion bombardment leads to the spraying of micro-roughness and hidden defects along grain boundaries and smoothing of microcracks. The edges of the burrs are sprayed on it, all irregularities are smoothed out, there are no small scratches. Precipitation of the carbide phase practically does not occur. The results of microhardness tests showed that on a sample treated in a low-temperature plasma with alternating current, the microhardness in the layer at a depth of up to 2 microns doubled from 3.8 to 7.6 GPa. The surface layer became denser compared to the surface layer of the untreated sample, since the indenter penetrated to a lower depth under the same load. The greatest consolidation occurred in the layer at a depth of up to 100 microns.

The study of the morphology and chemical composition of the surface layer sample showed that corrosion processes in the control sample, there are grain boundaries. In the sample processed in low-temperature plasma with the imposition of a variable component, they proceeded at the boundaries of the healed defect and the amorphous bond. Both the content of the main elements and their ratio in terms of a decrease in the amount of iron, chromium and an increase in the amount of carbon and especially oxygen have changed

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# INCREASING THE SELECTIVITY OF HYDROMETALLURGICAL PROCESSING OF OXIDIZED NICKEL ORES OF THE BURUKTALSKY DEPOSIT

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Oxidized nickel ores (ONR) account for about 60% of all nickel reserves in the world. The rest is represented by copper-nickel sulfides, which currently provide industrial production of Ni. The main area of nickel consumption (75-80%) is the production of stainless and special steels. According to the International Stainless Steel Forum (ISSF), stainless steel production increased by 16.9% in 2021, and nickel demand in this area will increase in the medium term. Another fast-growing area of the Ni market is its use in batteries for electric vehicles, energy storage systems in wind turbines and solar panels. In the modern world, with a continuous increase in resource consumption, the predominant part of the "balance raw materials" of nickel is rapidly depleted, while no new rich reserves of sulfide nickel ores have been identified. This expands the raw material base by involving relatively poor ores, as well as the development of deposits of oxidized nickel ores. At the same time, ONR are hypergenic and lie near the surface of the earth, causing a low cost of open-pit mining and making them promising.

On the territory of Russia, among the large ONR deposits, Buruktalskoye (Orenburg region) can be distinguished, in which significant reserves of nickel of the Russian Federation (1377 thousand tons) are concentrated. A technological scheme for complex hydrometallurgical processing of ferrous laterite nickel ores of the Buruktalskoye deposit with selective extraction of nickel and cobalt was developed at IMET RAS. It includes reduction roasting of ore and sulfuric acid leaching of the stub with the transfer of nickel and cobalt into solution, and their subsequent precipitation as a mixed Ni/Co hydroxide product (MHP). To intensify and increase the selectivity of leaching, the process is carried out in the presence of the complexing ammonia reagent  $(\text{NH}_4)_2\text{SO}_4$ .

*The work was performed according to the state task No. 075-00320-24-00.*





Section 4

# **RESOURCE SAVING, ENVIRONMENTAL SAFETY AND CHEMICAL-TECHNOLOGICAL PROCESSES IN CIRCULAR ECONOMY**

# APPLICATION OF MAGNETIC AND ELECTRICAL SEPARATION FOR BENEFICATION OF REDUCED LEUCOXENE CONCENTRATE OF THE YAREGSKOYE DEPOSIT

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In Russia, metallic titanium is produced at the VSMPO-AVISMA enterprise using the chlorine method, and pigment titanium dioxide is produced at the Crimean Titan enterprise using the sulfuric acid method. Imported ilmenite concentrates are used as raw materials. To solve the problem of raw material dependence, IMET RAS is conducting research aimed at processing the leucoxene concentrate of the Yaregskoye deposit to produce porous anosovite, suitable for the production of titanium and its pigment dioxide.

Leucoxene concentrate contains about 50%  $\text{TiO}_2$  and 40%  $\text{SiO}_2$ . Some quartz is present in the form of independent grains. The ferruginous anosovite and quartz formed as a result of the reduction have contrasting magnetic and electrical properties, which makes it possible to remove quartz grains using magnetic (MS) or electrostatic separation (ES). Separation was carried out on leucoxene concentrates reduced at 1400 °C in the presence of 5% reducing agent (carbon black). Before separation, the recovered concentrate was divided into several size classes on sieves.

As a result of the research, it was found that both with MS and with ES it is possible to separate quartz grains from grains of reduced leucoxene. However, better selectivity was achieved with ES. The reason for this is the presence of a small amount of reduced iron particles on quartz grains due to the formation of low-melting eutectics in the  $\text{FeO-SiO}_2$  system during reduction. In this case, quartz grains acquire bulk magnetic properties and local surface conductivity like titanium-containing grains. Such quartz grains have permanent magnetic properties and their separation is difficult even with the use of several MS cleanings. However, the conductive properties of the surface of quartz grains differ at different points. Therefore, if during the first ES a quartz grain came into contact with the drum with the conductive part of the surface and ended up in the concentrate, then during subsequent cleanings such grains may come into contact with the drum with a non-conductive surface and be released into the tailings.

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



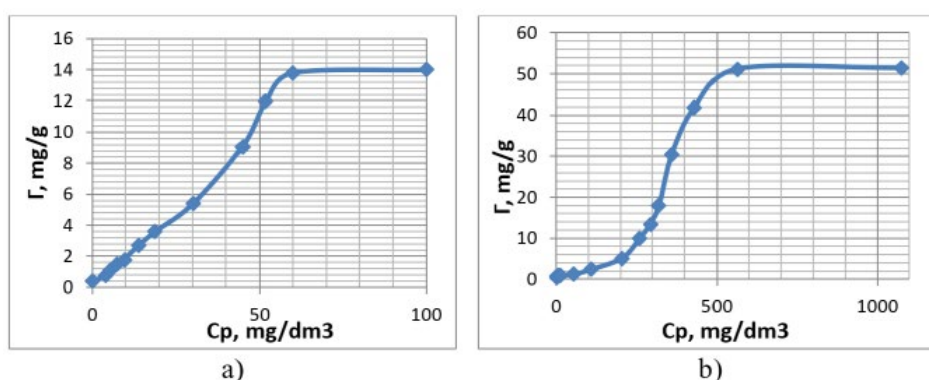
# SORPTION TREATMENT OF INDUSTRIAL WASTEWATER FROM HEAVY METAL IONS AND ORGANIC COMPOUNDS WITH MODIFIED BENTONITE

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Currently, different technologies are used to treat industrial wastewater. Adsorption water purification is recognized as one of the most promising technologies<sup>1</sup>. It is advisable to use modified bentonites as a sorption material<sup>2</sup>.

Based on the results of studies of bentonite modified with carbon nanotubes (CNTs), adsorption isotherms of  $\text{Fe}^{2+}$  ions and *o*-phenylenediamine (*o*-PDA) were obtained.



**Fig 1.** Adsorption isotherms of  $\text{Fe}^{2+}$  ions (a) and *o*-PDA (b) on bentonite modified with CNTs under static conditions

The characteristics of  $\text{Fe}^{2+}$  ions and *o*-PDA adsorption by bentonite modified with CNTs under static conditions were established.

**Table 1.** Characteristics of adsorption of  $\text{Fe}^{2+}$  ions and *o*-PDA ions

Substance	Static exchange capacity, SEC, mg/g	Interfacial distribution coefficient, $K_d$ , $\text{dm}^3/\text{mg}$	Adsorptiondrawaldegree, $S$ , %
$\text{Fe}^{2+}$ ions	$14,056 \pm 0,336$	$0,140 \pm 0,013$	$90,09 \pm 4,48$
<i>o</i> -PDA	$51,310 \pm 0,815$	$0,050 \pm 0,004$	$74,14 \pm 1,757$

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# PREPARATION OF THE SLUDGES FROM METALLIZATION SHAFT FURNACES FOR FURTHER METALLURGICAL TREATMENT

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The treatment of blast furnace gas from Midrex and Hyl furnaces is carried out in the scrubber wash units with sludge as a by-product. While the sludge is exposed to recycling process, it becomes viable to turn the existing production into a circular economy model. Iron content in the sludge accounts for 61...82%, and therefore considered as a valuable feed. Taking into account a current trend of sludge formation and its deposited volumes, an annual unloading of said material is feasible at a rate of 100-150 thousand tones within 20 years and longer. Mostly, the sludge is made up of fines with a high specific surface value and is represented as a slurry. Those sludge fines should be prepared for handling (in winter season as well) and dewatered for further utilization in the metallurgical treatment.

According to the studies conducted, a sludge dewatering up to the level of water mass fraction of 8% is feasible by means of thickeners and press filters. It is recommended to use coagulants in the course of thickening (for instance, a polyaluminum chloride by Aqua-RAS 30), which could reduce the thickener diameter by two-three times. It is proposed to perform a dewatering of sludge in the press filters. Filtration in the vacuum filters is inefficient even with intensification by means of anionic surfactant of Ferry type and/or heating by vapor. Mixing of dewatered sludge with lime up to a moisture level of 6.0... 6.5% (dosage of lime is 4%) allows for preventing a state of freezing under conditions of sub-zero temperature (of ambient air). Albeit, the iron mass fraction in the sludge gets down and prime costs get higher (due to addition of expensive lime). In the course of drying under 200°C, a moisture of sludge gets lower up to 4.5 for 17.3 minutes and under temperature of 400°C for ≈12.2 minutes; under temperature of 600°C for ≈8 minutes; under temperature of 800°C for ≈ 7 minutes. Specific flow rate of natural gas dedicated to drying process will be 5.3...6.5 nm<sup>3</sup>/t.

From a production process perspective, the thickening-filtration-drying scheme is considered optimal. This scheme provides with a max flexibility of production while preserving the high metallurgical properties of sludge.

# COMPLEX PROCESSING OF DEACTIVATED PLATINUM-RHENIUM CATALYSTS

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The production of high-quality gasoline is based on the catalytic reforming process using bimetallic catalysts, which are granular active aluminum oxide with platinum and rhenium distributed over its surface. Catalysts that have exhausted their service life are removed from the process. These catalysts contain platinum and rhenium in quantities from 0.25 – 0.4 wt. % for each component, which significantly exceeds the content of these metals in the ore raw materials traditionally used for their production.

Among the various fundamental methods for processing spent platinum-rhenium catalysts, preference was given to the option based on the sequential extraction of first rhenium, then platinum. Using the spent catalyst KR-108 as an example, the leaching of rhenium with dilute solutions of  $\text{H}_2\text{SO}_4$ ,  $\text{HCl}$ ,  $\text{NaCl}$ ,  $\text{NaClO}$ ,  $\text{H}_2\text{O}_2$ ,  $\text{NaHCO}_3$  was studied. It has been established that when using all these solutions, except for the  $\text{NaHCO}_3$  solution, along with rhenium, from 2,4 to 7,8 % of the platinum contained in the catalyst passes into the solutions. Only when the catalyst is treated with a 0,1 M  $\text{NaHCO}_3$  solution, platinum remains almost completely in the solid phase (no less than 99%), while 98-99 % of rhenium passes into the solution phase. It has been proven that it is possible to achieve complete transfer of platinum into solution by treating the catalyst with 6 M  $\text{HCl}$  solution with the addition of  $\text{H}_2\text{O}_2$  as an oxidizing agent only with complete dissolution of the carrier –  $\text{Al}_2\text{O}_3$ , preferably in two stages in countercurrent mode. It is proposed to extract  $\text{Re(VII)}$  from a solution after its leaching by acidifying the solution to pH 1,5–2,0 and sorption on a rhenium-selective anion exchange resin Purolite A170, followed by desorption with an ammonia solution and separation from the desorbate in the form of  $\text{NH}_4\text{ReO}_4$ , and platinum from the solution after complete decomposition catalyst by cementation on aluminum shavings. A basic technological scheme of the process has been developed, which provides for the sequential extraction of rhenium and platinum and the utilization of the catalyst base –  $\text{Al}_2\text{O}_3$ , in the form of an  $\text{AlCl}_3$  solution or in the form of a solid salt  $\text{AlCl}_3 \cdot 6\text{H}_2\text{O}$ .

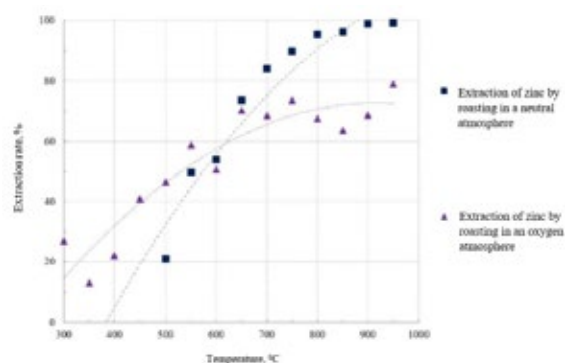
*The research was conducted at the expense of a grant from the Russian Science Foundation (project No. 21-79-30029)*

# RESEARCH ON CO-PROCESSING OF HALOGEN-CONTAINING WASTE

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Technogenic waste, despite the complexity of its processing, has the potential to be a source of secondary non-ferrous metals<sup>1</sup>. In particular, dust from the remelting of galvanized steel scrap contains organic compounds in addition to metals<sup>2</sup>. In the presented laboratory study, zinc was extracted from dust by chlorination of halogen-containing waste.



**Figure 1.** Dependence of zinc extraction into the gas phase during dust chlorination in an oxidizing and neutral atmosphere on the roast temperature (process duration 60 minutes, Zn/HCl ratio = 0.62)

Roasting the mixture at 950 °C led to the evaporation of about 80 wt.% zinc in an oxidizing atmosphere and more than 95 wt.% zinc in a neutral atmosphere. Energy dispersive X-ray spectroscopy of the cinder after firing in a neutral atmosphere showed that the dry residue of the material does not contain zinc.

O	Na	Mg	Al	Si	S	Cl	K	Ca	Cr	Mn	Fe	Total
30,80	2,75	0,70	0,30	1,50	0,75	12,50	1,20	5,60	0,30	2,60	41,00	100

**Table 1.** Result of elemental analysis of a cake sample after washing the cinder obtained by firing at 950 °C in a neutral atmosphere, wt.%

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# THERMODYNAMIC ANALYSIS OF THE DECOMPOSITION OF ZINC FERRITE DURING SULFATING ROASTING

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The difficulty of processing zinc-containing metallurgical waste is often explained by the presence of zinc ferrite,  $\text{Zn-Fe}_2\text{O}_4$ , in it. Therefore, the key task when processing such waste and industrial products is the destruction of  $\text{ZnFe}_2\text{O}_4$ . To assess the probability of this process occurring, thermodynamic calculations<sup>1</sup> of the decomposition of zinc ferrite during sulfating roasting were carried out, the results of which are presented in Table 1.

№	Reaction	$\Delta G$ , kJ/mol at t, °C		
		300	600	900
1	$3\text{ZnFe}_2\text{O}_4 + \text{Fe}_2(\text{SO}_4)_3 \cdot 9\text{H}_2\text{O} = 3\text{ZnSO}_4 + 4\text{Fe}_2\text{O}_3 + 9\text{H}_2\text{O}\uparrow$	-246,46	-430,97	-564,11
2	$\text{ZnFe}_2\text{O}_4 + \text{Fe}_2(\text{SO}_4)_3 \cdot 9\text{H}_2\text{O} = \text{ZnO} + 2\text{Fe}_2\text{O}_3 + 3\text{SO}_3\uparrow + 9\text{H}_2\text{O}\uparrow$	99,38	-249,91	-525,64
3	$\text{ZnFe}_2\text{O}_4 + \text{SO}_3\uparrow = \text{ZnSO}_4 + \text{Fe}_2\text{O}_3$	-109,15	-52,48	-3,83
4	$\text{ZnFe}_2\text{O}_4 + \text{SO}_2\uparrow + 0,5\text{O}_2\uparrow = \text{ZnSO}_4 + \text{Fe}_2\text{O}_3$	-154,06	-69,26	7,12
5	$\text{ZnFe}_2\text{O}_4 + \text{S} + 1,5\text{O}_2\uparrow = \text{ZnSO}_4 + \text{Fe}_2\text{O}_3$	-454,83	-367,02	-286,35
6	$\text{ZnFe}_2\text{O}_4 + \text{H}_2\text{SO}_4 = \text{ZnSO}_4 + \text{Fe}_2\text{O}_3 + \text{H}_2\text{O}\uparrow$	-92,34	-106,19	-121,77

**Table 1.** Change in free energy for the main sulfatization reactions during the decomposition of zinc ferrite

If we evaluate the magnitude of the change in the Gibbs free energy, the most probable decomposition of zinc ferrite is the solid-phase interaction of a mixture of hydrated iron sulfate (III) and excess  $\text{ZnFe}_2\text{O}_4$  according to reaction (1). When a stoichiometric amount of iron sulfate and franklinite enter into reaction (2), no sulfatization occurs. At temperatures up to 600 °C, according to reactions (3-4), franklinite decomposes in the event of its contact with gaseous  $\text{SO}_3$  and  $\text{SO}_2$  (subject to oxygen access). According to calculations, it is theoretically possible to sulfatize zinc with elemental sulfur (reaction (5)), which would require the presence of oxygen in the system, or with sulfuric acid vapor (reaction (6)) in the temperature range from 300 to 900 °C.

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## THE STUDY OF EMULSION GLASS MAT

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Improving product quality and safety depends on the nature of the raw materials used in the production process<sup>1</sup>.

Glass fiber is the most commonly used material in the manufacture of composite products. The fibrous glass filler gives strength and rigidity to the fiberglass.

The properties of glass fiber are determined by the structure and composition of the main component – glass. Currently, there are several hypotheses of the structure of glass, but the most common of them are the crystallite hypothesis and the reticulated glass structure theory. The composition of glass cannot be expressed by a specific formula, since glass is an alloy of oxides. In addition, the chemical composition of glass for the production of glass fiber is unstable and may vary depending on the melting conditions and the manufacturer.

In order to fully unlock the potential of the physico-mechanical properties of the glass composite, improve the surface adhesion between the matrix and the fiber, in order to prevent the formation of cracks resulting from the transfer of stresses from the polymer matrix to the glass fiber, the latter is coated with an oiling agent.

In this work, studies have been conducted to identify the chemical composition of the emulsion oiling agent and the component composition of glass, its effect on the structure, and possible changes in the physical and mechanical properties of glass mat, widely used in mechanical engineering for the production of products based on polyester glass composites in order to determine the optimal temperatures for the process of recycling of fiberglass plastic.

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# ISOLATION OF SOLUBLE CHLORELLA VULGARIS PROTEINS AS A BIOPOLYMER FOR NANOPARTICLE FORMATION WITH FUCOIDAN FOR USE AS AN ORGANIC DRUG DELIVERY SYSTEM FOR PIPERINE

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In light of the mounting disadvantages associated with the usage of chemical substances, researchers have turned to plants and algae as prospective drug delivery systems in green nanotechnology (Tripathi et al., 2017; Thakkar et al., 2010). While microalgae like fucoidan have been used to generate nanoparticles in conjunction with other substances, it is uncommon to employ chlorella soluble proteins and soluble polysaccharides of micro- and microalgae primarily to form nanoparticles, serving as a nanocarrier for piperine. Piperine is a type of naturally occurring functional active ingredient that has a spicy flavour and a range of pharmacological properties. The extraction procedure, detection technique, chemical modification, bioavailability, and physiological function are currently the main areas of study for piperine (Lingli, 2019). Despite this, there is little research in the literature on the use of piperine in a nanocarrier of soluble proteins and fucoidan derived from macro- and microalgae as drug delivery systems.

The goal is to understand the charge-driven self-assembly of chlorella-soluble proteins and fucoidan-coated nanoparticles. Using the self-assembled polyelectrolyte approach, stable nanoparticles of fucoidan-soluble chlorella protein would be synthesised as a nanocarrier for piperine, with different concentrations, pHs, and volumes of the encapsulated fucoidan and soluble chlorella proteins. The nanoparticles in this study will be made from two separate protein extracts of *Chlorella vulgaris* (flocculated and non-flocculated protein extracts) coated with fucoidan and will be investigated in terms of pegylation (PEG-600 and 1500), concentration, and pH (4.07, 5.5, and 7.0). Photon correlation spectroscopy (PCS), also known as DLS, would be used to characterise the nanoparticles, followed by qualitative analysis with FTIR spectroscopy. A linear regression model would be used to analyse the percentage of the release profile and Dpph would be used to measure the antioxidant activity using EPR and UV spectrophotometers.

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# REGENERATION OF ACID ETCHING SOLUTION FOR PRINTED BOARD PRODUCTION

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One of the promising solutions used in the manufacture of printed circuit boards is a copper chloride solution containing  $\text{CuCl}_2$  65-140 g/l (in terms of Cu),  $\text{HCl}$  90-160 g/l and  $\text{H}_2\text{O}_2$  25-30 g/l<sup>1-3</sup>. The initial solution used by Ufa Instrument-Making Production Association JSC for the manufacture of printed circuit boards uses a solution containing 80 g/l  $\text{CuCl}_2$  (in terms of Cu), 100 g/l  $\text{HCl}$  and 30 g/l  $\text{H}_2\text{O}_2$ . During the processing of printed circuit boards, the copper content in the solution increases. When the copper content reaches more than 140 g/l, the solution is waste. At the same time, it contains about 65 g/l  $\text{HCl}$  and about 14 g/l  $\text{H}_2\text{O}_2$ .

Purification of copper-containing wastewater by treating it with alkaline reagents to produce a sludge of copper hydroxide leads to losses of copper<sup>4</sup>.

The research study examined the electrochemical processing of copper-containing waste that is produced during the etching of printed circuit boards in an electrolyzer equipped with a cation-exchange membrane. It is demonstrated that these wastewaters undergo electrochemical processing, which results in the production of metallic copper, a reduction in wastewater concentration to 40 g/l of copper, and a concentration of hydrochloric acid to 180 g/l. Therefore, the final solution can be put back into production after the required modifications, creating a closed circuit and reducing the impact on the environment.

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# REGENERATION OF ETCHING SOLUTION FOR PRODUCTION OF TITANIUM PRODUCTS

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Titanium and its alloys are widely used in aviation, rocketry, mechanical engineering, shipbuilding, chemical engineering, medicine, etc.

The manufacture of titanium products, in particular the application of modifying coatings to its surface, is hampered by a strong oxide film. This film is removed using various methods. The method of treating titanium surfaces with acids<sup>1</sup> has become widespread. This leads to the formation of spent acid etching solution (SAS), which is a production waste. Existing methods for processing SAS lead to the production of precipitates of titanium hydroxide and substances containing fluorides. As a result, the problem of disposal of these sediments arises<sup>2-4</sup>.

The presented work presents the results of studies on the processing of SAS with the production of titanium hydroxide and a mixture of acids suitable for the preparation of an etching solution used in the production of titanium products.

It has been shown that by treating SAS with alkali to pH 7.6-7.8, almost 100% of titanium in the form of hydroxide is extracted from it. The filtrate obtained after separation of titanium hydroxide and containing sodium fluorides and chlorides was subjected to electrochemical processing in a membrane electrolyzer. This made it possible to obtain sodium hydroxide with a concentration of up to 370 g/l and a mixture of hydrofluoric and hydrochloric acids with a concentration of HF up to 66 g/l and HCl up to 63 g/l.

The resulting titanium hydroxide after calcination can be used as a filler in the paint and varnish industry. The mixture of acids obtained by electrochemical processing of the filtrate can also be used to prepare etching solutions.

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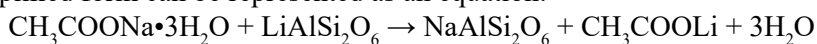
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# PRODUCTION OF LITHIUM CARBONATE FROM SPODUMENE

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Russia, which has significant reserves of lithium raw materials, does not have its own enterprises for its extraction and processing<sup>1,2</sup>. The main industrial method of processing spodumene to produce lithium compounds is the sulfuric acid method. Its disadvantages include a high consumption of 93% acid to extract more than 80% lithium and hardware requirements due to the aggressive environment of the process. Alternative methods of lithium extraction from spodumene<sup>3,4</sup> are being sought. Sintering of  $\beta$ -spodumene with organic sodium salts is a promising method for lithium extraction. The substitution of lithium for sodium in the spodumene occurs due to an ion exchange reaction, which in a simplified form can be represented as an equation:



The resulting water-soluble  $\text{CH}_3\text{COOLi}$  is leached with water, followed by treatment with a solution of sodium carbonate. As a result,  $\text{Li}_2\text{CO}_3$  falls out (Table 1).

**Table 1.** The content of the main impurities in  $\text{Li}_2\text{CO}_3$

№	Содержание, % мас								
	Li	Na	Mg	Al	Si	Ca	Fe	Sr	пр.
1	96,5	1,9	0,1	0,03	0,06	1,25	0,02	0,01	0,12
2	95,9	2,7	0,1	0,03	0,06	1,04	0,01	0,01	0,04
3	96,7	1,9	0,1	0,03	0,06	1,00	0,02	0,01	0,15

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# TECHNOLOGY FOR PURIFICATION OF PRODUCED WATER INTO BRINE FOR THE PURPOSE OF FURTHER USE IN THE PRODUCTION OF SODA ASH

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Produced waters are a constant companion of oil and gas fields. Huge volumes of wastewater with high concentrations of toxic substances are particularly likely to have a negative impact on the environment. Therefore, the purification of produced water is an urgent task<sup>1</sup>. Purified produced waters are a new source of mineral raw materials that can replace traditional types of raw materials in the production of soda ash.

The goal of the work was to find a way to purify the produced water of oil fields from petroleum products and calcium and magnesium salts for the production of soda ash.

Based on the studied ionic composition of produced water, it was found that it can be classified as brines and used to produce technical soda ash.

**Table 1.** Composition of produced water of PJSC Tatneft named after. V.D.Shashina

No. p / p	Defined component	Content, mg/dm <sup>3</sup>
1	Sodium	91866
2	Magnesium	3555
3	Calcium	16828
4	Chloride	151670
5	Petroleum products	1,05

It was proposed to carry out preliminary purification of the brine from traces of petroleum products and iron by passing through a layer of adsorbents - zeolite-coal-zeolite.

To purify produced water from impurities of calcium and magnesium salts, the soda-caustic method<sup>2</sup> was chosen.

A block diagram was proposed for the purification of produced water from oil fields into brine for the purpose of further use for the production of soda ash.

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# INTENSIFICATION OF HEAT AND MASS TRANSFER PROCESSES IN VORTEX APPARATUS

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Intensification of chemical technology processes such as absorption, desorption, evaporation, distillation is possible by using vortex devices. Vortex devices are used to intensify the purification of exhaust gases from toxic substances, such as vapors and mist of nitric acid, ammonia, for the absorption of ammonia in the production of soda ash, the absorption of sulfur trioxide in the production of sulfuric acid, low-waste concentration of spent sulfuric acid, extractive distillation of spent acid mixtures<sup>1</sup>. To increase the efficiency of acid mist collection, the vortex devices are equipped with fiber sleeve elements of the hose type. Designs of vortex devices have been developed, both with ascending and descending flow of gas and liquid phases<sup>2,3</sup>.

Long-term operation of vortex devices in industry has shown that in a vortex gas-liquid flow the efficiency of heat and mass transfer processes increases and reliable phase separation in a centrifugal field is ensured. At the same time, in contrast to packed and disc-type devices, vortex devices have a high throughput capacity for gas and liquid phases, are compact, and do not require pumps to circulate the liquid. Vortex devices with a downward flow of phases have low hydraulic resistance with high absorption efficiency.

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# TECHNOLOGY OF N(S)- AND NK(S)-FERTILIZERS FROM SPENT ACID MIXTURES IN PRODUCING NITROCELLULOSE AND ASSESSMENT OF THEIR AGROCHEMICAL EFFICIENCY

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The existing technology of regeneration of the spent acid mixtures – SAM ( $\text{H}_2\text{SO}_4 + \text{HNO}_3$ ) for the production of cellulose nitrates is ineffective [significant costs, an increase in the amount of toxic gas emissions into the atmosphere ( $\text{NO}_x$ , mist  $\text{H}_2\text{SO}_4 + \text{HNO}_3$ )]<sup>1</sup>. One of the ways to solve this problem is the processing of SAM into N(S)-fertilizer by neutralizing it with ammonia water<sup>2</sup>. The resulting product in this case is a mixture of ammonium sulfatonitrates (ASN) of various compositions  $[\text{NH}_4\text{NO}_3 \cdot 2(\text{NH}_4)_2\text{SO}_4, \text{NH}_4\text{NO}_3 \cdot 3(\text{NH}_4)_2\text{SO}_4]$  with an admixture of ammonium nitrate (AN). The fertilizer contains 2 forms of nitrogen and meets the requirements of TU 2181-036-00205311-08 «Ammonium nitrate containing sulfur» ( $\text{N}:\text{S} \approx 30\%:7\% \approx 1:0,23$  wt.) However, data on its agrochemical efficiency are not provided in the work.

The most promising method is our proposed method of processing SAM into NK(S)-fertilizer by neutralizing it with a mixture of  $\text{NH}_4\text{OH} + \text{KOH}$ <sup>3</sup>. In the neutralization product [60-70%  $(\text{NH}_4)_2\text{SO}_4 \cdot 2\text{NH}_4\text{NO}_3$  with an admixture of  $\text{KNO}_3$  and  $\text{K}_2\text{SO}_4$ ;  $\Sigma\text{NK} = 36-41\%$ ;  $\Sigma\text{NK(S)} = 46-51\%$ ] the ratio of batteries is optimal  $\text{N}:\text{K}_2\text{O}:\text{S} = 1:(0,6-1,1):(0,43-0,5)$  mass. (for most crops, the optimum is  $\text{N}:\text{K}_2\text{O} \approx 1:0,7$  wt.).

In vegetation experiments on gray forest soil ( $\text{N}:\text{P}_2\text{O}_5:\text{K}_2\text{O} = 56:298:121$  mg/kg), the weight of wheat grain when applying ammonium nitrate was 15,2 g/vessel (an increase of 198% to the control), and when applying N(S)-fertilizers ( $\text{ASN}:\text{AN} = 81\%:19\%$ ) was 17,3 g/vessel (an increase of 240% to the control). In the variant with the addition of NK(S)-fertilizer [ $\text{ASN}:(\text{NH}_4)_2\text{SO}_4:\text{K}_2\text{SO}_4 = 53\%:27\%:20\%$ ] the yield increase was relatively small (+205% to the control), which can be explained by the high content of  $\text{K}_2\text{O}$  in the initial soil (with additional potassium addition, the  $\text{N}:\text{K}_2\text{O}$  ratio is suboptimal).

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# COMPLEX PROCESSING OF OIL-CONTAINING WASTE: TECHNOLOGICAL ASPECTS AND ADVANTAGES

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Oil-containing waste (OCW) differs significantly from each other, both in dispersed and chemical composition and in physical properties. Therefore, today there is no universal technology with which it would be possible to process various types of OCW. A technology for complex processing of OCW was proposed at St. Petersburg State Technical University (Technical University). An installation consisting of five processing blocks interconnected in such a way that the products obtained using one technology (in one block) are raw materials or energy resources sold in other blocks was developed. This allows us to significantly reduce the costs of processing waste into useful products.

The first block is a pre-processing unit for OCW heated by steam, in which OCW is hydromechanically separated into more homogeneous components - hydrocarbons with a content of at least 75%, a mineral part - no more than 10%, and water using a tricanter. A granular hydrophobic additive for asphalt concrete mixtures is obtained from the mineral part in the second block. It is possible to obtain water-based fuel from water-cut oil at the third block. The fourth block makes it possible to obtain oxidized bitumen, which can be used as a road bitumen or as a binder for solid fuels, from heavy oil residues. At the fifth pyrolysis block, it is possible to obtain synthetic tar, semi-coke and hydrocarbon gases, which are burned to generate thermal energy, from a mixture of heavy oil residues with coal.

The entire amount of heat required for processing OCW, as well as part of the raw materials used (bitumen binder) is produced within the framework of one technology; this is an important feature of the complex technology for processing OCW. In addition, the power plant that produces electricity can operate using its own cheap fuel. It is possible to make all manufactured products profitable using a pricing policy for selling your own components.

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# ENVIRONMENTALLY FRIENDLY MULTIFUNCTIONAL MULTILAYER ORGANIC MINERAL FERTILIZERS

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To increase the efficiency of assimilation of nutrients and maintain soil fertility, a method on a plate granulator<sup>1</sup> for obtaining multifunctional organobiomineral fertilizers with prolonged action and containing living microorganisms<sup>2</sup> is proposed. Biocultures of *Bacillus subtilis*, *Bacillus amyloliquefaciens*, *Azotobacter vinelandii*, etc., immobilized on corn starch and having fungicidal and bactericidal effects, the ability to associative nitrogen fixation and providing protection from fungi, insects and other pests, were used.

Laboratory microbiological tests of fertilizers with *Bacillus subtilis* culture have shown that the number of viable microorganisms after granulation is about  $1.0 \cdot 10^7$  CFU/g. The introduction of this fertilizer into the soil at the rate of 100 kg /ha is equivalent to using traditional nitrogen fertilizer for spring fertilization of cereals in the amount of 100-150 kg/ha and liquid preparation «Бактофорт» (also containing *Bacillus subtilis*) at a rate of 2.0 l/ha. However, the use of granular organic fertilizer allows you to add all the components on a one-time basis and is technically easier than microdosing liquid ones.

Of particular interest are the mechanisms of mass transfer inside multilayer granules with microorganisms. The kinetics of the transfer of substances in structured media is complex and diverse<sup>3</sup>. It is important that in the soil inside the granule, over time, the mass conductivity of the transfer medium changes due to biodegradation, the concentration of microorganisms increases in the direction of its outer shell, the effect of prolonged action of the nitrogen-containing core is ensured, etc.

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# NITRIC ACID LEACHING OF CARBONACEOUS GOLD SULPHIDE CONCENTRATE IN THE PRESENCE OF SURFACTANTS

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In the world gold mining the interest in the involvement of difficult-to-process, refractory types of raw materials increases in the processing every year. First of all, this is due to the depletion of reserves of easily processed primary ores. An increase of low-grade, multicomponent, refractory ores, for which the use of traditional technologies is generally unprofitable or completely impossible, necessitates the development of new, more efficient methods of processing raw materials, ensuring high extraction rates of target components, and at the same time reducing production costs and the negative impact on environment.

In this work, studies were carried out on nitric acid leaching of carbonaceous gold sulfide concentrate in the presence of a surfactant. Technical sodium lignosulfonate (LS) was used as a surfactant. Table 1 presents the chemical composition of the studied concentrate.

Component	S	Fe	As	Si	Al	K	C <sub>init</sub>	C <sub>org</sub>	Au, ppm	Others
Mass. %	19.7	18.9	4.6	14.2	7.9	3.8	1.09	0.50	26.9	30

**Table 1** - Chemical composition of gold sulfide concentrate

Nitric acid leaching was carried out for 1 hour,  $T = 353 \text{ K}$ , ratio  $L:S = 5:1$ ,  $\text{HNO}_3$  concentration = 315 g/l,  $LS = 0.5 \text{ g/l}$ . In the process of nitric acid leaching almost complete oxidation of pyrite (98.4 %) and arsenopyrite (98.2 %) is observed, while organic carbon is oxidized and passivated when it is exposed by nitric acid and LS; the gold is concentrated in the cake. Next, the cake was subjected to cyanidation under standard conditions. After cyanidation, the cake was submitted for assay analysis for gold. The gold extraction rate was 90.3 %.

Further research will be aimed at optimizing the process to increase gold extraction.

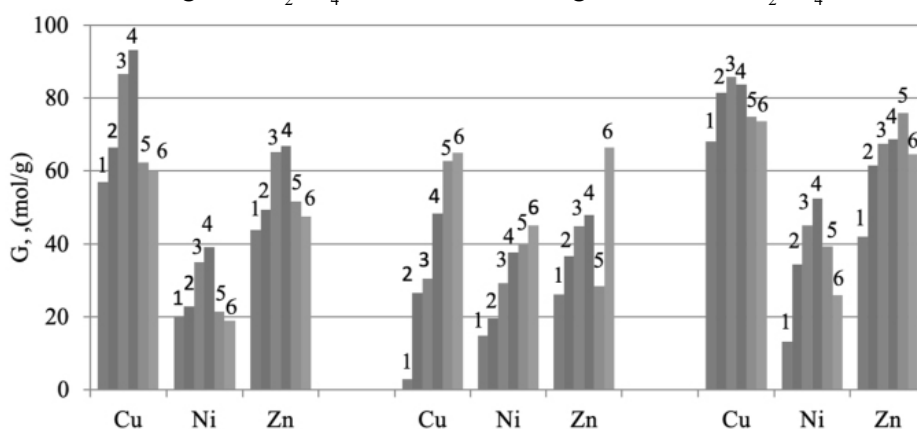
*The research was carried out within the framework of the State Assignment of the Russian Federation under the Grant № 075-03-2024-009/1 (FEUZ-2024-0010).*

# STUDY OF THE PROCESS OF EXTRACTION OF METAL IONS FROM ACIDIC SOLUTIONS BY SORPTION IN A REACTOR

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Sorption extraction of metals depends on the concentration of salts in the solution. This ability is influenced by the ionic strength of the salt in the wastewater solution. Higher sorption efficiency was noted in solutions of NaCl and Na<sub>2</sub>SO<sub>4</sub>. Sorption extraction of copper ions is higher in all electrolytes. The residual concentration of the Cu<sup>2+</sup> group is 0.032mg/l in NaCl solution, 0.45mg/l in Na<sub>2</sub>SO<sub>4</sub> solution and 0.12mg/l in NaCl + Na<sub>2</sub>SO<sub>4</sub> solution.



**Picture 1.** Dependence of the sorption of metal ions  $G$ , (mol/g) on the nature of the electrolyte.  
 pH = 2.5; time = 2 h; BAU-A = 10 g/l

Based on the experimental data presented in pic. 1, the following conclusion can be drawn: the sorption activity of  $G$  (mol/l) of metal depends on the concentration, as well as on the type of electrolyte solution. Higher sorption activity of  $G$  was found in a solution of NaCl electrolytes and a mixture of NaCl and Na<sub>2</sub>SO<sub>4</sub> in the concentration range of 50-150 g/l. In Na<sub>2</sub>SO<sub>4</sub> solution, the sorption activity of metals increases with increasing salt concentration.

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# METHODOLOGY OF CHEMICAL-BIOLOGICAL-SOIL SYSTEM ENGINEERING

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A standard chemical-technological system hierarchy determines the own technological waste and ecosphere chemical-technological load of technology. A scientific and technical direction «Chemical-biological-soil system engineering» was developed capable in providing: a main chemical product completely waste-free technology; a dispersed by-products recycling within the synthesized fine-aggregate architecture of the soil inner layer for a plants favorable development; and a food, fodder and row material economic use of the biological production obtained on the synthesized soil.

The objects of the chemical-biological-soil systems engineering: a main product chemical-technological system; a device for improving the geophysical and geochemical properties of soil by synthesizing the structure and architecture of its illuvial layer for the biological-soil recycling of bulk or granular by-product; a pulsed intra-soil sequential-discrete device for recycling of liquid by-product and/or soil moistening and plant nutrition; and a production of environmentally friendly biological product.

The new multidimensional chemical-biological-soil system includes subsystems: a main chemical-technological product making; a by-product preparing for recycling; and a soil and biological recycling of by-product.

The system involves the following operators: a main product making, a by-product preparation, a mechanical subsoil 20-50 cm layer milling with the introduction of waste; a pulsed sequential-discrete intra-soil moistening; and an agricultural production in crop rotation.

The socio-economic significance of a new multidimensional chemical-biological-soil system engineering is: an increase in the chemical product making resource-energy-efficiency, an environmentally safe recycling of by-products, a long-term production of environmentally friendly food, fodder, raw materials and an ensuring of population employment in the knowledge-intensive production sector.

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# AUTOCLAVE PURIFICATION OF COPPER CONCENTRATES FROM ARSENIC

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Currently, due to the intensive development of non-ferrous metal deposits, the reserves of rich and lightly enriched ores have been largely depleted, and there is a general trend towards a decrease in the metal content of mined ores. Increasingly, hard-to-enrich, thinly-deposited, low-quality, polymetallic and technogenic raw materials containing arsenic are involved in processing<sup>1,2</sup>.

The influence of oxidation duration and leaching temperature on the degree of opening of chalcopyrite, tennantite was investigated to maximise the dissolution of arsenic, iron and zinc. The experimental conditions and results are summarised in Table 1. After oxidation, a hydrothermal copper precipitation stage was carried out at 225 °C on non-oxidised sulphides.

№	t, °C	$\tau_{ox}$ , min	Cake output, %	$Cu_{conc}$ , g/dm <sup>3</sup>	Element, %					Extraction, %			
					S	Fe	Cu	As	Zn	Fe	Cu	As	Zn
1	223,2	20,0	57,1	1,0	45,4	20,7	29,9	1,2	0,4	55,7	2,2	76,4	95,3
2	186,9	20,0	85,8	0,3	42,2	27,3	20,2	3,0	1,4	14,8	0,6	11,2	74,7
3	220,0	30,0	28,0	10,0	42,2	19,7	25,2	0,6	0,3	79,9	59,6	94,5	98,5

**Table 1.** Experimental conditions and results

As a result, the arsenic recovery rate of 76 % was achieved, while the copper conversion into solution was only 2.2 %, at a temperature of 223 °C, oxidation time of 20 min.

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## UTILIZATION OF TECHNOLOGICAL SLUDGE OF “KOLA MMC”

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One of the problematic types of copper and nickel production waste is process sludge. Sludge formation occurs during liming of wastewater from the “Severonickel” Plant of Kola MMC. Liming process leads to the formation of insoluble nickel and copper compounds and their conversion into sludge. According to the results of the analysis, it is determined that the sludge consists mainly of calcium carbonate. Nickel concentration in the sludge depends on the depth of occurrence in the settling tank and can reach 22 %<sup>1</sup>.

The easiest way to return nickel to production is to send them for pyrometallurgical processing. However due to the closure of smelting facilities at “Pechenganickel”, this operation is currently only possible at the Polar Division of MMC “Norilsky Nickel”. To provide transportation of sludge to Norilsk, briquetting studies were carried out at the ICT KSC RAS. Current sludge from Kola MMC containing in wt. %: Ni-6.42, Cu-1.2, Co-0.21, Ca-22.7, SiO<sub>2</sub>-12.5. It is established that for obtaining conditioned briquettes the optimum moisture content of technological sludge should be 10-15 wt.%. Under such conditions, the strength of briquettes in 4 hours after pressing is 3.70-4.24 MPa. It is shown that to increase the strength of briquettes it is recommended to add lime or cement to the composition, and after manufacturing they should be kept at the temperature of 20±2 °C or dried to the residual humidity of 3-4 wt.%, which will increase the compressive strength up to 8.24-9.85 MPa.

An alternative method of sludge utilization is their hydrometallurgical processing. In response to sulfuric acid leaching from the sludge, solutions containing 16 g/L Ni were obtained, followed by technical nickel carbonate suitable for use in the main production of Kola MMC.

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# SORPTION OF Pb(II) BY BIOGENIC ALUMOSILICATE UNDER DYNAMIC CONDITIONS

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Previous research has demonstrated that aluminosilicates produced through hydrolytic precipitation from rice straw are effective materials for sorbing lead(II) from aqueous solutions under static conditions. The objective of this study was to investigate the absorption capacity of sodium aluminosilicate samples under dynamic conditions.

To achieve this, a model solution was passed through a fixed sorbent layer. The study varied the height of the sorption layer between 0.8–4.2 cm and used a flow rate of 1.5 ml/min. The point at which the extraction efficiency of Pb(II) dropped below 95% was considered the slippage of lead ions. The results are presented in the table.

**Table 1.** Dynamic parameters of Pb(II) sorption by sodium aluminosilicate

Parameters	Height of loading layer in the column, cm		
	0,8	1,6	4,2
Dynamic exchange capacity, mg/g	90,3	105,3	99,7
Total dynamic exchange capacity, mg/g	388,9	170,1	136,1
Time to slip, min	50	130	330
Height of working sorbent layer, cm	1,1	1,7	2,2
Sorbent capacity utilisation rate, %	63,8	60,0	9,4

Based on the presented data in the table, it can be observed that increasing the height of the sorption layer results in a decrease in the exchange capacity calculated per mass of the sorbent. Additionally, it increases the time to the appearance of slippage concentration of lead (II) ions, and consequently, the time of the protective effect of the sorption column. The optimal height of the column, taking into account the efficiency of sorbent capacity utilization at a flow rate of 1.5 ml/min, is between 1.7–2.2 cm. At lower heights, lead ions slip before the upper layer of the sorbent becomes saturated.

Therefore, studying the sorption of lead(II) ions in the dynamic regime allowed us to determine the effect of the sorbent layer height on the dynamic and total dynamic exchange capacity of biogenic sodium aluminosilicate. The minimum effective height of the sorbent layer is 1.7 cm.

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# CRYSTALLIZABILITY EVALUATION OF SLAGS TO SUBSTANTIATE THE EFFECTIVENESS OF JOINT PYROMETALLURGICAL PROCESSING OF SILICATE NICKEL AND COPPER PYRITE ORES

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In order to substantiate the possibility of obtaining glass-ceramics from glasses based on slags from joint smelting of silicate nickel and copper pyrite ores the crystallization ability of model samples (particle size  $<0.1$  mm) that are close in composition and structure to real prototypes was evaluated. Using the methods of differential scanning calorimetry (5–20 °C/min heating rate) and X-ray powder diffraction, it was established that in an inert atmosphere, crystallization is accompanied by the formation of products, the crystalline part (46.6–71.6 mass%) of which is represented by associations of pyroxenes and anorthite. The primary crystallizing phase is pyroxene. The transition from iron-free to iron-containing sample leads to a change in the composition of pyroxene from enstatite to pigeonite, a shift in the range of formation of these associations from 826–1018 to 728–874 °C, and additional (966–1068 °C) formation of silica. Kinetic analysis (Ozawa–Flynn–Wall and multivariate non-linear regression methods) showed sequential bulk nucleation of pyroxenes and anorthite with the formation of two- and one-dimensional nuclei by a chain mechanism, passing into diffusion-controlled two- and three-dimensional crystal growth. The activation energy of enstatite nucleation (670.7 kJ/mol) is significantly higher than for pigeonite (417.9 kJ/mol), for crystal growth (444 and 533.9 kJ/mol respectively) the reverse relationship is noted. Pyroxenes promote the heterogeneous nucleation of anorthite. The activation threshold for the release of the latter in iron-free sample (220 kJ/mol) is three times higher than in iron-containing one (76 kJ/mol). The formation of two- and one-dimensional silica nuclei in the bulk of glass is synchronized with their two-dimensional growth under conditions of diffusion deceleration. The results obtained can be used in the development of technologies for producing glass ceramics from various types of ores and technogenic raw materials.

*The work was carried out according to the State assignment for IMET UB RAS (State registration number of the topic: 122020100404-2).*

# REACTIVITY OF PHENOXYACETIC ACID ESTERS

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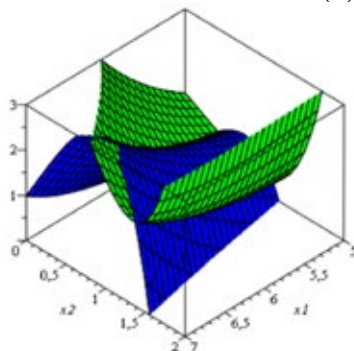
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Thanks to the wide range of practical properties, new products of organic synthesis do not lose their relevance<sup>1-3</sup>. Currently, the arsenal of use of drugs synthesized on the basis of aryloxyacetic acids is very wide. The presence of phenoxyacetate fragments determines phytohormonal and herbicidal properties. The dependence of the antimicrobial activity of alkylthioethylene glycol ethers of phenoxyacetic acid on the calculated energy values of the boundary molecular orbitals was revealed. Equations are obtained that describe the influence of the values of the boundary orbitals on the action of the substances considered.

$$\text{AMA} = 2.4423 \cdot 10^{-8} xI^9 - 1.0758 x2^4 + 0.069864 xI^2 x2 \quad (1)$$

$$\text{AMA} = 0.00038994 xI^5 + 0.39208 xI^5 - 0.012798 xI^3 x2 \quad (2)$$



**Figure 1.** Graph of the dependence of bactericidal (1) ( $R^2=0.93$ ) and fungicidal (2) ( $R^2=0.98$ ) properties on the energies of the boundary orbitals

The equations were used to predict the antimicrobial properties of S-containing ethylene glycol esters of phenoxyacetic acid.

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# HYDROMETALLURGICAL EXTRACTION OF INDIUM AND TIN FROM END-OF-LIFE DISPLAYS

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Indium-tin oxide (ITO), which is composed of 90%  $\text{In}_2\text{O}_3$  and 10%  $\text{SnO}_2$ , possesses unique properties such as electrical conductivity, optical transparency, and chemical stability. Due to these properties, ITO has found wide application in electronic devices such as screens, monitors, and touch panels. Indium is a rare element that is widely dispersed and has no deposits of its own. The indium content in glass substrates of displays is comparable to that in zinc concentrates obtained from sulphide ores. Therefore, end-of-life monitors are a promising secondary source of indium.

This work investigates the physicochemical features of ITO dissolution from the surface of glass substrates of end-of-life displays in sulfuric acid solutions. Leaching was carried out in a thermostated reactor at a temperature range of 298-353 K, with a sulfuric acid concentration of 0.05-0.5 M and a liquid-to-solid ratio of  $L:T = 10:1 \text{ cm}^3/\text{g}$ .

The dissolution rate of ITO was significantly affected by the concentration of  $\text{H}^+$  ions. During 60 minutes of leaching at low concentrations of sulfuric acid (0.05-0.1 M), the recovery of indium and tin reached 42-75% and 5-15%, respectively. Increasing the acid concentration to 0.2-0.5 M resulted in almost complete recovery of indium (98 %) and increased tin recovery to 25-53% in 60 minutes of leaching.

Raising the leaching temperature from 298 K to 353 K resulted in a significant increase in indium recovery, from 13.6% to 96.5%, within 60 minutes. The maximum tin recovery was achieved at 333 K, reaching 15%. However, increasing the temperature beyond 353 K led to a rapid decline in tin ion concentration in solution after only 10 minutes of leaching, likely due to tin hydrolysis.

Thus, this work demonstrates a high efficiency of sulfuric acid leaching for indium tin oxide. 98% of the indium is recovered in 60 minutes at 333 K.

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# MODELING OF CATHODE CATALYST ACTIVE SURFACE AREA DEGRADATION TO INCREASE FUEL CELL OPERATION RESOURCE

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A mathematical model of a platinum catalyst electrochemical active surface area degradation in a hydrogen-air (oxygen) fuel cell with a proton-exchange polymer electrolyte is presented.

The model considers the main mechanisms of platinum catalyst degradation<sup>1</sup>: platinum nanoparticles electrochemical dissolution, particles growth due to the precipitation and the migration, Ostwald ripening, platinum nanoparticles coagulation on the carbon support surface, platinum ions diffusion in the ionomer and their transfer into the membrane. The mathematical model is an integral-differential equations system, solved by the difference method.

$$\frac{\partial \varphi}{\partial t} + \frac{\partial \varphi \eta_1}{\partial l} + \frac{\partial \varphi \eta_2}{\partial l} = D_{Pt} \frac{\partial^2 \varphi}{\partial x^2} + \int_0^L K(\mu, \sqrt[3]{l^3 - \mu^3}) \varphi(\mu) \varphi(\sqrt[3]{l^3 - \mu^3}) d\mu - \varphi(l) \int_0^L K(\mu, l) \varphi(\mu) d\mu, \quad (1)$$

$$\frac{\partial c_{Pt^{2+}}}{\partial t} + v \frac{\partial c_{Pt^{2+}}}{\partial x} = D_{Pt^{2+}} \frac{\partial^2 c_{Pt^{2+}}}{\partial x^2} - 4\pi \frac{\rho_{Pt}}{M_{Pt}} \int_0^L \varphi(\eta_1 + \eta_2) l^2 dl. \quad (2)$$

The calculated data of the catalyst electrochemical active surface area correspond to the experimental ones.

The influence of individual mechanisms on degradation as a whole has been studied. It has been revealed that the contribution of the coalescence mechanism to the overall process of catalyst degradation is predominant. The operation resource of the fuel cell has been predicted, and ways to increase it have been proposed.

The work is performed in the framework of the development program «Priority-2030» of D. I. Mendeleev Russian University of Chemical Technology.

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# SYNTHESIS OF MENTHOL FROM CITRUS WASTE

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Total production of citrus fruits can be estimated as more than 100 million t/year, that results in the annual accumulation of about 10 million t of waste<sup>1</sup>. There are different ways to involve citrus pulp, cake, and seeds in processing, but most of the waste with a high concentration of essential oils remains unclaimed. Currently, waste recycling for economic sustainability is of great interest.

The aim of this work is to develop an efficient continuous method for converting a citrus waste component (cital) into a valuable commercial product (menthol) in the presence of nickel containing catalyst.

Synthesis of menthol from citral involves a set of sequential conversions: citral → citronellal → isopulegol → menthol. Presence of nanodispersed metal particles is necessary for hydrogenation at the initial and final stages, while acid sites are required for the cyclization of citronellal into isopulegol at the intermediate stage. In this work a bifunctional Ni catalyst was developed, supported on H-Beta-38 zeolite, with the addition of various binders for the preparation of mechanically strong extrudates and carrying out the reaction in a continuous mode. Ni catalysts were synthesized using clay material - bentonite (a) and zeolite (b), as well as their mixtures (bentonite – 30 %) (c) as support and studied in the hydrogenation of citral at various temperatures, pH<sub>2</sub> and solvents. It was shown that cyclization of Ni/bentonite does not proceed; whereas the conversion of citral occurs through hydrogenation into 3,7-dimethyloctanol-1. According to IR spectroscopy data with pyridine, bentonite has a lower concentration of acid sites than beta-zeolite (19 and 31 μmol/g, respectively) that affect the route of citral transformation. At the same time, addition of bentonite up to 30 wt. %, which has a higher mesoporosity, allows creating a well-developed structure with a higher content of mesopores, which ensures a more selective conversion of citral into menthol<sup>2</sup>.

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# TECHNOLOGY OF OBJECTS LIQUIDATION ACCUMULATED ENVIRONMENTAL DAMAGE FOR COPPER AND COBALT MINES

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Currently in Russia has developed paradoxical situation when with an acute shortage of mineral resources, especially for non-ferrous and rare metals, huge volumes of unextinguished reserves of copper-zinc ores related to mines transferred to wet conservation, are abandoned. Thus, the authors propose the technology which makes it possible to remove the contradiction between the need to eliminate objects of accumulated environmental damage (OED) for copper-zinc mines under wet conservation and the presence of unextinguished reserves. In this case are used the actual processes of in-situ leaching and subsequent cavitation treatment of spewing acid mine water (AMW).

The proposed technology is based on the controlled transformation of the phase composition of CRW at the post-operational stage of the life cycle of the mine, allowing to obtain treated water and sludge, which is a marketable product, with minimal unit costs.

The proposed technological scheme of copper and cobalt ore deposits mining at the post-exploitation stage of the life cycle includes in-situ leaching of unexploited ore reserves, as well as cavitation treatment and neutralization of CRW spilling from mothballed mines with extraction of sludge to be sent for further processing<sup>1</sup>.

There is «auto-acidification» of spouting solutions due to oxidation of pyrite which eliminates the consumption of sulfuric acid. The formed iron sulfate in the presence of sulfuric acid is easily oxidized by air into iron oxide sulfate.

The precipitate obtained after cavitation is nanosized metal oxides, has a porous hydrogel structure and sorbs heavy metal ions on its surface<sup>2</sup>. In the process of cavitation with iron (II) solution with simultaneous oxidation of the reaction mixture by air oxygen, mixed oxides of heavy metal ions and iron - ferrites with the general formula  $Me_nFe_{3-n}O_4$  are formed on the surface of heavy metal hydroxides.

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# FROM THE LAB BENCH TO SCALING-UP PRODUCING CELLULOSE HYDROGELS. PROS AND CONS

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The purpose of technology transfer is to reproduce the laboratory process under semi- or industrial conditions defined during the development of products in laboratory conditions.

Hydrogels derived from biopolymers are currently viewed as three-dimensional (3D) materials with the ability to absorb large amounts of water or solvents, which maintain their dimensional stability. The cellulose biopolymer defines the basic structure of many plants. Cellulose-based hydrogels have gained a great popularity in biomedical area, pharmaceutical industry and agriculture. Cellulose hydrogels are generally prepared with 4 main steps, each consisting of sub-steps. Initially, native cellulose is dissolved in the solvents and then gelation of the dissolved system can take place either by physical linking (physical gelation) or by chemical linking (chemical gelation).

The only company in the world producing cellulose hydrogels named

GrowDex® hydrogels is UPM Biomedical (Finland). In our case, to use lab-to-process experience in the scaling it was necessary to take into account the differences in the behaviour of the cellulose samples during the dissolution and gelation processes. The powder samples prepared from sulphite hardwood and softwood pulps, short-length flax fibres and waste paper.

The first attempt to scale up the lab producing the hydrogels was made taking to the account the main stages of the process. However, the flowchart had some weak points. To overcome them, some additional devices to be utilised. Particularly important are the reconstruction of the mixer, which has to be adapted for each pulp sample, the addition of a filter press to the filtration chamber and a pumping device with different capacities. These improvements are economically costly and can be implemented with the support of design, thorough calculation, financial, and technical assistance. This suggests that scaling up the process of producing cellulose hydrogels has serious «Pros» and equally important «Cons». Which of these outweighs, is a matter of further research and time.

# GROWING CONIFEROUS PLANTS IN VERTICAL GREENHOUSES

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To carry out work on compensatory reforestation and reclamation of technogenically disturbed territories, a large amount of planting material for coniferous plants with a closed root system (CRS) is needed. Vertical greenhouses are one of the promising technologies for growing seedlings with CRS.

Comparative studies were conducted at Kemerovo State University on the cultivation of seedlings from Scots pine in classical and vertical greenhouses. An analysis of the results showed that in hydroponic conditions, seedlings are characterized by more intensive growth and a more developed root system (Table 1). To optimize energy costs, climate loads and reduce initial costs during implementation, it is preferable to use light intensity indicators at the level of 180 mmol/sec/m<sup>2</sup> (Table 2).

**Table 1.** Biometric indicators of scots pine seedlings

	Growing period, days from stratification (from germination)	Seedling height, average value, cm	Error of the average value, ± cm
Classical greenhouses	60 (46)	2,3	0,1
Vertical greenhouses	60 (46)	2,7	0,1

**Table 2.** The effect of lighting intensity on the height of seedlings of scots pine

Light, mmol/sec/ m <sup>2</sup>	Growing period, days from stratification (from germination)	Seedling height, average value, cm	Error of the average value, ± cm
250	53(41)	2,3	0,1
180	53(41)	2,0	0,1

The use of modern technologies will increase the yield of standard seedlings from CRS per unit area, due to the intensification of planting material cultivation in fully controlled conditions.

## VERTICAL FARMS

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Vertical farms are a modern automated intelligent system for growing plants using the hydroponics method. The main advantages:

- the possibility of year-round cultivation of plants, regardless of natural conditions;
- the use of artificial intelligence and machine vision in order to create optimal schemes for mineral nutrition, lighting, and maintaining the required temperature and humidity conditions;
- reduction of water consumption by 95 % relative to traditional agricultural production;
- a closed cycle of air exchange in the growing rooms, which allows to eliminate the occurrence of pests and phytopathologies, reducing the use of pesticides, herbicides and insecticides;
- production capacity (the possibility of placement within cities).



**Figure 1.** Vertical farms

Currently, Kemerovo State University is developing a technology for growing coniferous plants with a closed root system in vertical greenhouses for compensatory reforestation and reclamation of technogenically disturbed territories.



# USING THE SOLUBILITY DIAGRAM $\text{KCl-MgCl}_2\text{-CaCl}_2\text{-H}_2\text{O}$ IN TECHNOLOGY FOR EXTRACTION OF CHEMICAL COMPOUNDS

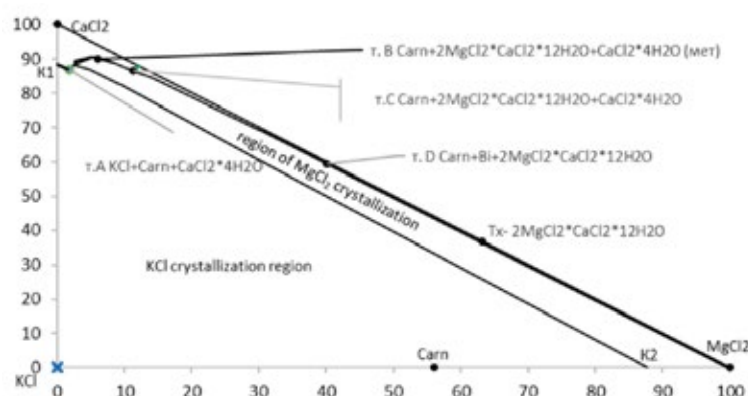
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Recently, the problem of processing hydromineral raw materials has acquired great importance. To extract compounds such as  $\text{KCl}$ ,  $\text{MgCl}_2$ ,  $\text{CaCl}_2$  from underground formation waters, halurgical methods based on evaporation of solutions and crystallization of salts can be used. The theoretical justification and prediction of the parameters of the crystallization stage is based on the consideration of solubility diagrams, which make it possible to determine the compositions of equilibrium phases.<sup>1</sup>

Figure 1 shows an anhydrous projection of the solubility diagram of the  $\text{KCl-MgCl}_2\text{-CaCl}_2\text{-H}_2\text{O}$  system, constructed from reference data.<sup>2</sup>



**Figure 1.**  $\text{KCl-MgCl}_2\text{-CaCl}_2\text{-H}_2\text{O}$  solubility diagram.

Using the general principles of reading the presented solubility diagram, the work describes the processes occurring during the processing of hydromineral raw materials of a given chemical composition and selects optimal conditions for the extraction of chemical products of the required quality.

# THE USE OF ULTRASOUND IN HALITE WASTE TREATMENT TECHNOLOGY

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In the process of processing potassium ores, a fairly large amount of so-called halite waste is formed, which is a very rich concentrate of sodium chloride with a main substance content of at least 93%. The possibility of further processing of halite concentrate to obtain target products is complicated by the content of calcium sulfate impurities, which have a negative impact on both the process equipment and the quality of the resulting inorganic products and compounds. Analysis of halite waste, presented in the form of samples of quarry salt and halite dump, showed a number of specific differences in the localization and modification of calcium sulfate caused by waste storage conditions<sup>1</sup>. Thus, long-term storage of quarry salt in open areas promotes the process of hydration of calcium sulfate and the formation of its dihydrate modification, and constant exposure to ambient temperature and precipitation leads to occlusive capture of poorly soluble calcium sulfate particles by aggregated halite crystals, which makes their removal difficult during hydromechanical cleaning and reagent processing. Conducted studies on the influence of physical impact on the treated aqueous suspension of halite in the form of ultrasonic radiation have shown the possibility of getting rid of a large proportion of calcium sulfate impurities without additional reagent treatment of solutions. The optimal technological parameters for the duration and intensity of ultrasonic and hydromechanical effects on the treated environment have been found. The high efficiency of using ultrasonic treatment as a tool for cleaning halite dumps from calcium sulfate impurities has been proven<sup>2</sup>. The technology of sodium chloride brines and technical salt with a residual content of calcium sulfate impurities of less than 0,5% wt. was proposed.

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# INFLUENCE OF TEMPERATURE REGIME ON DESORPTION OF CORROSIVE GASES FROM WATER IN PACKED APPARATUSES

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The report describes the processes of desorption of dissolved corrosive gases ( $\text{CO}_2$  and  $\text{O}_2$ ) from water by air in packed apparatuses. For example, desorption of  $\text{CO}_2$  from water occurs using atmospheric air, which, depending on the time of year and operating conditions of desorbers (decarbonizers), can have different temperatures and moisture content. Typically, in traditional calculations of decarbonizers, the calculation of mass transfer efficiency is carried out based on the initial temperatures of water and air and without taking into account humidity.

Water is supplied for decarbonization with an initial temperature of 40-70°C. The  $\text{CO}_2$  content in water can be in the range of 100-400 mg/kg, and the required concentration after decarbonization is less than 4 mg/kg.

To numerically model the  $\text{CO}_2$  concentration profile in water and the temperatures of water and air along the packed bed height in a counterflow decarbonizer, the present work uses a system of partial differential equations of mass and heat transfer, in which the interactions between phases (air and water film on a random packing) are taken into account in the form of local interphase sources of mass and heat<sup>1</sup>. Under given conditions at the inlet of water and air, the numerical solution determines the  $\text{CO}_2$  concentration in water and air at the outlet, as well as the temperatures of water and air. Taking into account the obtained temperature profiles, during the solution process the thermophysical properties of water and air are updated (mainly density, viscosity, heat capacity and coefficients of thermal conductivity and molecular diffusion).

As a result of mathematical modeling, it was found that not taking into account the temperature profiles of water and air gives an error in determining the height of the packing up to 10-12%. For example, at an initial water temperature of 60 °C and air 20 °C, in the process of heat and mass transfer in a layer of random packing, we reduce the water temperature to 50 °C, and increase the air temperature to 58 °C with a water irrigation density of 70 m<sup>3</sup>/(m<sup>2</sup>h) and an air speed of 0.75 m/s.

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# HEAT TRANSFER EFFICIENCY IN COUNTERFLOW APPARATUSES WITH INTENSIFIERS OF THE HEATING PROCESS OF HIGH VISCOSITY MEDIA

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The report describes plate heat exchangers, as well as the «pipe-in-pipe» type heat exchangers, where high viscosity media (fuel oil, lubrication oils, etc.) are heated through a separating wall with heating water vapor or hot water. Moreover, in the channel where the viscous medium moves, there are surface (protrusions, knurling, etc.) or volumetric (small irregular elements) heat transfer intensifiers. Surface intensifiers provide a transition from laminar to turbulent motion at Reynolds numbers  $Re > 500-1000$ , and volumetric intensifiers at  $Re > 50$ . Due to the turbulization of the viscous medium, there is a significant increase in heat transfer coefficients (by 5–20 times) and, accordingly, heat transmission, which allows significant reduction of weight and size of heat exchangers.

To calculate the heat transfer efficiency in apparatuses with intensifiers, a mathematical model for calculating the thermal efficiency is developed. The mathematical model is based on the hydrodynamic structure of the flow, where the heating medium is conditionally divided into a number of consecutive cells of complete mixing. The number of cells depends on the value of the modified Peclet number (Bodenstein number), which characterizes the back mixing of the coolant. As a result of solving the equations of the cell model, an expression is obtained in an explicit form for calculating the thermal efficiency of the process in channels with intensifiers, where the main parameters are the thermal number of transfer units and the number of complete mixing cells<sup>1</sup>. Graphic dependences of the thermal efficiency of heating industrial oil in a heat exchanger with volumetric intensifiers are obtained. The influence of back mixing of heated oil on the efficiency of heat transfer is established. A comparison with the laminar flow regime is shown, i.e. without intensifiers. The developed mathematical model can be used in the design or modernization of heat exchangers.

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# HYBRID BARO-ELECTROMEMBRANE TECHNOLOGY FOR ALTERNATIVE ENERGY

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Currently, there is great interest in alternative energy generation technologies. The hybrid osmosis system with back pressure (PRO) is a new technology that uses the potential between the difference in salinity of water to generate energy [1]. In reverse osmosis (RO) and PRO [2-3] enters a membrane module with a membrane for removing salt, and then exits through an energy recovery device

The purpose of this work was to obtain electrical energy using hybrid technology based on marine reverse osmosis and reverse electrodialysis (RED).

A membrane unit with ion exchange membranes and an industrial marine reverse osmosis plant (permeate capacity 1-1.5 m<sup>3</sup>/h) were selected for the reverse electrodialysis process. An imitation of seawater with a concentration of 15 g/l NaCl was selected as the initial solution for desalination by marine reverse osmosis. During the study of the reverse osmosis plant, permeate with a sodium chloride salt content of 40 mg/l and NaCl concentrate with a concentration of 20 g/l were obtained. Subsequently, the concentrated solution is used to extract electricity by mixing two solutions of different concentrations in RED.

The hybrid baro-electromembrane technological scheme allows the production of purified water at a low price, while acting as an alternative source of electricity.

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# OPTIMIZATION OF AUTOMATIC EMISSION CONTROL AT CHEMICAL ENTERPRISES

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The legislation requirements on equipping stationary emission sources of the 1st category objects with continuous emission monitoring systems (CEMS), as well as difficulties associated with installation and maintenance of these systems, have led enterprises to seek the most optimal solutions:

- unification of CEMS used within the same enterprise/holding;
- use of the most universal and modern analytical methods;
- optimization of the number of sources and parameters that require automatic control.

One of the promising directions for the development of automatic emission control is the application of mathematical modeling of process indicators to determine parameters of pollutant emissions (commonly referred to as predictive emission monitoring systems – PEMS)<sup>1</sup>. When selecting facilities for implementing PEMS, it is essential to consider the following requirements: a high level of automated process control equipment, and the availability of historical data on process parameters (data source for modeling); consideration of the technological specifics of the process (for the implementation of the PEMS, it is necessary to select a process with sustainable technological indicators, the quality of raw materials, materials and products); design features of the emission source (the technical ability to equip the emission source on which it is planned to implement the PEMS, with an instrumental CEMS – used to train the model in real time); the ability to organize the process of data collection and analysis in real time.

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# FLOTATION TREATMENT OF OILY EFFLUENTS IN AN INDUSTRIAL APPARATUS

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One of the most important tasks of ensuring the environmental safety of production cycles at oil refineries is the purification of industrial wastewater from oily compounds. Solving this problem simultaneously creates the possibility of reuse of purified water in technological processes. At the same time, the main feature of the purification process is the large volume of wastewater.

In such conditions, the most effective method of removing petroleum products from wastewater can be the flotation process, which in practice can be quite simply organized in large-sized apparatuses. However, when creating engineering methods for calculating industrial processes, the problem of large-scale transition inevitably arises, which does not allow directly transferring the results of laboratory and pilot studies to industrial-sized devices. Therefore, the results obtained during the operation of real flotation plants are of particular value. They make it possible to adjust the model representations of the process, taking into account the nature of the movement of working media in a large-diameter apparatus, which makes it possible to develop methods for calculating industrial devices, bypassing the stages of laboratory research.

In this paper, data from the long-term operation of the flotation plant at the Kirishi ORP were used to simulate the process of cleaning oily wastewater in a flotation device with a diameter of 14.6 m. It was shown that the mathematical model of the process can be reduced to a one-dimensional convective diffusion equation, in which the scale effect is taken into account using the effective mixing coefficient  $D_{ef}$ , which clearly depends on the transverse heterogeneity of the distribution of hydrodynamic quantities. A comparison of the calculated and actual values of the degree of wastewater purification confirmed the adequacy of the model representations to the real process, which gives grounds to use them in the development of engineering methods for calculating industrial technological processes and related equipment.

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# CERAMIC COMPOSITES BASED ON ZIRCON: PREPARATION AND PROPERTIES

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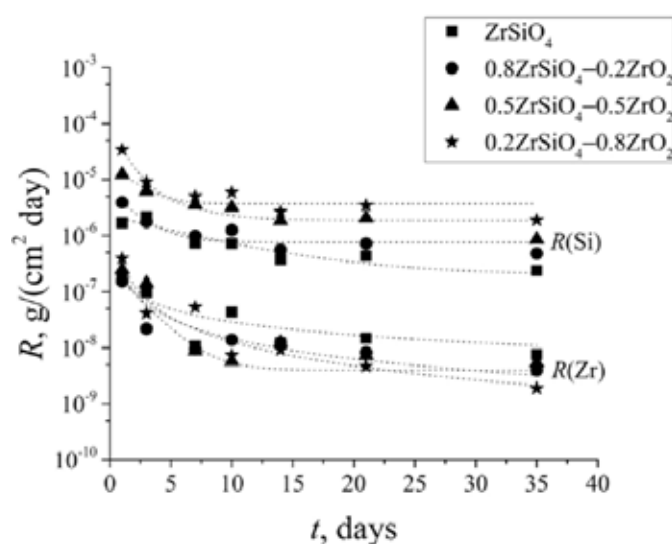
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The work is devoted to the development of physicochemical principles for fabrication of ceramic matrices from zircon-based composites with additives of zirconia and hafnia, and the study of their physicochemical properties.

As a result of the work, highly dispersed precursor powders were synthesized by the original methodology, and dense chemically resistant ceramic compositions  $(1-x)\text{ZrSiO}_4-x\text{ZrO}_2$  and  $(1-x)\text{ZrSiO}_4-x\text{HfO}_2$  were obtained by sintering them.

Ceramic samples exhibited low porosity and high chemical resistance in distilled water (Fig.)1.



**Figure 1.** The dependence of the leaching rate  $R$  of silicon and zirconium from ceramic matrices  $\text{ZrSiO}_4$ ,  $0.8\text{ZrSiO}_4-0.2\text{ZrO}_2$ ,  $0.5\text{ZrSiO}_4-0.5\text{ZrO}_2$  and  $0.2\text{ZrSiO}_4-0.8\text{ZrO}_2$  on contact time  $t$  in distilled water.

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# RED PHOSPHORUS BIODEGRADATION BY STRAIN *ASPERGILLUS NIGER* F-4815D

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Earlier studies have shown the ability of microorganisms, mainly the black aspergillus fungi *Aspergillus niger*, to oxidize to harmless phosphate ions a substance of the first hazard class white phosphorus. Red phosphorus is much less toxic, but more thermodynamically stable, and this makes it difficult to metabolize enzymatically. Nevertheless, more recent studies have shown that red phosphorus serves as a source of a nutrient for the same fungi that neutralize white phosphorus. The descriptions of the experiments, however, were mostly qualitative in nature. Quantification of biodegradation is essential, and the present work shows the first quantitative data on the biodegradation of red phosphorus by *A. niger* F-4815D. These data indicate a significant increase in the rate of red phosphorus oxidation, expressed through the accumulation of phosphate ions, the final product of oxidation, under the influence of the metabolism of *Aspergillus* growing in culture medium. Compared with the control, sterile medium containing red phosphorus, the rate increases by a factor of 1.25. The difference is insignificant, but reliable and appearing in each repetition of the experiment. We can assume that this difference would have been even higher. But the red phosphorus under study turned out to be originally contaminated with phosphoric acid. Probably it oxidized during storage. Because *Aspergillus* originally grew in phosphate-enriched medium, the activity of the red phosphorus biodegradation process was reduced compared to what was theoretically possible. Nevertheless, the presented work is the first documented study confirming red phosphorus biodegradation.

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## DISPOSAL AND RECYCLING OF KHOVU-AKSY DUMPS

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Technological wastes of Tuvakobalt Combine, namely sludge dumps of Khovu-Aksy were accumulated during 20 years of its operation. They differ significantly from the dumps of other non-ferrous metallurgy enterprises both in chemical and mineral composition and in their higher arsenic content (up to 6 % wt. %). During the storage period the contents of the dumps have undergone significant changes and by their composition are carbonate-silicate with increased content of calcium and iron. Secondary minerals, products of hypergenesis are represented mainly by arsenates of the vivianite group. The dumps represent a serious environmental hazard for the region.

As a result of a large volume of research a complex technology of neutralization and processing of waste sludge was developed, including low-temperature roasting of charge (mixture of sludge with soda ash), aqueous leaching of cinder with arsenic transfer into solution and acid precipitation of arsenic from solution in the form of trisulfide (auripigment). In this case, the degree of arsenic extraction into solution was 92 %, and the degree of arsenic precipitation from solution was 99.5 %. The obtained arsenic sulfide precipitate appears to be a compact low-soluble product, which can be used in antifouling coatings of marine hulls and structures, as well as in woodworking and agriculture<sup>1</sup>.

The cake of aqueous dearsenization of the cinder was used in subsequent studies as a possible recycled material in the initial charge for the production of ceramic products. The results of the conducted experiments showed the possibility of using cake as a melting agent, an important component of the charge for the production of ceramic materials.

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# MODIFICATION OF RIGID PVC WASTE WITH SAN COPOLYMER

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Rigid PVC waste is generated at the site of renovation of residential and industrial buildings (siding). It is not difficult to select long products and piece goods (containers) at the site where municipal solid waste is processed. A well-known method for recycling them into products is extrusion.

An attempt was made to process them by injection molding.

The research objects were obtained according to the following scheme: crushed siding (10 kg) + dibutyl phthalate (1.5 kg) = PVCR → + SAN (granules) → mixing → granulation → melt flow index (MFI 190 °C, 98 N, 6 min) → casting under pressure of standard samples (TPA DH 3224) → tensile yield strength, strength and elongation at break ( $\sigma_1$ ,  $\sigma_2$  and  $\varepsilon$ , 20 mm/min), conditional bending strength ( $\sigma_3$ , 10 mm/min up to a bending value of 6 mm), heat resistance according to Vicat (TV, 50 °C/hour) and other indicators (table).

**Table 1.** Properties of PVCR + SAN mixtures

Index	PVCR	SAN content, %					SAN
		10	15	20	25	30	
MFI, g/10 min	0,3	0,5	0,9	1,5	2,3	4,5	10,2
$\sigma_1$ , MPa	40,2	42,9	44,4	47,0	46,5	48,1	нет
$\sigma_2$ , MPa	18,3	32,1	29,4	28,9	28,5	30,1	65
$\varepsilon_{pp}$ , %	29	26	24	28	21	30	3
$\sigma_3$ , MPa	45	45	47	44	45	46	70
$T_v$ , °C	55	60	63	66	68	69	100
NB*	33	11	10	6	4	3	1
*NB – number of bends of standard samples before breaking (360°)							

Of interest is a composition containing 15% SAN. Granulation of the composition is possible by cutting granules on an air-cooled extruder head, but the strand method is better. The optimum temperature for injection molding is 170 °C.

*The work was carried out with financial support from the Ministry of Science and Education of the Russian Federation within the framework of the scientific project «Laboratory of Smart Materials and Technologies», project N FSSM-2024-0005.*

# ABOUT VELOCITY AND SEQUENCE OF BIO-OXIDATION OF THE SPECIFIC ORGANIC IMPURITIES OF COKE & BY-PRODUCT PLANT EFFLUENTS

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As it was found the process of bio-destruction of main impurities of coke plant (CP) effluents (E) is going on in a distinct sequence, i.e. phenols – rhodanides – ammonia. The indicated above impurities differ in duration of oxidation limited by the development and velocity of growth of bacteria culture responsible for the destruction of the same<sup>1</sup>. Similar information about the velocity and sequence of bio-oxidation of numerous organic impurities of CPE is not revealed which is required for solving problems of decreasing of secondary contamination of E.

The aim of work is the recovery of accumulative cultures in static conditions and the establishment of sequence of bio-oxidation of the specific contaminants (impurities) of CPE. The results are presented in Table 1.

**Table 1.** The results of investigation of velocity (V) of bio-oxidation of organic contaminants in the process of biological treatment of CPE

Contaminant of E	Content, mg/l	V, mg/day	Content, mg/l	V, mg/day
1. Oxybenzol	607,3	15,96	662,8	7,22
2. Resorcin	330,8	6,26	300,1	3,76
3. Toluene	210,9	3,65	238,5	0,70
4. Benzene	251,5	2,22	230,9	2,30
5. Pyridine	80,1	1,96	111,6	0,93
6. Quinoline	83,3	1,48	72,3	0,56
7. Ethylbenzol	26,5	0,51	34,3	0,18
8. Hydrochinon	3,2	0,17	12,7	0,10
9. Naphthalene	10,0	0,12	8,9	0,18
10. o-xylene	118,2	-0,04	162,1	-0,22
11. m-,p-xylene	845,5	-2,58	1057,6	-2,89

Thus, for the first time obtained are data concerning sequence of bacterial oxidation of the specific organic impurities of CPE in relation to the nature of the same.

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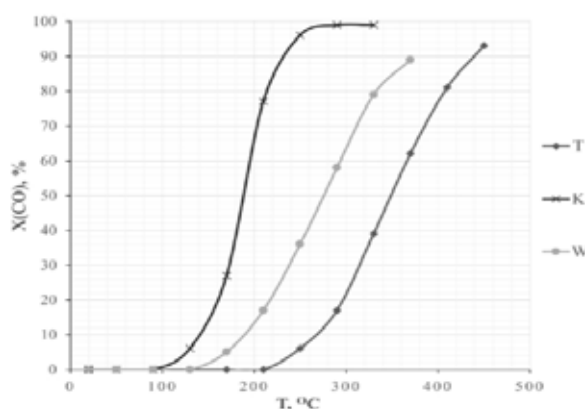
# ACTIVITY OF BLOCK CATALYSTS ON CERAMIC AND METAL SUPPORTS IN CO OXIDATION

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Carbon monoxide CO is released in large quantities by chemical and thermal power industries and transport. In order to comply with environmental standards, additional oxidation of CO to CO<sub>2</sub> is required.

Cu, Co, Ce catalysts on metal (honeycomb and cartridge) and ceramic (honeycomb) carriers with low flow resistance compared to granular ones<sup>1</sup> were chosen as oxidation catalysts. The metal block of the honeycomb structure (W) is made of steel foil X23YU5, the cartridge block (T) is made of steel shavings 12X18N10, and the ceramic carrier (K) is made of cordierite. The activity of the products was determined on a flow stand ( $C_0 = 0,44\%$ ,  $\tau = 0,24$  c,  $\varphi = 70\%$ ),  $C_{CO}$  was monitored by reaction gas chromatography on a GC-TsVET-100.



**Figure 1.** Dependence of the degree of CO conversion on temperature

**Table 1.** Main comparative characteristics of catalysts

Catalyst	The weight of the cat. coverage (g) in 1 cm <sup>3</sup> of the unit, g/cm <sup>3</sup>	Productivity, $\frac{g(CO)}{h \cdot g(cat.)}$	Temperature at X(CO) – 90%, °C
T	0,038	333 (330 oC)	440
K	0,041	636 (330 oC)	370
W	0,136	240 (330 oC)	230

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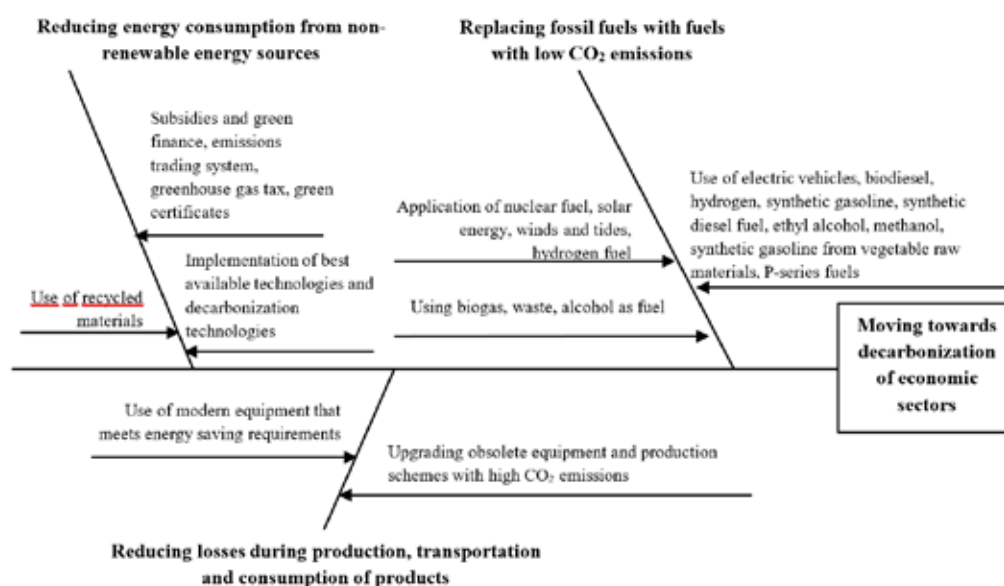
# TOOLKIT FOR REGULATING GREEN DEVELOPMENT IN CONDITIONS OF CIRCULAR ECONOMY

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Within the framework of the Industry 4.0 concept, the transition from a linear model of the economy to a circular one, aimed at energy saving, regenerative environmentally friendly production, circulation and consumption, is becoming increasingly relevant. Within the framework of the circular economy (CE), the priority has been given to the direction of low-carbon transformation, implemented through the management of carbon emissions, the introduction of an emissions trading system, subsidies and financing of «green» projects. The study analyzes the main directions of decarbonization of economic sectors and proposes tools that combine administrative and economic measures to create a roadmap for their development (figure).



**Figure 1.** Toolkit for decarbonization of economic sectors based on CE principles

# INNOVATIVE ENERGY- AND RESOURCE- SAVING «GREEN TECHNOLOGIES» («WASTE TO INCOME»)

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Green technologies are innovations based on the principles of sustainable development and reuse of recycled material resources. They cover all spheres of the economy: energy, industry, transport, construction, agriculture. They are introduced into the entire chain of company activities, including, in addition to production, consumption, management and methods of organizing production. Green technologies can significantly reduce the consumption of natural resources and increase the use of by-products.

At this stage, we have proposed ways and techniques to reduce the formation and disposal of solid municipal and industrial waste (MSW) into consumer goods to reduce the volume of natural resources consumed. Scientifically based strategies have been developed to create highly effective technologies to reduce water pollution, restore land fertility, reduce the generation and disposal of waste to obtain useful products of national economic importance from MSW I and II hazard classes:

- \* Technological scheme for the extraction of iron and zinc oxides from iron and zinc containing galvanic sludge (GS) by acid-base dissolution-precipitation to obtain pigments - fillers and oil paints based on them (zinc white, red lead).

- \* A method for recycling nickel-containing HS to obtain  $\text{Ni}(\text{OH})_2$  hydroxide, used in the production of nickel oxide electrodes of Ni-Cd and Fe-Ni batteries. The electrodes were tested at PJSC «Plant of Autonomous Current Sources» (Saratov).

- \* Technology for extracting metallic nickel from nickel-containing galvanic waste by electrochemical method.

- \* A technology has been developed for the ferritization of iron-containing GS for the production and modification of nano-sized and nanostructured magnetic powders with high adsorption capacity for the production of magnetosorbents for cleaning water and soil from oil pollution.

- \* Methods have been proposed for purifying wastewater and natural waters and soils from various pollutants (oil pollutants, heavy metals, surfactants) using phytosorbents and composite sorbents developed on the basis of agricultural waste to reduce the negative impact of pollutants on the environment.

# MULTISCALE MODELING OF HEAT-MASS-EXCHANGE-CHEMICAL PROCESS FOR PROCESSING TECHNOGENIC WASTE ORE RAW MATERIALS AT MINING AND PROCESSING PLANTS

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The mining and processing industries produce technogenic waste with a complex and heterogeneous polymineral composition. To reuse this waste in beneficiation processes, a comprehensive assessment of processing is necessary<sup>1</sup>. This is because rock-forming minerals undergo physical and chemical transformations during heating, which alters the structure of the raw material and its thermophysical properties. Thermally activated processes are determined by kinetic laws, so the thermophysical properties of the ore material under investigation acquire a complex temperature-time and temperature-concentration dependence. Therefore, comprehensive theoretical and experimental research of the chemical, technological, and thermophysical properties of mining and processing waste is necessary<sup>2</sup>. The research findings can be applied to current strategies for developing energy-efficient directions in energy-intensive industries. Reusing technogenic mining waste in production processes reduces production costs and increases the energy resource efficiency of ore enrichment<sup>3</sup>.

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*The work was performed under the state assignment, project No. FSWF-2023-0012.*

# PROPERTIES OF MIXTURES OF RECYCLED ABS PLASTICS AND PVC PLASTIC COMPOUND

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Mixtures involving acrylonitrile butadiene styrene plastics (ABS plastics) and polyvinyl chloride plastics can be formed at the stage of crushing waste from their processing. Mixtures can be classified according to the two-stage «floating-settling» method, however, this requires additional production space and certain considerable labor costs.

It was interesting to evaluate the possibilities of processing such mixtures directly using model systems involving real secondary polymers: ABS-2020 and PVC-compound OM-40.

Standard samples were obtained by injection molding of pre-granulated mixtures of the specified materials.

The introduction of ABS-2020 into the composition of OM-40 in an amount of 25 % leads to a sharp increase in its melt flow index and a decrease in elongation at break, which is most likely due to the diffusion of the plasticizer into the ABS medium (table).

**Table 1.** Properties of mixtures of recycled ABS-2020 and PVC compound OM-40

Index	OM-40	ABS-2020 content, %			ABS-2020
		25	50	75	
Melt flow index (200 °C, 5 min, 49 H), g/10 min	2,4	22,4	9,4	2,5	2,6
Tensile yield strength, MPa	No	No	No	31,2	52,1
Tensile strength, MPa	13,5	13,8	17,5	23,0	40,9
Elongation at break, %	480	90	25	22	10
Charpy impact strength without notch, kJ/m <sup>2</sup>	> 90	> 90	> 90	> 90	> 90
Shoulder blade shrinkage N 2 (GOST 11262)	2,6	0,7	0,7	0,8	0,7

It is advisable to introduce secondary OM-40 into the secondary ABS-2020. The mechanical properties of the material containing 25 % OM-40 correspond to the level of impact-resistant polystyrene.

*The work was carried out with financial support from the Ministry of Science and Education of the Russian Federation within the framework of the scientific project «Laboratory of Smart Materials and Technologies», project N FSSM-2024-0005.*

# ECOLOGICAL MONITORING OF OPERATING AND RELATED MUNICIPAL SOLID WASTE LANDFILLS

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A system for environmental monitoring of emissions from existing and reclaimed municipal solid waste (MSW) landfills has been developed, which automatically generates models of chemical, technological and hydrodynamic processes occurring in the body of the landfill. The environmental monitoring system uses three ways to measure the state of the landfill: by installing autonomous monitoring stations for gas emissions directly on the territory of the landfill to control point zones; using aerial drones (UAVs) to measure methane emissions and the temperature of the entire body surface of the landfill; using manual measurements by operators to verify the accuracy of autonomous and unmanned inspection systems. This is necessary for further forecasting the environmental hazard indicators of the controlled site<sup>1</sup>.

All data that comes to the server from autonomous monitoring stations is displayed on a special website on the Internet.

The developed system for monitoring gas emissions from MSW landfills allows for remote continuous operational monitoring in real time at the landfill due to installed temperature and gas sensors<sup>2</sup>. In addition, the system can monitor the condition of large areas of landfills based on methane emissions, as well as provide landfill operators with gas distribution maps and information about locations of possible gas leaks.

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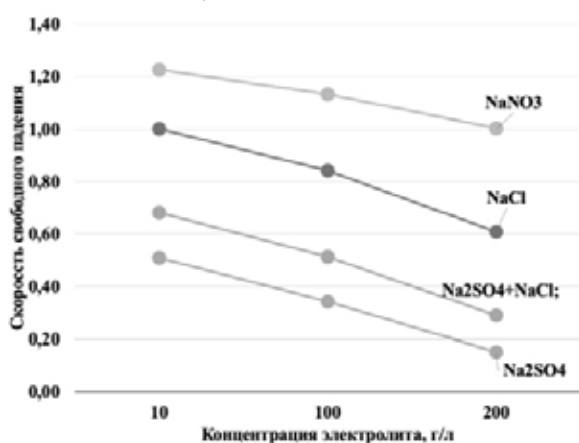


# STUDY OF THE INFLUENCE OF THE PHYSICO-CHEMICAL PROPERTIES OF ELECTROLYTES AND THE DISPERSED PHASE ON THE EFFICIENCY OF SEDIMENTATION EXTRACTION OF HEAVY METAL IONS

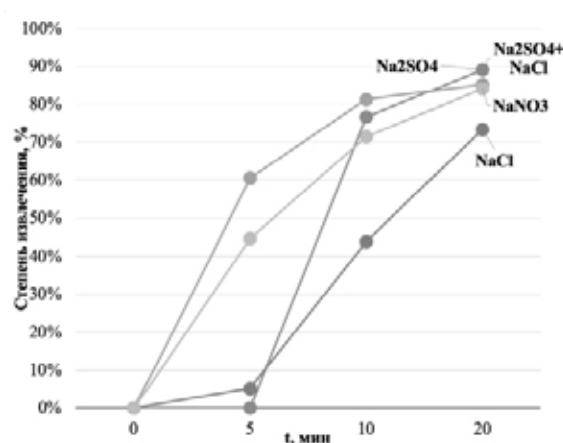
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The influence of the physico-chemical properties of electrolyte solutions on the degree of extraction of heavy metal ions in a multicomponent system from electrolyte solutions by sedimentation methods in the presence of electrolytes of various nature and concentration has been studied. The studies were carried out in solutions containing Fe (III), Ni (II), Cu (II), Pb (II) and Zn (II) ions with additives of electrolytes NaCl, NaNO<sub>3</sub> and Na<sub>2</sub>SO<sub>4</sub> ( $C_{\Sigma el} = 10$  g/l, 100 g/l and 200 g/l) at pH 9.8–10.1<sup>1</sup>. For laminar motion conditions, the free fall velocity  $V_0$ , m/s, was calculated using the Stokes formula:  $V_0 = (g \cdot (\delta - \Delta) \cdot d^2) / 18 \cdot \mu$ .



**Picture 1.** Dependence of the free fall velocity on the concentration of various electrolytes



**Picture 2.** Dependence of the degree of extraction on the duration of sedimentation, with  $\Sigma_{\text{electrolyte}} = 100$  g/l

It was found that at a lower concentration of the salt background and a lower concentration of heavy metal ions, the degree of extraction is greater than at other values.

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# LUMINESCENT SENSORY SYSTEMS FOR ECOTOXICANTS CONTROL IN NATURAL WATERS AND INDUSTRIAL WASTEWATER

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The development of industry, transport, and agriculture leads to a widespread increase in the burden on the environment. The priority pollutants that require ongoing monitoring are polycyclic aromatic hydrocarbons (PAHs). These substances are highly toxic and have carcinogenic and mutagenic properties.

Widely used PAHs analysis methods in analytical practice are chromatographic and mass-spectrometric methods. Luminescence spectroscopy methods have certain advantages. Since the development of sensor technologies is relevant for modern analytical chemistry, we have proposed a luminescent sensor system for the PAHs determination. The sensor system is based on recording solid-phase PAHs luminescence (phosphorescence) directly in the surfactant-modified viscose phase of a sorbent.<sup>1,2</sup> The sensor system allows the PAHs determination with high sensitivity, relative selectivity and low detection limits. These characteristics are especially important for PAHs analysis in natural waters, where it be present in trace amounts. However, even at such low concentrations, PAHs can have carcinogenic and mutagenic effects on organisms.

Luminescent methods are also very promising for the industrial wastewater analysis, in particular, oil-containing wastewater. We have proposed a luminescent sensor system for the wastewater treatment efficiency monitoring.<sup>3</sup> When analyzing PAHs complex mixtures broad fluorescence bands overlap usually interferes with the identification of individual components. The method selectivity was increased by using the synchronous technique of excitation and fluorescence spectra scanning with a constant wavelength shift.

The developed sensor systems can be successfully used to PAHs and petroleum products identify in ecotoxics environmental monitoring in environment water and in monitoring of industrial wastewater content.

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# COMPUTER SYSTEM FOR BIG DATA PROCESSING TO PREDICT AND CONTROL THE QUALITY OF MULTI-ASSORTMENT POLYMERIC FILMS

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A wide range of polymeric films, large volumes, high accumulation rates and a variety of sources of film production data and at the same time the incompleteness of this data complicate the control of film quality, which is subject to stringent requirements<sup>1</sup>. The solution to the problem is to develop a computer system that is based on the integration of machine learning models and deterministic mathematical models and generates advice on controlling the quality of films of various types produced on lines of different configurations.

The system includes a module for data loading and primary processing, a module for calculating unmonitored quality indices of extrudate and polymeric film, a data analysis module, a module for predicting film quality indices, a module for generating control advice, and a data visualization module. Integration of modules and system adjustments are carried out using a data bank of film types, line configurations and production parameters. The operator enters the line number and time interval of downloaded data. Data is transformed, filtered, structured. The destruction index and mixing degree of extrudate, thickness variation and shrinkage degree of film are calculated using mathematical models of the main production stages<sup>2</sup>. The complete data set is assessed for normality to select a processing method: regression analysis with data normality; recurrent neural network, adaptive boosting otherwise (depending on the amount of data, requirements for accuracy and cost-effectiveness of the forecast). Predicted values of quality indices are calculated using the predictor and displayed as trends. The system allows you to create areas of polymeric film quality indices. These areas show combinations of control actions that ensure specified quality indices when recycling production waste (edges and defective areas of the film).

Testing of the system based on data from the production of pharmaceutical and food films based on polyvinyl chloride over a month at factories in Russia and Germany has confirmed its operability and efficiency due to resource saving while reducing the mass of non-returnable waste and increasing the yield of quality film.

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# VIRTUAL SIMULATOR FOR RESOURCE-SAVING CONTROL OF FLEXIBLE MULTI-ASSORTMENT PRODUCTION OF POLYMERIC FILMS

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The flexibility and multi-assortment nature of the production of polymeric films (PF), characterized by a large number of parameters and connections between them, requires an increase in the efficiency of operator training through the use of computer simulators. They are necessary to develop control skills when immersing trainees in a simulated (using VR technologies) production environment<sup>1</sup>. Therefore, it is relevant to develop a virtual simulator for training control when readjusting to new types and requirements for quality of PF.

The simulator allows trainees, by varying control actions (CA) at the main stages, to ensure the specified quality of the extrudate and PF. The type of film and the requirements for its quality, the configuration of the line, the regulatory ranges of CA and the training time are given in the scenario generated by the instructor. The production simulation system is the core of the simulator, allowing for active learning. It includes mathematical models (MM) of the stages of extrudate preparation and calendering, film cooling for calculating quality indices (QI), databases of PF, lines, technological regulations for implementing different training scenarios, interactive 3D models of line unit control panels. MM of stages are adjusted to variable configurations of units (extruders of various types, calenders, take-off and cooling devices), implementing a cellular approach to modeling<sup>2</sup>. For CA that are entered by the trainee using VR helmet controllers, the QI of the extrudate and PF are calculated using MM. The calculated and required values of QI are displayed as trends. The moments of change in CA, the values of CA and QI, the percentage of deviations of QI from the specified values are recorded in the training protocol. According to the protocol, the instructor assesses the development of skills (by analyzing the percentage of deviations of QI) taking into account the proportion of training time spent.

Testing of the simulator using data from the industrial production of rigid packaging films based on polyvinyl chloride has confirmed its operability and effectiveness by reducing operator training time.

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# FEATURES OF EXTRACTION OF COBALT AND LITHIUM COMPOUNDS BY MULTISTAGE METHODS FROM SPENT CURRENT SOURCES

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Currently, lithium-ion batteries (LIBs) are used in various industries. However, used power sources must be recycled, since they contain valuable components in the form of compounds of cobalt, lithium, and other metals<sup>1</sup>. When such waste is disposed of, toxic substances (dimethoxyethane, propylene carbonate)<sup>2</sup> are also released. Comprehensive studies of the physical and chemical processes occurring at various stages of LIB processing were carried out. The patterns of influence of crushing and grinding processes on the efficiency of recycling have been identified, and a mathematical description of the kinetics of the leaching process from mechanically activated powders has been proposed<sup>3</sup>.

The Kurchatov Chemical Research Complex (IREA) has developed a comprehensive technology for processing spent LIBs, consisting of the following stages: 1) discharging LIBs in saline solutions; 2) opening the LIB in a shredder; 3) selection of metal and polymer inclusions; 4) grinding of cathode and anode materials to a particle size of <3 mm; 5) grinding with mechanical activation with a particle size of 20–100 microns; 6) leaching in the «liquid–solid» system; 7) extraction in a «liquid–liquid» system to obtain a powdery sediment containing the target components.

Based on the research results, a pilot plant for LIB processing with a capacity of 20 kg/h for feedstock was developed. It ensures the recycling of all components included in the batteries. It allows you to obtain various valuable components in the form of compounds of cobalt, lithium, nickel, manganese and utilize metal and polymer materials.

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# DISPERSANTS AND HERDERS. CHEMICAL TREATING AGENTS FOR OIL SPILL RESPONSE AT THE WATER SURFACE

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Oil spill response (OSR) at the water surface is carried out using four techniques: mechanical, physico-chemical, thermal and biological. Mechanical containment or recovery still remains a priority in the Russian Federation. The main disadvantage of this technique is its low efficiency. It is hard to collect more than 30% of spilled oil or petroleum products<sup>1,2</sup>. *In situ* burning requires compliance with special fire prevention and safety measures and is therefore rarely (if ever) used. Application of biological agents depends significantly on environmental conditions. Sorbents are the preferential physico-chemical treating agents despite the obvious unhandiness associated with necessity of their collection from the water surface and subsequent waste disposal.

Application of dispersants and herders may become a worthy alternative to the methods described above or at least one of the stages of combined OSR technologies (final treatment of water areas with dispersants, pre-treatment of oil spills with herders).

The effectiveness of dispersants and herder, including those that developed by the authors, was determined in this work at laboratory level. The effectiveness was tested using different types of oil and petroleum products in various hydrometeorological conditions: air temperature, water temperature, water salinity, wave levels. Particular attention was paid to the influence of oil weathering processes on the chemical agent effectiveness. Additionally, the optimal values of DOR/HOR (dispersant-to-oil or herder-to-oil ratio) were assessed.

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# INTENSIFICATION OF PROCESSING TECHNOLOGY FOR TECHNOGENIC WASTE FROM EKIBASTUZ COAL BURNING USING $\text{NaCl-H}_2\text{SO}_4\text{-H}_2\text{O}$ SOLUTIONS

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The intensification of technology for processing fly-ash from Ekibastuz coal solves the problem of transition to a waste-free production process and makes it possible to deal with existing commercial waste.

The increased ash content of Ekibastuz coal leads to the significant accumulation of technogenic waste. The chemical composition of fly-ash during the combustion of these coals corresponds to the  $\text{MeO-Al}_2\text{O}_3\text{-SiO}_2$  system (where Me is Fe, Ca, Mg), with average percentages of components: 61,5  $\text{SiO}_2$ ; 27,3  $\text{Al}_2\text{O}_3$ ; 5,65  $\text{FeO}$ ; 1,17  $\text{CaO}$ ; 0,49  $\text{MgO}$ . Valuable impurities of these wastes are gallium and yttrium.

An analysis of known technologies for processing fly-ash from coal combustion has shown that both pyrometallurgical and hydrometallurgical methods do not allow achieving the efficiency of using raw materials, as a result of which they have not been widely used.

In the course of work, the synthesis of model ash samples was carried out and the kinetics of the dissolution of industrial and model samples were studied.

The distribution of ash components from the combustion of Ekibastuz coals in interaction with  $\text{NaCl-H}_2\text{SO}_4\text{-H}_2\text{O}$  solutions depending on the temperature and composition of the solutions has been studied.

Recommendations have been developed for the disposal of industrial waste (using the example of fly-ash from burning Ekibastuz coal), with the extraction of gallium and the production of an aluminum sulfate acid catalyst.

A method has been proposed for intensifying the technology of ash processing of Ekibastuz coal using  $\text{NaCl-H}_2\text{SO}_4\text{-H}_2\text{O}$  solutions, which allows increasing gallium extraction to 69%, switching to waste-free production and recycling existing technogenic waste.

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# STUDY OF THE COMPOSITION AND PROPERTIES OF TECHNOGENIC WASTE FROM BURNING EKIBASUTZ COALS

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To increase the extraction of gallium from technogenic waste from the combustion of Ekibastuz coals, the kinetics of interactions of simple and complex oxides of  $\text{MeO-Al}_2\text{O}_3\text{-SiO}_2$  (where Me - Fe, Ca, Mg) with aqueous solutions of the  $\text{NaCl-H}_2\text{SO}_4$  system were studied.

The dependences of the physicochemical properties of solutions of the  $\text{NaCl-H}_2\text{SO}_4\text{-H}_2\text{O}$  system on temperature and the  $\text{NaCl-H}_2\text{SO}_4$  ratio are studied.

The equilibrium pressure and composition of the gas phase over solutions of the  $\text{NaCl-H}_2\text{SO}_4\text{-H}_2\text{O}$  system is calculated by thermodynamic modeling.

The kinetic parameters of the dissolution of  $\text{MeO-Al}_2\text{O}_3\text{-SiO}_2$  oxides (where Me – Mg, Ca, Fe, Al) in  $\text{NaCl-H}_2\text{SO}_4\text{-H}_2\text{O}$  solutions at a total molar concentration of  $\text{NaCl+H}_2\text{SO}_4$  equal to 2 mol/l have been determined.

To clarify the parameters of gallium concentration and impurity distribution, a series of studies was performed, including ash leaching in a solution of  $\text{NaCl-H}_2\text{SO}_4\text{-H}_2\text{O}$  with the precipitation of gallium, aluminum and iron.

The use of  $\text{NaCl-H}_2\text{SO}_4\text{-H}_2\text{O}$  solutions for gallium extraction during the processing of ash from the combustion of Ekibastuz coals has advantages over the use of pure sulfuric acid solutions. These advantages include increased extraction of gallium and macro components, as well as the possibility of using technogenic and difficult-to-implement reagents.

The research results confirmed the possibility of two-stage gallium concentration at the leaching and neutralization stages. The main impurities that reduce the enrichment rate are aluminum and iron (III), and the extraction of gallium during neutralization increases to 69%.

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# SORPTION MATERIAL BASED ON CHITOSAN AND POLYURETHANE FOAM IN OIL SPILL REMOVAL TECHNOLOGY

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The work investigated the possibility of using the sorption material PPUel-30-KhK based on elastic polyurethane foam and crushed chitosan, soluble in acid in an amount of 30% of the total mass, to remove oil spills, which has an absorption capacity of up to 14.0 g/g.<sup>1</sup> The ecological friendliness of the developed sorption material is confirmed by its ability to be reused multiple times (up to 24 times) after squeezing out the absorbed product without significant changes in oil capacity, which allows for reduced costs of its usage, decreased waste during spill clean-up, and the regeneration of a large portion of the absorbed product. The sorption material can be produced both in stationary conditions and in emergency situations. Technological schemes have been developed for both scenarios<sup>3</sup>.

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# THE EFFECT OF THE NATURE OF THE ALKALINE REAGENT ON THE DISPERSION OF SOLID KERATIN HYDROLYSATES

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Solid keratin in the form of waste from livestock and poultry enterprises is a valuable protein-containing raw material that can be used to produce various products, including protein foaming agent for the manufacture of foam concrete. Before preparing this useful product, keratin-containing waste is subjected to alkaline hydrolysis to obtain hydrolysates containing particles of different sizes: large and small complexes or proteins, peptides, amino acids, depending on the alkaline reagent used, its content in the hydrolyzing solution and the depth of hydrolysis. It is also necessary to know the dispersion interval for hydrolysates corresponding to the foaming agent with the required specific gravity, multiplicity and foam stability.

In this work, the turbidimetric method was used to determine the particle size and dispersion of solid keratin hydrolysates obtained by hydrolysis of solid keratin - test raw materials (RCS) in an alkaline medium. Sodium hydroxide and sulfide were used as an alkaline reagent individually and in a mixture with calcium hydroxide in various ratios with RCS, while the water content remained constant – 0.168 mol H<sub>2</sub>O/g of RCS.

When using sodium hydroxide in an amount of (3.2-4.9)·mmol NaOH/g RCS colloidal systems with a dispersion of  $(0.640 \div 1.73) \cdot 10^7 \text{ m}^{-1}$  were obtained, which is typical for large proteins. With an increase in the content of sodium hydroxide, the dispersion increases to values corresponding to small complexes, amino acid residues. The values of the degree of dispersion in protein hydrolysates obtained in the presence of sodium sulfide in the amount of  $(2.09 \div 2.68) \cdot \text{mmol Na}_2\text{S/g}$  of RCS, corresponded to those for large complexes (fragments, components of a protein molecule), namely  $(0.234 \div 0.300) \cdot 10^7 \text{ m}^{-1}$ . An increase in the content of sodium sulfide leads to an increase in the dispersion to values characteristic of large proteins. The use of calcium hydroxide in small amounts in a mixture with sodium hydroxide and sulfide makes it possible to expand the range of quantitative ratios to obtain dispersion values corresponding to large proteins.

Foaming agents prepared on hydrolysates with high concentrations of alkaline reagents are characterized by a higher foam specific gravity, but with lower values of foam multiplicity and stability.

# CHEMICAL DEPOLYMERIZATION OF POLYCARBONATES IN THE MONOETHANOLAMINE AND ETHYLENEDIAMINE MEDIUM

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The volume of polycarbonate production is constantly growing due to their wide range of applications and high consumer properties. Polycarbonates are popular materials in various industries, construction, packaging and other fields, which contributes to an increase in demand and production.

Research on the recycling of polycarbonates is important in the modern world, where the problem of environmental pollution is becoming more and more urgent. Polycarbonates are widely used in the manufacture of various products such as plastic tableware, packaging, automotive parts and many others. However, after use, these materials often turn into garbage, which can pollute nature. Research on the recycling of polycarbonates allows us to find ways to reuse these materials, which reduces the amount of waste and reduces the negative impact on the environment. In addition, the recycling of polycarbonates allows you to save natural resources and reduce the cost of producing new materials.

The B3LYP/6-311++G(df,p) method was used to study the model reaction of polycarbonate depolymerization - the non-catalytic and base-catalyzed interaction of diethyl carbonate with methylamine. It has been shown that non-catalytic reactions proceed through a large activation barrier. A significant decrease in the activation barrier occurs during catalysis with sodium hydroxide.

The process of chemical depolymerization of polycarbonate based on diphenylolpropane in a monoethanolamine medium has been studied. It has been shown that the main degradation product is diphenylolpropane. The carbonate fragment is converted into oxazolidine-2-oh. The process can be catalyzed by sodium hydroxide. The process also proceeds faster when exposed to microwave radiation.

The process of polycarbonate based on diphenylolpropane in an ethylenediamine medium has been studied. It has been shown that the main degradation product is also diphenylolpropane. In this case, the carbonate fragment is converted into ethylene urea.

# ANALYSIS OF THE DEVELOPMENT OF ENTERPRISES OF THE RUSSIAN CHEMICAL COMPLEX TAKING INTO ACCOUNT THE PRINCIPLES OF CLOSED-CYCLE ECONOMICS

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The results of the federal project on the transition to a closed-cycle economy include the modernization of production, the development of non-raw materials industries and the greening of products. The chemical industry of the Russian Federation ensures the achievement of the specified indicators<sup>1</sup>. When creating and modernizing enterprises, they adhere to the principles of the best available technologies to increase the energy and resource efficiency of technological processes, minimize emissions, and recover secondary resources<sup>2</sup>.

For the chemical industry, the economy should be formed at each production site and relate to the rational and efficient use of resources through the introduction of full-cycle technologies, for example, using waste gases as fuel<sup>3</sup>. Emission minimization should be focused on systemic environmental regulation based on scientifically based calculations of emission<sup>4</sup>. It is also crucial to obtain products of competitive quality and the development of high-quality industries with the receipt of goods of maximum added value<sup>5</sup>.

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# REARRANGEMENT OF THE RODENTICIDAL SUBSTANCE BROMADIOLONE DURING SOLUBILIZATION IN PRODUCTION CONDITIONS

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Bromadiolone is a rodenticide with a second-generation anticoagulant mechanism of action, widely used since the 80s of the last century in agriculture and medical deratization. In finished compositions (poisoned baits, gels and foams) it is used in fairly low concentrations (up to 0.0025%). In this case, the path of the substance to the final composition is divided into three stages: at the first, a concentrated (up to 20%) «premix» is prepared in DMSO, at the second stage, the «premix» is diluted to 0.25% in more technologically advanced glycol solvents, and at the final stage – 0.25% solutions of the substance serve as the basis for the manufacture of final formulations.

Under production conditions, when heated during the production of the «premix» a precipitate appears, the formation of which was associated with the possible thermolysis of bromadiolone. However, it was found that the phase composition of the precipitate is complex and includes salicylic acid, triacetone triperoxide (which forces us to reconsider the requirements for fire and explosion safety of production) and a substance containing a  $\gamma$ -butyrolactone fragment. It has been suggested that the latter compound is a solvated form of bromadiolone with a solvent (DMSO), similar to another anticoagulant, Warfarin<sup>1</sup>. However, the presence of the coumarin ring was not confirmed, while the isolated crystalline phase P21/c:  $a = 34.0$ ,  $b = 5.3$ ,  $c = 10.0$  Å,  $\beta = 93^\circ$ ,  $Z = 4$  (preliminarily) indeed contains  $\gamma$ -butyrolactone with bulk substituents in the 3rd and 5th positions. The regrouping route is not clear, but facts indicate the need to review safety standards and the conditions for obtaining the «premix».

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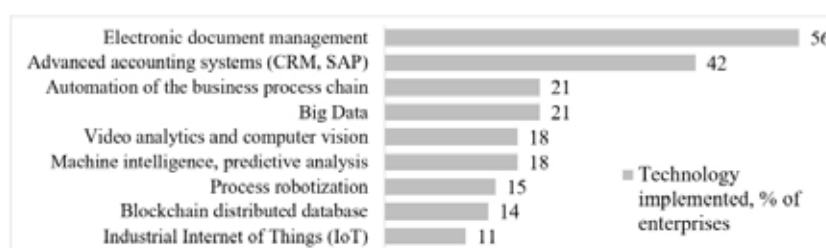
# LOGISTICS DIGITAL TRANSFORMATION IN RUSSIA OIL AND GAS CHEMICAL COMPLEX

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The logistics digital transformation processes in Russians petrochemical industry is aimed at forming a unified digital supply chain. This requires the development of a methodology and the creation of an industry-specific software platform. Many companies face the problem of «digital chaos» due to a non-standardized approach.

In this regard, first of all, the digital transformation requires a systematic analysis of business processes with the identification of complex areas to assess the response from innovation. Secondly, the digital technologies choice should be aligned with the objectives of process modernization, in view of the software used and ready-made industry practices: IoT provides information on transport location and cargo tracking; AI and ML can optimize delivery routes and automate inventory management; Big Data provides information on deliveries, cargo traceability, inventory levels; robots can perform packing, sorting and unloading of cargo; cloud technologies simplify data exchange between participants in the logistics chain.



**Figure 1.** The digital technologies introduction at Russian enterprises

The digital logistics trends include increasing the use of robots and automated systems, the development of analytical capabilities and AI algorithms to optimize operations. Digital technologies are becoming more and more understandable and accessible, enabling them to be utilized by small and medium-sized enterprises.

*The research was carried out within the framework of the «Advanced Engineering School «Promkhimtech» project.*

# IDENTIFICATION OF OPTIMAL PARAMETERS OF THE PYROLYSIS PROCESS OF POLYESTER FIBERGLASS

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The range of polymer composite materials is extensive today, but unsaturated polyester resins in combination with glass fibers have proven themselves well in modern industry. They are available in various forms, while having low cost and increased mechanical properties.

Although polyester fiberglass plastics have many successful applications in engineering, construction and energy, however, their end-of-life disposal is a difficult task to realize on an industrial scale. Until now, enterprises have used these materials without having proper information about their disposal method, since for decades landfills and incineration have been two popular ways to dispose of waste. The lack of technological advances in the creation of efficient and cost-effective recycling of polyester fiberglass is currently becoming increasingly important and is seen as a key obstacle to the development or even further use of composite materials in some markets. To develop new markets, it is necessary to use modern methods of recycling polyester fiberglass, including pyrolysis, which allows waste to be disposed of, but at the same time receive additional processed products (raw materials, energy).

On the territory of «Promtechnopark» GC KSC is developing and implementing an environmental waste recycling project program<sup>1</sup>.

In this work, studies have been conducted to identify the optimal parameters of recycling polyester fiberglass at the developed innovative pyrolysis plant.

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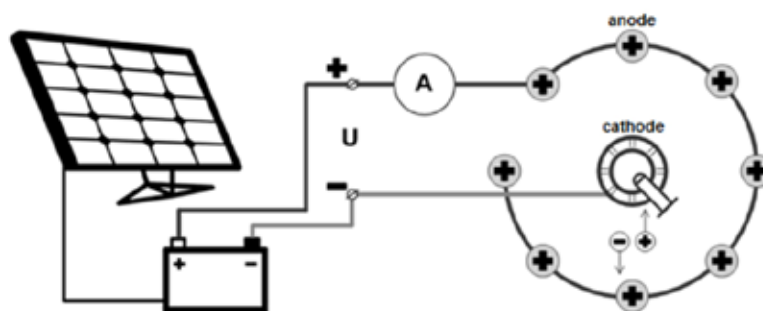
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# ELECTROCHEMICAL CLEANING OF TECHNOGENICALLY POLLUTED TERRITORIES WITH AN ENERGY-EFFICIENT AUTONOMOUS POWER SUPPLY

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The electrochemical method of technogenically polluted territories cleaning is a set of electrokinetic reactions due to the directional movement of pollutants in the liquid or solid phase to one of the electrodes<sup>1</sup>. A decrease in the concentration of pollutants occurs due to direct oxidation with oxygen, chlorine-containing substances in the anode region, fenton-like reactions with the formation of hydrogen peroxide and subsequent formation of hydroxyl radicals. Electrochemical reactions occur throughout the interelectrode volume due to the presence of electrical conductivity. It is shown that to purify 1 kg of pollutants, it is necessary to pass  $\sim 10^7$  C of electric charges<sup>2</sup>. At the same time, energy consumption at a voltage of  $U \approx 12$  V will amount to 120 MJ. Considering that the average power of solar panels is  $P \approx 160$  W/m<sup>2</sup>, it will take 18 days to clean this amount of pollutants from a 1 m<sup>2</sup> panel. The use of solar energy for the electrical supply of electrochemical soil treatment plants allows us to offer autonomous structures that do not require connection to electrical networks



**Figure 1.** Installation scheme with an autonomous power supply

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# PROCESSES OF SUBSTANCES TRANSFER DURING ELECTROCHEMICAL CLEANING OF TECHNOGENICALLY CONTAMINATED SOILS

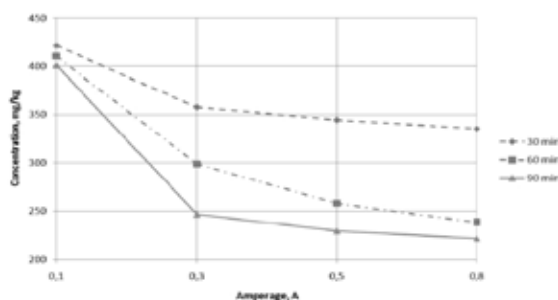
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Electrochemical soil treatment is one of the energy-efficient, environmentally friendly technologies for damaged environments remediation<sup>1</sup>. An important area of research is the study of the specifics of substance transfer during the electrochemical treatment of contaminated soils, which makes it possible to determine the main technological parameters and, accordingly, adapt the operating modes of cleaning plants in order to increase their efficiency<sup>2</sup>.

A theoretical and experimental study of the processes of transfer of solvated ions by pollutant molecules was carried out. Dependencies that describe the relationship between the change in the mass of the pollutants and the parameters that determine the rate of the transfer process were obtained. It has been shown that the rate of decrease in the pollutants concentration is determined by the volume of solvated ions moving in the interelectrode space<sup>3</sup>.



**Figure 1.** The nature of the reduction in the concentration of petroleum products in the cleaned soil

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# PROPERTIES OF THE PLANTS DERIVED BIODIESEL AND THE POSSIBILITY OF IT'S APPLICATION IN THE INDUSTRIAL EXPLOSIVES

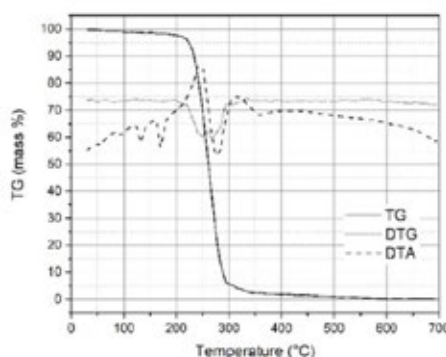
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Biodiesel fuel (BF) is a promising renewable energy resource, which can significantly decrease both greenhouse gases emissions, and the amount of different harmful substances, that are being formed during the combustion of the fossil fuels<sup>1</sup>. New mixed explosives with BF are especially relevant for mining in arctic regions due to the strict legislative environmental requirements<sup>2</sup>. It is established, that the use of BF as a fuel for mixes with ammonium nitrate gives practically no negative effects on the detonation parameters<sup>3</sup>.

Differential thermal analysis of the mixture of porous ammonium nitrate and BF (Fig. 1) allowed us to establish, that the exothermic decomposition of the sample can be observed in the temperature range from 200 to 300 °C. The curves obtained are similar to those for ANFO, which indicates the possibility of using BT as a fuel in mixtures with ammonium nitrate.



**Fig. 1.** Curves of differential thermal analysis of a mixture of ammonium nitrate with biodiesel fuel.

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# SECONDARY USE OF WASTE FROM ATROSPIRA PLATENSIS BIOMASS PRODUCTION IN PLANT CULTIVATION

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Cyanobacteria *Arthospira platensis* (spirulina) are considered a promising raw material for the production of various types of products (food items, dietary supplements, cosmetic products, biofuels, etc.). Consequently, there is an increase in their production in isolated bioreactors, which involves the consumption of large amounts of water<sup>1-3</sup>. The reuse of spent culture medium is limited; therefore, researching the possibility of secondary use of such waste is an environmentally justified and promising direction<sup>4-6</sup>.

At Kursk State University, in close collaboration with LLC «BIOSOLYAR MSU» work is being conducted to develop a technology for obtaining a plant cultivation preparation from the spent culture medium of cyanobacteria *Arthospira platensis* biomass cultivation. Laboratory and field research have yielded results that indicate the potential of the developed preparation as an inducer of resistance and a growth regulator for cultivated plants.

Currently, the compositions of such preparations are not standardized, on one hand, due to the lack of clear identification of the components that determine their properties, and on the other hand, due to changes that may occur in their composition during storage<sup>7</sup>. In this regard, the study pays special attention to the identification and quantitative determination of generalized physicochemical indicators that could characterize the quality of the new preparation.

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# COMPATIBILITY OF PETROLEUM PRODUCTS WITH ANTICORROSIVE COATINGS OF STORAGE FACILITIES

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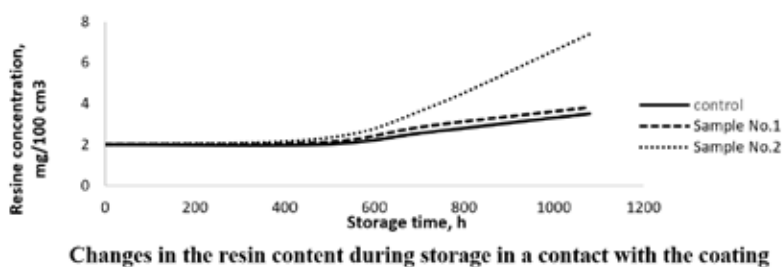
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A necessary requirement for anticorrosive coatings of tanks is the absence of their influence on the quality of petroleum products during storage.

Chemical transformations during the process of interaction of petroleum hydrocarbons or various types of functional additives to them with coating materials

are the main reasons of changes in the quality of petroleum products. Exposure to an aggressive environment can contribute to the destruction of coatings due to washouts and dissolution. The presence of water, mechanical impurities and microorganisms in the oil product/coating zone is a catalyst for various, primarily oxidative reactions that cause a changes in the quality of petroleum products.

Studies of the compatibility of petroleum products with anticorrosion coatings performed under conditions of accelerated aging at elevated temperatures made it possible for various types of oils and fuels to establish indicators that make it possible to assess the influence of coatings on changes in their physico-chemical properties. The control samples were subjected to accelerated aging without contact with coating materials.



**Figure 1.** Changes in the resin content during storage in a contact with the coating

To assess the compatibility of gasoline with anticorrosive coatings, it is necessary to determine the following indicators: the concentration of actual resins, chemical stability by the proportion of absorbed oxygen, acidity, content of water-soluble acids and alkalines<sup>1</sup>.

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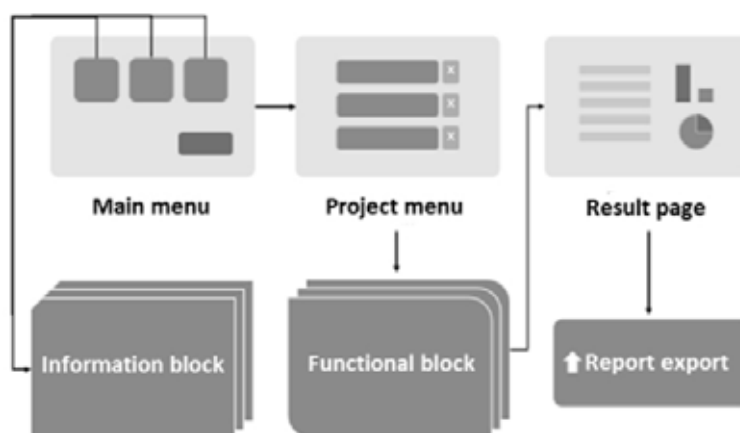
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# COMPUTATIONAL APPROACH TO ASSESSING COMPLIANCE OF CHEMICAL PROCESSES WITH PRINCIPLES OF GREEN CHEMISTRY

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Modern society is facing an urgent need for the development of innovative high-tech approaches to implement chemical processes and careful planning of syntheses aimed at minimizing negative impact on the environment<sup>1</sup>. This paper presents the process of developing the functional part of software for assessing chemical processes using numerical indicators based on the 12 principles of green chemistry. For each principle of green chemistry a mathematical formula has been developed to calculate indicators that allow to compare chemical-technological processes. The algorithms are based on known mass indicators of the process, taking into account specific coefficients that influence the ecological efficiency of the process. The initial formulas were developed taking into account available data from regulatory documents of the Russian Federation, including GOST 32419-2022 «Classification of the Hazard of Chemical Products. General Requirements»<sup>2</sup>. The created mathematical algorithms provide the ability to compare the environmental efficiency and safety of various chemical processes aimed at obtaining the same chemical product.



**Figure 1.** Block diagram of the software functionality

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# LOW-TEMPERATURE AUTOCLAVE OXIDATION OF POLYMETALLIC SULFIDE CONCENTRATES

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At present, there is a trend towards integrated processing of mineral raw materials of the deposits being developed<sup>1</sup>. A promising way of processing polymetallic raw materials is autoclave hydrometallurgy<sup>2</sup>. Low-temperature autoclave leaching allows oxidizing sulfur from sulfides into elemental sulfur and leaving it in the leaching cake.

For the studies, mixtures of chalcopyrite and pyrite concentrates were prepared until the  $\text{FeS}_2/\text{CuFeS}_2$  ratio = 1 and 2 were achieved. Autoclave oxidation was carried out at 105 °C, 0.7 MPa  $\text{O}_2$ , 100 g/dm<sup>3</sup>  $\text{H}_2\text{SO}_4$ , 5 g/dm<sup>3</sup> Cu (II), 7 g/dm<sup>3</sup> Fe (III). The leaching cake compositions are presented in Table 1.

Cake	Cu	Fe	S
Pyrite concentrate	0.03	32.31	54.36
$\text{FeS}_2/\text{CuFeS}_2 = 1$	11.74	25.59	48.27
$\text{FeS}_2/\text{CuFeS}_2 = 2$	4.74	25.01	59.39

**Table 1.** Leach cake compositions, %

As a result, it was possible to increase the oxidation degree of pyrite by 25% when chalcopyrite was added to the system and the ratio  $\text{FeS}_2/\text{CuFeS}_2 = 2$ . Oxidation degree of chalcopyrite did not exceed 35 %. For further processing of the cake, a hydrothermal treatment process is recommended to enrich the cake for copper and further purify it from impurities.

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*The study was carried out within the framework of the RF Government Order under Grant No. 075-03-2024-009/1 (FEUZ-2024-0010).*

# APPLICATION OF 3D MODELING IN A CLOSED SCIENTIFIC AND PRODUCTION CYCLE OF FINE CHEMISTRY

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As part of the innovative development of the closed scientific and industrial complex of fine chemistry, work has been carried out to create digital twins of one of the leading enterprises of fine chemistry JSC «EKOS-1» and the Fine Chemistry Scientific Center created on its basis. At the first stage, a 3D model of the «EKOS-1»<sup>1</sup> warehouse was created, including 6 warehouses of raw materials and finished products.

Using Autodesk Revit software, 3D models of warehouses were built, as well as their internal component. All models are as similar as possible to the original objects and provide the creation of a virtual warehouse space, its visualization, optimization of logistics and interactive interaction with the consumer. Many 3D models of special equipment have been created: loaders, racks, pallets, containers, etc.

The analytical department of the Scientific Center, according to the analytical service «EKOS-1», develops common approaches to quality control, as well as the development of optimal algorithms for the analysis of raw materials, finished products and intermediates. On the basis of the Blender software, the development of digital twins of analytical laboratories<sup>2</sup>, including many 3D models of individual elements, has been carried out. The elements include analytical instruments, auxiliary equipment, furniture and electronics.

Digital twins enhance the quality of analytical research. By modeling real-world conditions, they give a complete picture of the behavior of the system and allow to make informed decisions on optimizing the work of existing analytical laboratories and designing new ones. In addition, the developed 3D models are used for marketing work promoting analytical services to prospective customers.

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# RESOURCE-SAVING WATER MANAGEMENT CALS-SYSTEM FOR FINE CHEMISTRY ENTERPRISES

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A systematization of water resources management tasks at three levels of hierarchy is proposed: country, industry, enterprise<sup>1</sup>. At the country level, one of the main problems is water supply to the economy, including industrial enterprises. At the lower level of analysis, the main subsystems of the enterprise's water management are proposed<sup>1</sup>.

An integrated water management system has been developed for one of the leading fine chemistry enterprises, JSC «EKOS-1»<sup>2</sup>. The modular structure of the system includes 6 local subsystems: circulating water supply; steam generation, condensate collection and treatment; obtaining demineralised water; obtaining high-purity water; collection and purification of contaminated water; hot water supply. Nine types of water flows are analyzed: main water, concentrate, recycled water (direct and return), osmotic water, saturated steam, domestic and industrial wastewater, highly pure water, hot water. The system allows to increase resource efficiency and energy efficiency of production and reduce the negative impact of the enterprise on the environment. The development was carried out on the basis of a promising computer support system - CALS technology<sup>2</sup>.

For the three main stages of the system (recirculating water supply, production of demineralized water, steam generation and condensate treatment), water treatment problems (combat scale, corrosion and biological fouling) using reagents produced by JSC «EKOS-1» were considered and solved<sup>3</sup>. The positive experience gained in organizing the corrective water-chemical regime of thermal power equipment at the JSC «EKOS-1» plant allows to recommend the introduction and replication of technologies at other enterprises in the industry.

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# ENVIRONMENTALLY SAFE USE OF EXPIRED DRUGS AS ANTI-CORROSIVE MATERIALS

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Medicines enter the environment during the disposal of expired and unused medicines, residues and waste from medical institutions, waste from the pharmaceutical industry, and from wastewater treatment plants. According to WHO, this poses a threat to public health and the environment, as it leads to contamination of drinking water and the destruction of beneficial bacteria and other aquatic organisms. One method of solving the problem of improper disposal of drugs is the possibility of using them as metal corrosion inhibitors.

It is known that the most effective corrosion inhibitors are organic compounds whose molecules contain unsaturated bonds, aromatic rings and heteroatoms, such as O, N, S, etc. Expired drugs have a similar structure to organic inhibitors and can be used as such. Similar studies have been conducted abroad for more than ten years, summarized in a number of reviews<sup>1-2</sup>.

We used a gravimetric method to study the protective effectiveness of the expired drug omeprazole ((RS)-5-methoxy-2-[(4-methoxy-3,5-dimethylpyridin-2-yl)methylsulfinyl]-1H-benzimidazole) against corrosion of St3 carbon steel in 1 N solutions of sulfuric and hydrochloric acids and in a model stratum water containing 400 mg/L H<sub>2</sub>S. The protective effect of omeprazole reaches 90% at a concentration of 40 mg/l in acid solutions and 80% at a concentration of 60 mg/l in a hydrogen sulfide environment.

The expired drug drotaverine (1-(3,4-diethoxybenzylidene)-6,7-diethoxy-1,2,3,4-tetrahydroisoquinoline) at a concentration of 80 mg/l exhibits a protective effectiveness against corrosion of St3 steel equal to 95% in a 1 N solution of sulfuric acid and 82% in a 1 N solution of hydrochloric acid at 20°C, and at 80°C - 96%. Interestingly, protective drug concentrations are significantly lower than the values typical for target organic inhibitors. The results obtained were confirmed by polarization and impedance measurements.

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# PHYSICAL AND CHEMICAL STUDIES OF PROCESSING SOME TYPES OF MINERAL ALUMINUM-CONTAINING RAW MATERIALS

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In our country, the only global problem is environmental protection and the reasonable use of water and mineral resources. Sources of centralized water supply are surface and underground waters. Most of them are associated with processing to remove excess impurities using various coagulants. An urgent task is to find raw materials for their production<sup>1,2</sup>. Such raw material sources include Kanash clay from the Chuvash deposit.

The main clay minerals are quartz (70,82%), albite (5,19%), kaolinite (4,45%), prochlorite (3,82%), ekepgitite (2,97%), perovskite (2,97%). Chemical analysis performed by atomic emission spectrometry with induction plasma showed that Kanash clay contains on average, %: 18,20  $\text{Al}_2\text{O}_3$ ; 7,54  $\text{Fe}_2\text{O}_3$ ; 55,40  $\text{SiO}_2$ ; 0,15  $\text{MgO}$ ; 0,05; 0,05  $\text{CaO}$ ; 0,10  $\text{TiO}_2$ ; 0,01  $\text{Na}_2\text{O}$ ; 0,01  $\text{Cr}_2\text{O}_3$ ; 0,01  $\text{CuO}$ . It does not contain harmful impurities such as Sr, Be, Pb, etc., and Mn, Cr, Na, Cu, Ti are present in small quantities and do not have a significant effect on the composition of the resulting coagulants.

The optimal conditions for processing Kanash clay are sulfatizing firing at a temperature of 175°C for 1 hour, followed by leaching of specs into aqueous solutions. The degree of extraction of clay components into the aqueous solution was, %: 75  $\text{Al}_2\text{O}_3$ , 90  $\text{Fe}_2\text{O}_3$ , 15  $\text{SiO}_2$ . The degree of extraction of components into hydrochloric acid solutions from clay calcined at 650°C was, %: 42  $\text{Al}_2\text{O}_3$ , 73  $\text{Fe}_2\text{O}_3$ , 14  $\text{SiO}_2$ .

The resulting solutions containing sulfates and chlorides of aluminum and iron can be recommended for use as various mixed coagulants for the purification of drinking or waste water.

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# SCIENTIFIC BASICS AND DEVELOPMENT OF ALKALINE-CHLORINE AND ACID-CHLORINE TECHNOLOGICAL SCHEME FOR COMPLEX PROCESSING OF ALUMINUM-CONTAINING RAW MATERIALS

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Physico-chemical studies of the chlorination process of aluminum-containing raw materials have been carried out. The raw materials for the production of aluminum chloride can be nephelines, bauxite, kaolin clay, coal preparation and coal mining waste, shale, etc. The production of aluminum chloride is one of the main problems in chlorine technology for the production of aluminum, which is caused by the chlorination of aluminum oxide, which has a high reactivity towards chlorine. Aluminum oxide was obtained by calcination of aluminum hydroxide isolated by carbonization and decomposition of aluminate solutions.

Aluminum hydroxide, released by carbonization of an aluminate solution at 40°C, is represented by bayerite. Decomposition aluminum hydroxide has a gibbsite structure<sup>1</sup>.

When acid enriching carbonaceous rock, alumina was obtained, isolated by calcination of crystalline hydrates: aluminum sulfate, chloride and nitrate. The polymorphism of chemically pure grade aluminum oxide has been studied. and crude alumina isolated after thermal decomposition of various crystalline hydrates of aluminum salts<sup>1</sup>.

Alkali- and acid-chlorine technological schemes for the complex processing of aluminum-containing raw materials have been developed, consisting of two main stages - the production of aluminum chloride and its electrolysis. The chlorine method of aluminum production has the following advantages: the possibility of direct and efficient conversion of the starting material into chlorides; significant energy savings, the use of graphite non-consumable electrodes in the electrolysis of aluminum chloride, the abandonment of expensive cryolite and fluorine-containing salts<sup>2</sup>.

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

# REAGENTS FOR WATER PURIFICATION FROM THIN OIL FILMS

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Crude oil or petroleum product (CO/PP) spills response in water areas is a technologically complex, multi-stage process. In general, CO/PP spills response begins with the installation of booms. Then the oil is collect by oil skimmers, after which the remaining oil is treat with sorbents or dispersants and, at the final stage, with biological products. In Arctic conditions, the site of an oil or petroleum product spill due to natural and climatic conditions is often not accessible to equipment or it arrives very late. This leads to an increase in the spill area and a decrease in film thickness. However, the minimum thickness of the pumped-out layer of CO/PP in water for most skimmers is not less than 1 mm. The lack of possibility of mechanical cleaning of the water area leads to the further spread of O/PP water and, consequently, to a manifold increase in environmental damage.

A promising solution for combating thin films of CO/PP is the use of oil collector reagents (OCR), under the influence of which a thin oil film (less than 1 mm thick) is contracted to a layer of 1–5 mm, and the spill area is reduced many times over. Known commercially available imported OCR contain components that are difficult to biodegrade. Materials used in oil spill response in the Arctic are subject to increased requirements related to minimizing the impact on the environment. In this regard, it was of interest to develop domestic OCR based on environmentally friendly components.

Two two-component OCR compositions were developed, consisting of natural components and monohydric alcohol, classified as hazard class 4. It has been experimentally established that the developed OCR are non-toxic, capable of reducing the area of the CO/PP film by 96–97% and increasing the thickness from 0.1 mm to 2.6 mm, which is sufficient for the subsequent effective removal of the CO/PP film from the water area.

*The study was supported by the Russian Science Foundation grant No. 22-13-00410, <https://rscf.ru/project/22-13-00410/>.*

# EXTRACTION OF NICKEL FROM SPENT CATALYSTS FOR OIL DEMETALLIZATION

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Catalysts designed for oil demetallization consist of molybdenum and aluminum compounds. During the oil refining process, the porphyrins contained in it are destroyed, as a result of which the catalysts are enriched with nickel and vanadium. The processing of spent catalysts has been organized at the Balause LLP enterprise. During processing, ammonium metavanadate and calcium molybdate are obtained. Vanadium pentoxide is obtained from ammonium metavanadate, and ferromolybdenum is obtained from calcium molybdate. The insoluble residue contains mainly nickel compounds (up to 40% NiO) and aluminum.

In the framework of this work, studies have been conducted on the technology of obtaining ferronickel from the residue of a spent catalyst after leaching vanadium and molybdenum from it. For this purpose, a series of reduction melts was carried out in the Tamman furnace and on the two-electrode arc furnace of the Laboratory of Ferroalloy Production of I.P. Bardin TsNIIchermet. During the research, the optimal composition of the charge and melting conditions were selected. Smelting was carried out using coal and ferrosilicon grade FS75 as a reducing agent. Using the diagrams of the state of the oxide systems, the optimal composition of the slag was selected.

During the experiments, an increased content of sulfur and phosphorus was found in the obtained ferronickel samples. Therefore, it is recommended to refine the hydrometallurgical stage of the technology with the separation of harmful impurities. The nickel content in ferronickel exceeded 30%. Before loading into the furnace, it is recommended to sift the insoluble leaching residue of the spent catalyst, and pre-compress its fine fraction (to obtain briquettes).

The developed hardware scheme for nickel extraction from the insoluble leaching residue of the spent catalyst for oil demetallization includes a feedstock preparation department, a limestone preparation and firing workshop, a smelting department, a ferroalloy and slag cutting department.

## FOR THE COMPLEX PROCESSING OF PRODUCTION AND ENRICHMENT WASTE (CHP ASH, SLAG TAILS, STUBS)

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Currently, a large amount of waste from production and enrichment has been accumulated (for example, CHP ash, pyrite stubs, slag tails, etc.). So, at Almalyk MMC, 580 - 650 thousand tons of slag tails are formed annually during flotation of copper smelting slag (33-34% SiO<sub>2</sub>, 32-38% Fe, 1-2% CaO, 1% MgO, 0.3-0.5% Cu, 0.8-1.0 Zn, 0.3 Pb). About 110 million tons of stale copper slag have been accumulated in the Ural region, including 26 million tons at the Mednogorsk MSC (27-34% SiO<sub>2</sub>, 34-42% Fe, 5.4-6.7% CaO, 1.6-2.4% Al<sub>2</sub>O<sub>3</sub>, 0.4-1.6% Cu, 1.7-1.9 Zn, 1.7-2.5 S). In Russia, more than 2.5 billion have been accumulated in dumps tons of ash and slag waste from thermal power plants with an annual increase of about 25 million tons (50-64% SiO<sub>2</sub>, 18-30% Al<sub>2</sub>O<sub>3</sub>, 4-15% Fe<sub>2</sub>O<sub>3</sub>, 2-10% CaO, 0.5-3.0% MgO). All these materials mainly consist of silicon, aluminum and iron compounds, and Mg, Ca, Cu, Ni, Zn, Au, Ag, As, S, P. are also present in their composition.

As a rule, the methods of processing ash and slag, slag tails, pyrite stubs mentioned in publications and research reports are aimed at obtaining non-ferrous metals (Au, Ag, Cu, Zn). Such technologies make it possible to extract a small amount of valuable components, but not to recycle the dumps completely. Within the framework of this work, a solution to the problem of waste disposal is proposed by obtaining iron and silicon-containing products from them (iron concentrate, cast iron, steel, ferrosilicon, ferrosilicon aluminum). In addition to the preliminary extraction of non-ferrous metals, it is necessary to study the possibility of iron separation, the use of silicate residue for the production of building materials and products, solid phase reduction, etc.

We carried out research and pre-design technical and economic calculations for the processing of pyrite stumps of the Priargunsky PGHO, which showed the possibility of their cost-effective processing to obtain marketable products. Preliminary calculations have shown that 1 ton of ferrosilicoaluminium can be obtained from 2.4 tons of TPP ash and 1 ton of coke. Slag tails of copper production after pretreatment can be considered as raw materials for the production of cast iron and ferrosilicon. Thus, waste from production and enrichment can be considered as man-made raw materials for the production of marketable products.



# COMPARATIVE ANALYSIS OF THE STATE OF ATMOSPHERIC AIR IN THE MOSCOW REGION

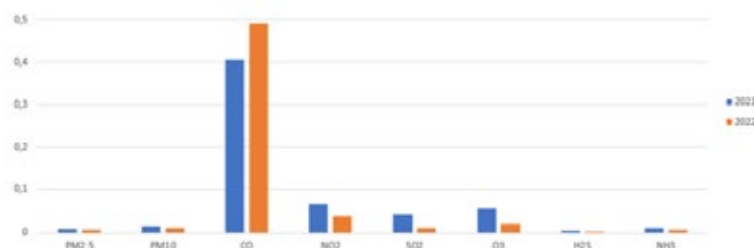
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Regular monitoring of atmospheric air pollution is carried out throughout the Moscow region in 57 urban districts through 374 observation posts around the clock for 11 pollutants (further – «P»): carbon monoxide, nitrogen dioxide, nitrogen oxide, sulfur dioxide, hydrogen sulfide, ammonia, suspended substances, suspended particles PM10, 2.5, ozone, methane.

In 2022, the average annual concentrations of these pollutants did not exceed the established hygienic standards and were: carbon monoxide – 0.2 MPC<sub>ss</sub>, nitrogen dioxide – 0.4 MPC<sub>ss</sub>, suspended particles PM10 – 0.2 MPC<sub>ss</sub>, PM2.5 – 0.2 MPC<sub>ss</sub>, sulfur dioxide – 0.2 MPC<sub>ss</sub>, ozone – 0.2 MPC<sub>ss</sub>, ammonia – 0.05 MPC<sub>ss</sub>, hydrogen sulfide – at the level of 0.001 mg/m<sup>3</sup>. Compared to 2021, the indicator values of «P» generally decreased by 33% for PM2.5 suspended particles, by 31% for PM10 suspended particles, by 44% for nitrogen dioxide, by 77.5% for sulfur dioxide, by 75% for hydrogen sulfide and by 46% for ammonia. Carbon monoxide concentrations increased slightly. According to the complex indicator of the air pollution index (API), the level of atmospheric air pollution is assessed as low (API - 2.6).

The main source of pollutants in all cities of the Moscow region is transport. It causes high spatial and temporal heterogeneity of pollutant concentrations: maximum values of «P» was observed near highways, minimum values of «P» was observed in residential and natural areas. In addition to transport, the formation of increased concentrations of pollutants was influenced by unfavorable weather conditions observed in the summer months.



# MODELING AS A FORECASTING METHOD MIGRATION OF POLLUTANTS IN THE ATMOSPHERE

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Anthropogenic impact on the atmosphere necessitates the control of its physic-chemical parameters and the study of the migration of pollutants in it. One of the modern and promising tools for solving such problems is mathematical modeling.

Since the atmosphere is characterized by a complex multicomponent composition and a variety of physic-chemical processes occurring in it, the general approach to modeling should be formulated on the basis of kinetic equations for spatiotemporal functions, taking into account the nature of the sources of emission of pollutants and their chemical nature, the efficiency of their accumulation and life expectancy in the atmosphere, as well as a variety of physic-chemical processes occurring in it.

We have attempted to use kinetic equations that allow us to assess with the greatest probability the influence of various factors on the processes of pollutant propagation in the atmosphere.

The object of the study was a thermal power plant located on the territory of Tula.

The author conducted local monitoring of emissions into the atmosphere as a result of the activities of this enterprise and estimated the concentration levels of atmospheric aerosols in them, selected at different dispersations from the source of emissions of pollutants of organic and inorganic origin. The obtained results were used as a data bank for modeling.

When developing the model, the influence of adiabatic factors, the intensity of thermal and ultraviolet radiation, the location of emission sources and its parametric concentrations of matter at the considered point, as well as the metrological characteristics of the compartments, of which the wind speed was one, were also taken into account.

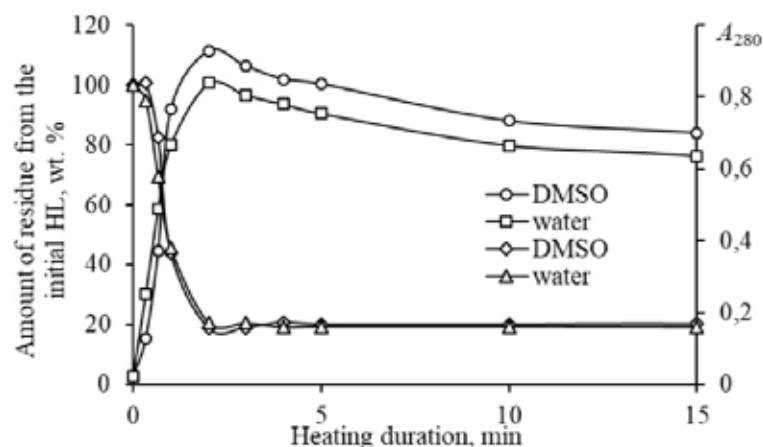
# NITRATION OF HYDROLYSIS LIGNIN WITH NITRIC ACID IN WATER-DIMETHYL SULFOXIDE AND IN AQUEOUS MEDIUM

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The study of lignins and their use has received increasing attention due to the prospect of abandoning the use of petrochemical feedstocks in favor of renewable resources in some areas.<sup>1</sup> It has been shown previously that nitration of hydrolysis lignin (HL) and Klason lignin with nitric acid upon heating with dimethyl sulfoxide (DMSO) resulted in their complete depolymerization to water-soluble products.<sup>2</sup>

In this work, we show that when extractive-free HL was treated at 100 °C with DMSO-nitric acid mixture of 4:1 by volume and liquor-to-HL ratio of 10, all lignin passed into the added alkaline solution after 2 min, only cellulose residue (about 20 %) remained. A similar result was obtained when DMSO was replaced by water. However, in this case, the products soluble in the alkaline solution had lower absorbance, which indicates their stronger degradation in water medium than in the mixture with DMSO (Figure 1).



**Figure 1.** Dependence of the amount of HL residue on the initial amount of HL and the absorbance at 280 nm of the reaction products transferred to the alkaline solution on the heating duration at 100 °C of HL with nitric acid in mixtures with water and with DMSO

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# ON THE ISSUE OF AN INTEGRATED APPROACH TO HYDROMETALLURGICAL PROCESSING OF DOMESTIC HIGH-QUARTZ TITANIUM CONCENTRATES WITH THE POSSIBILITY OF CONCOMITANT SYNTHESIS OF ACICULAR WOLLASTONITE

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The largest titanium deposits, Yaregskoye and Pyzhemskoye, are located in the Komi Republic on Timan. Their common distinguishing feature is their complex polymineral composition and high quartz content (up to 40% in enriched concentrates). Processing of such highly quartz raw materials is associated with significant difficulties. And to involve such titanium raw materials, it is necessary to create an innovative processing technology that ensures maximum extraction of valuable components and production of the largest variety of products from a unit volume of ore matter with less environmental stress. A new method for hydrometallurgical enrichment of quartz-titanium concentrates using lime milk with the participation of NaOH was proposed at IMET RAS. As a result, artificial rutile and acicular wollastonite are obtained, providing for the waste-free use of quartz for the associated synthesis of silicate products.

The most promising and manageable method for producing synthetic wollastonite is the dehydration of calcium hydrosilicates (CSH) obtained by hydrothermal treatment of calcium and silicon-containing components. At the same time, depending on the structural features of the initial silica and its size, the conditions for the synthesis of CSH and the habitus of the synthesized wollastonite change.

In quartz-titanium concentrates, almost all quartz is represented in a finely dispersed state, located inside titanium grains, which are represented as a thin network of rutile with a thickness of about a micron. It is worth noting that during the geological formation of sandstones, the pores of the grains were filled with ultrafine quartz formed from dissolved silica brought by hydrothermal solutions. This makes it possible to obtain acicular wollastonite during hydrothermal enrichment of concentrates, which does not require many hours of exposure and elevated temperatures.

*The work was performed according to the state task No. 075-00320-24-00.*





Section 5

# **CHEMISTRY OF FOSSIL AND RENEWABLE HYDROCARBON RESOURCES**

# WOOD WASTE TO ENERGY: BEECH WOOD PYROLYSIS FOR BIOFUEL PRODUCTION

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Nowadays, it is so important exploring the viability of using agricultural and forestry wastes as a sustainable feedstock which can improve energy security, lower CO<sub>2</sub> emissions, mitigate ecological problems and promote economic growth<sup>1-2</sup>. Taking into account all these points, in this research the potential of beech wood residues as a feedstock for biofuel production was investigated. Pyrolysis method in a fixed bed reactor was applied to study the capability for the conversion of beech wood wastes into biogas, bio-oil (liquid product) and bio-char at two different temperature values 420°C and 540°C in order to investigate how the temperature which is one of the main parameters, impact on biofuel distribution and product yields. The results of this study clearly shows that the yields of liquid and bio-char enhanced from 47.9% to 60.1% and 21.2% to 28.5%, accordingly, with decreasing temperature from 540°C to 420°C while bio-gas fraction reduced from 30.4% to 12.7%.

GC analysis of biogases shows that compared to the pyrolysis gas at 540°C, which has 43% methane, the pyrolytic gas at 420°C contains more methane gas, roundly 53% which validate its effectiveness as a fuel for generator applications.

In summary, the analysis results of products properties depicts that the bio-products (generated from beech residues) potential to offer environmentally-friendly and sustainable replacement for traditional fossil fuels in chemical manufacturing industries and mainly in energy generation.

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# THE INFLUENCE OF COMBINING METHODS OF OIL MECHANOCHEMICAL ACTIVATION ON THE CHARACTERISTICS OF REFINED PRODUCTS

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Increasing the depth of oil processing with increasing yield of distillate fractions is achieved by modifying (activating) through the creation of mixed oil systems or by the influence of physical methods on oil dispersive systems<sup>1-6</sup>. Research on the influence of cavitation treatment of oil, both using hydrodynamic cavitation in the DA-1 apparatus and in the apparatus with a vortex layer (AVS) of ferromagnetic elements, showed an increase in the yield of light fuel fractions NK-350 °C by 10% relative, with simultaneous reduction in the density and viscosity of oil. The most effective impact for reducing the density of oil was found to be the combination of DA-1 (at a compression pressure of 40 MPa) + AVS, with the density decreasing from 887.5 to 885.2 kg/m<sup>3</sup>. The most noticeable decrease in viscosity occurs during processing in DA-1 at a compression pressure of 30 MPa, with the value decreasing from 42.5 to 33.2 m<sup>2</sup>/s.

According to the results of chromatographymass spectrometry analysis of fuel fractions, it has been revealed that mechano-chemical processes have a significant influence on the structural-group and chemical composition of oil and its fractions. It has been demonstrated that combining activation methods leads to changes in the ratio between paraffins and aromatic hydrocarbons in the composition of petroleum product.

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# IMPROVING THE QUALITY OF DIESEL FUEL USING BIODIESEL ESTERS

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It is known that to improve the quality of diesel fuels, it is necessary to include in their composition various environmentally friendly additives obtained from alternative raw materials<sup>1,2</sup>. Among them, a special place is occupied by oxygen-containing additives of plant origin, the so-called biodiesel esters obtained from fatty acids of vegetable oils<sup>3</sup>.

In this work, a mixture of propyl esters of fatty acids of soybean oil (PEFASO) and acetyl glycerin (AG) was studied as an oxygen-containing additive when added to the hydrotreated diesel fraction (HDF) in an amount of 10% at an ester ratio of 1:1 and the physicochemical properties were studied the resulting compound. It was found that by adding a 10% mixture of PEFASO and AG to the HDF composition, the quality indicators of the resulting compound improve. Thus, if in HDF the contents of sulfur and aromatic hydrocarbons are 0.0310% and 16.0%, respectively, then in the resulting compound the values of these indicators are reduced to 0.0279% and 14.4%, respectively. In addition, an increase in the cetane number and flash point of the resulting compound is observed. If the cetane number of HDF is 46 points and the flash point is 67°C, then in the fuel compound these values increase by 3 points and 7°C, respectively. Also, unlike HDF, the wear scar diameter for a 10% compound is reduced to 0.476 mm. Based on the data obtained, PEFASO and AG can be recommended as resource-saving and anti-wear additives to diesel fuel.

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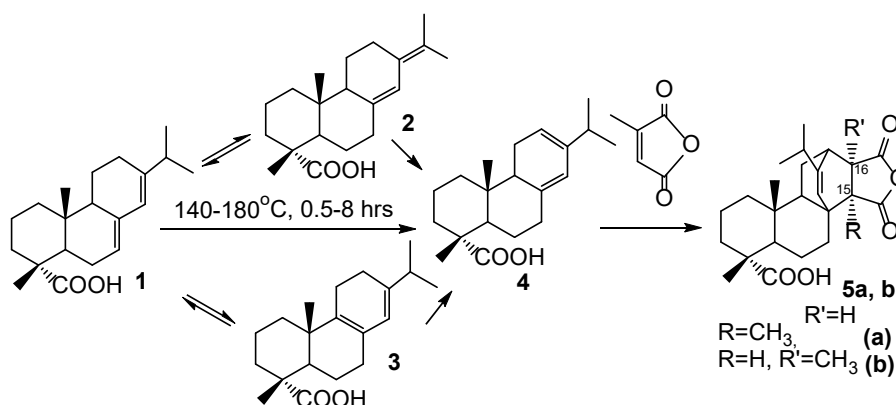
# NEW GREEN CHEMISTRY PRODUCTS BASED ON ROSIN AND CITRACONIC ANHYDRIDE

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Modern concepts of “green chemistry” and sustainable development require the evolution of chemical technologies toward production of chemicals using renewable plant raw materials<sup>1</sup>.

The interaction of rosin and citraconic anhydride at 140–180°C for 0.5–8 hours was studied, including the use of catalytic additives H<sub>2</sub>SO<sub>4</sub>, MgCl<sub>2</sub>, AlCl<sub>3</sub>, FeCl<sub>3</sub>. It has been established that as a result of the interconversion of resin acids of abietic type (abietic acid **1**, neoabietic acid **2**, palustric acid **3**) into levopimaric acid **4**, which irreversibly enters into the Diels-Alder reaction, the formation of adducts of rosin and citraconic anhydride occurs, containing up to ~70% (180°C, 4–8 h, 1–2% H<sub>2</sub>SO<sub>4</sub>) of citraconopimaric acid (in the form of an equimolar mixture of two isomers C<sup>15</sup>-CH<sub>3</sub> **5a** and C<sup>16</sup>-CH<sub>3</sub> **5b**)<sup>2</sup>.



Based on the C<sup>15</sup>-CH<sub>3</sub> isomer of citraconopimaric acid **5a**, a number of individual derivatives – esters, amides, and imides were obtained. Rosin-citraconic anhydride adducts and their derivatives (imides) are effective modifiers of unfilled and filled industrial rubber compounds<sup>3</sup>.

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# OPTIMIZATION OF COKE FINES MAGNETIC SEPARATION PARAMETERS

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The method of magnetic separation of<sup>1</sup> coke fines obtained from Kuzbass coals (content of sulfur, phosphorus, volatile substances, carbon, other impurities  $\leq 1\%$ ,  $\leq 0.6\%$ ,  $\leq 3\%$ , up to 94%, up to 3% respectively; ash content  $\leq 20\%$ ; moisture  $\leq 24\%$ ; mass fraction of lumps over 10 mm  $\leq 10\%$ )<sup>3,4</sup> and in huge quantities accumulated at coke-chemical enterprises of the region<sup>2,3</sup> with the help of neodymium magnet N52, in order to enrich it for more efficient and rational use. The highly magnetic fraction of coke breeze is of interest from the point of view of its use as a component for the production of sinter ores.

We analyzed the influence of the degree of coke fines grinding on the yield and composition of fractions (magnetic/non-magnetic); analyzed the chemical composition of ash of the obtained fractions; analyzed the ash content before and after separation; evaluated the moisture limits at which the separation of coke fines without drying is possible. Two separation modes were used – without and with preliminary grinding (particle diameter from 0, 05 to 0,2 mm).

The optimal mode of separation (fraction size up to 0.2 mm; moisture content up to 10% (without preliminary drying)) was determined, which allows to achieve ash content reduction up to  $8.8 \pm 0.3\%$  (ash content of initial coke fines without magnetic separation  $-14.3 \pm 0.22\%$ ) with enriched product yield up to 91%.

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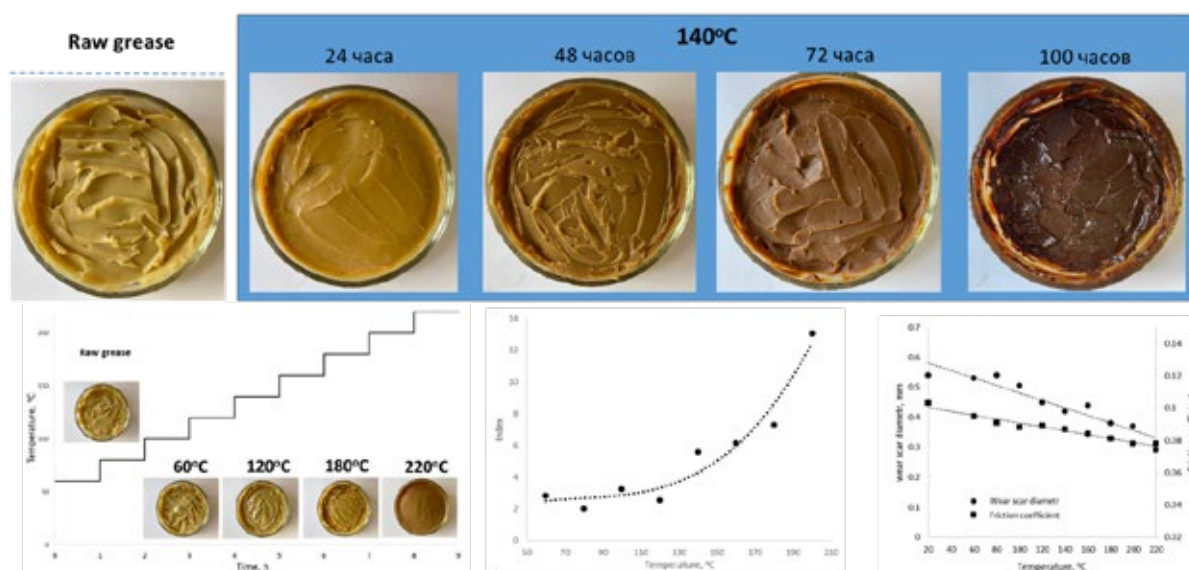
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# THERMAL STABILITY OF UREA GREASES

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The operation of modern industrial equipment at elevated temperatures, such as roller bearings in continuous casting mills, requires the use of lubricants that are thermally stable and have long-term durability. In units where friction occurs under high thermal stress, greases with synthetic base oil thickened with different types of diureas have proven to be effective. These lubricants provide excellent protection against wear and tear, ensuring efficient operation of the equipment.



**Figure.** The study of thermal degradation of urea grease based on a synthetic base oil (PAO-4).

As part of a comprehensive research project carried out at TIPS RAS, the features of changes in the main properties of synthetic urea greases were studied. The focus of the research was on changes in its basic properties, such as dropping point, ultimate strength, oil separation, and tribological characteristics. These changes were observed under critical conditions, including an increase in temperature (from room temperature to 220 °C) and thermal treatment at high temperature (140 °C for 100 hours). The study used the method of infrared spectroscopy to analyze the process of thermal decomposition of the thickener during thermal treatment. The results of this research have high practical significance for the development of new lubricant with improved performance characteristics.

*The work was carried out within the framework of the State assignment for the Topchiev Institute of Petrochemical Synthesis, Russian Academy of Sciences.*



# OPPORTUNITIES FOR INCREASING EFFICIENCY CAVITATION PROCESSING OF OIL RAW MATERIALS

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Unconventional methods of modifying petroleum feedstock to increase its processing potential are of great interest<sup>1</sup>. One of these promising methods is cavitation treatment<sup>2</sup>, the possibility of intensifying the impact on oil disperse systems may determine the further direction of development of this area.

The purpose of the study was to study the influence of factors influencing the efficiency of hydrodynamic cavitation treatment of petroleum feedstock. The effectiveness of the treatment was assessed by the increment in the yield of fractions boiling up to 400 °C after treatment.

Empirical mathematical models of the dependence of changes in the yield of target fractions on processing conditions were constructed. A linear relationship was established between the yield of target fractions and processing pressure, the correlation coefficient of which exceeded 0.98. The influence of the number of processing cycles on this indicator had a more complex power-law character with saturation. After 5 acts of exposure, virtually no changes were observed. Thus, changing the treatment pressure allows you to influence the treatment efficiency more significantly than the number of exposure cycles.

It has been shown that efficiency depends not only on the processing mode (number of cycles and impact power), but also on the gas content of the processed raw material. Blowing various gases (air, hydrogen, propane-butane fraction) of oil raw material objects in order to vary their gas content and subsequent processing led to an increase in the efficiency of cavitation effects.

The combination of observed effects made it possible to confirm the assumption of an increase in the number of cavitation nuclei as a fundamental factor in increasing the efficiency of processing with increasing gas content of the raw material.

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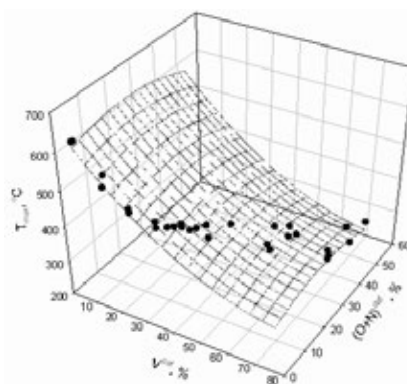
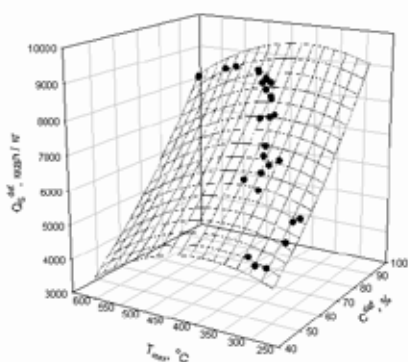


# IDENTIFICATION OF NEW RELATIONSHIPS TO ASSESS THE QUALITY OF SOLID FUELS

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Earlier, on the basis of derivatography and pyrolysis data, linear regression equations have been proposed describing the relationship ( $R = 0.917-0.975$ ) between the yield of the primary pyrolysis tar ( $CM^{daf}$ ) at a temperature  $T_{max}$  (from the derivatogram) with the  $C^{daf}$  content for the entire series of solid fuels, including coal generators - coal precursors ( $C^{daf} = 44.3-59.0\%$ ) and coals of the series brown to anthracite metamorphisms ( $C^{daf} = 62.4-93.7\%$ )<sup>1</sup>. The proposed approach yielded new relationships between  $C^{daf}$ ,  $T_{max}$  and the heat of combustion ( $Q_s^{daf}$ ) of solid fuels, their elemental and technical analyses ( $V^{daf}$ ,  $O+N^{daf}$ )<sup>2</sup>.



**Figure 1.** (left) A graphical representation of the surface corresponding to the two-parameter equation  $Q_s^{daf} = f(C^{daf}, T_{max})$  with the experimental points plotted ( $R = 0.979$ ):

$$Q_s^{daf} = -(3535.8 \pm 1244.0) + (95.7 \pm 10.1)C^{daf} + (18.2 \pm 7.0)T_{max} - (0.022 \pm 0.002)(T_{max})^2.$$

**Figure 2.** (right) A graphical representation of the surface corresponding to the two-parameter equation  $T_{max} = f(V^{daf}, O+N^{daf})$  with the experimental points plotted ( $R = 0.956$ ):

$$T_{max} = (600.1 \pm 13.8) - (4.94 \pm 0.65)V^{daf} + (1.86 \pm 1.0)(O+N^{daf}).$$

The use of these equations in practical terms will allow, already at the stage of preparation, to obtain additional information on the composition and structural features of solid fuels and determine ways of their further use in various technological processes.

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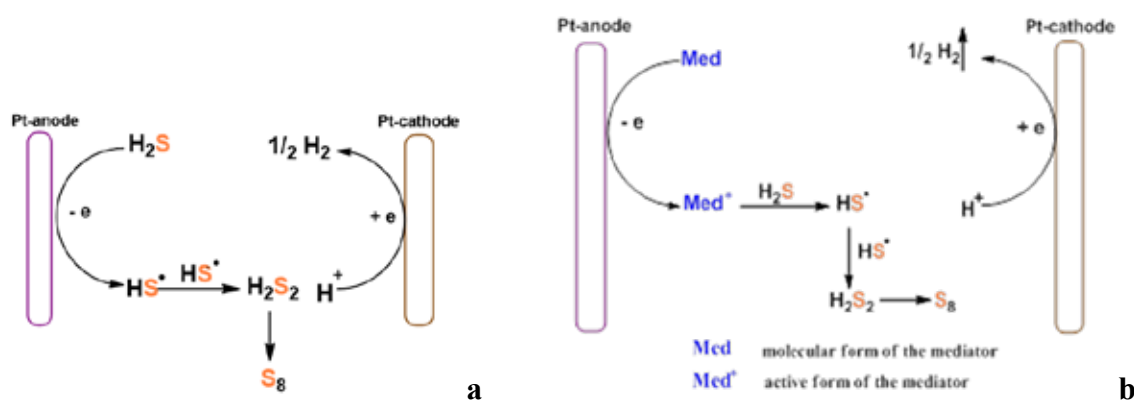
# AN ENVIRONMENTALLY FRIENDLY METHOD FOR PRODUCING HYDROGEN AND SULFUR UNDER THE CONDITIONS OF ELECTROOXIDATION OF HYDROGEN SULFIDE

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Hydrogen is the most versatile and environmentally friendly fuel. There is a continuous search for new ways to produce hydrogen, mainly from renewable resources. One of the practically inexhaustible sources of hydrogen is hydrogen sulfide, the reserves of which are very large in nature and in industrial processes for processing gas, gas condensate and oil. There are a number of thermal and catalytic methods for producing hydrogen from hydrogen sulfide.<sup>1-4</sup>

The work proposes an electrochemical method for the decomposition of hydrogen sulfide under conditions of its direct (a) and mediator (b) oxidation in organic solvents (CH<sub>3</sub>CN, CH<sub>2</sub>Cl<sub>2</sub>, N-methylpyrrolidone).



In the case of direct electrosynthesis of hydrogen, its yield varied from 19.2 to 44.0% vol., and the maximum value was achieved in N-methylpyrrolidone. The efficiency of H<sub>2</sub>S transformations was influenced by the nature of the background electrolyte (n-Bu<sub>4</sub>NClO<sub>4</sub>, NaClO<sub>4</sub>). The sulfur yield under these conditions was 20.3-46.6% wt. Organic (DABCO, methyl-substituted triphenylamine, methyl- and bromo-substituted triphenylphosphines) and inorganic (tetrabutylammonium bromide) compounds, as well as metal complexes Cr(V), Sn(IV) with redox-active ligands were used as mediators that made it possible to reduce energy costs for the synthesis of hydrogen.

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# COMPOSITES OF MICRO- OR NANOSIZED MFI ZEOLITES AND SILICON CARBIDE SYNTHESIZED BY HYDROTHERMAL-MICROWAVE METHOD – NEW CATALYSTS FOR THE CONVERSION OF RAPESEED OIL TO PETROCHEMICALS

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The use of microwave irradiation is an effective approach to the synthesis of zeolite-containing materials of various morphologies.<sup>1</sup> In the presented work, composites containing micro- or nanosized MFI zeolite particles (ZSM-5) in proton form and silicon carbide<sup>2,3</sup> were synthesized using the hydrothermal-microwave method. Synthesized HMFI/SiC and “nano”HMFI/SiC composites were tested for the first time in rapeseed oil conversion to “green” hydrocarbons and motor fuel components. Catalytic experiments were carried out in a flow-type reactor at 450-600 °C and atmospheric pressure.

It has been established that as a result of the conversion of rapeseed oil at 450 °C on the “nano”HMFI/SiC composite, a yield of liquid hydrocarbon products of 66 wt.% is achieved, and on HMFI/SiC - 59 wt.%. At the same time, a higher yield of aromatic hydrocarbons was achieved on the HMFI/SiC composite - 32 wt.%, and on “nano” HMFI/SiC their yield was 19 wt.%. At 600 °C on both catalysts the yield of C<sub>2</sub>-C<sub>4</sub> olefins increased, reaching 36 wt.% on “nano”HMFI/SiC, which is two times higher than on the HMFI/SiC composite.

Thus, the materials HMFI/SiC and “nano” HMFI/SiC synthesized by the hydrothermal microwave method are promising catalysts for the conversion of rapeseed oil to hydrocarbons - components of motor fuels, as well as into C<sub>2</sub>-C<sub>4</sub> olefins and aromatic hydrocarbons - valuable petrochemicals.

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*The work was carried out within the framework of the State Assignment of the TIPS RAS.*

# WASTE-FREE METHOD FOR PRODUCING OLEIC AND ACETIC ACIDS FROM RAPESEED OIL IN SUB- AND SUPERCRITICAL WATER CONDITIONS

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Oleic acid (OA) is a key product in the production of modern lubricants. The main source of OA is rapeseed oil containing 65-68% OA in triglycerides, from which OA is isolated by alkaline hydrolysis followed by fractionation. The process is energy-intensive and labor-intensive, accompanied by the formation of significant amounts of polluted wastewater.

The possibility of eliminating these disadvantages was studied within the framework of a hydrothermal process in sub- and supercritical water conditions ( $T=573-653$  K,  $p=30$  MPa) in a batch plant<sup>1</sup>. Unlike traditional hydrolysis, in the hydrothermal process there is an *in situ* change in the acid composition of the hydrolyzate as a result of the conversion of linoleic acid into oleic acid with the possibility of its selective isolation with a degree of purity (95%, at  $T=573$  K, water-oil ratio 2:1, process duration 30 min.), close to an individual product that does not require special cleaning for use for technical purposes. This is confirmed by direct oxidation of the hydrolyzate into azelaic acid with a yield exceeding the natural content of OA in the oil. Water effluent containing organic pollutants is converted to acetic acid by the action of  $H_2O_2$  under hydrothermal conditions. The acid was isolated preparatively and identified by IR and liquid chromatography. The fact of a change in the fatty acid composition of the oil has been recorded for the first time.

The mechanism of the hydrothermal process was studied based on the analysis of the products of the transformation of individual linoleic acid.

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Экологические проблемы планеты становятся все более значимыми и тревожащими, поэтому инновации, которые помогали бы эти проблемы решить, не просто привлекают интерес, а приобретают поистине глобальную актуальность. Сохранение окружающей среды и природных ресурсов для будущих поколений – суть новой этики прогресса.

## ПРОГРЕСС, БЕЗОПАСНЫЙ ДЛЯ ПРИРОДЫ

Компания «ФосАгро» – лидер российской химической промышленности выступила с инициативой создания фонда для финансовой и научной поддержки перспективных ученых-химиков, в сферу интересов которых попадают охрана окружающей среды, здравоохранение, продовольствие, повышение энергоэффективности и рациональное использование природных ресурсов.

В 2013 году между ЮНЕСКО, Международным союзом теоретической и прикладной химии (IUPAC) и компанией «ФосАгро» было подписано соглашение о партнерстве в создании программы грантов для ученых, занимающихся так называемой «зеленой химией». Предметом этого направления в науке является создание производственных технологий и материалов, безопасных для природы и человека.

Так родился проект «Зеленая химия для жизни», помогающий талантливой молодежи не только материальными средствами для

продолжения исследовательской работы и реализации проектов, но и плодотворным общением со старшими коллегами – видными современными химиками, и организацией информационного обмена в научной среде. Это первый проект в истории ЮНЕСКО и ООН, реализуемый за счет средств российского бизнеса. ФосАгро выделила более \$2,5 млн на развитие и реализацию проекта.

## ТРИНАДЦАТЬ МУДРЕЦОВ

Отбор заявок на участие в проекте – обязанность компетентного жюри, в которое входят 13 ученых из 11 стран. Проект-победитель должен соответствовать нескольким критериям. Оцениваются его научная новизна, глобальная и локальная значимость, соответствие принципам «зеленой химии», компетентность молодого ученого и его команды, оснащенность института и лабораторий, в которых предполагается вести проект. Качество работ очень высокое, и членам жюри приходится порой вступать в длительные диспуты по той или иной кандидатуре.

## НАУЧНЫЙ ПОИСК БЕЗ ГРАНИЦ

В 2016 году был учрежден специальный грант за исследования в области применения фосфогипса. В 2019 году в штаб-квартире ЮНЕСКО в Париже в рамках открытия Года Периодической таблицы химических элементов было принято решение продлить грантовую программу «Зеленая химия для жизни».

Проблемы экологического характера, к сожалению, есть во всем мире, и во всем мире есть ученые, которые предлагают решения для многих из этих проблем методами и технологиями «зеленой химии». Это наглядно демонстрирует география проекта «Зеленая химия для жизни». За время реализации программы на рассмотрение жюри поступило более 1000 заявок, 55 грантов было присуждено молодым ученым из 33 стран. Самый главный результат грантовой программы – практическое применение разработок молодых исследователей.





## ЖИЗНЬ ПОСЛЕ ГРАНТА

Дважды за первые 10 лет существования проекта победителями конкурса становились ученые из России. Одна из них – Галина Калашникова, заведующая лабораторией синтеза и исследования минералоподобных функциональных материалов Центра наноматериаловедения ФИЦ КНЦ РАН. В 2019 году грант «Зеленая химия для жизни» был присужден проекту «Разработка универсального и экологичного метода гранулирования синтетических титаносиликатных материалов (сорбентов, катализаторов, регенерируемых матриц), полученных на основе отходов региональных горно-обогатительных и металлургических производств».

### Галина Калашникова:

– В рамках проекта удалось опробовать 5 разных методов грануляции для новых материалов с широким функционалом свойств (сорбенты, катализаторы для органического синтеза, керамические матрицы), которые мы синтезируем именно в нашей лаборатории. Мы смогли выбрать наиболее подходящий метод получения гранул для каждого из них, а также приоритетные нетоксичные связующие. Полученные гранулы были опробованы в качестве сорбентов для очистки жидких радиоактивных отходов от радиоизотопов  $^{137}\text{Cs}$  и  $^{90}\text{Sr}$  совместно с лабораторией хроматографии радиоактивных элементов и станцией переработки радиоактивных отходов Института физической химии и электрохимии им. А. Н. Фрумкина РАН.

Работа по проекту продолжается, несмотря на окончание действия гранта. Все полученные средства были потрачены только на выполнение основной задачи, благодаря чему мы приобрели необходимое оборудование, получили хороший опыт в работе с зарубежными коллегами и выстроили приоритетные направления дальнейшей совместной работы со многими научно-исследовательскими организациями.

Хочется пожелать организаторам конкурса еще больше новых проектов, которые были бы направлены на самые острые вопросы взаимосвязи экологии и современной промышленности.





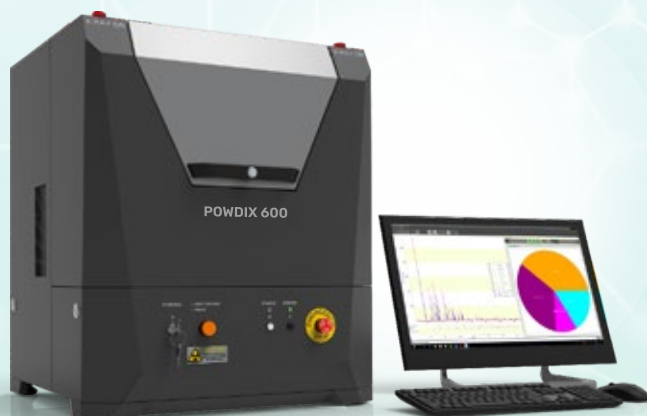
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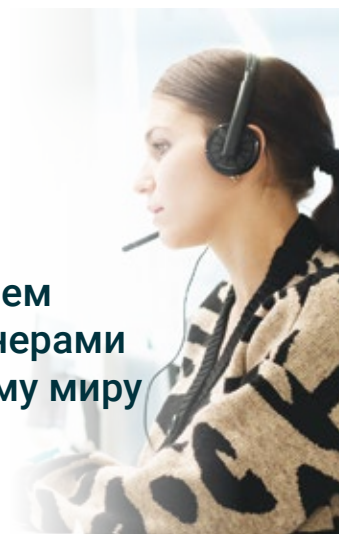
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