XXII МЕНДЕЛЕЕВСКИЙ СЪЕЗД ПО ОБЩЕЙ И ПРИКЛАДНОЙ ХИМИИ, СЕКЦИЯ 1. КЛЮЧЕВЫЕ И ЗАОЧНЫЕ ДОКЛАДЫ. СБОРНИК ТЕЗИСОВ

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XXII MENDELEEV CONGRESS ON GENERAL AND APPLIED CHEMISTRY, SECTION 1. KEYNOTE AND CORRESPONDENCE REPORTS. BOOK OF ABSTRACTS

research works

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В книге представлены ключевые и заочные научные доклады секции 1 XXII Менделеевского съезда по общей и прикладной химии (под эгидой ИЮПАК, 2024, 7–12 октября, федеральная территория «Сириус»). Для специалистов-химиков.

Keynote and correspondence scientific reports of the Section 1, XXII Mendeleev Congress on General and Applied Chemistry (under the auspices of IUPAC, 2024, October 7–12, Sirius Federal Territory), are presented in the book. The book is intended for specialists-chemists.

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NOVEL ELECTRODE MATERIALS FOR METAL-ION BATTERIES

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Lithium-ion batteries, originally developed for portable devices, are already widely used as stationary energy storage devices, in electric vehicles, etc. Rapid progress in the mass use of metal-ion batteries is intensifying the search for new electrode materials for Na- and K-ion batteries as a possible alternative to the already developed lithium-ion technology. Similar to lithium-ion intercalation systems, Na/K-based mixed oxides and polyanionic compounds are being intensively studied as potential cathodes with the aim of achieving high specific energy and cycling stability. Layered oxides are characterized by higher volumetric energy densities, however, polyanionic materials generally exhibit higher specific power, better cyclic and thermal stability due to covalently bonded structural frameworks. Polyanionic compounds are also characterized by a wide variety of crystal structures, which significantly expands the playground of the search for new materials with electrochemical characteristics attractive for practical applications. Additional benefits are expected from the synergistic effect of combining different anions (such as $(PO_4)^{3-}$ and F^-) in the crystal structure.

An overview of the research on novel phosphates and fluoride-phosphates as prospective electrode materials for the Na/K-ion batteries will be presented with a special emphasis on the interrelation between composition, synthesis conditions, crystal structure and electrochemical properties of the materials intended for practical applications.

METALLOIMIDAZOLS – NEW CLASS OF ORGANIC HETEROCYCLES

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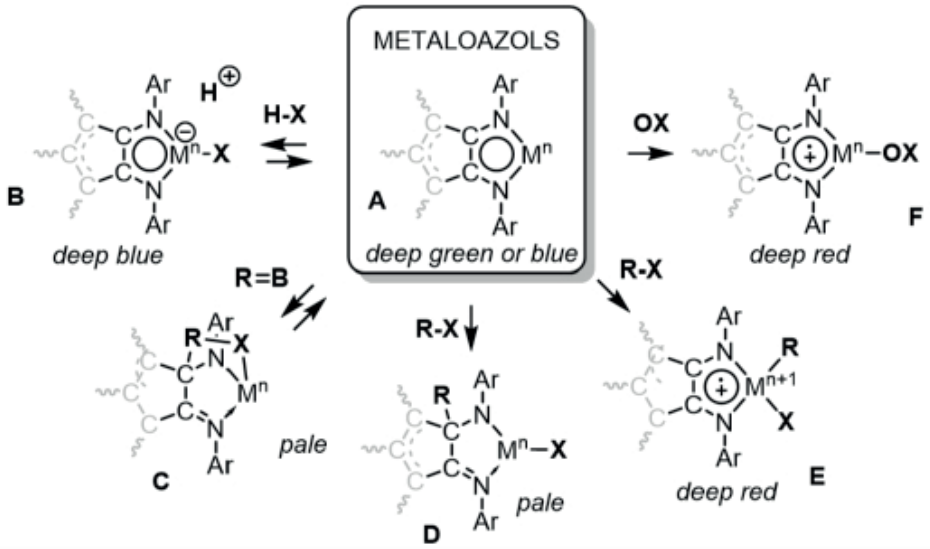
A two-electron reduction of diazadienes, ArN=C(R)–C(R)=NAr, by metals affords five-membered metal-nitrogen heterocycles – metalloimidazolls (MIAs). Conjugation of p_z orbitals of all five atoms in the cycles in these compounds provides for the formation of a π system. The properties of MIAs differ significantly of those of acyclic metal bisamides, $(R_2N)_2M$, as well as of metal-free azols. In contrast to the formers, all the MIAs (structural types **A, B, E** and **F**) are intensively colored; their solutions absorb in different regions of a visible spectrum. Some of them, as for instance **E** and **F**, reveal also absorption in the IR region. 2+4 (Cyclo)addition reactions destroy the conjugation within the cycles and, as the consequence, affords pale products **C** and **D**.



Involvement of the metal orbitals in the formation of the frontier molecular orbitals in MIDs causes an increase of their energy and, as a consequence, to a lowering of the ionization potential. Therefore all the MIDs represent highly reactive species that are reactive even towards unreactive molecules such as CO_2.

The study has been supported by the Russian Science Foundation, project 24-13-00369.

COLLOIDAL QUANTUM DOTS – A NEW CLASS OF PHOSPHORS

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In 2023, Munji Bavendi, Louis Bruce and Alexey Ekimov were awarded the Nobel Prize in Chemistry for the discovery and synthesis of quantum dots. As stated in the press release of the Nobel Committee, "one of the exciting and unusual properties of quantum dots is that they create light of different colors depending on the particle size, while maintaining the atomic structure unchanged".

Quantum dots (QD) are semiconductor nanocrystals, the properties of which can be adjusted depending on their based on the quantum size effect discovered by Bruce and Ekimov, and Bavendi developed a chemical synthesis process that allows to obtain nanoparticles of the same size and quality. All this marked the beginning of the creation of a fundamentally new class of phosphors, the luminescent properties of which are determined by the average size of nanoparticles of a crystalline semiconductor, variable within 2-10 nm, while the width of the luminescence spectrum of a single nanoparticle at room temperature is only 20-30 nm, and the position of the nanoparticle spectrum can vary within the order of 100 nm relative to the band gap of a massive semiconductor.

Thus, a rather limited set of luminescent quantum dots based on semiconductors such as AIIBVI, AIIIBV or AIVBVI easily cover the spectral range from 350 to 3500 nm only by varying their size. Unlike organic molecular phosphors, QD has significantly greater thermal stability, photostability and, in addition, has a number of functional advantages, thanks to which they are already being used in photodetectors, light-emitting diodes, displays, solar panels, optical amplifiers, lasers, in chemo- and biosensors, in biomedical diagnostics. A more distant prospect of using QD is related to molecular electronics and quantum computing. In addition to the quantum-dimensional effect, a number of new physical phenomena were discovered in QD, such as multi-exciton generation, the effect of fluorescence blinking, inhomogeneous spectral broadening, etc.

In this overview report examines in detail the fundamental principles of the luminescent properties of QD, discusses the problems and prospects of their application.

The work was carried out with the financial support of the Russian National Fund, project 21-73-20245.

MATERIALS FOR CHEMICAL CURRENT SOURCES

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In recent years, the main trends in the energy sector have become energy conservation and the transition to environmentally friendly, renewable energy sources. However, the possibilities for using solar, wind and water energy are characterized by significant variability, primarily due to daily and seasonal fluctuations. To ensure a constant energy supply, energy storage devices are also needed, the main of which are metal-ion batteries and the hydrogen cycle. In Russia, as in a number of other technologically developed countries, a program for the development of hydrogen energy has been adopted and the construction of several large factories for the production of lithium-ion batteries has begun. This report reviews current trends and advances in materials for advanced chemical power sources.

The desire for stable operation of lithium-ion batteries has led to the replacement of lithium anodes with carbon ones, which prevent the formation of dendrites. However, this significantly limits the energy intensity of the batteries, and a return to lithium electrodes is being considered as an opportunity to increase it. A necessary condition for ensuring their safety is the use of solid electrolytes (inorganic polymer or composite). The development of such electrolytes, along with new cathode materials, is becoming a key challenge for the creation of a new generation of lithium batteries.

The main objectives of modern hydrogen energy are the environmentally friendly production of relatively cheap hydrogen, its transportation to the point of consumption and the creation of stably operating fuel cells, characterized by tolerance to low humidity and carbon monoxide impurities. Catalysts and membrane materials must play a key role in solving these problems. Similar problems must be solved when developing other promising current sources, which have received significant attention in recent years - flow batteries and reverse electrodialysis units. Materials for them are also being developed by Russian scientists.

The work was carried out with the financial support of the RSF, project 21-73-20229.

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 İRC 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 İRC 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^--, Cl^-- and Na^+-forms. AMP in the OH^--form sorbs less chromium (VI) than in the chloride form. A similar picture is observed during sorption with Amberlite İRC 748. The Na-form sorbs Cr (VI) ions more preferentially than the H^+-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

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The equilibrium condition and kinetics of the sorption of Cu^{2+}, Zn^{2+}, Co^{2+}, Ni^{2+}, Cd^{2+}, Pb^{2+} ions with Diaion PK 208 ($-SO_2OH$) and DiaionWK 100 (-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^{2+}/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 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 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: $\boldsymbol{D_0 = d^2(ekT/h)exp(\Delta S/R):ekT/h=1,69.10^{13}sec^{-1}, d=0.5\ nm.}$ 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 Cu^{2+}-Diaion WK 100.

MECHANISM OF PSEUDOTHIOHYDANTOIN FORMATION

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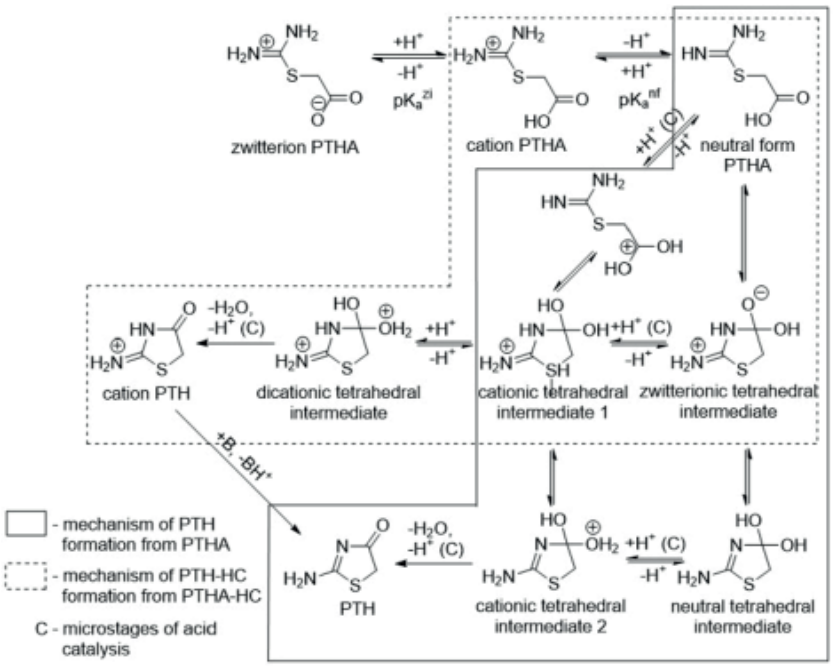
The previously proposed mechanisms for the cyclization of pseudothiohydantoic acid (PTHA) to pseudothiohydantoin (PTH) and its hydrochloride (PTHA-HC) to pseudothiohydantoin hydrochloride (PTH-HC)[1,2] are not complete and not entirely accurate. Detailed cyclization mechanisms consistent with experimental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

Only the minor[2] 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.[1] 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.

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ANODE POLARIZATION OF Pb-Ag-Sb ALLOYS IN THE KCl-$PbCl_2$ 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-$PbCl_2$ 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-$PbCl_2$(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:

$$Pb_{(Pb\text{-}Ag\text{-}Sbi)} \leftrightarrow Pb^{2+} + 2e. \qquad (1)$$

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:

$$Sb_{(Pb\text{-}Ag\text{-}Sb)} \leftrightarrow Sb^{3+} + 3e. \qquad (2)$$

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:

$$Ag_{(Ag\text{-}Sb)} \leftrightarrow Ag^{+} + e. \qquad (3)$$

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

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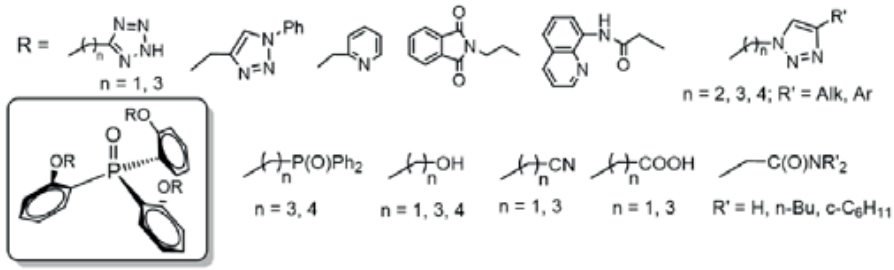
New tripodal phosphine oxides modified by functional groups promising as O,N ligands for *d*- and *f*- elements have been synthesized. Complexes of the compounds with lanthanides and actinides have been prepared. The structure of the ligands and their complexes in solid state and solution has been studied.



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 α-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.[1]

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*- $Gd_2(HCit)_2^0$ and $Gd_2Cit_2^{2-}$ hexanuclear *hexakis*- $Gd_6(OH)_2Cit_6^{8-}$ and $Gd_6(OH)_3Cit_6^{9-}$ citrate gadolinium(III) complexes were described, the formation of which can be considered typical for M^{3+} (Al^{3+}, Ga^{3+}, In^{3+})—citric acid systems.

In the gadolinium(III)—*xylo*-trihydroxyglutaric acid system, polynuclear complexes of the composition $Gd_2(H_3Thgl)(H_2Thgl)^+$, $Gd_4HxThgl_4$ and $Gd_4HxThgl_8$ 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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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[1]. 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[1-3]. The new model (M) is based on a limitation (L) of time of looking (t_L) after R-nuclei (Ñ) of an element (E), on a substitution of nuclei Ñ, which didn't decay during a certain t_L, by nuclei-equivalents (NE). R doesn't have NE-decays even during $t>>t_L$: the NE-nature is other. There is a conclusion by Prof. M. Bunge[2] 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 $s_0=s_1+s_{1\text{-}2}+\Delta s$: s_1 – with Ñ which decayed during t_1, $s_{1\text{-}2}$ – during $(t_1;t_2]$, there is no decay in Δs during t_2. So A in s_1, $s_{1\text{-}2}$ are with Ñ, in Δs – with their NE. For $t<t_0$ it's an exact prognosis of P. "The statistics increases" by a large k of parallel P: $s_0=s_{0,1}+..+s_{0,k}$, etc.

Further, Ñ, its NE are collectives of p^+, n^0. Their charges are[2] 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 Ñ 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 $s_1+s_{1\text{-}2}>0$. Thus, A-mass of ^{25}N consists of A with Ñ (Q=Z=7), A with NE (Q=7, Z=0). A in $s_1+s_{1\text{-}2}$ consist of nitrogen atoms, A in Δs – 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}N, have electrons and chemistry (EC) of N, Nu-a from ^{30}F have EC of F, etc. Nu-positions (Nu-p) from ^{25}N are in gr.15, in periods 1-7. Nu-p in PT are minor[1,3].

R with not little $T_{1/2}$ have $s_1+s_{1\text{-}2}\approx 0$. Their A in Δs 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_{IUPAC}-cells, so for its P-zone[2] [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[1], V.A.Funtikov[4], J.P.Cid Ugalde et al. recognized it as innovation.

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ON SOME PROPERTIES OF FERRATES

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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[1] 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.

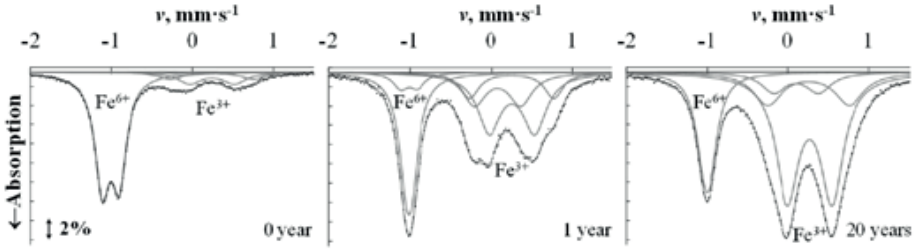

Figure 1. Room-temperature Mossbauer spectra of a sample of $K3Na(FeO_4)_2$ at three stages of its decomposition.

Another way of decomposition is shown by the solid Na_4FeO_4, which disproportionates at room temperature[2]. 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[3].

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PHOTO- AND IONOCHROMIC ACYLOTROPIC SYSTEMS

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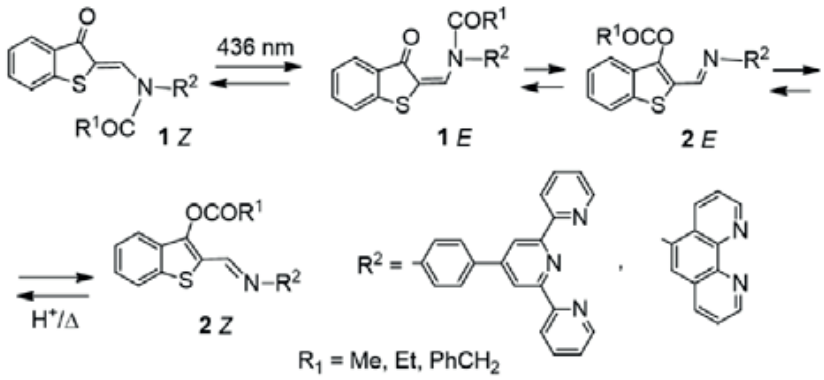
Photoacylotropic enaminoketones of the benzo[*b*]thiophene series con-taining terpyridine and phenanthroline groups have been synthesized. They represent polyfunctional on-off-on switches of optical and fluorescent properties.[1,2]



The three-step mechanism of photoinitiated rearrangement has been characterized in detail by IR, ^{1}H and ^{13}C NMR spectroscopy, HRMS, XRD analysis and DFT calculations. The emission modula-tion is realized by sequential exposure to light/H^{+} or by sequential addition of Fe^{2+}/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 $LBeB_9H_9C_2H_2$ 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 THERMOSTABILE 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 Mn_4O_5Ca. 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 Li+ as counter cations in the catalyst synthesis.

In this communication we studied by X-ray spectroscopy the structure of a new complex $Li_3[Ru_2(\mu\text{-}N)Cl_8{\cdot}2H_2O]$ **(1)**, and photocatalytic water oxidation reaction in the presence of electron acceptor $K_2S_2O_8$, photosensitizer (bpy)3$RuCl_2$ 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 $Li_4[Ru_2(\mu\text{-}O)Cl_{10}{\cdot}2H_2O]$. Complex **1** is stable in acidic solutions. In IR spectrum of 1 the maximal peak with ν = 1075 cm-1 (Ru-N-Ru) persists for several days.

The initial rate of the process w_o 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 correspons to the cation $Ru4N_2O^{5+}$. This cation is catalyst for four-electron oxidation of water to O_2: 2 [Ru^{IV}-N-Ru^{IV}] + 2 H_2O = 2 [Ru^{III}-N-Ru^{III}] + O_2 + 4 H^+. Maximal catalyst turnover number TON = 360, quantum yield O_2 Φ = 0.51 higher in its oxygen analog $Li_4[Ru_2(\mu\text{-}O)Cl_{10}{\cdot}2H_2O]$ (TON = 240, Φ = 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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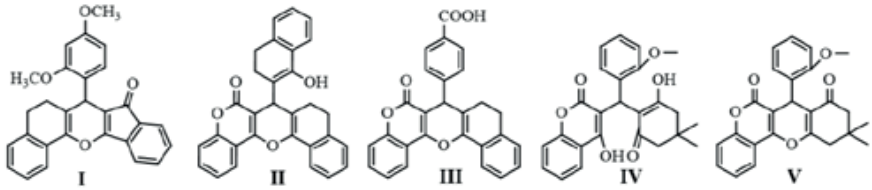
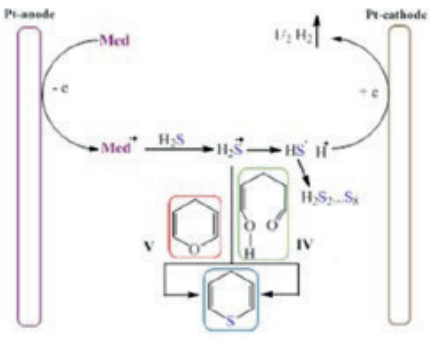
Interest in multifunctional heterocyclic compounds is due to their pharmacological activity towards various biological targets of a living organism, which makes it possible to create multi-purpose drugs based on them.[1,2] Electrosynthesis is a convenient and simple way to replace a heteroatom in the 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.[3] 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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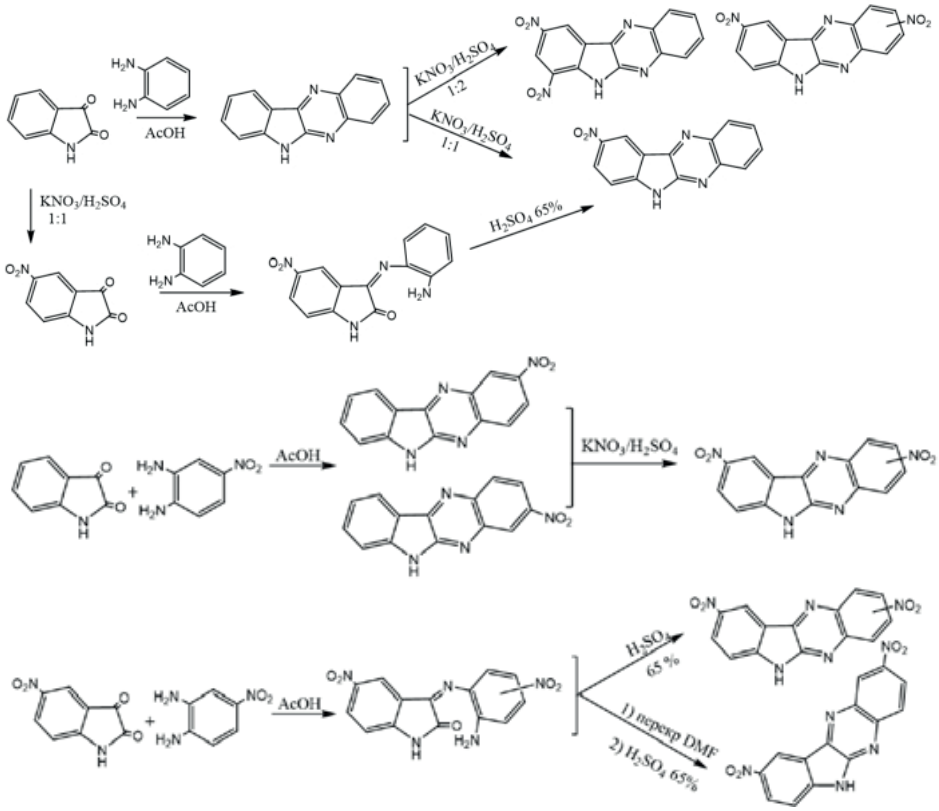
The conditions for the preparation of nitro-substituted 6H-indolo[2,3-b]quinoxaline derivatives, which are valuable precursors in the synthesis of the corresponding amines containing the 6H-indolo[2,3-b]quinoxaline fragment, have been studied and optimized. Amines obtained by reduction of nitro compounds 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

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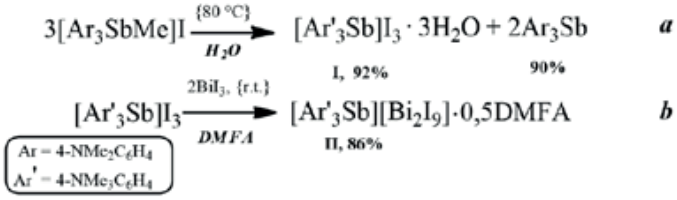
Functionalization of aromatic rings of organoantimony compounds determines the possibility of constructing complex organic structures based on them. The selective activation of reactive centers of such compounds is of particular interest.[1] For organoantimony compounds, we have demonstrated for the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

$^{Me2N}Ar_3Sb–Me \rightarrow {}^{Me3N}Ar_3Sb$ (scheme a).



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

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

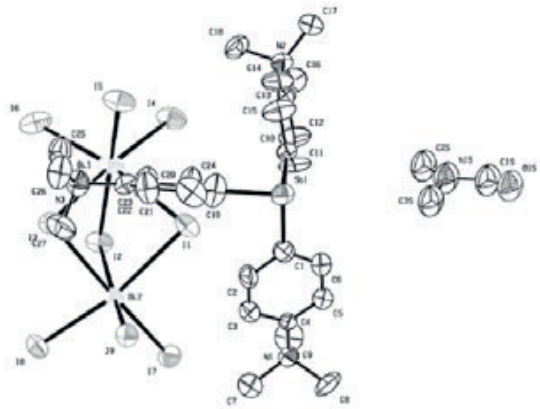


Figure 1. *ORTEP* representation of the structure of complex **II** in the crystal (p = 0.3).

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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.[1] 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.[2]

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

Compound $[2,6\text{-}(MeO)_2C_6H_3]_3Bi$ crystallizes in the monoclinic syngony. According to the X-ray diffraction data in $[2,6\text{-}(MeO)_2C_6H_3]_3Bi$, 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 μ-oxo-bis[(perchlorato)tri-*p*-tolylbismuth] were synthesized by the reaction of tri-*p*-tolylbismuth dibro-mide with silver perchlorate and its hydrate.[3] The reaction of silver perchlo-rate with other organo-bismuth compounds remains a poorly studied meth-od 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 con-tained the absorption bands with maximums at 1099 [$\nu_{as}(ClO_2)$], 1016 [$\nu_s(ClO_2)$], 891 [$\nu_s(ClO_2)$], 623 [ν_s (ClO_2)] 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[1], 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).

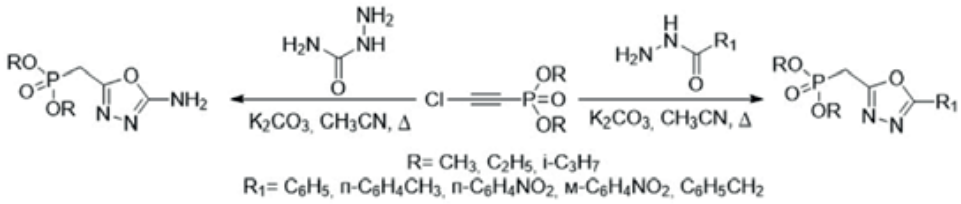

Figure 1. Reaction of dialkyl chloroacetylene phosphonate with semicarbazide and acid hydrazides

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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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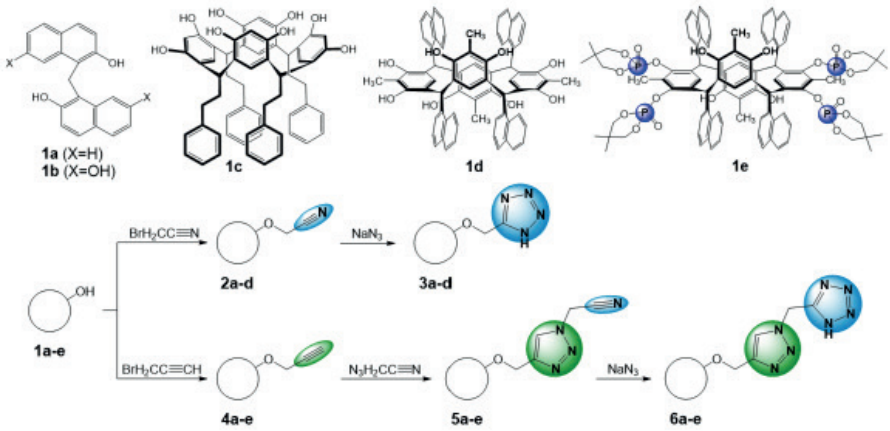
The pathways for successive modification of 1,1'-dinaphthylmethanes **1a,b**, *rccc* tetra-C-phenethyl-calix[4] resorcinarene **1c**, *rctt* tetra-C-naphthyl-calix[4]resorcinarenes **1d,e** were developed. In the result of their implementation the series of new polyazole derivatives differing in structure of polycyclic platform and containing some functional branches oriented in a certain way in space with tetrazole, triazole[1] 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*- (Cu^{2+}, Ag^{+}) and *f*- (Tb^{3+}, Yb^{3+}) metal cations was studied.

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

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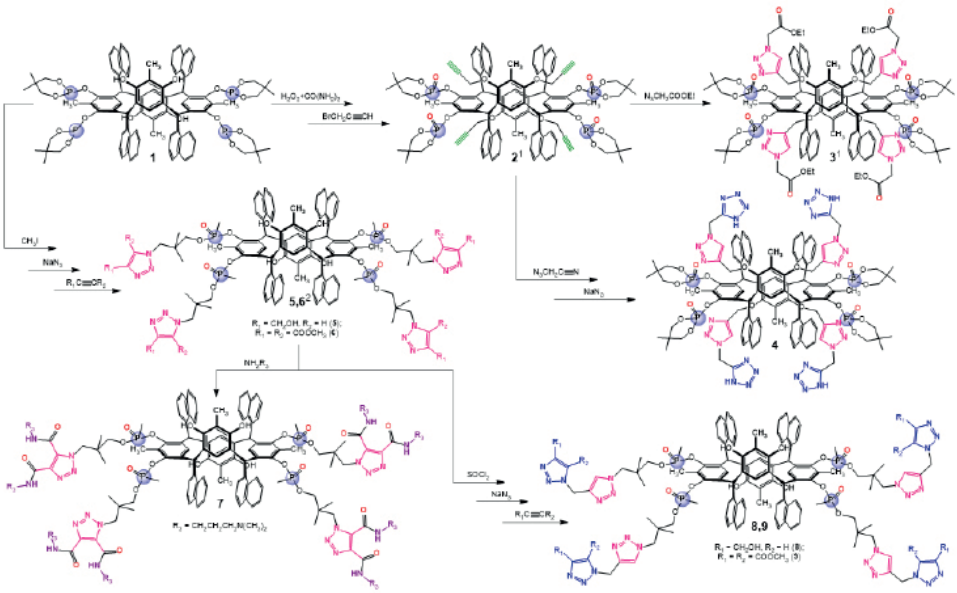
The approaches for synthesis of polytopic derivatives of *rctt ortho*-methyl-tetra-*C*-naphthyl-calix[4]resorcinare **1** containing active functional sites with predefined orientation relative to the macrocycle core were developed. Both considered routes based on use of bifunctional reagents with terminal 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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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),[1] instead of incineration, we propose the introduction of its methylene derivative (MDH)[2] into fine organic synthesis. The reaction of MDH with tethracyanoethylated 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,[3,4] according to the scheme presented below (Figure 1):

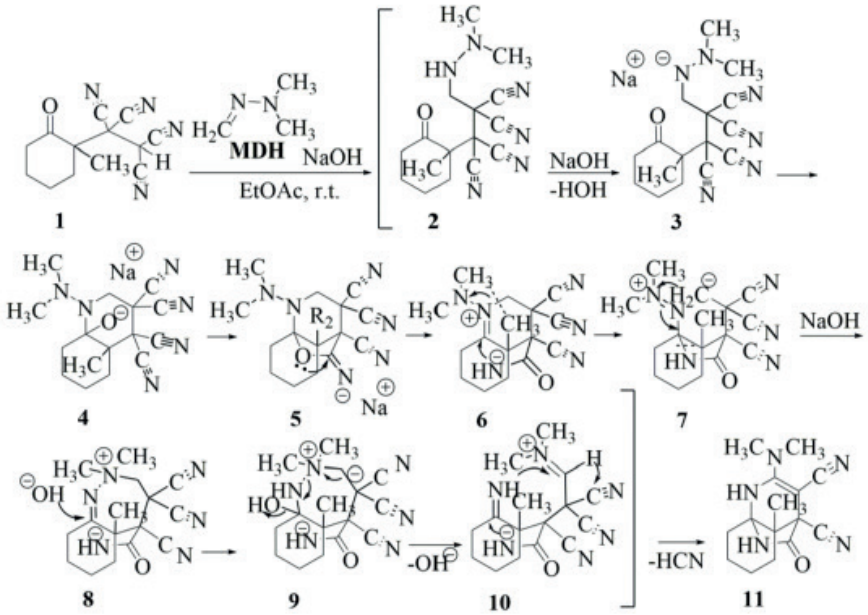

Figure 1. The proposed synthesis scheme is 8a,4-(epiminomethano)quinoline-3,4-dicarbonitrile

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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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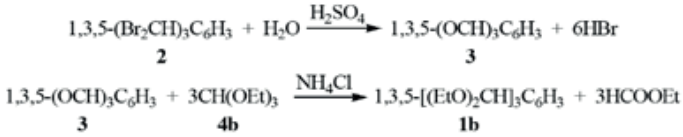
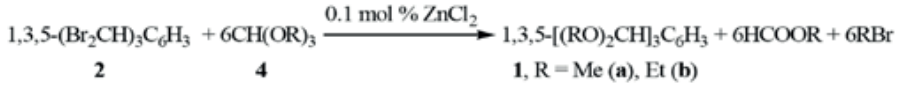
Aromatic polyaldehydes and their acetals are used in the preparation of bac-tericidal compositions for disinfection and sterilization. The work1 describes a two-stage method for the synthesis of 1,3,5-benzenetricarbaldehyde hexaethyl triacetal **1b**: 1) hydrolysis of 1,3,5-tris(dibromomethyl)benzene **2** into 1,3,5-benzenetricarbaldehyde **3** using an aqueous solution of sulfuric acid; 2) acetali-zation of aldehyde **3** with triethyl orthoformate **4b**.

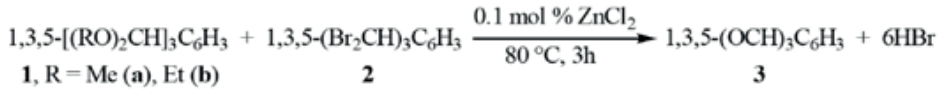


The disadvantages of the method are the use of sulfuric acid during the hy-drolysis of hexabromide **2** and the evolution of hydrogen bromide. They cor-rode the equipment. The goal of this work is to develop methods for the synthesis of compounds **1** and **3** that do not have the above disadvantages.

Previously, we developed a method for producing acetals directly from ben-zalhalides[2]. 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 $ZnCl_2$ at 80 ºC for **3** hours, an aldehyde is formed.



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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[1].

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[2].

The chemical analysis of the products was carried out using certain techniques[3]. 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_2SO_4	$CaSO_4$	Na_2CO_3	$CaCO_3$	H_2O	
E_1^4	24,38	0,911	20,29	–	54,4190	Te+Gb+ Br
E_2^4	28,42	–	30,14	0,0058	41,4342	Na·1+ Br +Pr
E_3^4	15,19	0,824	–	0,0067	83,9793	5Ca·Na·3+Gp+Cc
E_4^4	16,98	0,783	21,18	–	61,0570	Gb+ Br +5Ca·Na·3
E_5^4	–	0,544	33,72	0,0091	65,7200	5Ca·Na·3+Cc+Pr
E_6^4	–	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.

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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^{2+} in complex with 2,9-dimethyl-1,10-phenanthroline (CUPRAC assay) and on Fe^{3+} 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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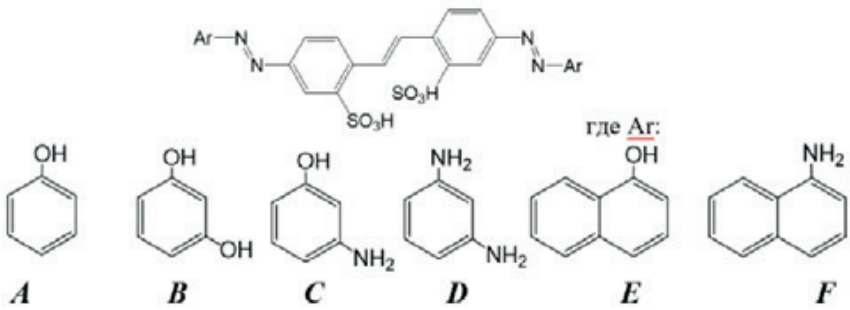
Using the Allium test plant test system based on the Allium cepa plant - onion (Stuttgarten variety), the mutagenic, mitosis-modifying and toxic effects of textile materials dyed with a number of known and new stilbene halochromic dyes, obtained during the study, were studied, intended for the manufacture 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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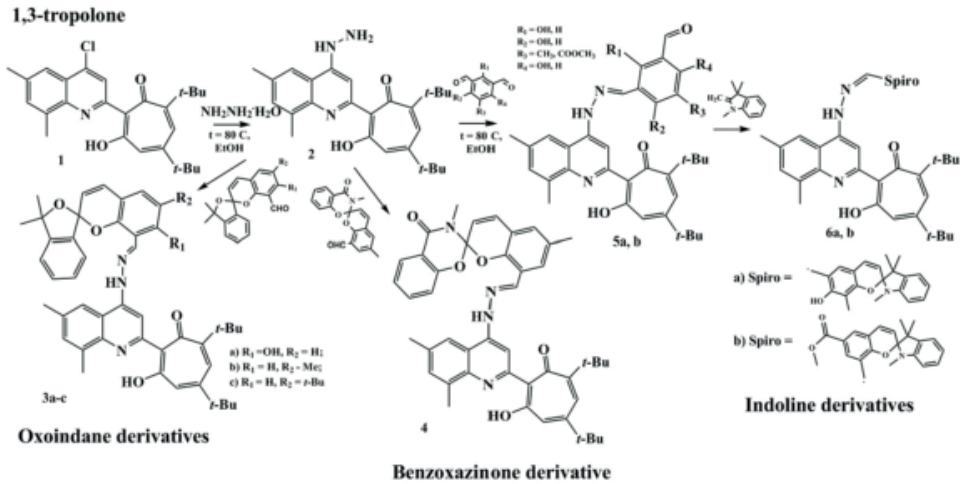
The targeted obtaining of medicines with therapeutic and diagnostic effects is an significant task of theranostics and set the challenge to chemists to synthesize molecular tandems based on photochromic and bioactive compounds.

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[1,2].



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

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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

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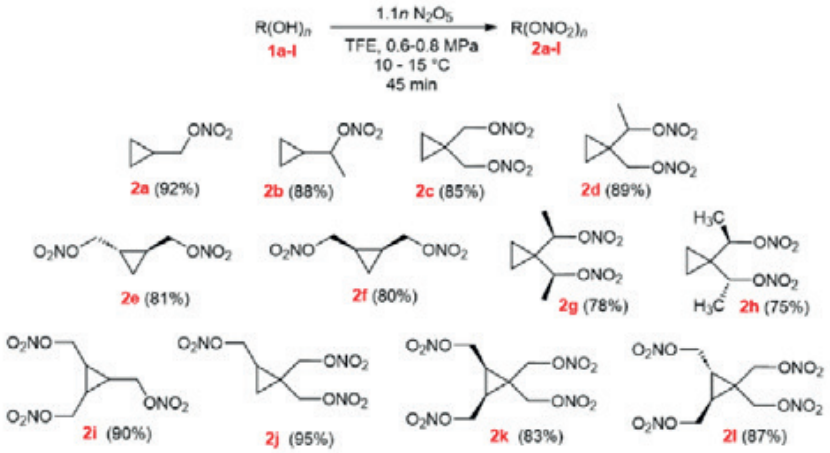
[c] M. V. Lomonosov Moscow State University, Leninskiye Gory 1, Moscow, 119991, RF

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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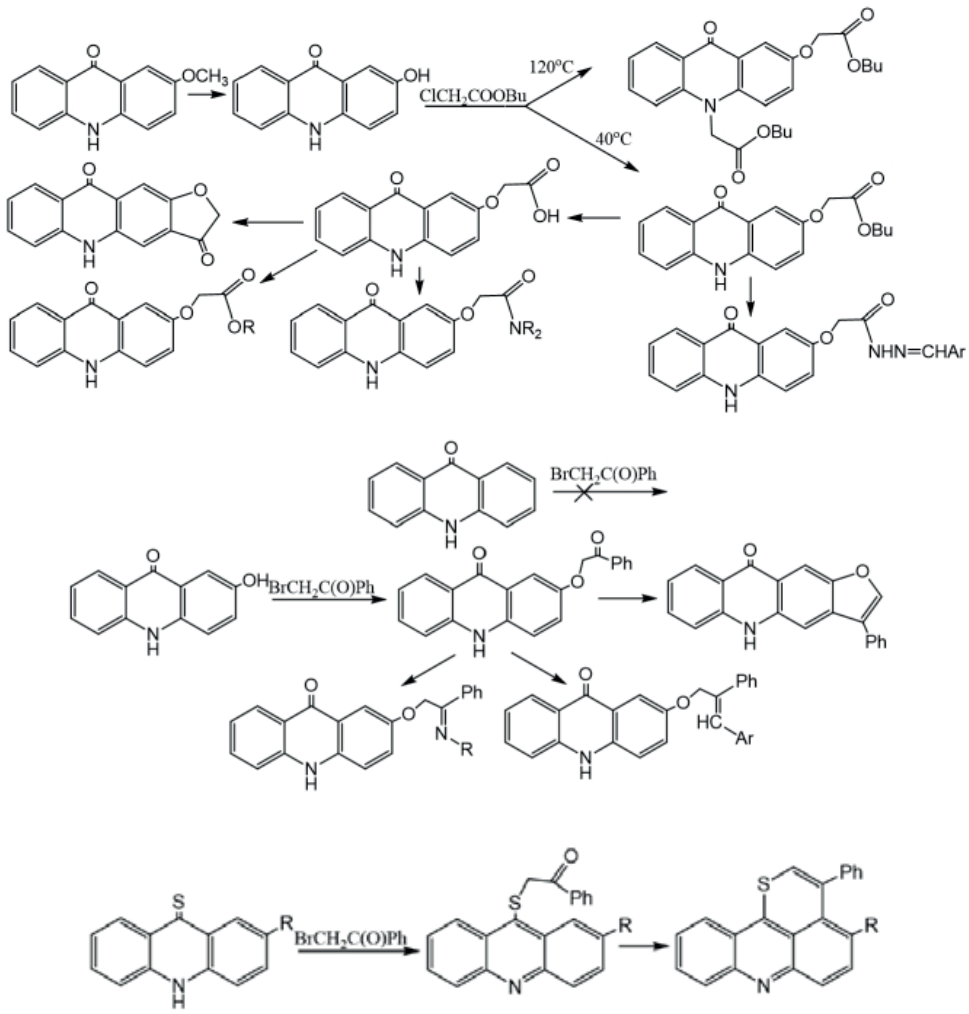
In order to synthesize new precursors for the production of biologically active compounds, the conditions for alkylation of 9-acridanone and its hydroxy derivatives, as well as 9-acridanione with butyl ester of monochloroacetic acid and phenacyl bromide were studied and optimized. For the obtained alkylation 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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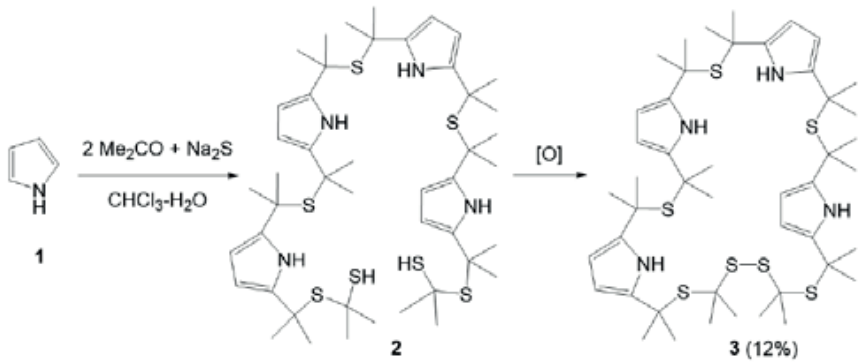
Porphyrin derivatives form supramolecular assemblies with proteins and are of interest as a therapy for cancer.[1,2]

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 ^{1}H, ^{13}C NMR.

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The work was carried out within the framework of the state assignment of the Institute of Scientific Research of the Federal Research Center of the RAS FMRS-2022-0079, 2022–2024.

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.[1]

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.[2] 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 $Ti(\eta^5:\eta^1\text{-}CpCMe_2CB_{10}H_{10}C)_2$ within the traditional Mulliken approach. Moreover, the vast majority of these methods describe well the molecular architecture and electric dipole moment of the complex.[3] 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.[1] The present contribution will be a reflection of on-going systematic research[2-8] 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. ($Eh_{\nu} \propto \Delta E_{redox}$), 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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The financial support under the state contract 124013000686-3 is gratefully acknowledged.

MONO-IMINOACENAPHTHENONE LIGANDS: RESEARCH TRENDS

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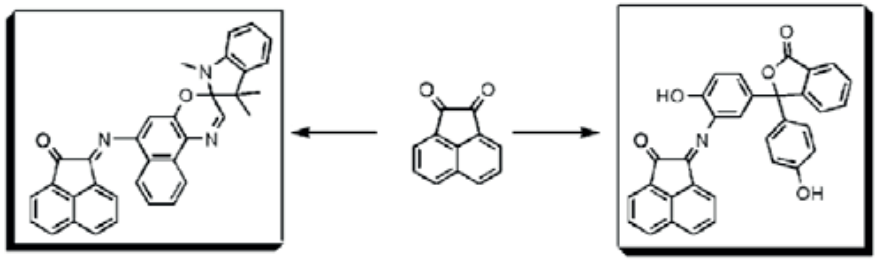
Mono-iminoacenaphthenones (Ar-MIAN) have been shown to occupy an intermediate position between o-quinones and 1,2-bis-iminoacenaphthenes (Ar-BIAN). Their properties, primarily steric and redox, are intermediate in this series.[1,2]

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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The work was carried out with the financial support of the Russian Science Foundation, project 23-23-00474.

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[1] (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[2]. These potential parameters were tested when calculating the properties of the gold macrocrystal in the article[3].

The following properties were calculated: Debye temperature (Θ), the first (γ) and second (q) Grüneisen parameters, elastic modulus (B_T), thermal expansion coefficient (α_p), product of $\alpha_p \cdot B_T$, heat capacity (C), specific (per unit area) surface energy (σ), derivative of the σ function over temperature ($\sigma'(T)$), and the melting point (T_m). The pressure derivatives of these functions were also studied: $\Theta'(P)$, $B'(P)$, $\alpha_p'(P)$, $C'(P)$, $\sigma'(T)$, и $T_m'(P)$. When calculating the functions σ, $\sigma'(T)$ and $\sigma'(P)$, the method from[4] was used, and when calculating $T_m(P)$ and $T_m'(P)$ – the method from article5 was used.

It was shown that under any P-T-conditions the following functions decrease under isomorphic-isothermal-isobaric reduction of the nanocrystal size: Θ, q, B_T, T_m. In doing so, the next functions increase: $\Theta'(P)$, γ, α_p, $|\alpha_p'(P)|$, $C(P)$, $|C'(P)|$, $|\sigma'(T)|$. It is shown that other properties: $\alpha_p \cdot B_T$, $B'(P)$, σ, $\sigma'(T)$, $T_m'(P)$, 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[1], an expression for the Lindemann parameter has been obtained. For a single-component crystal with an Einstein vibrational spectrum, it has the form:

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

where $<u^2>^{1/2}$ is the root-mean-square deviation of an atom in a crystal, $c = [6k_pV/(\pi N)]^{1/3}$ 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, Θ 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[2] 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 main focus in cluster research is on the structural approach. The random nature of these unstable formations has not been sufficiently studied. A general picture of the relationship of clusters with the main aggregate states of matter as a special subclass of crystal-mobile particles identified for the solid state with equilibrium defects of the crystal lattice was obtained. In liquid and gas, they take the simplest rounded shape with dense packing of particles with zero-crystalline dimensions in diameter, area and volume in comparison with structural totals – coordination numbers.

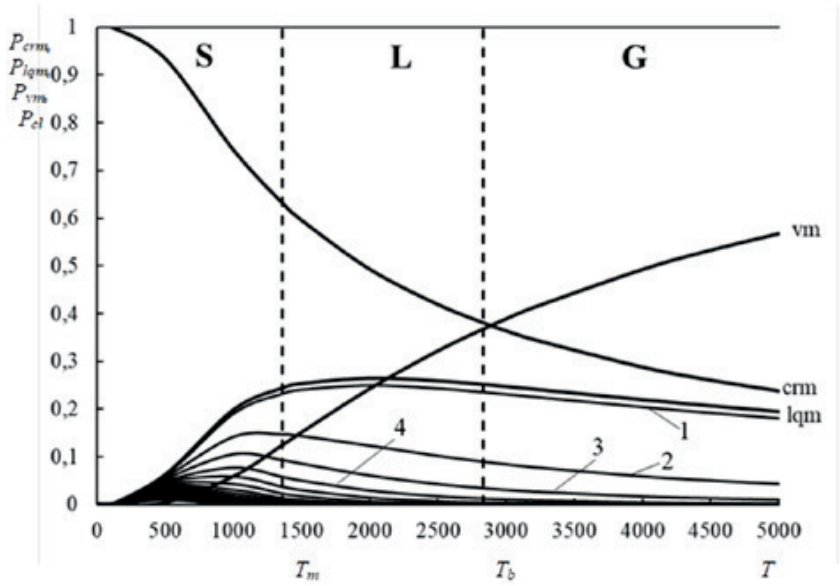

Figure. Temperature dependence of the fraction of crystal-mobile (crm), liquid-mobile (lqm), vapor-mobile (vm) and cluster (1, 2, 3, 4…) particles with a temperature shift of the maximum fraction of clusters.

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

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The Boltzmann distribution for the kinetic energy of chaotic (thermal) particle motion served as a tool for stochastic development of clusters; 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*-); author's distribution of clusters by the number n of *crm*-particles included in them $P_{cl,n} = (1 - P_{crm})$; 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 was used to interconnect all shares of chaotized particles[1] – P_{crm}, P_{lqm}, P_{vm} и 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.

1. .
2. .
3. .
4. .
5. $P_{crm} + P_{lqm} + P_{vm} = 1$.
6. .
7.
8. .
9. $P_{crm,m} = 1 - e^{-1} \approx 0{,}632$.
10. $s = s_n + R_n$.
11. .
12. $n_\rho = \ln\rho/\ln P_{crm}$.
13. .
14. .

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IRON(II) BROMIDE MONO(IMINO)ACEANTHRENONE COMPLEX

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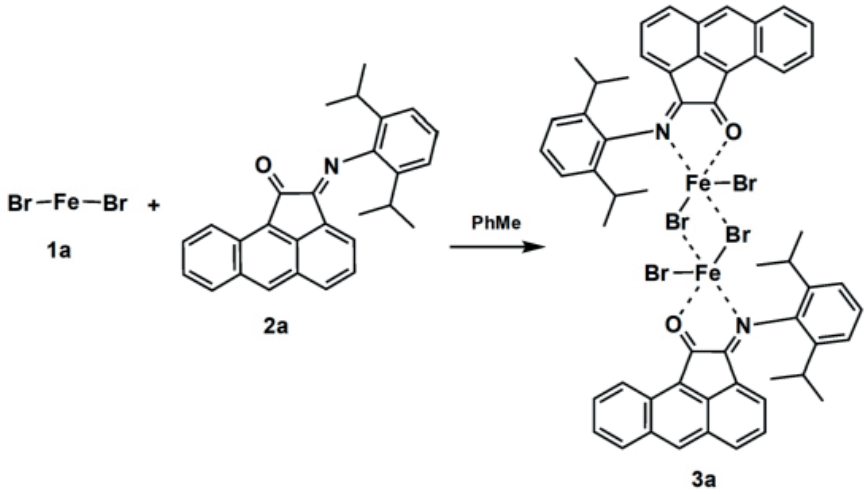
Iron(II) bromide (**1a**) reacts with (E)-2-(2,6-diisopropylphenylimino)aceanthrylen-1(2H)-one (**2a**) in toluene at 423 K (in a sealed degassed ampoule no traces of moisture) to form dark red crystals. According to X-ray diffraction data, coordination complex bis((2-(2,6-diisopropylphenylimino)aceanthrylen-1(2H)-one)irondibromide)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



The work was supported RSF (№ 23-13-00139) and carried out use "Analytical Center of the IOMC RAS", "Ensuring the development of the material and technical infrastructure of the centers for collective use of scientific equipment "(RF----2296.61321X0017, N 075-15-2021-670).

FULLERENE 2-ETHOXYETHYLPYRAZINE-2-CARBOXYLATES

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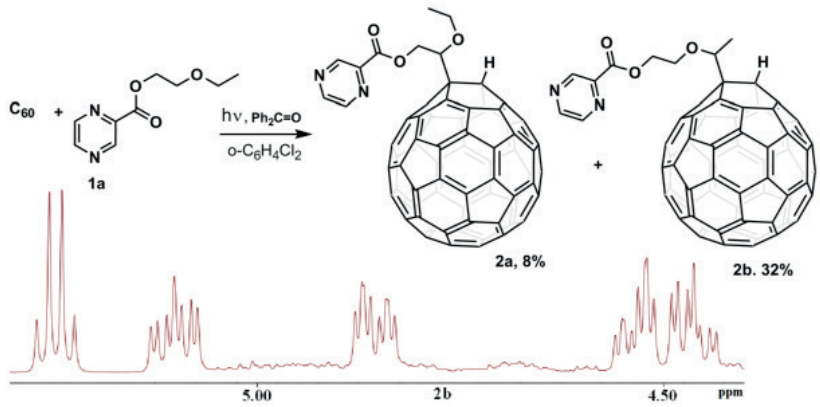
C_{60} reacts with 2-ethoxyethylpyrazine-2-carboxylate (**1a**) at the presence of benzophenone in o-dichlorobenzene at 293 K to form 1-(1-ethoxy-2-((pyrazine-2-carbonyl)oxy)ethyl)-1,2-dihydrofullerene (**2a**) and 1-(1-(2-((pyrazine-2-carbonyl)oxy)ethoxy)ethyl)-1,2-dihydrofullerene (**2b**). The CH_3 signal of **2a** (t, δ=1.56 ppm) and **2b** (d, δ=2.34 ppm, J=6.3 Hz) is shifted downfield compared to 1a (t, δ=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, δ=5.25 ppm) is in a stronger magnetic field compared to **2a** (dd, δ=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-caboxylate 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 H_3AsO_4 - H_2O 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 H_3AsO_4-H_2O are practically absent in literature. Therefore, to increase the yield of AsH_3 at electrochemical production from arsenic acid aqueous solutions, it is necessary to study the thermal properties in the system H_3AsO_4-H_2O. The measurements of the specific heat capacity of the H_3AsO_4-H_2O solutions by adiabatic calorimetry are presented in this work.

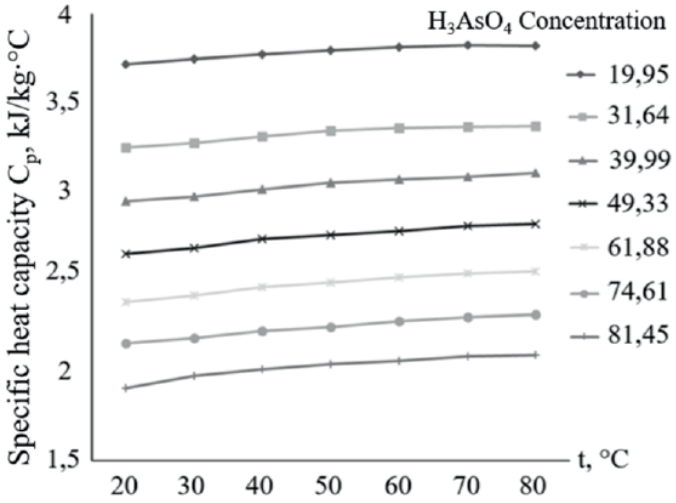

Fig. 1. Dependence of the specific heat capacity C_p of arsenic acid solutions on temperature at different arcenic acid concentrations, mas. %.

It has been found that the C_p of solutions in the H_3AsO_4-H_2O 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. % H_3AsO_4 increases as well as the heat capacity of water, which is characterized by a monotonic increase.

This work was supported by the Ministry of Science and Higher Education of the Russian Federation as part of the State Assignment of the Kurnakov Institute of General and Inorganic Chemistry of the Russian Academy of Sciences.

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-benzylmethylamine, 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.

This work was supported by the Science Committee of the Ministry of Science and High Education within the framework of the targeted funding program № BR21882220 "Synthesis and creation of technologies for fertilizers, compositions, preparations and materials of multifunctional action for use on desert and degraded lands" (2023-2025).

STUDY OF THE PHASE COMPLEX OF THE $Na,K||SO_4,CO_3,HCO_3,F\text{-}H_2O$ SYSTEM AT 25°C IN THE REGION OF VILLOMITE CRYSTALLIZATION

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The process of recycling liquid waste from industrial aluminum production[1] is determined by the regularities patterns of phase equilibria in the six-component water-salt system $Na,K||SO_4,CO_3,HCO_3,F\text{-}H_2O$, 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[2].

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 byo divariant fields[3].

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.

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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 ρ 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^3.

On the basis of the data obtained, the apparent molar values of Φ_c and Φ_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 $\overline{C^0_{p\,2}}$ and $\overline{V}_2^o$ are shown in the table.

$\overline{C^0_{p\,2}}/\overline{V}_2^o$	$X_{МП}$						
	0,00	0,10	0,33	0,50	0,75	0,90	1,00
NH_4Br	-67/42,9	-73/44,8	10/42,9	54/39,5	105/35,0	115/33,0	98/32,9
NH_4I	-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 $\overline{C^0_{p\,2}}$ J/mole·K and volumes $\overline{V}_2^o$ cm^3/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 $\overline{C^0_{p,i}}$ and volume $\overline{V^0_i}$ of alkali metal and ammonium ions in mixtures of N-methylpyrrolidone (MP)-water. The values $\overline{C^0_{p,i}}$ and $\overline{V^0_i}$ 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 NH^{4+} and Rb^+ ions, which means that the values of the other components are close, the difference in values $\overline{C^0_{p,i}}$ and $\overline{V^0_i}$ makes it possible to determine the contribution $\Delta_{sp.int.}C^0_{p,i}$ and $\Delta_{sp.int.}V^0_i$ of the ammonium ion for all compositions of the MP-water mixture.

	$X_{МП}$						
	0,00	0,10	0,33	0,50	0,75	0,90	1,00
$\Delta_{sp.int.}C^0_{p,i}$ ±10 J/mole·K	30	2	-7	-5	-8	-9	-28
$\Delta_{sp.int.}V^0_i$ ±1,0 cm3/mole	4,1	3,5	0,2	0,2	-0,7	-0,2	2,9

Table. The contribution to the values of $\overline{C^0_{p,i}}$ and $\overline{V^0_i}$ 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 NH^{4+} - solvent interactions is insignificant and noticeable only in two ranges of mixture compositions, where the values $\Delta_{sp.int.}C^0_{p,i}$ and $\Delta_{sp.int.}V^0_i$ exceed the error of their determination. In almost the entire range of $0,1<X_{МП}<0,9$ 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 $Na^+, Ca^{2+}, Al^{3+}//SO_4^{2-}, HCO_3^- - H_2O$

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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 $Na^+,Ca^{2+},Al^{3+}//SO_4^{2-}$, HCO^{3-}–H_2O 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[1]. Full information about the translation method can be seen in works [2].

The f ive-component mutual system $Na^+,Ca^{2+},Al^{3+}//SO_4^{2-}$, HCO^{3-}–H_2O at 273 K includes the following four-component systems with equilibrium solid phases at non-invariant points:

1) $NaHCO_3$-$Ca(HCO_3)_2$-$Al(HCO_3)_3$-H_2O: E_1^4=Nh+CaH+AlH.
2) Na_2SO_4-$CaSO_4$-$Al2(SO_4)_3$-H_2O: E_2^4 =Mib+Gp+Al·18.
3) $Ca^{2+},Al^{3+}||SO_4^{2-},HCO_3$-$H_2O$: E_3^4=Gp+CaH+ AlH; E_4^4=Gp+AlH+Al·18.
4) $Na^+,Al|^{3+}||SO_4^{2-},HCO_3$-$H_2O$: E_5^4=Nh+AlH+Mib; E_6^4=Mib+AlH+Al·18.
5) $Na^+,Ca^{2+}||SO_4^{2-},HCO_3$-$H_2O$: E_7^4=Mib+Nh+Gp; E_8^4=Nh+CaH+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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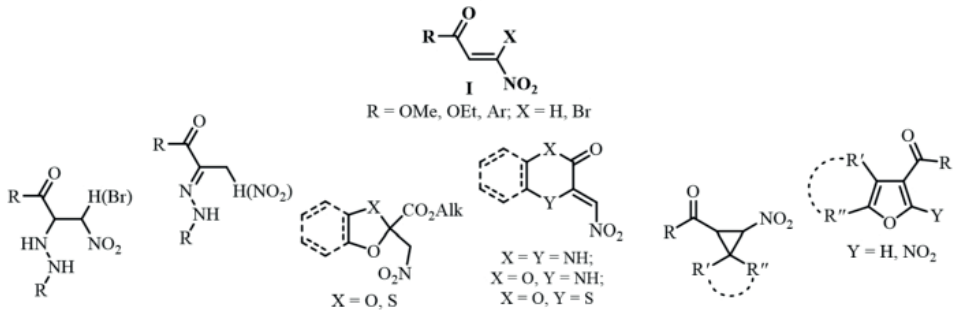
β-Carbonyl containing nitro- and *gem*-bromonitroethenes are highly reactive compounds that combine several electrophilic centers in their structure. They are interesting objects of theoretical organic chemistry, as well as convenient reagents for the synthesis of polyfunctional acyclic nitro compounds, as well as carbo- and heterocyclic structures.

We have studied the behavior of alkoxycarbonyl(aroyl)-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_2 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_2 or HBr and isomerization of the resulting C=C bond;
- elimination of HBr and heterocyclization via the Ad_N or S_N 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[1]. 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[2] (Fig. 1).

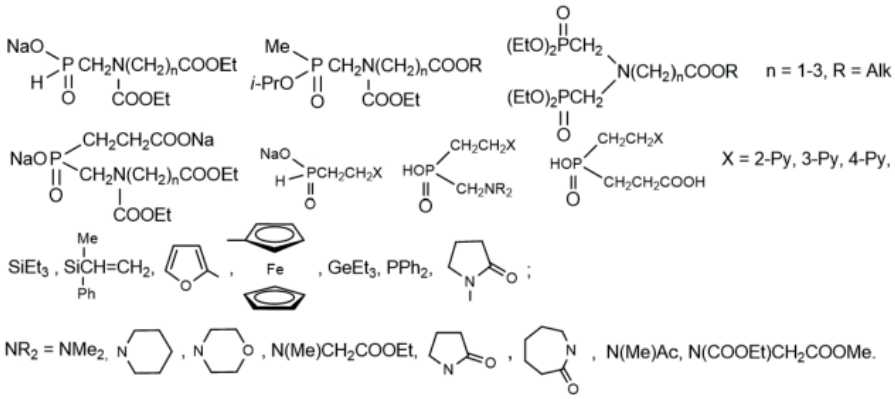

Figure 1. Functionalized phosphorus-containing amino acids and their analogues

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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[1]. 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, Γ_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»[2].

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

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

In the sample $SH_{HA + PEG\text{-}6000}$ due to a charge decrease during the interac-tion of –COOH groups with ethoxy groups of PEG, the n value decreases and the parameter increases. In the sample $SH_{HA + CG}$ both parameters de-crease due to an increase in the total charge of the macromolecule (–COOH and $–NH_2$ groups). In the sample $SH_{HA + PEG\text{-}6000 + CG}$ due to the larger molecu-lar 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 ad-sorption 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

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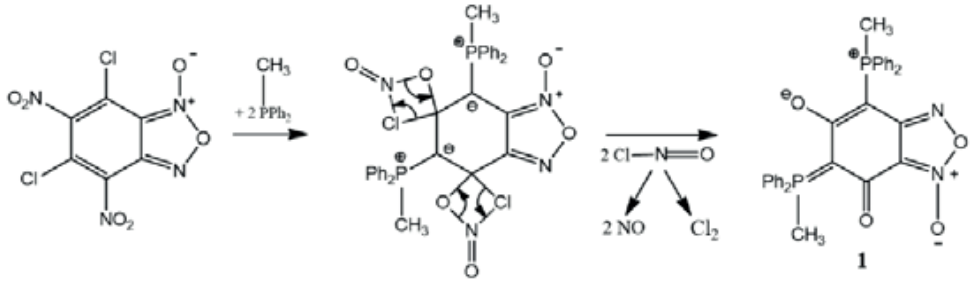
Reactions of tertiary phosphines: methyldiphenylphosphine, 1,2-bis(diphenylphosphino)ethane and 1,3-bis(diphenylphosphino)propane with 5,7-dichloro-4,6-dinitrobenzofuroxane proceed by nucleophilic aromatic substitution of chlorine atoms and nitro groups in the six-membered ring of the latter heterocycle. The structure of phosphorylation products has been proved by EPR, IR, NMR^{31}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 establishedethane and 1,3-bis(diphenylphosphino)propane, as shown in Figure 1.

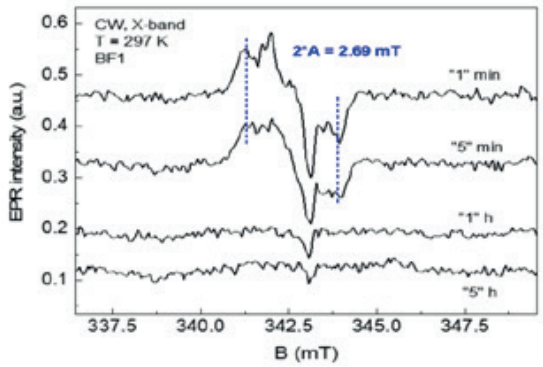


Figure 1. EPR spectral studies of reaction mixture of product 1 for 5 hours, bound NO radical and its parameters (Bruker Elexys E 580)

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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[1,2]. The present work is devoted to synthesis and consideration of structure and properties for a complex compound $[Pr(AAP)_6](ClO_4)_3$ (**1**) (AAP is 4-aminoantipyrine) in comparison with a preliminary studied $[Pr(AP)_6](ClO_4)_3$ (**2**) (AP – antipyrine). The complex compound (**1**) was prepared from $Pr(ClO_4)_3.6H_2O$ 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**) crystalizes in a trigonal system (sp. gr. *R*–3. $a = b = 13.9327(4)$, $c = 33.1320$ Å, $\alpha = \beta = 90$, $\gamma = 120°$, $V = 5569.9(3)$ Å^3) and is isostructural with the compound (**2**)[3], 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 $Pr(ClO_4)_3.6H_2O$. Elucidation of the cytotoxicity – composition – structure regularities for the mentioned compounds (**1**) and (**2**) are in progress[4].

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PHOSPHONIUM ENOLATES: KINETICS OF THEIR FORMATION AND APPLICATION IN ORGANOCATALYSIS

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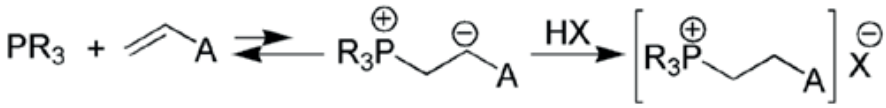
Phosphonium enolates are key intermediates of phosphine-catalyzed reactions.[1] The kinetics of phosphonium enolates formation in the reaction of tertiary phosphines with unsaturated electrophilic compounds was studied. The reactions are acid-dependent, and due to the short lifetime of phosphonium enolate 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 β-conjugated to α-umpolung addition.

For the activated alkenes with locked s-*cis* geometry, the effect of anchimeric assistance was determined.[2] 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 α-methylene-γ-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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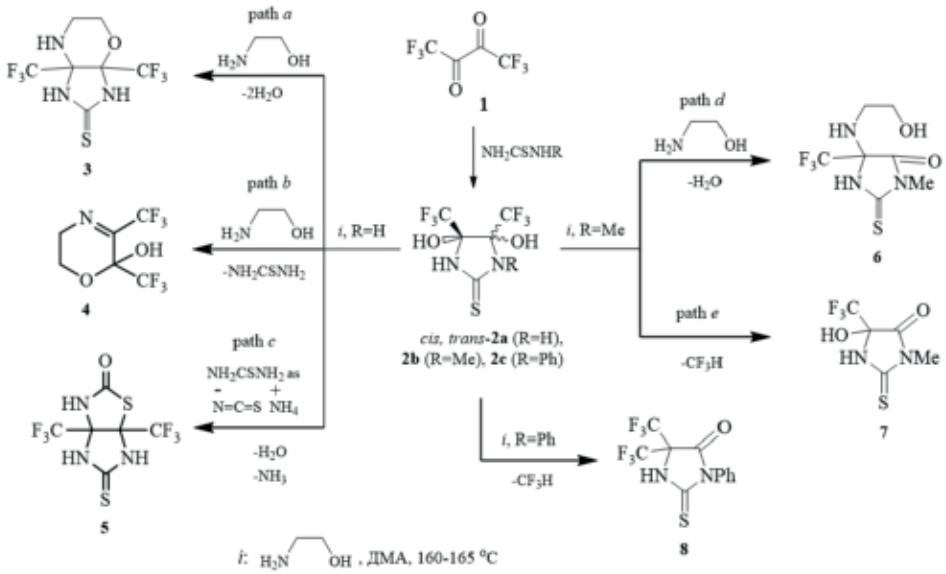
The reaction of perfluorobiacetyl **1** with thiourea (TU) and substituted TU produced imidazolidine-2-thiones **2a-c** (scheme 1). Unlike non-fluorinated analo¬gues, compound **2a**, when interacting with 2-aminoethanol (2-AE), gives only a small amount of the condensation product, imidazooxazine **3** (scheme 1, pathway *a*). The main product of the reaction is compound **5** (pathway *c*). When imidazoli¬dine 2b interacts with 2-AE, unexpected products are obtained: thioxohydantoins **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 AMINOALKYLTRIAZOLTHIOLS

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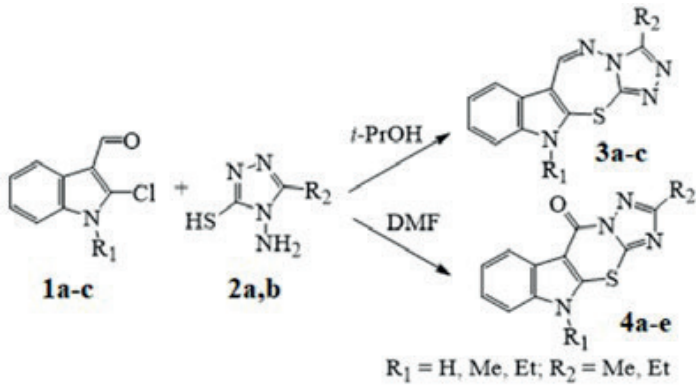
The indole system plays a key role in vital compounds such as hormones, alkaloids and proteins. Indole derivatives are widely used in medicine as antiviral, anti-inflammatory, antiemetic, antitumor agents, etc.[1,2]

To expand the range of such fused heterocyclic compounds with possible biological activity, the reactions of 2-chloro-indole-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) [1,2].



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** [1,2].

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

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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[1]. 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[2] 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^2
	Intensity	Efficiency	
Freundlich	n = 2,61	K_F = 12,8	0,9866
Langmuir	K_L = 2,46 дм^3/г	Q_e = 0,12 г/г	0,9729
Temkin	K_T =73,7	∞ = 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[3], 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^3 per 100 cm^3 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 coordi-nation 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 complex-ation is determined by a significant set of factors, the contribution of which is also very variable[1-2].

Complexation in ternary systems containing nickel(II) cations, polyamin-opolycarboxylate ligands (ethylenediaminetetraacetic Edta and diethylenetri-aminepentaacetic 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, electro-static interaction of protonated amine cations and Dtpa anions occurred with the formation of ion pairs which complicated the process of intraspher-ical 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, γ_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 γ_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[1]. It is shown that salts of ethoxyaminogumic acids, possessing the functions of an anionic, cationic and non-ionogenic surfactants, increase surface activity at NaCl concentrations up to 1.0 mol/l.

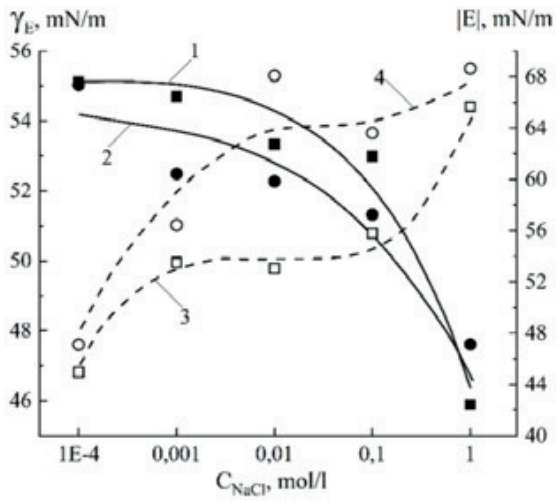

Figure. Effect of NaCl concentration on γ_E (1, 2) and |E| (3, 4) parameters of sodium ethoxy aminogumate solutions at the air interface, $SH_{HA+PEG-6000+urea}$ (1, 3) and $SH_{HA+PEG-6000+cyanguanidine}$ (2, 4).

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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.

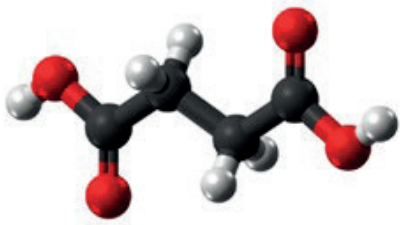

Figure 1. Chemical formula of succinic acid

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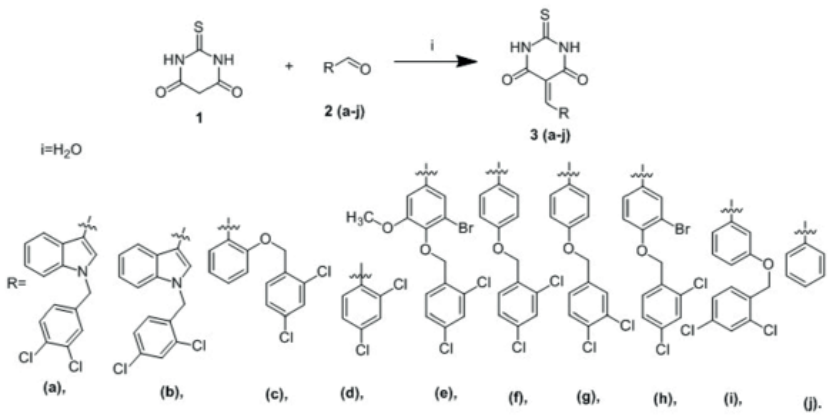
Thiobarbituric acid derivatives are widely used as active pharmaceutical ingredients of drugs. We have obtained new 5-substituted 2-thioxodihydropyrimidine-4,6(1*H*,5*H*)-diones **3 (a-j)** by reacting thiobarbituric acid **1** with the corresponding substituted benzaldehydes **2 (a-j)** by boiling in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

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

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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:

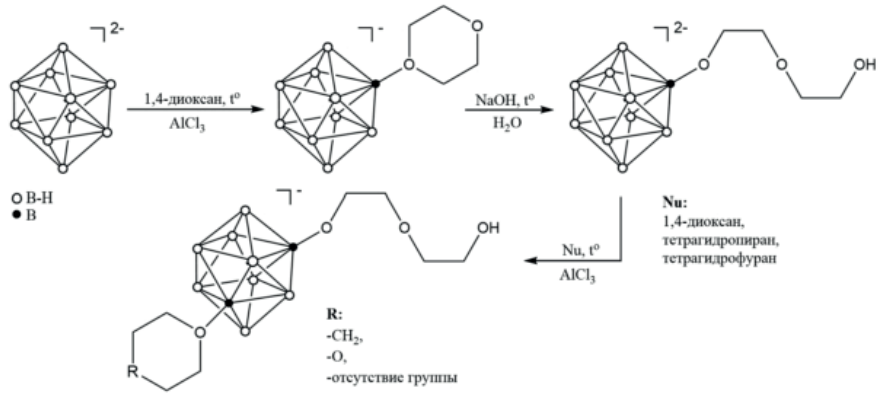

Fig. 1. Scheme of synthesis of heterofunctional disubstituted derivatives of anion $[B_{10}H_{10}]^{2-}$.

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

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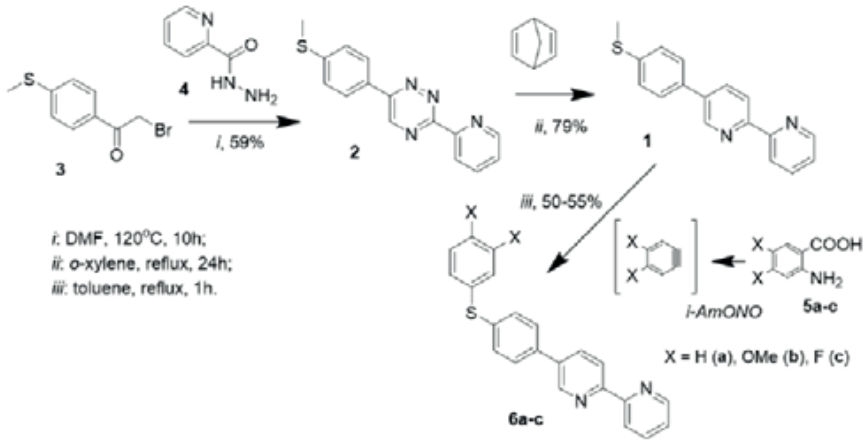
A convenient method for the preparation of 5-aryl-2,2′-bipyridines with para-arylsulfanyl group in an aromatic substituent was proposed. The synthesis was performed using in situ generated aryne intermediates without the use of complex experimental procedures and expensive reagents/catalysts. The structure 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 ^{1}H,^{19}F, and ^{13}C NMR spectroscopy, mass spectrometry, and elemental analysis. In addition, the structure of product 6a was additionally confirmed by X-ray diffraction data.

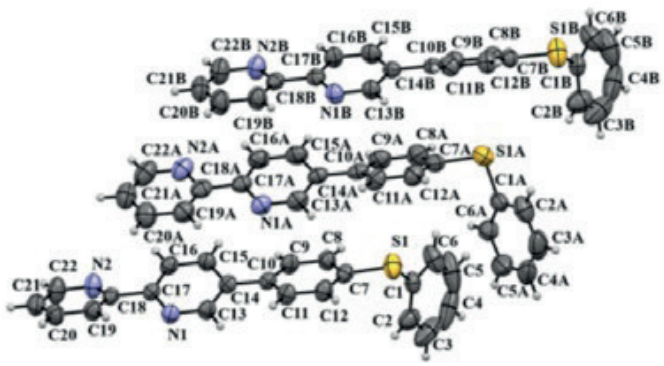


Fig. 1. General view of molecule of compound **6a** in crystal.

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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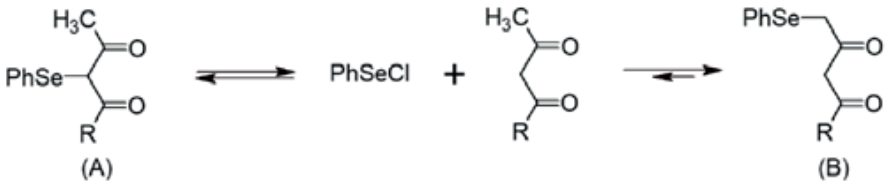
The reaction of PhSeCl with diketones having two reaction centers (at the central carbon atom and in the side substituent) occurs in both directions, with the first direction being predominantly realized. In the presence of releasing hydrogen chloride, the reaction is reversible and a dynamic equilibrium 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+ 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.[1]

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CYMANTHRENYLALKYL 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.[1] 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.[2]

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.

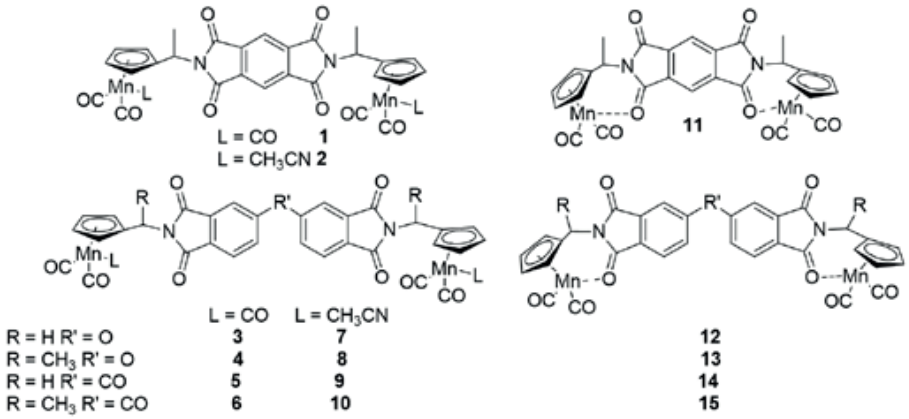

Figure 1. Complexes based on cymantrenealkyl diimides.

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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 $Zn(CH_3COO)_2 \cdot 2H_2O$ 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 C_2H_5OH:H_2O:HCl:sopanines 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).

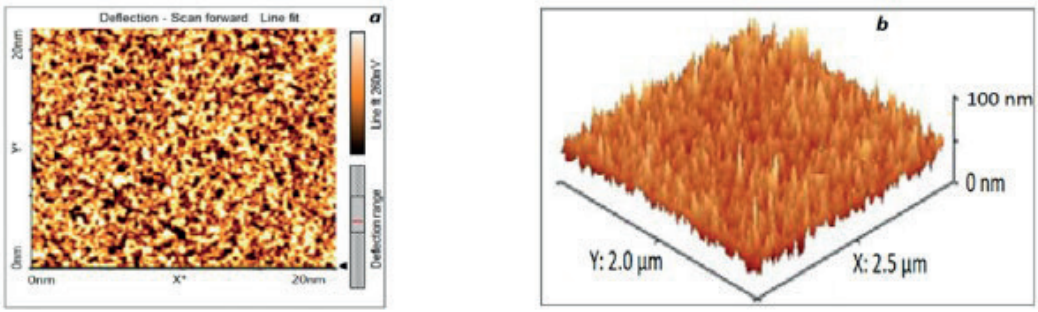

Fig.1. An atomic force microscope image of a ZnO film and its 3D view

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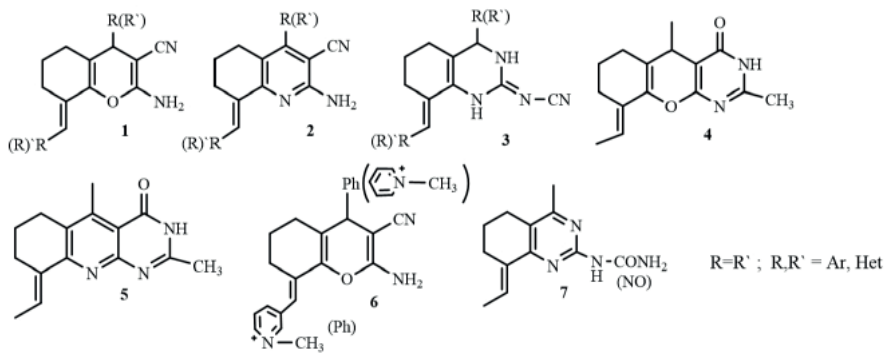
The "green chemistry" methodology is widely used in the design of hybrid "drug-like" systems, including key nitrogen- and oxygen-containing heterocycles.

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 heteroannelation 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[1].

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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Our research group is actively developing catalysts for the production of biodegradable polymers[1-2], as well as functionalized polymers[3] 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 ^{1}H and ^{13}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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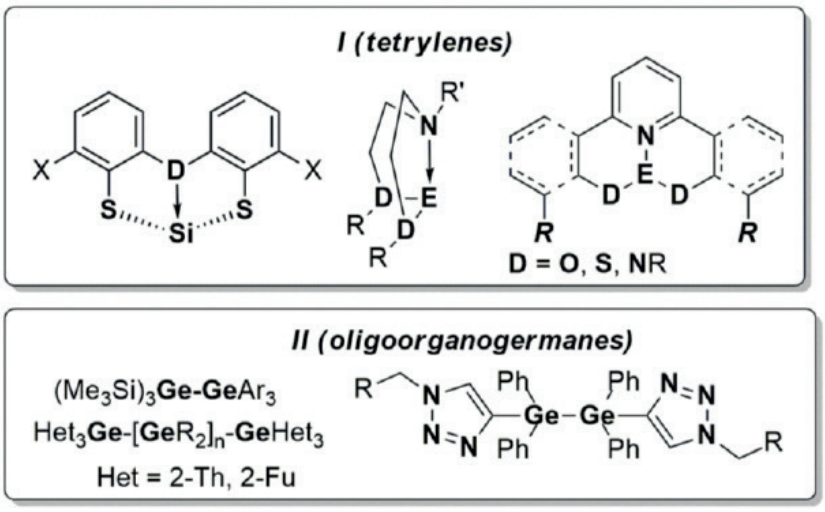
Nowadays, derivatives of Group 14 elements (E = Si, Ge, Sn),[1] intensively investigated worldwide, which is caused by both fundamental interest (possibility of synthesis) and their applications due to unique properties (catalytic, coordination, optical, semiconductor, synthetic, biological).

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



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

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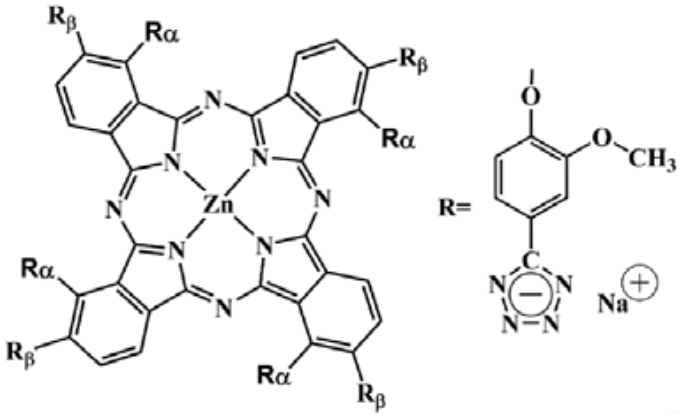
Metal phthalocyanines are potential photosensitizers for photodynamic therapy of cancer (PDT).[1] A limitation to the use of such macroheterocycles is their insolubility in water. A solution to this problem is the introduction of hydrophilic groups such as sulfo-, carboxy- or quaternary amino groups.[2] Tetrazoles, unique pharmacophoric heterocycles with high acidity, can act as a bioisosteric analogue of the carboxyl group.[3] 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	λ_{max} (log ε) (DMSO)	λ_{max} (log ε) (H_2O)	Φ_Δ (DMSO)	Φ_Δ (H_2O)	PD, % (DMSO)	PD, % (H_2O)
α-ZnPcR$_4$	702 (5.09)	697 (4.98)	64.07	76.74	8.02	5.07
β-ZnPcR$_4$	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 (λ_{max}), high quantum yields of singlet oxygen generation (ΦΔ) and a low percentage of photodestruction (PD), the synthesized compounds can be promising photosensitizers for PDT.

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Editorial [От и.о. главного редактора]

This book of abstracts is an abridged and corrected paper edition of the e-book of abstracts of the XXII Mendeleev Congress in seven volumes which is published on the official website mendeleevcongress.ru. The abridgement was made for quantities of report types, of sections and symposia, so this book has reports of two types, of one section. The correction was made, first of all, for post addresses in data of many reports. The minimum correction was made for the general Congress information and for headings of some reports: only the grossest misprints in headings were corrected.

This editorial's rest contains analyses, is in Russian below. In brief, due to the fact that the graphic design of the Congress raised questions in the community of Congress participants and beyond it and that these questions still remain unanswered, the acting editor-in-chief analyzes versions known to him, refutes them, puts forward and proves his own version. Thus, he proves that this design is entirely related to the modern state of the concept of periodicity which contains equations, with the most advanced type of Periodic Tables (PT), even if it is still not generally recognized as such. Thus, designers of the Congress recognized the permanent-radius variant of MLPT ('Multilayered' PT) as the most advanced type of PT rightfully and conveyed images of all six circular structures of this variant (based on the Pyykkö model) and its apparent dynamics artistically. It consists of just six circular structures of equal radii, with no gaps, with single-cell sectors, first combined in pairs (A+B, C1+C2, D1+D2) and then combined into the whole system to form the whole sequence of positions of chemical elements (E) in it, displayed mathematically by matrices consisting of E-positions. The structure of this MLPT variant can be represented as a flat ring or a circle. The acting editor-in-chief explains the black and coloured circular symbols of the Congress.

Данный сборник тезисов представляет собой сокращённое и исправленное книжное переиздание электронного англоязычного сборника тезисов докладов XXII Менделеевского съезда в семи томах, опубликованного на официальном сайте съезда mendeleevcongress.ru. Сокращение сборника в семи томах коснулось типов докладов и числа секций и симпозиумов съезда, так что в данный сборник вошли доклады только двух типов и только одной секции. Исправление коснулось, прежде всего, почтовых адресов научных учреждений многих докладчиков. В минимальной степени исправление коснулось заглавий отдельных докладов в части наиболее грубых опечаток. Улучшены вступительные разделы с общими сведениями о съезде.

Редакторское исправление не коснулось текстов тезисов докладов даже в части наиболее грубых опечаток. Попадание их в сборник в семи томах было связано, не исключено, с тем, что секция 1 съезда относилась к русскоязычным, так что англоязычный текст тезисов при наличии его русскоязычной версии оценивался Программным комитетом, не исключено,

менее внимательно. Графическое оформление настоящего сборника, по сравнению со сборником в семи томах, изменено.

Графическое оформление съезда в целом вызвало вопросы в сообществе участников съезда и за его пределами, и они до сих пор остаются без ответов. Преемственность графического оформления предшествующих съездов видна здесь далеко не во всём. Непонимание оформления, включая эмблему с чёрным кругом и видеозаставку (ВЗ) съезда на церемонии его открытия (mendeleevcongress.ru/video/), породило, помимо прочего, версии, порочащие замысел оформителей. Одна из чьих-то таких версий об эмблеме состоит в том, что это якобы малоизменённая сердцевина известного памятника Д.И.Менделееву и Периодической системе (ПС) в Братиславе, круг в проекции. Так, отсутствие в эмблеме окружения сердцевины памятника, то есть варианта ПС, созданного скульптором в виде «изящной дуги с лучами», якобы намекает на негативное отношение оформителей съезда ко всем непрямоугольным вариантам ПС. Сторонники версии видят даже такой аргумент в её пользу: цифры в эмблеме расположены углом в виде римской цифры L (50), а 50 лет – возраст памятника. Чья-то альтернативная версия состоит в том, что одноцветный круг эмблемы съезда рождён эмблемой НТУ «Сириус» с одноцветными кругами, а его чёрный цвет якобы символизирует ночной мрак – отражение мифа об открытии Д.И.Менделеевым ПС во время ночного сна. Так, цвет эмблемы якобы свидетельствует о восторженном отношении оформителей к широкому распространению красивых мифов об истории химии. Чья-то иная версия состоит в том, что чёрный круг – якобы нефть в чашке Петри (ЧП). Так, эмблема якобы намекает на то, что важность решения задач химии, связанных с нефтью, намного выше важности решения остальных задач химии и что иной взгляд на это осуждается. Это кем-то усматривается и в «превращении совмещающихся ЧП в ЧП с чёрным содержимым» (конечная стадия ВЗ). Ещё одна чья-то версия состоит в том, что в оформлении мы видим шары, а не круги или цилиндры, и это связано с событиями эпохи Менделеева начала XX в., когда господствовала атомная модель Томсона, а явление изотопии не было известно. Так, три совмещающиеся в ВЗ пары цветных шаров – это известные в те годы «аномальные в знаке изменения атомных масс» пары элементов Ar+K, Co+Ni, Te+I, а чёрный шар с портретом Менделеева – это символ любого элемента, «удовлетворяющего менделеевской формулировке Периодического закона». Сторонники этой версии оформления съезда упоминают научные события, описанные в литературе (Макареня А.А. «Д.И.Менделеев и физико-химические науки», изд. 2-е, М.: Энергоиздат, 1982, с.218): «*Безуспешны были попытки многих учёных исправить эту «нелепость». Многократно определялись атомные веса таких двойников, иногда ошибочно находили кажущееся соответствие «…». В 1905 г. Менделеев отказался от подобной нивелировки и решительно исправил принятые ранее и введённые в таблицу значения. Так, атомный вес аргона он исправляет с 38 на 39,9, никеля – с 59 на 58,7, теллура – со 127 на 127,6, йода – со 127 на 126,97*». Так, ВЗ и эмблема якобы намекают на

оправдание оформителями этой «нивелировки» экспериментальных данных, сделанной до 1905 г. и поддержавшей веру в общий закон, а чёрный цвет всех совмещённых элементов и эмблемы символизирует неразвитость атомной физики в то время – «тайну атомов, покрытую мраком». Целый ряд чьих-то иных версий приписывает замыслу оформителей завуалированную эпатирующую демонстрацию недопустимой символики, усматриваемой в строго чёрном фоне в круге, «напоминающем чёрную метку пиратов, их чёрный флаг», в белых очертаниях головы не в профиль в сочетании с белой цифрой X во главе угла из цифр в эмблеме. Так, один из намёков в эмблеме состоит якобы в одобрении смерти дискуссий вокруг научного вклада великого учёного или вокруг того, в какой момент истории Периодический закон стал по-настоящему законом. Потому эмблема якобы имеет целью напомнить устрашающую символику пиратских банд, соединений СС с костями в виде «X» (или без них) и черепом, которая и является недопустимой. «Чёрная метка» якобы не мнима и адресована сверхактивным участникам этих дискуссий. Такие намёки кем-то усматриваются и в превращении в чёрный круг совмещающихся цветных кругов (конечная стадия ВЗ). Создатели версий могут учитывать, что современные научные мероприятия не всегда защищены от неуместных намёков и демонстраций. Распространение этих версий без их опровержения может привести к частичному забвению съезда в мире, к ущербу репутации его организаторам и участникам, не осудившим это оформление.

Сторонники всех вышеприведённых версий оформления правы в том, что зрителя не удовлетворяет версия, связанная с доминирующим абстракционизмом: зритель желает разгадать загадку оформителей, связанную с химией. В связи с вышесказанным об оформлении и.о. главного редактора сборника (далее – редактор) приводит ниже собственный анализ с выводами, позволяющий полностью исправить ситуацию. В итоге он обосновывает собственную версию и в ходе анализа попутно делает вытекающие выводы о перечисленных выше версиях.

Вначале возникает вопрос, что мы видим в ВЗ – цветные геометрические круги, или же шары-элементы, или же ЧП с содержимым, образы которых угадываются в кругах. ЧП – символ биологии, а не химии. Если всё же допустить, что мы видим именно ЧП, то из ВЗ видно, что этих чашек шесть, их радиусы равны, каждая из них имеет парную: парные ЧП имеют плоскость симметрии, общую для всех пар. Также видно, что ЧП каждой пары устремляются к плоскости симметрии, происходит их «совмещение». Заметим, что настоящие ЧП, с содержимым или пустые, должны иметь высоту, но зритель видит её отсутствие, игнорируя иллюзорные тени. Далее, ЧП при использовании не вращают, но вступительная стадия ВЗ изображает их равномерное вращение, физически невозможное по ряду причин, что также говорит о том, что это не ЧП. Кроме того, «взвешенные тела, осадки и т.д.» в ЧП должны смещаться в результате быстрого движения ЧП, но и этого не видно. Наконец, невозможно

технически весь свободный объём в ЧП заполнить окрашенным раствором, вытеснив весь воздух, но при движении ЧП не видно признаков наличия газа в них. Значит, ЧП и их содержимое ненастоящие, мы видим цветные геометрические круги. При этом образ ЧП создан, видимо, лишь для того, чтобы зритель, «глаз которого лабораторный образ радует неизмеримо больше, чем математическая фигура», мог видеть такой образ в цветном круге. Вышеупомянутая «нефтяная» версия представляется сомнительной уже исходя из программы съезда, а выполненная часть анализа ВЗ склоняет к выводу об отсутствии настоящих «лабораторных тем» в оформлении, включая тему нефти в ЧП. Вышеупомянутая «элементная» версия оказывается при этом опровергнутой, так как шары отсутствуют: объём не виден, а содержимое не напоминает электроны Томсона.

Из ВЗ также видно, что из этих «совмещений» попарно цветных кругов образуется «совмещение» всех шести кругов, становящееся чёрным кругом с белыми очертаниями головы Д.И.Менделеева. Редактор излагает ниже основу собственной версии, чтобы сразу объяснить это.

Наиболее узнаваемым в мире открытием Д.И.Менделеева, имя которого с почтением носит съезд, является ПС (или PT – Periodic Table). Исходя из этого и из всей истории Международного года Периодической таблицы (IYPT, 2019 г.) предположим, что оформление нового съезда целиком связано с современным съезду состоянием учения о периодичности в химии, с наиболее совершенным видом ПС, пусть и всё ещё не общепризнанным в качестве такового. Так, по праву признавая наиболее совершенным видом ПС постояннорадиусный вариант MLPT (‘Multilayered’ PT), оформители съезда художественным путём передали образы всех шести круговых структур этого варианта (исходя из модели Пююкке) и его кажущуюся динамику. Он состоит как раз из шести круговых структур равных радиусов, не имеющих разрывов, с одноячеечными секторами, совмещаемых сначала попарно (A+B, C1+C2, D1+D2), а затем совмещаемых в единую систему с образованием единой последовательности позиций химических элементов (Э) в ней, отображаемой математически матрицами, состоящими из позиций Э. Круговую структуру этого варианта MLPT можно изображать как плоским кольцом, так и кругом. При общепринятой передаче разными цветами Э, относящихся к разным блокам (s-, p- и т.д.), единая система MLPT обнаруживает каждый цвет без разрывов в нём на плоскости, и этот факт упрощённо отражён оформителями окраской шести кругов, запоминающейся чётким разделением цветов, отсутствием разрывов в каждом цвете. Смешения Э и цветов в MLPT нет, но результат вышеописанного совмещения представлен в эмблеме именно как смешение цветов при растворении красок, и это оформительское решение вполне уместно. При помещении водорастворимых красок (красной, жёлтой, синей, зелёной и др.) в пробирку с водой цвет такого раствора стремится к чёрному, и поэтому, по проясняющемуся замыслу оформителей, совмещение всех шести кругов в MLPT становится именно чёрным кругом. Так, эмблема и ВЗ уже во многом объяснены. При этом белый цвет головы и надписей в круге

вызван необходимостью выбора цвета, контрастирующего с чёрным. Что касается ракурса белой головы не в профиль, то за этим, видимо, стояло желание заимствовать портрет, являвшийся частью официальной эмблемы Года IYPT. Заимствование новой эмблемой портрета той эмблемы – ещё одно свидетельство прямой связи новой эмблемы с темой ПС, причём на церемонии открытия съезда в историческом видео при упоминании XXI съезда (2019 г.) эмблема IYPT была показана в новом виде – в чёрном круге (на самом XXI съезде использовались лишь тёмный фон с «сеткой» ПС).

«Трёхцветный» вариант чёрной эмблемы (его смысл теснейшим образом должен быть связан со смыслом этой эмблемы) создан оформителями путём замены чёрного цвета цветовым переливом (синий, розовый, голубой цвета). По-видимому, это связано с получением MLPT широкой в мире известности, роста признания в мировом профессорском сообществе на IV Международной конференции по ПС «Mendeleev 150» (ИТМО, 2019 г.), оформление которой (как и церемонии открытия Года IYPT) включало эти три основных цвета, их перелив. Этот вариант эмблемы окончательно опровергает вышеупомянутые «нефтяную», «мифоцентричную» и «устрашающие» версии. «Скульптурная» версия опровергается уже тем фактом, что оформители выбрали всё же не тот портрет учёного, который запечатлён памятником. И даже дуга с Э в символике РХО им. Д.И.Менделеева, одного из организаторов съезда, говорит о том, что выражать негатив к непрямоугольным вариантам ПС никто не мог. Разрабатываемая же редактором версия находит лишь подтверждения, и их оставшаяся часть представлена ниже.

Возникает вопрос, почему эти три пары кругов выстроены оформителями не в одной плоскости (одна пара над другой, как в MLPT), а в параллельных плоскостях (одна пара впереди другой). Дело в том, что при создании ВЗ, очевидно, было технически проще изобразить «процесс совмещения» из такого построения: совмещённые пары кругов заслоняют одна другую для зрителя, и показ «процесса последующего совмещения» пар становится необязательным. Вопрос о выборе оформителями цветов этих кругов – ненастоящего содержимого ненастоящих ЧП – объяснён выше не полностью: связь с MLPT видна, но видны и отличия. И они находят объяснения. Так, именно для зрелищности цвета «жидких сред» в разных ЧП сделаны разными, причём близкими к цветам квадратов (полос спектра) в эмблеме IUPAC. При этом цвет «содержимого» в ЧП сделан белым, и это соответствует цвету букв в квадратах эмблемы IUPAC. Раскрыть загадки деталей ВЗ подчас трудно и не всегда важно, но связь с MLPT можно усмотреть везде: даже в музыкальном сопровождении к ВЗ «M-L-P-T» угадывается многократно, как ничто другое. Во вращении же кругов (вступительная стадия ВЗ) можно усмотреть следующее: структуры MLPT «переместятся в целом в направлении, на которое указывает это вращение», но на деле никаких движений в MLPT нет, зритель это знает, так что оформители, добавляя любую вымышленную ими динамику в ВЗ, не

обманывают зрителя. Кроме динамической ВЗ, оформителями создана и статическая ВЗ (она показана в кратких «видеоотчётах» об отдельных днях съезда и т.д.). Она состоит из быстро сменяющих друг друга изображений этих шести кругов, сменяемых в конце эмблемой съезда. Это художественный образ MLPT без кажущейся динамики. Подтверждение своей версии редактор видит и в том, что в конце церемонии открытия руководителем съезда академиком Цивадзе А.Ю. было рассказано об истории признания ПС в научном мире, триумфе ПС, об инициировании проведения Года IYPT. Эта тема, очевидно, была намеренно выбрана для освещения её непосредственно перед моментом открытия съезда. Далее, ПС – наиболее узнаваемое в мире российское открытие в области химии, так что для празднования 300-летия РАН в рамках международного химического съезда весьма логичен выбор символики, изображающей ПС (пусть и не самый известный вариант ПС). Наконец, открыто связывать символику съезда с научными открытиями одного из докладчиков – редактора данного сборника – могло быть, возможно, не вполне дипломатичным жестом по отношению к остальным докладчикам, потому символика съезда и оставалась загадкой. Чтобы усложнить разгадку, всё остальное оформление, включая мелкие детали ВЗ, сборник из семи томов, сайт съезда в целом, территорию, где проходил съезд, и т.д., было выполнено с доминированием абстракционизма. При этом возможно, что идея «подобрать круг для эмблемы съезда из мира химии» возникла изначально при взгляде на эмблему НТУ «Сириус».

Что же касается самого доклада редактора, который уже был утверждён Программным комитетом съезда, когда вся данная символика съезда ещё не была опубликована и, по всей видимости, ещё не была создана (сайт съезда имел полностью иное оформление), то этот новаторский доклад окончательно превратил наиболее современное учение о периодичности в химии, включающее MLPT, в высокоразвитое учение. Он размещён на странице 20, перепечатан крупным шрифтом для облегчения чтения ниже (Appendix). Мы видим, в докладе структура MLPT не подверглась пересмотру (пересмотру подверглись теоретические основы логического выделения Nu-частиц). Сохранение всех представлений об MLPT при дальнейшем развитии учения о периодичности в докладе, не исключено, могло послужить дополнительным вдохновляющим фактором для создания нового оформления съезда, которому и был посвящён данный разбор.

Редактор будет признателен читателям за замечания, предложения, благодарности за максимальную защиту авторских прав докладчиков, просит направлять их по адресам istinayubukayev@yandex.ru, istinayubukayev@yahoo.com (Yury V. Bukayev – Букаев Юрий Вячеславович).

The acting editor-in-chief will be grateful for criticisms, offers, thanks for the maximum defending of authors' rights, he asks to send them to addresses: istinayubukayev@yandex.ru, istinayubukayev@yahoo.com.

Yury Vyacheslavovich Bukayev, the acting editor-in-chief

Appendix [Приложение]

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[1-3]. The new model (M) is based on a limitation (L) of time of looking (t_L) after R-nuclei (Ñ) of an element (E), on a substitution of nuclei Ñ, which didn't decay during a certain t_L, by nuclei-equivalents (NE). R doesn't have NE-decays even during $t>>t_L$: the NE-nature is other. There is a conclusion by Prof. M. Bunge[2] 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 Ñ which decayed during t_1, s_{1-2} – during $(t_1;t_2]$, there is no decay in Δs during t_2. So A in s_1, s_{1-2} are with Ñ, in Δs – with their NE. For $t<t_0$ it's an exact prognosis of P. "The statistics increases" by a large k of parallel P: $s_0=s_{0,1}+..+s_{0,k}$, etc.

Further, Ñ, its NE are collectives of p^+, n^0. Their charges are[2] 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 Ñ 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}N consists of A with Ñ (Q=Z=7), A with NE (Q=7, Z=0). A in s_1+s_{1-2} consist of nitrogen atoms, A in Δs – 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}N, have electrons and chemistry (EC) of N, Nu-a from ^{30}F have EC of F, etc. Nu-positions (Nu-p) from ^{25}N are in gr.15, in periods 1-7. Nu-p in PT are minor[1,3].

R with not little $T_{1/2}$ have $s_1+s_{1-2}\approx 0$. Their A in Δs 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_{IUPAC}-cells, so for its P-zone[2] [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[1], V.A.Funtikov[4], J.P.Cid Ugalde et al. recognized it as innovation.

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ВЫЯВЛЕНИЕ Т-ФАКТОРОВ ПРИ ВЫДЕЛЕНИИ Nu-ЧАСТИЦ

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Описан новый угол зрения на стабильный (S) и радионуклид (R), важны следствия[1-3]. В основе модели (М) – ограничение (L) времени наблюдения (t_L) за R-ядрами (Ñ) элемента (Э), замена ядрами-эквивалентами (NE) ядер Ñ, не распавшихся за данное t_L. Распада NE у R нет и за $t>>t_L$: природа NE иная. О пользе таких М и теорий – вывод проф. М. Бунге[2,с.38]. Из описания выпадут лишь R с особо малыми $T_{1/2}$: Э не выпадут. Для простых R-частиц (А) в камере есть наглядный процесс (П) с L в $t=t_2$: $t_0=0$ – начало ионизации A^0 потоком и автовыключение его источника, t_1 – начало рекомбинации $A^+ + e^-$, t_2 – её конец и автозапуск новой химстадии. При $t=t_2$ сумма А в П – $s_0=s_1+s_{1-2}+\Delta s$: s_1 – с Ñ, распавшимися за t_1, s_{1-2} – за (t1;t2], в Δs распада нет за t_2. Потому А в s_1, s_{1-2} – с Ñ, а в Δs – с их NE. При $t<t_0$ это точный прогноз П. Большим k параллельных П «набирается статистика»: s0=s0,1+..+s0,k , и т.д.

Ñ и его NE – коллективы p^+, n^0. Их заряды равны[2] Q=Z+q, где Z – общий заряд «реальных R-» (RR) p^+ коллектива (они могут обрести изменённый коллектив (ИК) или превратиться), q – «эквивалентных R-» (ER) p^+ его (не могут ни то, ни другое). Все p^+ у ядра Ñ – RR: q=0, Q=Z. У его NE – ER: Z=0, Q=q. Далее, у одних R (где $T_{1/2}$ малы) при $t=t_2$ $s_1+s_{1-2}>0$. Так, m(А ^{25}N) – из А с Ñ (Q=Z=7), А с NE (Q=7, Z=0). А в s_1+s_{1-2} – из атомов азота, А в Δs – из Nu(-a) – атомов нульбеккерелия (Z=0 – признак, а Nu – символ Э с 0 Бк): у Nu-a, выделенных так из ^{25}N, электроны и химия (ЭХ) азота, у Nu-a из ^{30}F ЭХ фтора, и т.д. Позиции (Nu-п) Nu, выделенного из ^{25}N, – в гр.15, в периодах 1-7. Nu-п в ПС младшие[1,3]. У прочих R ($T_{1/2}$ не малы): $s_1+s_{1-2}\approx 0$. И их А в Δs состоят из Nu. Nu – изо всех Э с учётом Т-факторов (t_L,$T_{1/2}$ у R).

Формула Q=Z+q верна и для S: его «реальные S-» p^+ не обретают ИК, не превращаются, «эквивалентных» p^+ нет, q=0, Q=Z. NE и Nu нет. Далее, раз Nu из R – и в пустые ячейки $ПС_{IUPAC}$, то в её П-зоне[2] [Z=1; Z=56]: $G_{(pas. groups\ in\ a\ period)}=Z+D_{(pas.\ rel.\ positions)}-18N_{(group\ rep.\ pas.)}$. Новаторство признали профессора Степанов Н.Ф.(МГУ)[1], Фунтиков В.А.(БФУ)[4], Cid Ugalde J.P.(USaCh) и др.

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