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**Editors:** Nodar Lekishvili, Professor, Doctor of Chemical Sciences  
Ioseb Chikvaidze, Professor, Doctor of Chemical Sciences

**Executive secretary:** Khatuna Barbakadze, Doctor of Chemistry

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## A B S T R A C T S

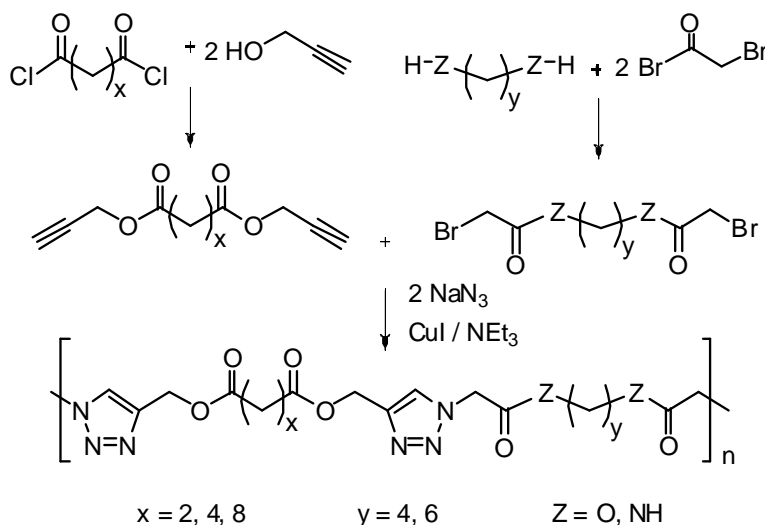
### SYNTHESIS OF NEW BIODEGRADABLE “CLICK” POLYMERS BEARING 1,2,3-TRIAZOLE RINGS IN THE BACKBONE

**Tengiz Kantaria\*, Temur Kantaria, Nino Kupatadze, Nino Zavrashvili,  
David Tugushi and Ramaz Katsarava**

Institute of Chemistry and Molecular Engineering, Agricultural University of Georgia, Kakha Bendukidze University Campus, # 240 David Aghmashenebeli Alley, Tbilisi, Georgia;

\*t.kantaria@agruni.edu.ge

The use of click chemistry in polymer science is a quickly emerging field of research. The copper(I) catalyzed azide–alkyne cycloaddition (CuAAC) click reaction has already been exploited for the synthesis of end-functionalized polymers, block copolymers, cyclic polymers, dendrimers, cross-linked materials, etc. Surprisingly, there are only few papers on the application of CuAAC click reaction in step-growth polymerization (SGP) as a chain propagation reaction, and, to our best knowledge, there are limited publications on the synthesis of aliphatic triazole-linked AA-BB-type ester polymers by CuAAC click SGP.



**Scheme 1.** Synthesis of 1,2,3-triazole containing polyesters and poly(ester amide)s

In the present work we have carried out a systematic study for optimizing the CuAAC c SGP reaction for the synthesis of clicking polyesters in terms of solvent, catalyst, catalyst's activator (ligand), monomers concentration, duration and temperature of various steps of one pot reaction. Comparing the clicking polyester's molecular weights and yields the best parameters for the click SGP

were found as: a solvent - N-Methyl-2-pyrrolidone, a catalyst – CuI, a ligand –  $\text{NEt}_3$ , a monomers concentration – 0.6 mol/L, duration of bis-azide formation step – 3 h (at room temperature), duration of SGP – 15 h, temperature of the click SGP reaction – 0° C. The established optimal conditions of the CuAAC-based SGP reaction was applied to the synthesis of a series of high-molecular-weight ( $M_w$  up to 73,000 Da) 1,2,3-triazole cycles-containing “clicking” polyesters and poly(ester amide)s (Scheme 1) which reveal improved thermal properties compared to their regular analogues. The new polymers are promising for practical applications in medicine, agriculture, and food industry as biodegradable (bioresorbable) materials, as environmentally friendly biomaterials, etc. Furthermore, one of the important advantages of the developed CuAAC click SGP is the possibility of quaternization of 1,2,3-triazole cycles of the resulting polymers which opens a way to cationic polymers – both water soluble ones and cross-linked cationic hydrogels promising for numerous biomedical applications.

**Acknowledgement:** This work was supported by the joint grant № 6298 from the Science and Technology Center in Ukraine (STCU) and Shota Rustaveli National Science Foundation of Georgia (SRNSF).

## ANTIMICROBIAL COATINGS BASED ON BIOACTIVE NANO PARTICLES

**Kh. Barbakadze<sup>1,2,3\*</sup>, G. Lekishvili<sup>1</sup>, B. Arziani<sup>1</sup>, N. Lekishvili<sup>2</sup>, W. Brostow<sup>3</sup>**

<sup>1</sup>Tbilisi State Medical University, Faculty of Pharmacy, Department of Medical Chemistry  
33, Vazha Pshavela., 0186 Tbilisi, Georgia; \*kh.barakadze@tsmu.edu

<sup>2</sup>Institute of Inorganic-Organic Compounds and Nontraditional Materials, Faculty of Exact and Natural Sciences, Tbilisi State University, 3, Ilia Chavchavadze Ave., 0179 Tbilisi, Georgia;  
nodar.lekishvili@tsu.ge

<sup>3</sup>Laboratory of Advanced Polymers & Optimized Materials (LAPOM), Department of Materials Science and Engineering and Department of Physics, University of North Texas, 3940 North Elm Street, Denton TX 76207, USA; www.unt.edu/LAPOM/; wkbrostow@gmail.com

The effects of pathogenic microorganisms constitute global hazards for humanity and the environment. These microorganisms appear in natural systems and form complicated aggregates on the surfaces of various natural and synthetic polymers resulting in irreversible deterioration and non-controlled biodegradation that cause significant economic losses to industry and pose serious threats to cultural heritage (historic monuments, archeological patterns, museum exhibits, etc.) as well [1, 2].

An important option in mitigation biodegradation is in formation of polymerbased hybrid materials, taking advantage of the best properties of each component, decreasing or eliminating their drawbacks, and achieving synergic effects. Low scratch and wear resistance and also environmental degradation have hindered many important applications and long-term performance of polymer materials [3, 4].



Thus, it is essential to achieve prolonged maintaining of their physical and mechanical properties (isothermal aging stability, strength, tribological characteristics, etc.) in operational conditions. Improved features which affect on the operational characteristics of the hybrid materials will reduce the risk of bio-damaging caused by biodestructors and effectively provides inhibition of growth of harmful microorganisms on materials surfaces and allow their applications as functional coatings, adhesives, membranes, optics, fuel and solar cells, sensors, medical products and materials, etc. [4].

The main concept of the following research consisted in creation of bioactive hybrid materials against wide spectrum of biodestructors. For creation of “*Short-time*” active composites polyurethanes were selected as a base of polymeric matrix of inorganic-organic hybrid materials. Silicon-organic oligomers act as plasticizers and improve elasticity, thermal stability, hydrophobicity of polymers. They also improve forming homogeneous films and adhesion of the composites to various substrates [5]. Thus, polyorganosiloxanes with functional groups at silicon atom were used for modification of basic polymers. As a bioactive components were chosen micro- and nano-sized particles of available biogenic metals (antimony, arsenic).

Thermophysical properties of the obtained polymer composites and corresponding antimicrobial coatings were studied by the differential scanning calorimetric (DSC) and thermogravimetric (TGA) analysis methods. All materials studied are amorphous, melting transitions are not visible. Almost all hybrids have glass transition regions beginning in the range between 49 and 58°C. This is important for the use of coatings for protection of museum exhibits since the optical clarity at room temperature and above is assured. Thermal stability of the modified hybrids increases with respect to the pure polymeric matrices. Herewith resistance to thermal degradation is enhanced and weight loss is shifted to higher temperatures as the amount of polyorganosiloxanes increase and further is improved by addition of bioactive components.

Tribological properties of hybrids are related to their composition. The sliding wear (SWD) of the samples was determined by multiple scratching along the same groove at a constant force using a micro scratch tester. The modification mainly causes gradual decrease of sliding wear with respect to pure polymers, improvement of viscoelastic recovery (75-90%), lowering of dynamic friction and also increasing of hydrophobicity. Progressive scratch testing with linearly increased load (1.0 N-30.0N) was performed to study scratch resistance of researched materials. As was shown, modification does improve scratch resistance depending on the modifier type and quantity with respect to pure polymers.

The study of surface morphology of obtained composites (SEM) confirmed that by modification wear resistance of polymer composites is increased. Thus, it is possible to achieve both lower friction and a higher scratch resistance with definite concentration of modifiers.

Created antimicrobial polymer materials show improved mechanical, tribological and thermal properties and provide the prolonged exploitation of the protected materials and wares. This on the other hand will economize material resources. Herewith elimination of unfavorable factors which affect on the operational characteristics and surface morphology of the hybrid materials reduce the risk of bio-damaging caused by biodestructors and effectively provides inhibition of growth of harmful microorganisms on materials surfaces.

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## BRITTLINESS AND FLEXIBILITY OF POLYMERS DEFINED BY EQUATIONS

**W. Brostow<sup>1\*</sup>, H. Faltynowicz<sup>2</sup>, O. Gencel<sup>1,3</sup> and N. Hnatchuk<sup>1</sup>**

<sup>1</sup>Laboratory of Advanced Polymers & Optimized Materials (LAPOM), Department of Materials Science and Engineering, University of North Texas, 3940 North Elm Street, Denton, TX 76207, USA

\*wkbrostow@gmail.com; hnatnm@gmail.com; konradb09@gmail.com

<sup>2</sup> Faculty of Chemistry, Wrocław University of Science and Technology, ul. Gdańska 7/9, 50-344

Wrocław, Poland; hanna.faltynowicz@pwr.edu.pl

<sup>3</sup>Department of Civil Engineering, College of Engineering, Bartın University, Bartın 74100, Turkey;

osmangencel@gmail.com

For a long time polymers and polymer-based materials (PBMs) were described qualitatively using terms such as „brittleness“ and „flexibility“. We have defined brittleness  $B$  of polymers and PBMs as follows [1, 2]:

$$B = 1/\varepsilon_b E' \quad (1)$$

where  $E'$  is the storage modulus determined in dynamic mechanical testing [2] and  $\varepsilon_b$  is the tensile strain at break at the same temperature.

In 2019 we have also defined polymer flexibility  $Y$  by an equation [3]:

$$Y = V_{sp}/(\sum_i^n U_{bi}) \quad (2)$$

Here  $V_{sp}$  is the specific volume of a given polymer in  $\text{cm}^3/\text{g}$  at a specified temperature while  $\sum_i^n U_{bi}$  is the sum of the strengths of bonds in the monomer.

Connections of both B and Y to a variety of properties have been demonstrated and will be discussed at the Conference.

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## **BIODEGRADABLE NANOPARTICLES BASED ON PSEUDO-PROTEINS FOR OCULAR DRUG DELIVERY**

**Tem. Kantaria<sup>1</sup>, W.. Zhang<sup>2</sup>, Ten. Kantaria<sup>1\*</sup>, N, Eter<sup>2</sup>, P. Heiduschka<sup>2</sup>,  
D. Tugushi<sup>1</sup>, R. Katsarava<sup>1</sup>**

<sup>1</sup> Institute of Chemistry and Molecular Engineering, Agricultural University of Georgia  
Tbilisi, Georgia

<sup>2</sup> Research lab of the Department of Ophthalmology, University of Münster Medical School  
Münster, Germany; \*tkant2015@agrni.edu.ge

Drug delivery in case of chronic eye diseases, such as age-related macular degeneration, glaucoma and diabetic retinopathy remains a challenge, as these diseases are becoming increasingly prevalent in the aging population [1]. Ocular barriers make it difficult to deliver effective drug concentrations to the back of the eye when non-invasive routes such as topical or systemic administration are taken [2]. Only very low drug concentrations are achieved in the retina and choroid after topical administration due to the short retention time of drops on the ocular surface, the presence of tissue barriers (cornea, conjunctiva, etc.), and the aqueous flow inside the eye [3]. One way to achieve drug delivery that is investigated currently is topical administration of drug-loaded polymeric nanoparticles (NPs) that are able to penetrate ocular barriers. The purpose of this study is optimal preparation of NPs made from pseudo-proteins and evaluation of their ability to penetrate ocular tissues.

Pseudo-protein based biodegradable NPs of various types were prepared by nanoprecipitation of the polymer composed of L-leucine, 1,6-hexanediol and sebacic acid (8L6). Arginine-based cationic polyester amides 8R6 and comb-like polyester amide containing lateral PEG-2000 chains along with 8L6 anchoring fragments in the backbones were used to construct positively charged and PEGylated NPs. They were loaded with fluorescein diacetate (FDA) or rhodamine 6G (Rh6G) as fluorescent probes. Suspensions of the NPs were given to cultivated microglial cells and RPE cells as well as topically on eyes of C57BL/6 mice. Penetration of NPs into the eyes was checked by fluorescence analysis.

Fluorescently tagged NPs were prepared, and their properties were characterized. Cultured microglial cells and RPE cells took up the NPs. After topical administration, penetration of NPs into the cornea of the eyes could be clearly shown. Small amounts of fluorescent dyes were also found in the lens, the retina and the sclera depending on the type of NPs. The results show that the new pseudo-protein-based NPs penetrate ocular tissues after topical administration and are internalized by the cells. This raises confidence that the NPs may be useful carriers of therapeutic agents for ocular delivery.

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## WEATHERING OF GREENHOUSES PLASTIC FILMS IN DIFFERENT EXPOSURE PERIODS

**A. Abdelhafidi, S.F. Chabira, N.H. Benmiloud, Y. Wassima, M. Sebaa**

University of Ammar TelidjiLaghouat; Mechanics laboratory (Ime); Algeria

\* abdelhafidiasma@yahoo.com; s.chabira@lagh-univ.dz; nh.benmiloud@lagh-univ.dz  
w.yagoubi@lagh-univ.dz; sebaamed2014@gmail.com

Analysis of the IR spectra of weathered films exposed at different periods of the year reveals that, the main regions of the IR spectrum affected by solar irradiation and temperature variation are the complex carbonyls and unsaturations composite absorption bands. Their respective kinetics vary in different manner according to the period at which the exposure is started. Curve fitting has been performed to refine the analysis of the IR spectra and to identify all the chemical species constituting the complex absorption bands.

The analysis of the results let appears that whatever the exposure period of the year is, it does not affect the type of developing products, but it has strong effect on their kinetic rate of formation. The warm season is the more effective in terms of carbonyl formation and crystallinity index. This indicates that the Norrish type I (NI) process is very important in this season and it adds to the Norrish type II (NII) process. Both contribute to the carbonyl and vinyl groups formation via chain scission reactions; however, the NII process is active during all the period of the year.

## **NEW APPROACH TO STOP GLOBAL WARMING** **(New Planet Technology of the Green Revolution)**

**R. Gakhokidze**

Iv. Javakhishvili Tbilisi State University, 3, Ilia Chavchavadze Ave., 0179 Tbilisi, Georgia  
ramaz.gakhokidze@tsu.ge

Global warming – the biggest and most serious problem we are facing in this century – is the phenomenon due to which global temperatures are increasing. During the last century the temperature of the Earth increased by one degree. Global warming affects everyone living on the Earth, as it is happening right now all around us. Global warming effect can cause serious damage to cities and towns, as extreme weather is becoming more and more a problem because of strong hurricanes and tornadoes, droughts and flooding occur. The increase in temperature caused the melting of ice and, accordingly, the rise of the level of the world ocean. Together with global warming, the risk of destruction of living organisms sharply increases. Global warming consequences, including the loss of life, economic disruption and population dislocation are growing each year. We can no longer afford to ignore global warming. It is a serious problem that needs to be stopped. One of the reasons for climate changes is the growth of the amount of carbon dioxide causing the so-called greenhouse effect.

Many methods and concepts of dealing with preventing carbon dioxide from entering the atmosphere have been proposed. The projects for saving the world from global warming are being actively carried out all over the world. According to one of the mentioned projects, the disposition of millions of 60cm diameter lenses around the Earth will cause the reflection of sun rays and, accordingly, the decrease of sun radiation. Pursuant to another project, across the Earth the layer of cosmic vessels or small particles should be created, which should cover the tropics and this will result in climate softening. But for the realization of this project colossal sums of money are required: 500 billion dollars are needed for the disposition of cosmic spaceships and in the case of small particles from 6 to 200 trillion dollars are required [see R. Gakhokidze, *The Problem of Global Warming and Ways for its Solution*. In: *Priorities of the Sustainable Development of Agriculture*, Tbilisi, TSU Press, 2012].

Concentration of carbon dioxide in the atmosphere is naturally regulated by numerous processes. The movement of carbon between the atmosphere and the land is dominated by natural processes such as plant photosynthesis. While these natural processes can absorb some of the net 6,1 billion metric tons of anthropogenic carbon dioxide emission produced each year, an estimated 3,2 billion metric tons is added to the atmosphere annually. The Earth's positive imbalance between emission and absorption results in the accumulation of carbon dioxide in the atmosphere.

Due to the increase of the chlorophyll level and intensification of photosynthetic activity, one of the most effective results of Biorag use is the acceleration of growth and development of plants (e.g. of wood plant by 4-5 years) and growth of the total size of leaf surface by 482%, whereas, according to the literature data, that parameter is only 15-17%. With the use of

bioenergyactivators on 1 million hectares, up to 30 million tons of carbon dioxide will be removed from the atmosphere by green plants each year. According to the literature data, in the same area the evasion of only 1 million ton of carbon dioxide is possible (<http://www.kiev.trade.gov.pl.uk/download/life/f.9149/>).

## **ADSORPTION PROCESSES IN SORBENTS**

**T. Marsagishvili\*, M. Machavariani, G. Tatishvili, Z. Samkharadze**

Iv. Javakhishvili Tbilisi State University, R. Agladze Institute of Inorganic Chemistry and Electrochemistry; Georgia 0186 Tbilisi, 11 Mindeli Str.

\*tamaz.marsagishvili@gmail.com

The development of modern technology requires the creation of materials with specified properties. The development of sorbents, which are one of the most important elements for many industries and for environment protection, also belongs to this type of tasks.

The manufacture and use of sorbents require a clear understanding of what tasks the sorbent will be designed for. We will consider more or less general approaches for describing processes that occur when using sorbents. First of all, a sorbent is a solid body with many channels and cavities through which liquid with impurity particles, atoms, molecules, ions can flow. Deposition (adsorption) of particles from which it is necessary to clean this liquid, takes place on the walls of channels and cavities.

As a rule, the liquid that must be purified from impurities is polar. The liquid enters the channels and cavities of the sorbent either under the influence of gravitational forces, or using high pressure from an external source. In both cases, during the movement of the liquid in the channels and cavities of the sorbent, sedimentation (physical or chemical adsorption) of impurities takes place on the walls of the channels and cavities of the sorbent.

Within the framework of the general quantum theory of particle adsorption on a solid surface, the probability of the corresponding process can be calculated.

In the framework of the given project the following tasks will be realized:

1. Adsorption and desorption processes on the solid surface;
2. Charge transfer processes from adsorbed particle on solid surface;
3. Effects of frequency dispersion of the solid in the kinetics of the charge transfer processes;
4. Effects of spatial dispersion of the solid in the kinetics of the charge transfer processes;

Solution of these tasks allows search of the new methods of description of mesoscopic materials and processes on the surface and depth of these materials. Solid may be described by the polarization field, description will be quantum. The properties of the solid will be defined by correlation functions (quantum-statistical average values at nonzero temperature) of polarization operator.



**Results:**

1. Analytic expressions for probability of adsorption or desorption processes, as with formation (bond rupture) of the chemical bond – chemical adsorption, so without formation of the chemical bond – physical adsorption, on the surface of the solid for adsorption and desorption processes will be obtained. Analytic dependences of characteristic parameters of the processes on the temperature, distribution of the electronic density on the adsorbable particles and close to the solid surface, vibration spectrum of adsorbable particle, etc. will be obtained.
2. Analytical expressions for the rate constant of the process will be obtained for the charge transfer processes from the adsorbed particle to solid surface. The analytic dependences of the characteristic parameters of the processes on the temperature, distribution of the electronic density on the adsorbable particles and close to the solid surface and on the particle from which (on which) takes place charge transfer, vibration spectra of adsorbable particle and particle-reagent, etc. will be obtained.
3. Effects of frequency dispersion of the solid in the kinetics of the charge transfer processes. Realization of investigation of atomic-molecular transformation on the solid surface with consideration of quantum character of the charge transfer during these transformations is not possible without considering frequency dispersion effects of the researched solid. The effects of frequency dispersion will be taken into account in terms of absorption spectrum of the solid.
4. Effects of spatial dispersion of the solid in the kinetics of the charge transfer processes. Model functions for polarization operators' correlation functions of the solid will be suggested for taking into account of spatial dispersion effects. The kinetic parameters of the charge transfer process will be calculated with taking into consideration these model functions.

**OBTAINING OF SOME FUNCTIONALIZED POLYMERS AND MATERIALS WITH SPECIFIC PROPERTIES BASED ON THEM**

**N. Lekishvili<sup>1\*</sup>, Kh. Barbakadze<sup>2</sup>, W. Brostow<sup>3</sup>**

<sup>1</sup>Iv. Javakhishvili Tbilisi State University, Institute of Nontraditional Compounds and Inorganic-Organic Materials, Faculty of Exact and Natural Sciences. I. Chavchavadze Ave., 3, 0179 Tbilisi, Georgia; \*nodar@lekishvili.info

<sup>2</sup>Tbilisi State Medical University, Faculty of Pharmacy, Department of Medical Chemistry, 33, Vazha Pshavela Ave., 0186 Tbilisi, Georgia; kh.barakadze@tsmu.edu

<sup>3</sup>Laboratory of Advanced Polymers & Optimized Materials (LAPOM), Department of Materials Science and Engineering and Department of Physics, University of North Texas, 3940 North Elm Street, Denton TX 76207, USA; www.unt.edu/LAPOM/; wkbrostow@gmail.com

One of the applicable functionalized fluorine-organic polymers and poly(oligo)organosiloxanes are developed. The general regularities of their obtaining and reaction conditions are established.

The synthesized polymers and oligomers are used for production of various important technical compositions and materials with specific properties: polymer varnishes, antimicrobial, antibiocoorrosive and anticorrosive coatings, water-repellents, hydrophobizers and other materials with specific properties. They are also successfully used as modifiers of the other organic and element-organic oligomers, polymers and materials on their basis.

The phase transition temperatures of some elaborated materials are determined. Their thermal stability, water resistance and tribological properties are studied.

In this report also are discussed practically more important and technologically justified methods for obtaining of polyfunctional siliconorganic oligomers and polymers with various structures of main chains.

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## **LiMe<sub>x</sub>Ni<sub>0.5-x</sub>Mn<sub>1.5</sub>O<sub>4</sub>-type COMPOUNDS AS PROMISING CATHODE MATERIALS FOR Li-ION BATTERIES**

**E. Kachibaia, T. Paikidze, Sh.\*Japaridze**

R. Agladze Institute of Inorganic Chemistry and Electrochemistry at Ivane Javakhishvili Tbilisi State University Tbilisi, Georgia; 11 Mindeli str. 0186, Tbilisi, Georgia; \*japaridzeshukri@yahoo.com

Nowadays, almost all portable electricity operated equipment has reached significant success due to development of Li-ion batteries. Their application has led to improved (increasing) performance of mobile phones, laptops, cameras, etc., and provided the practical use in electric vehicles and even small aircrafts. Today these materials are the subject of intense study and development internationally. Lithium-ion accumulators (LIA) have undeniable advantages due to the high activity of lithium, the lowest self-discharge and sufficiently high safety. LIA have high electrochemical characteristics, which still are being improving.



The operation of LIA is mostly impacted by the properties of cathode materials. The increasing interest towards the development of alternative sources of energy prompts the issue of elaborating and studying the cathode materials for high-voltage power sources based on LIB. In this case, the production of nanostructured materials becomes urgent.

The purpose of the presented work was creation of relatively cheap and environmentally acceptable nanostructure, high voltage cation substituted spinel type compounds –  $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ , and their derivatives  $\text{LiMe}_x\text{Ni}_{0.5-x}\text{Mn}_{1.5}\text{O}_4$  (where Me - is doping metal –Co, Cr and others,  $0 < x \leq 0.4$ ) as promising cathode materials for power consuming lithium-ion accumulators (LIA). As a result of carried out investigation the following problems have been addressed: 1. optimization of crystallization conditions for spinels with given composition; 2. development of physical and chemical basis for production of multidoped, phase pure, nanostructure  $\text{LiMe}_x\text{Ni}_{0.5-x}\text{Mn}_{1.5}\text{O}_4$  (Me = Co, Cr, Co+Cr, Al, Zn etc.) spinel type compounds with cubic syngony, using manganese, dopants (Co, Cr, Al, Zn) and lithium acetate. Samples were obtained by a relatively low-temperature method, based on thermal decomposition of eutectic mixtures of Li, Mn, Ni and dopants acetates [1]. X-ray studies of samples were carried out using DRON-3 diffractometer in the focused  $\text{CuK}\alpha$  radiation. The phase identification was carried out using diffractometric data for nonorganic compounds along with latest corresponding literature data. Evaluation of coherent scattering regions (d. nm) was carried out by the Debye-Scherrer formula:  $d = 0,9\lambda / \beta \cdot \cos\theta$ , where  $\lambda$  is wave length,  $\beta$  is line broadening at half the maximum intensity,  $\theta$  - diffraction angle. Particle size of synthesized samples was calculated using transmission electron microscope (TEM). Thermogravimetric studies were carried out using Q-1000°C derivatograph with simultaneous recording of T, TG, DTA and DTG curves. Chemical analysis of the samples was determined by atomic absorption method, as well as by traditional methods of chemical analysis. The results of the performed researches confirmed that by Li-Cr-Ni-Mn and Li-Co-Ni-Mn eutectic mixtures calcination temperature optimization it is possible to prepare phase-pure, nanoscale  $\text{LiMe}_x\text{Ni}_{0.5-x}\text{Mn}_{1.5}\text{O}_4$  type (Me = Cr, Co) samples with cubic structure. In this case, already at 200°C beginning of structurization is fixed, and the final formation of the spinel structure takes place at 350°C. Samples, prepared at 500°C and 700°C, represent phase pure cubic nanoscale spinel ( $d \sim 10 \div 25$  nm). The double doping of  $\text{LiMn}_2\text{O}_4$  spinel can promote increasing of spinels stability both in the synthesis process and in the cycling stage. Substitution of Ni in  $\text{LiMe}_x\text{Ni}_{0.5-x}\text{Mn}_{1.5}\text{O}_4$  by Co/Cr or other metals can trigger significant structural and electrochemical changes, such as structural transformation during extraction and increase of lithium diffusion rate.

Cathode materials developed on the bases of nanostructure spinels with particle size 10-20 nm, characterized by large specific surface, good crystallization, etc., due to high kinetic characteristics of nanostructure, will be able to generate high power and should be used as a promising cathode material of high capacity next generation Li-ion batteries, which provide energy for electric vehicles (EV) and hybrid electric vehicles (HEV) [2].

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2. E. Kachbaia et al. Russian Journal of Electrochemistry. 2009, 45, 175.

## THE INITIAL STAGE OF ELECTRODEPOSITION OF MANGANESE DIOXIDE ON A PLATINUM ELECTRODE

G. Tsagareli, S. Makhatadze and M. Soselia\*

R. Agladze Institute of Inorganic Chemistry and Electrochemistry at Iv. Javakishvili Tbilisi State University  
11 Mindeli str. 0186, Tbilisi, Georgia; \*marina.soselia@tsu.ge

The prospect of using manganese dioxide (MD) as electrodes for a supercapacitor is associated with the production of its film with nanoscale grains and pores. Therefore, the initial stage of electrodeposition of the film on the electrode surface is of great interest. To study this process, a platinum ring-disc electrode was used. The voltammogram was recorded in a solution of  $2 \cdot 10^{-2}$  M  $\text{MnSO}_4$  + 0,35 M  $\text{Na}_2\text{SO}_4$  + 0,05 M  $\text{H}_2\text{SO}_4$ , at an electrode rotation speed of 250 rpm and a potential sweep of 0.6 V / min. A potential was established on the ring at which reduction of Mn(III) ions is possible. Under these conditions, two peaks were observed on the anodic polarization curve, and on the ring a peak of the chronoamperometric curve of the cathodic reduction of Mn(III). The maximum of a peak on the ring coincided with the minimum on the disk. In the literature, the first peak observed on the disk is associated with the formation of MD, and the second with the oxidation of MnOOH, which is formed upon the interaction of Mn(II) with MD from solution. We believe that the first steep rise in the voltammogram is associated with the growth of MD nuclei, which determines the speed of the process. The decrease after the passage of the first peak is due to the cessation of nucleation and Mn(III) ions are fixed on the ring, which are formed on the surface of the disk of an uncoated MD. The second rise observed on the disk is apparently associated with the growth of nuclei along their perimeter at the Pt/MnO<sub>2</sub> boundary. An increase in the perimeter of nuclei should lead to an increase in current in itself, and not because of an increase in potential. As the nuclei merge, the current should decrease and reach a stationary value when the surface of the MD electrode is completely covered. In this case, the deposition process of MD proceeds already at the surface of growing dioxide. Such a mechanism of the process is confirmed by the following experiment. When the voltammogram was taken, the potential sweep was stopped at the potential of the first peak, and an i-t curve was recorded under potentiostatic conditions. The chronoamperogram repeated the course of the voltammogram, and the second rise in current was really not a consequence of the increase in potential. In this case, a peak of cathodic reduction of Mn(III) was observed on the ring, which also coincided with the minimum of the i-t curve of the disk. After passing the maximum, the current on the i-t curve gradually decreased and reached a stationary value. The corresponding current on the ring decreased markedly and did not change in time even if the potential sweep on the disk was resumed. Obviously, under these conditions, Mn(III) was formed as a result of the chemical interaction of Mn(II) with MD. Since the surface of the disk was completely covered with a MD film, the current on the ring remained unchanged.

**Acknowledgment:** The work was fulfilled with the financial support of the Shota Rustaveli National Science Foundation of Georgia within the framework of the Fundamental grant № FR17\_478.

## SELECTION OF COMPOSITIONS FOR BINDING RADIONUCLIDES

**K. Kochiashvili, M. Stephanishvili, R. Uridia, T. Dgebuadze, N. Kavtaradze\*,  
L. Dolidze, I. Mikadze**

Petre Melikishvili Institute of Physical and Organic Chemistry at Ivane Javakhishvili Tbilisi State University, Tbilisi, Georgia; \*kavtaradze\_n@hotmail.com

Decontamination of sites polluted with radionuclides is an important problem. In Georgia the most contaminated places with radionuclides are identified. Chemical and microbiological technologies belong to the modern methods for the purification of soils from radionuclides. For this purpose, some bacteria and fungi are selected that accumulate radionuclides, phytoremediation is also possible. For implementation of these methods, quantity of radionuclides in soils must be determined, as well as type of soil and acidity should be defined. For binding radionuclides representatives of different taxonomic groups can be used. Some strains of bacteria can reduce water-soluble sulfates to water insoluble sulfides.

Various methods used for radionuclide fixation are considered. Usually researchers use certain techniques, possibilities of which are partly limited. Therefore, our approach is perspective; it considers synergetic usage of different methods for achievement of maximal positive effect. Use of modified forms of humic acids, stimulation of local microorganisms and creation of geochemical barriers using acceptable natural raw materials will allow us to develop comprehensive and rational model for effective fixation of radionuclides in the soil. It should be noted that during the development of each method and preparation innovative technologies will be used.

Our group has selected certain strains of microorganisms. For the purpose of bioremediation, local microorganisms isolated from samples taken from extreme environments are studied: thermal sources, drains of iron and sulfur rocks, rocky breeds, etc. These microorganisms were identified in the laboratory at genus level: Cyanobacteria, Ironbacteria, Sulfur bacteria, Purple Bacteria Nitrogen-fixing bacteria. The acidity of soil samples artificially contaminated with various metals ( $\text{Pb}^{+2}$ ,  $\text{Cr}^{+2}$ ,  $\text{Cd}^{+2}$ ,  $\text{Sr}^{+2}$ ,  $\text{Ni}^{+2}$ ,  $\text{Cu}^{+2}$ ) have also been determined (varies 7.5-8.3). Soils of the same mass have been taken to form model samples. Each sample was contaminated with aqueous solutions of soluble heavy metal salts (0.1 N). Soil sample uncontaminated with heavy metals is taken as a control.

Considering the results of conducted works, development of modified forms of humic acids, stimulation of local microorganisms and creation of geochemical barriers using local natural raw materials is recommended. It is advisable to continue research on the development of an integrated and rational model of the purification of soils contaminated with heavy metals.

# EFFECTS OF HEAT TREATMENT ON PRECURSOR FOR THE SYNTHESIS OF TL-1223 SUPERCONDUCTORS

**T. Lobzhanidze<sup>1\*</sup>, I. Metskhvarishvili<sup>2,3</sup>, G. Dgebuadze<sup>2</sup>, B. Bendeliani<sup>2,3</sup>,  
M. Metskhvarishvili<sup>3</sup>, M. Rusia<sup>1</sup>, V. Gabunia<sup>2,4</sup>, K. Komakhidze<sup>2</sup>**

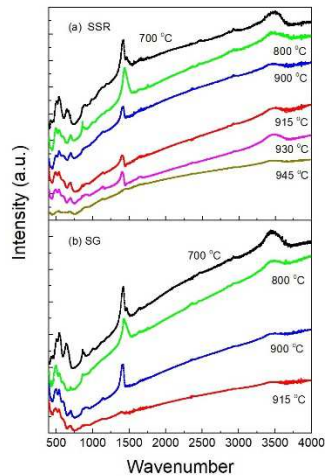
<sup>1</sup>Ivane Javakhishvili Tbilisi State University, Department of Chemistry, Faculty of Exact and Natural Sciences, 0179 Tbilisi, Georgia; \*t.lobzhanidze@tsu.ge

<sup>2</sup>Ilia Vekua Sukhumi Institute of Physics and Technology, Department of Cryogenic Technique and Technologies, 0186 Tbilisi, Georgia

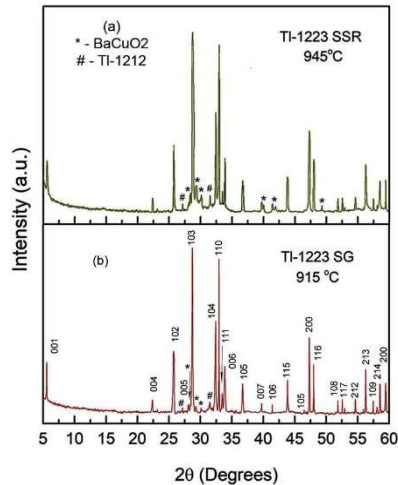
<sup>3</sup>Georgian Technical University, Faculty of Informatics and Control Systems, 0175 Tbilisi, Georgia

<sup>4</sup>Petre Melikishvili Institute of Physical and Organic Chemistry of the Iv. Javakhishvili Tbilisi State University, Jikia str 5, 0186, Tbilisi, Georgia

Mercury- and thallium-based superconductors having the highest critical temperature, when Hg-1223 are prepared at ambient conditions  $T_c \approx 135$  K [1] and  $T_c \approx 164$  K at under high pressures (30 GPa) [2]. Transition temperature nonsubstituted phase of Tl-1223 is  $T_c \approx 115$  K [3] and  $T_c \approx 130$  K at pressures (3.5 GPa) [4]. The formula unit and crystal structure of the  $TlBa_2Ca_{n-1}Cu_nO_{2n+2+\delta}$  system similar to that of the  $HgBa_2Ca_{n-1}Cu_nO_{2n+2+\delta}$  system, where ( $n$ ) is the number of adjacent Cu-O layers. Mercury- and thallium are very toxic, volatile at high temperature and what is more important for this family, to achieve high purity superconductivity phase, critically depends on the used precursor and synthesis conditions. Preparation of high purity and reaction ability precursor, in the various articles, was solved by diverse methods.



**Figure 1.** IR analysis of  $Ba_2Ca_2Cu_3O_y$  after annealing in flowing oxygen partial pressure of 0.5 bar: for SSR-precursor at 700°C-945°C (a) and for SG-precursor at 700°C-915°C (b).



**Figure 2.** XRD patterns of the  $TlBa_2Ca_2Cu_3O_{8+\delta}$  samples, prepared on the best precursor powders of both methods: (a) SSR synthesized at 945°C and (b) SG synthesized at 915°C temperatures.

We have presented the preparation of Tl-1223 high-temperature superconductors by sealed quartz tube technique. For the synthesis samples, we used the two-step method. In the first stage were prepared, multiphase precursors in the second stage where  $Tl_2O_3$  was added. Precursors were prepared by two methods, sol-gel, and solid-state reaction methods and examined the influence of heat treatment on precursors. These results showed that to obtain high-purity precursors for SG methods sufficiently heat treatments at  $915^\circ C$  temperatures and for SSR methods  $945^\circ C$ . The diamagnetic onset temperature of the superconducting transition for the samples prepared by precursors SG at  $915^\circ C$  and SSR at  $945^\circ C$  is about  $T=120$  K and full screening of applied *ac* magnetic fields observed at  $T \approx 102$  K and  $T \approx 92$  K, respectively. The unlike SG method in SSR samples clearly shows a two-step decrease with *T*, which reflects the flux shielding from and between the grains. As a result, we could conclude that the SG method demonstrated as a successful alternative to SSR methods allowing a faster production of the precursor powders, without any carbonate contamination.

**Acknowledgements:** this work was supported by Shota Rustaveli National Science Foundation (SRNSF), grant number: FR/261/6-260/14, Project title: Sol-gel Methods and Polymerization for synthesized Tl-based Polycrystalline Superconductors.

## **ECOLOGICAL SITUATION IN THE WORLD AND IN GEORGIA DURING AND AFTER THE PANDEMIC**

**E. Bakradze<sup>1\*</sup>, L. Shavliashvili<sup>2</sup>, G. Kuchava<sup>1</sup>, M. Arabidze<sup>1</sup>, N. Buachidze<sup>2</sup>, G. Kordzakhia<sup>1</sup>**

<sup>1</sup> National Environment Agency of the Ministry of Environment and Natural Resources  
Protection of Georgia; \*h.bakradze@gmail.com

<sup>2</sup> Institute of Hydrometeorology, Georgian Technical University

In this report the impact of covid-19 pre- and post-pandemic periods on the ecological state of the world and Georgia is discussed.

The level of real spread of the virus in Georgia; has been studied Concentrations of nitrogen dioxide and PM particles in the atmospheric air in Tbilisi and its surrounding area.

The trend of changing the concentrations of PM<sub>2.5</sub> and PM<sub>10</sub> in the rhythm of the usual life of the city and force majeure situations is discussed.

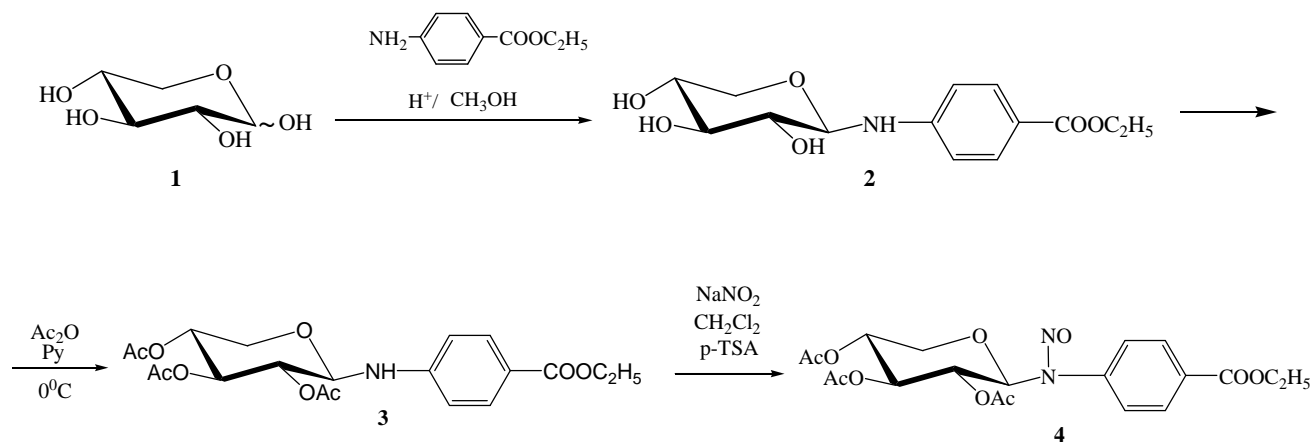
## SYNTHESIS OF NITROSO (N=O) GROUP CONTAINING D-XILOPYRANOSYLAMINE

N. Sidamonidze, R. Vardiashvili, K. Onashvili, R. Gakhokidze

Ivane Javakhishvili Tbilisi State University  
3, Ilia Chavchavadze ave., 0179 Tbilisi, Georgia

It is known that nitric oxide is involved in many physiological and pathological processes. It acts as a vasodilator, participates in the function of the immune system, the nervous system, regulates apoptosis and cell proliferation. In this respect, the synthesis of Nitroso (N = O) group containing carbohydrate derivatives and study of their biological activity is a promising research direction to obtain new type biologically and pharmacologically active compounds.

The goal of present investigation consist in synthesis of nitroso group (N=O) containing N-glycosilamines. As an initial substance in the given work has been used the products of condensation of D-xyloze (1) with 4-aminobenzoic acid ethyl ester, N-β-(4-aminobenzoic acid ethyl ester)-β-D-xylopyranozylamin (2). By acetylation and further nitrozylation of N-arylxyloseamine corresponding N-β-N-nitroso-(4-aminobenzoic acid ethyl ester)-2,3,4,6-tetra-O-acetyl-D-xylopyranosylamine (4) has been obtained at the first time. Reactions proceeds according to the following scheme:



The structures of obtained compounds were established by physical-chemical methods of analysis.

Determination of biological activity potential of synthesized substances have been carried out with the help of computer program PASS Online. By assessment of structure-activity relationships the effect of nitroso (-N-N = O) group on the biological activity spectrum of synthesized N-glycoside have been revealed. The results of the study will enable us providing selection of the most prospective compounds from the set of synthesized samples.



# INVESTIGATION OF NEW TRIBOLOGICAL NANOCOMPOSITES BASED ON PTFE MATRIX FILLED WITH FE-DOPED CARBON NANOPARTICLES

**L. Gventsadze<sup>1\*</sup>, E. Kutelia<sup>1</sup>, D. Gventsadze<sup>2</sup>**

<sup>1</sup>Republic Centre for Structure Researches of Georgian Technical University  
77, Kostava str., Tbilisi 0175, Georgia

<sup>2</sup>R. Dvali Institute of Machine Mechanics, 10 Mindeli str., Tbilisi 0186, Georgia  
[\\*lika.gventsadze@gmail.com](mailto:lika.gventsadze@gmail.com)

The present work is dealing with the study of a nano-compositional material which was obtained on the basis of PTFE with 2.5÷10wt% of core-shell type Fe-doped carbon nano-tubes and carbon nano-particles as fillers (1,2). The PTFE samples without the fillers were prepared too. Weight wear, friction coefficient and temperature were measured after passing some velocity steps, and afterwards the linear wear was calculated. The obtained results have shown that the incorporation of about 2,5÷5wt% of Fe-doped CNTs into PTFE matrix drastically improves the antifrictional properties in comparison to the unfilled PTFE. Namely, the wear resistance of these nanocompositions increased by the factor of 500-150 in the range of friction velocities 0.25÷1.25 m/sec. Increase of the filler portion up to 10wt% transforms the obtained nanocomposite from antifrictional to friction material with the enhanced coefficient of friction up to 0.32, but with the unexpectedly ultra-low wear.

**Table 1.** Summary of tribological test results for the three developed new (PTFE + Fe-dop.CNPs) nanocomposites and the two reference materials

Friction speed V, m/s	Unfilled (PTFE)			PTFE + 2.5 mass% Fe-dop.CNT			PTFE + 5 mass% Fe-dop.CNT			PTFE +10 mass% Fe-dop.CNT			“Superfluvis”		
	T, °C	f	I,10 <sup>-9</sup>	T, °C	f	I,10 <sup>-9</sup>	T, °C	f	I,10 <sup>-9</sup>	T, °C	f	I,10 <sup>-9</sup>	T, °C	f	I,10 <sup>-9</sup>
0.25	40	0.14	892	50	0.21	1,79	45	0.18	1.82	45	0.19	1.84	70	0.18	10.0
0.38	62	0.14	310	70	0.23	1.20	60	0.19	1.21	100	0.23	1.22	75	0.13	9.0
0.62	85	0.13	123	135	0.25	1.44	90	0.19	0.73	160	0.25	0.5	125	0.15	12.0
0.87	120	0.13	158	200	0.25	2.56	200	0.21	1.56	215	0.26	1.57	180	0.15	11.0
1.25	180	0.14	330	240	0.21	28,76	230	0.21	6.90	280	0.32	5.89	180	0.14	6.0

SEM-EDX analyses of the worn surfaces of the tested nanocomposites and the cast iron samples after working as a tribological pair, revealed some favorable effects of the Fe-doped CNTs filler on the formation mechanism of a transfer film and its role in promoting very low wear of the obtained new nanocomposites.

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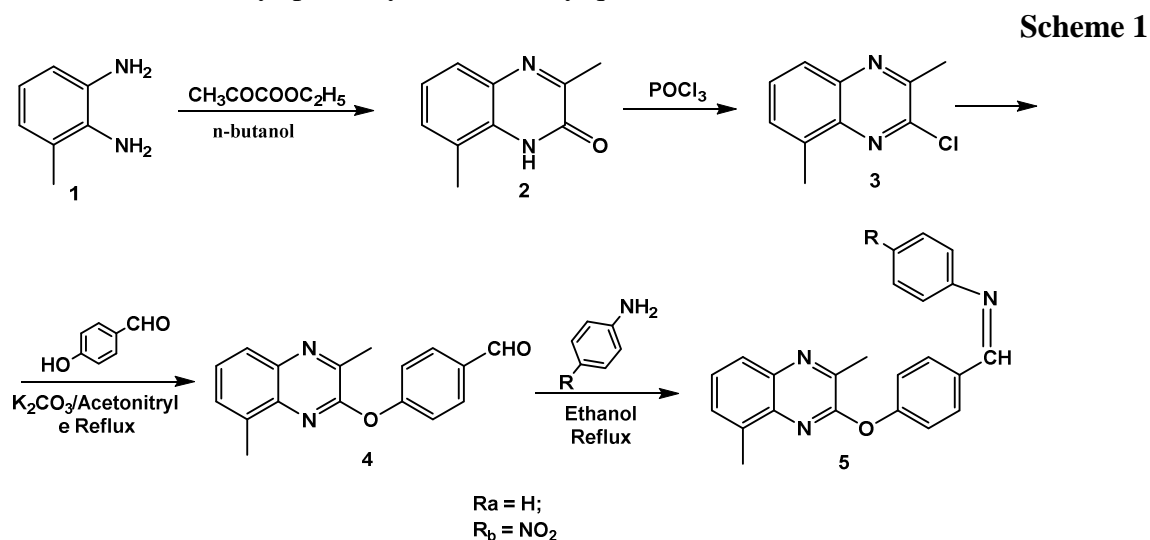
## SYNTHESIS AND STUDY OF N-((4-(3,8-DIMETHYLQUINOXALIN-2-YLOXY)PHENYL)METHYLENE)BENZENAMINE

**L. Tlashadze, E. Katsadze, S. Samsoniya**

Ivane Javakhishvili Tbilisi State University, Faculty of Exact and Natural Sciences  
Department of Chemistry; 3, Ilia Chavchavadze Ave., 0179 Tbilisi, Georgia

Quinoxaline derivatives have different pharmacological activities such as bacteriocides and insecticides [1], antibacterial [2,], antifungal [2, 3], antitubercular [4], analgesic [5] and anti-inflammatory [6]. In the light of these facts we decided to synthesize some new quinoxaline derivatives incorporating aromatic aldehyde attached to a 3,8-dimethylquinoxalin-2(1H)-one nucleus with an ether linkage followed by the treatment with aromatic amine to afford Schiff bases in the hope of obtaining better antimicrobial agents.

The chemical synthesis (Scheme 1) was initiated with the reaction of 3-methylbenzene-1,2-diamine (1) with ethyl pyruvate in n-butanol to yield 3,8-dimethylquinoxalin-2(1H)-one (2), which on treatment with POCl<sub>3</sub> yielded 3-chloro-2,5-dimethylquinoxaline (3). A mixture of compound 3 and 4-hydroxy benzaldehyde was next refluxed in acetonitrile for 20 hours to afford 4-((3,8-dimethylquinoxalin-2-yl)oxy)benzaldehyde (4) as an intermediate. Mixtures of compound 4 and various substituted aromatic amines were refluxed in ethanol to afford 2-[4-(substituted benziminomethyl)phenoxy]-3,8-dimethylquinoxalines 5a,b.





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## SYNTHESIS OF A NEW HYBRID (AZO AND SPIRO) PHOTOCHROMIC COMPOUND

**K. Meskhidze<sup>1,2</sup>, T. Bukia<sup>1,2\*</sup>, S. Akhobadze<sup>2</sup>, J. Maisuradze<sup>2</sup>**

<sup>1</sup>Ivane Javakhishvili Tbilisi State University, Faculty of Exact and Natural Sciences,  
3, Ilia Chavchavadze Ave., Tbilisi, Georgia

<sup>2</sup>Institute of Cybernetics, Vladimir Chavchanidze Georgian Technical University  
Tbilisi, Georgia; \* tinatini.bukia@tsu.ge

Spiropyrans (spirochromens) are an important class of organic photochromic compound. Bistable molecules and molecular ensembles can exist in two different, thermodynamically stable states. Transferring from one state into another occurs through different stimulators (light, heat, mechanical stress, electrical and magnetic fields, etc). An uncolored spiropyran molecule with volumetric structure by the expose with ultraviolet light, converts into a coplanar, colored merocyanine form with a high dipole moment. Such bipolar molecules easily self-organize in a certain area, i. e. form nanoparticles. [1-3].

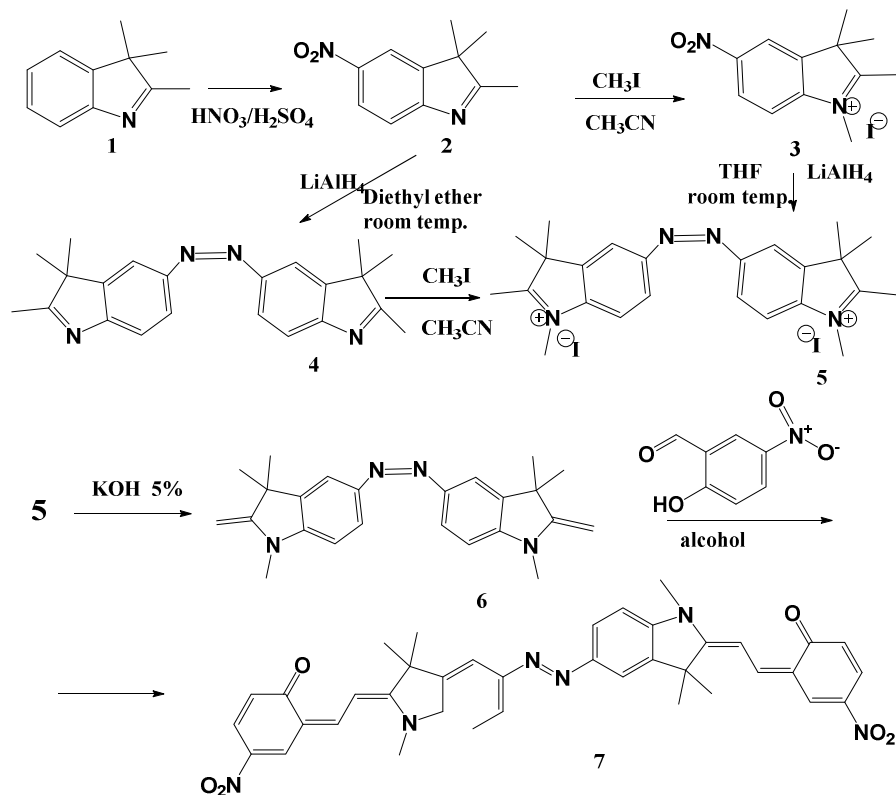
Perspectives to use spiropyrans to design new photo controlled molecular equipment and biological materials, logic valves and sensors are not exhausted. Therefore, today, active investigation to design and study compounds with new properties (by maintaining the existing ones) are underway.

It is interesting to combine spiropyran with other photochromic compounds so that maintain the important properties of both classes.

For this purpose, we have selected a diazo group, which, after irradiation of the sample by incorporating the formed spiropyran conjugated chain, will cause (or lead to) a sharp change in the maximum absorption, which has been confirmed.

We synthesized a new hybrid (azo and spiro) photochromic compound according to the given scheme. We first synthesized the starting compound - 5-nitro-2,3,3-trimethylindolenine (2) by nitration of 2,3,3-trimethylindolenine (1)[4]. With further reduction with  $\text{LiAlH}_4$ , in the area of

absolute diethyl ether, at room temperature, was obtained compound **4** with a high-yield (99%). Quaternization of the formed compound **4** with  $\text{CH}_3\text{I}$  was performed in a shallow ampoule at 80-82°C in the acetonitrile area and quaternized salt **5** was isolated. We obtained the same compound **5** in the second way, namely, we first conducted quaternation of compound **2** with  $\text{CH}_3\text{I}$  at an acetonitrile at 25-30 °C. With further reduction of compound **3** with  $\text{LiAlH}_4$  in the area of tetrahydrofuran compound **5** is formed. By the treatment of obtained compound **5** with alkaline solutions forms compound **6**, which reacts with 5-nitro salicylic aldehyde and gives a compound **7**, the maximum absorption of which in the alcohol area is 660 nm (the maximum absorption of similar spiropyranes is 540 nm). Presumably, it represents spiropyrane.



The structures of the synthesized compounds are determined by infrared and NMR spectral data. The final product is being studied.

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## SYNTHESIS OF FIVE RING CONTAINING HETEROCYCLIC COMPOUND- 1-ACETYL-1H,11H-2,3-DIHYDROPYRROLO- [3',2':5,6]INDOLO[2,3-B]QUINOXALINE

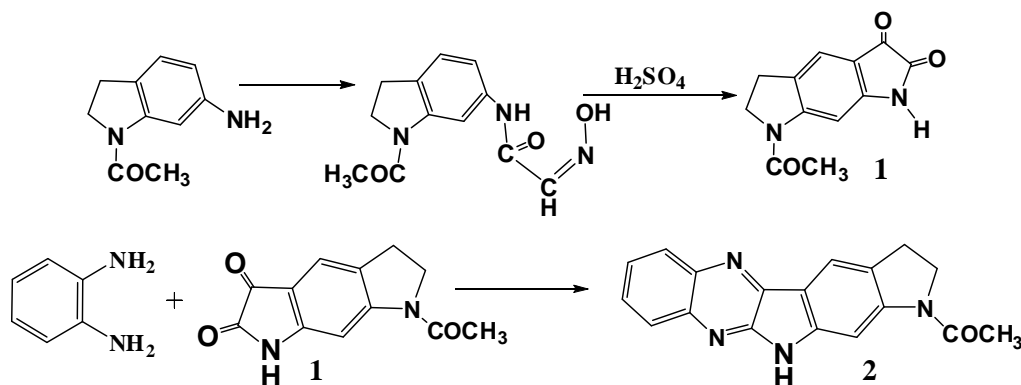
**L. Bobokhidze\*, D. Kajrishvili, I. Chikvaidze**

<sup>1</sup>Ivane Javakhishvili Tbilisi State University, Faculty of Exact and Natural Sciences  
3, Iliia Chavchavadze Ave., Tbilisi, Georgia.

\*likobobokhidze1992@gmail.com

Indoloquinoxalines are receiving considerable interest due to their significant biological activities. The compounds of this class are combined with two strong, heterocyclic rings such as indole and quinoxaline. 6H-Indolo[2,3-b]quinoxaline and its derivatives represent an important series of DNA intercalating agents and are endowed with potent antiviral and cytotoxic activities. For example, compound B-220 (2,3-dimethyl-6-(2-dimethylaminoethyl)-6H-indolo[2,3-b]quinoxaline) has been reported to show remarkable activity against herpes virus.

To improve synthetic anticancer compounds we have decided to continue research in the field of indoloquinoxalines. In particular, we set our goal to synthesize five ring containing heterocyclic compound, dihydropyrroloindoloquinoxaline, as a potential DNA intercalator. As a result, one of the first representative of this class, 1-acetyl-1H,11H-2,3-dihydropyrrolo-[3',2':5,6]indolo[2,3-b]quinoxaline has been synthesized. The methods of synthesis are based on the classical reactions. The first stage, which includes to produce dihydropyrroloisatine (1), is carried out with Sandmeyer traditional reaction. The target product (2) has been synthesized by cyclocondensation reaction between dihydropyrroloisatine (1) and o-phenyldiamine in acetic acid.



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## TRANSITION METAL COMPLEXES WITH SPECIFIC STRUCTURES AND PROPERTIES

N. Kutalia

San Diego State University Georgia; nika.kutalia19@gmail.com

In science, it is a frequent occasion when some particular compounds possess structures and properties that cannot be explained by the existing models. The remedy of the situation arises by developing new models and arguments that may answer many questions. Valence Bond theory (VB) explicated many bizarre behaviors of compounds, but it could not provide the arguments for the diamagnetic properties of O<sub>2</sub>. Then Molecular Orbital (MO) Theory arose which was able to explain almost everything. However, as every model in science, it has its limits. When we think about some specific compounds and materials with peculiar and particular properties the first thing that may come into our minds are transition metal complexes. Even the first row of transition metal complexes form very specific compounds without any general trends. Even in many cases, oxidation states deduced from some particular formulas may be misleading, e.g. MoCl<sub>2</sub> which may be thought of as Mo (II) compound, in reality, the compound exists as a metal-cluster unit [Mo<sub>6</sub>Cl<sub>8</sub>]<sup>4+</sup>(Cl<sup>-</sup>)<sub>4</sub>.

According to Valence Shell Electron Pair Repulsion (VSEPR) theory, the number of electron pairs surrounding the central atom determines the geometry and structure of compounds, and as a result, we have a full description and generalizations of many compounds. For transition metal complexes, whether we use the Kepert's and Werner's models attain the general trends associated with the d block metal complexes. For example, the same metal d<sup>8</sup> complex of Ni<sup>2+</sup> coordinates with Cl<sup>-</sup> to make a tetrahedral [Ni(Cl<sub>4</sub>)]<sup>2-</sup>, but the complex of [Ni(CN<sub>4</sub>)]<sup>2-</sup> is square-planar. Also, d<sup>2</sup>, d<sup>3</sup>, d<sup>4</sup>, etc. metal complexes with H<sub>2</sub>O associated with octahedral coordination geometry. We can find many examples in d block metal chemistry where the previous models just flawed.

The main goal of the research is to analyze the crystal and ligand field theories with the aid of MO theory to make a suitable model for explaining the unusual behaviors, properties, and structures for many compounds of materials in chemistry.

The development of symmetry operations, and the Ligand Group Orbital (LGO) approach, made it possible for MO theory to explain the unusual structure for B<sub>2</sub>H<sub>6</sub> (which is characterized with 3 centered 2 electrons (3c2e) bonds), and many other compounds. Why do d<sup>0</sup>, and d<sup>1</sup> metal complexes such as [W(Me<sub>6</sub>)] are trigonal prismatic? What are tripodal ligands, and how do they reflect on the structures and geometries for some compounds? These and even the magnetic and electronic properties of compounds can be explained by the combination of MO and crystal field theory which is the main purpose and goal of the research.

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## **DEVELOPMENT AND APPLICATION OF BIOACTIVE METALLOCENE HYBRID DERIVATIVES**

**Kh. Barbakadze<sup>\*</sup>, B. Arziani, G. Lekishvili**

Tbilisi State Medical University, Faculty of Pharmacy, Department of Medical Chemistry  
33, Vazha Pshavela Ave., 0186 Tbilisi, Georgia; \*kh.barakadze@tsmu.edu

Organometallic ligands provide a convenient route to the synthesis of heterometallic complexes. Due to the high stability of metallocenes have become versatile building blocks for the synthesis of compounds with tailor-made properties. Ferrocene-containing complexes are currently receiving much attention associated with their widespread utility, e.g. in organic synthesis, production of fine chemicals, homogeneous catalysis, and materials chemistry. An important feature of these potential ligands is their flexibility: the bidentate representatives can adapt as chelating groups to different geometric requirements of a given metal center and act as bridging ligands.

Ferrocenyl compounds have shown potential as both antibacterial and antifungal agents. Based on its unique properties such as stability, aromaticity, lipophilicity, low toxicity and redox activity, the ferrocene core is an attractive pharmacophore for drug design. At the same time, several drugs containing the adamantane moiety are currently commercially available. They mostly used in the prevention of viral diseases and as drugs in the treatment of Parkinson disease. Introduce of immunotropic and membranotropic spatial carbocyclic groups in the molecule of bioactive compounds frequently provoke the shortening of preparation toxicity and reinforcement of pharmacological action.

Design of novel classes of hybrid compounds with antimicrobial activity containing polycarbocyclic and metallocene structures and some biogenic elements have been carried out. By using of the data of IR and NMR spectral, thermal (TGA, DTA) and elemental analysis and by molar conductivity the structure of the obtained compounds have been established. By using model systems and semi empirical quantum-chemical AM1 method the electronic structure and complex forming capacity of obtained ligands have been established. It was shown that the organic ligand behaved as cyclic-bidentate through the electro donor carbonyl oxygen and the NH<sub>2</sub>- or azomethyne nitrogen atoms.

Quantitative structure-properties relationships (QSRR/QSAR) based on experimental data for construction of models of dependences of physical properties of biologically active metallocene hybrid derivatives based on spatial alicyclic polyfunctional group and some biogenic metals have been studied. Several sets of molecular descriptors have been used. Presence of the dataset outliers was controlled by using PCA; to ascertain the quality of models cross-validation has been used. Based on the performed research, one concludes that the best models have been acquired by the use of the GETWAY description of obtained compounds has been carried out.

Virtual bioscreening and activity towards various microorganisms of the obtained compounds have been studied. Microbiological study of the investigated compounds confirmed the evaluated virtual concepts. Area of their application has been established.

## **EXTRACTION OF QUERCETIN FROM ONION SKIN (*ALLIUM CERA*) BY GRADUAL CLEANING AND STANDARD METHOD**

**N. Chaganava\*, Kh. Barbakadze, G. Lekishvili, B. Arziani**

Tbilisi State Medical University, Faculty of Pharmacy, Department of Medical Chemistry  
33, Vazha Pshavela Ave., 0186 Tbilisi, Georgia; \*n.chaganava@tsmu.edu

In recent years, quercetin has attracted attention due to its antioxidant, anticancer and antimutagenic activity, antihyperglycemic/antidiabetic efficacy [1, 2]. Quercetin is a natural flavonoid found in fruits and vegetables in the form of aglycone or glycosides. It is known that onion (*Allium cera*) is one of the most common raw materials in terms of quercetin content. Various methods have been used to isolate quercetin from the latter, including standard method of solvent extraction, microwave method, ultrasonic extraction, and extraction with supercritical fluids [3, 4].

A simple and affordable, standard method of extraction was selected to extract quercetin from brown onion leaves. The results of the separation of quercetin with different solvents (acetone, methanol, ethanol, ethyl acetate) in a series of experiments showed that in order to increase purity and yield, it is recommended to boil onion leaves in water in the first stage, and ethyl acetate (250 ml) is the optimal solvent. However, the extraction efficiency increases during the fermentation process of the solvent at 4 hours. It should be noted that increasing the volume of the solvent and the duration of the process does not significantly affect the results obtained.

Thus, by the standard method used to excrete of quercetin was determined the optimal conditions for extraction (temperature, different solvent, duration of the experiment) to increase the quercetin yield and especially the purity.

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## **ADSORPTIVE REMOVAL OF THE FREQUENTLY USED FLUOROQUINOLONE ANTIBIOTIC – MOXIFLOXACIN HYDROCHLORIDE FROM WASTEWATERS USING NATURAL ZEOLITE**

**I. Rubashvili\*, L. Eprikashvili, T. Kordzakhia, M. Zautashvili,  
N. Pirtskhalava, M. Dzagania**

Petre Melikishvili Institute of Physical and Organic Chemistry,  
Ivane Javakhishvili Tbilisi State University, Tbilisi, Georgia  
31a, Anna Politkovskaya Str, 0179 Tbilisi, Georgia  
\*rubashvili@yahoo.fr

Residual antibiotics pollution has become one of the most serious environmental problems today. Antibiotics from hospitals and drug factories represent a potential risk for human health and environment. Therefore, it has been a great exigency to develop some efficient and cost-effective treatment methods and technologies for antibiotics removal from industrial and household contaminated water. There is the most utilised technique - adsorption which has the unique properties of flexibility, effectiveness, superior performance and the robustness for consecutive cycles.

The present research concerns the adsorption of the frequently used fluoroquinolone (FQ) antibiotic – moxifloxacin hydrochloride on natural zeolite – clinoptilolite (CL) and its acid-modified form (H-CL) at various operational conditions using two static and dynamic methods and to demonstrate that adsorption by natural zeolite has an economically feasible means of antibiotics removal.



The local natural zeolite with the zeolitic phase content - 55-65 % – clinoptilolite was obtained from Khandaki, Kartli region, Georgia. After milling the adsorbent in powdered form was washed with deionized water and dried under nitrogen flow at 300°C for 3 hours. For obtaining a modified H-form of natural clinoptilolite was treated with acidic solution (2M HCl solution). For study of adsorption dynamic process there was used the specially constructed laboratory dynamic type equipment with fixed bed adsorption glass column packed by powdered zeolite adsorbent and chromatography pump at constant temperature of 20°C. The upper and lower parts of column contained plastic pellets to compact the bed and avoid a dead volume and channeling. The concentration of adsorbate in influent and effluent stream was determined using the previously developed and validated effective and sensitive HPLC method. The limit of quantitation of the method is 0.05µg/mL. The chromatographic analysis was performed using LC-20AD Prominence Shimadzu HPLC System (Japan) and a column - Agilent SB-C18 4.6 x 250 mm, 5 µm (USA).

Crystal structural changes of natural clinoptilolite after the acid treatment to obtain clinoptilolite acid-modified H-form was investigated using XRD analysis. The results were shown an increase in the relative content of Si/Al ratio in zeolite framework and pore opening compared to CL.

The breakthrough curves for adsorption of the FQ antibiotic on zeolite adsorbent – CL and H-CL in terms of the effluent to influent concentrations ratio,  $C/C_0$ , versus the contact time –  $\tau$ , min were investigated by carrying out a set of fixed bed experiments at different pH values, flow rates and concentrations of the inlet FQ antibiotic solution at constant temperature of 20°C. In order to measure the adsorption, the removal efficiency - R, % of moxifloxacin hydrochloride and the adsorption capacity – q, mg/g were calculated. For explanation of the mechanism of adsorptive removal of moxifloxacin hydrochloride and the interaction of zeolite adsorbent with the FQ antibiotic was studied using the most commonly used Langmuir and Freundlich adsorption models. The obtained results show that isotherm has a good correlation ( $R^2 > 0.9$ ) and define a monolayer adsorption. The adsorption mechanism mainly composed of electrostatic interaction between the adsorbent surface and adsorbate.

The experimental data show that the high value of the volumetric flow rate, the inlet concentration of the antibiotic solution and the pH value accelerates breakthrough of adsorbates and correspondingly reduces the adsorption capacities. The capacities of moxifloxacin hydrochloride adsorption are strongly dependent on the volumetric flow rate and the inlet concentration of the FQ antibiotic solution. The value of pH does not have a significant influence on the adsorption process. The removal efficiency increased with a decrease in the concentration of adsorbate solution. The amount of FQ antibiotic adsorbed per unit mass of zeolite as a function of the contact time of each adsorbate with adsorbent, the structure, the molecular weight and the concentration of FQ antibiotic in solution.

Hence, the selected zeolites – CL and H-CL with hydrophilic pores have a greater affinity for adsorbing FQ antibiotic pollutant in aqueous solution. The developed adsorption laboratory



technology has been effectively applied for removal of the frequently used fluoroquinolone antibiotics from aqueous solutions. This research confirms that natural zeolite is competitive adsorbent in terms of cheapness, shape selectivity and adsorption efficacy.

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## **SYNTHESIS OF SOME QUINOXALHYDRAZONE**

**I. Jinikashvili\*, G. Lekishvili, B. Arziani**

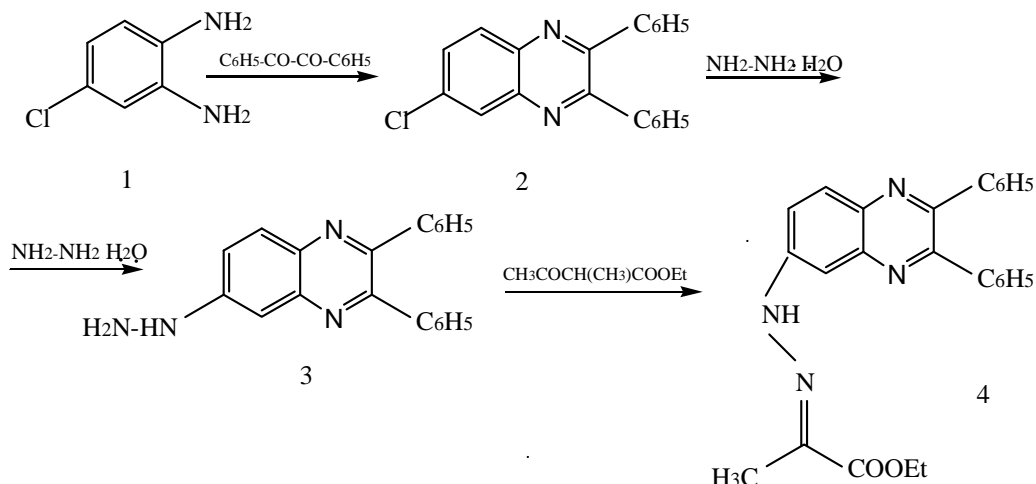
Tbilisi State Medical University, Faculty of Pharmacy, Department of Medical Chemistry  
33, Vazha Pshavela Ave., 0186 Tbilisi, Georgia; i.jinikashvili@tsmu.edu

As of today a total quantity of medications exceeded hundred thousands and more than a half from here falls on the heterocyclic compounds. That's why it seems that heterocycles are the structural units predetermining biological activity of most important medicinal preparations (cardiac drugs, anticarcinogens, antibiotics, curative alkaloids, their antagonists etc.). According to requirements of practical medicine an increasingly attention is paid to the synthesis of new heterocyclic compounds, study of their properties and biological activity. The interest is getting higher toward such heterocyclic systems, that contain two or more heterocyclic fragment in the molecule. Research of such polyheteroaromatic compounds turned to be important and fruitful not only from the viewpoint of development of heterocyclic compound chemistry, but also from practical point of view, since it promotes discovery of new effective medicinal preparations and their practical implementation.

There is relatively scarce information on biological activity of quinoxaline and other heterocycles containing two nitrogens, as well as on their use as medications. Antimalarial and sulfanylamide preparations prepared on the basis of quinoxaline due to their insufficient solubility or toxicity can't satisfy the requirements raised to chemotherapeutic preparations[1-2]. But it should be noted that modification of similar compounds through insertion of functional groups of different nature into their structure, creates definite basis for avoidance of these shortcomings and from the viewpoint of improvement of preparation properties[3-4].

Proceeding from the above mentioned, in order to create medicinal preparations of some pharmacological action we deemed topical to conduct synthesis and study of pyrroloquinoxalines of new condensed heterocyclic systems. These compounds are distinguished by the fact that indole fragment in them is annelated by heterocycle containing two heteroatoms that substantially extend the possibility of task-oriented synthesis of new, effective biologically active substances.

Our objective was obtaining quinoxalhydrazone according to the following scheme:



By condensation of 4-chlorophenylenediamine(1) with benzyl, 6-chloro-2,3-diphenylquinoxaline(2) was obtained in its interaction with hydrazine hydrate, 2,3-diphenyl-6-quinoxalylhydrazine (3) was obtained, which reacts with ethyl pyruvic acid to form the corresponding hydrazone (4).

Composition and structure of synthesized compounds is determined by element analysis and physical methods of investigation.

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## RECOVERY OF PECTIN AND PENTACYCLIC TRITERPENOIDS FROM APPLE POMACE

**A. Kalatozishvili, M. Chkhaidze, M. Khachidze, M. Buzariashvili, I. Rubashvili**

Petre Melikishvili Institute of Physical and Organic Chemistry of Ivane Javakhishvili  
Tbilisi State University, 31a, Anna Politkovskaya Str, 0179 Tbilisi, Georgia

Apple pomace is the primary by-product of apple juice production. The uses of apple pomace can be classified either as waste reduction strategy, or obtaining a high value product or both.

The production of pectin and pentacyclic triterpenoids-ursolic (UA) and oleanolic acids (OA) is considered the most reasonable way of utilization both from an economic and from

an ecological point of view. The main objectives of this study were to establish a stepwise recovery process for pectin and pentacyclic triterpenoids.

Pectin is a soluble viscous fermentable fiber and common additive in the food industry which functions as a gelling agent, emulsifier and thickener in various food products such as confectionery, bakery jellies, yoghurts and beverages.

In the recent years, one group of natural products called pentacyclic triterpenoids has attracted a lot of attention due to its unique and strong biological and pharmacological activities. The main pentacyclic triterpenes namely isomeric triterpene acids - oleanolic acid (OA) and ursolic acid (UA) are found in many medicinal herbs, fruits and vegetables as the free acid or aglycones. In apples they are found as free acids. The above-mentioned compounds have low toxicity and a wide variety of reported and approved pharmacological activities, including anticancer, chemopreventive, hepatoprotective, antiviral, antibacterial, anti-inflammatory, anticonvulsant, antiatherosclerotic, antidiabetic, antioxidant, immunomodulatory and gastroprotective properties. Therefore, the efficient and high-yield extraction of pectin and triterpene acids from raw materials has great significance and practicability.

Apple pomace was provided by LTD "Samegobro" and LTD "Achinebuli". The selection of suitable extraction technique for stepwise extraction of bioactive substances from agro-industrial waste materials depends on the nature and physical-chemical properties of the compounds, the quality of extracts and the yield; as well as on the conditions, the existence of appropriate analytical method of quantitative determination and economic expediency of the laboratory process. The technique should be reproducible, fast, simple, inexpensive and eco-friendly as possible. There are few attempts at using sequential stepwise extraction method for recycling apple pomace.

The two-stage simple and fast extraction method of pectin and triterpene acids were developed.

Pectin was extracted under reflux in a condensation system at 97<sup>0</sup>C for 1h. and dilute citric acid (pH 2.5) as the solvent. Hot acid extract was pressed and filtrate was cooled to 40<sup>0</sup>C. The apple pectin was precipitate by ethanol.

Two types of sonication - Jy92-Iidn ultrasonic homogenizer (probe-type) (China) and dual-frequency ultrasonic bath DW-5200DTS (bath-type) (China) were used for UAE. The ultrasound frequency was 25 kHz; the temperature was controlled at 25±2°C during ultrasonication; Three different solvents (acetone, isopropanol, ethanol) were used for ultrasonic extraction of UA and OA.

The results obtained with the extraction process indicate that the effects of the extraction time, the polarity and volume of extraction solvent and the sample size of raw material on the extraction efficiency are significant for both target compounds. The maximal extraction yields of OA and UA - 1.535 mg/g and 4.585 mg/g, respectively achieved at the following extraction parameters: the ultrasound frequency - 25 kHz; the sample/solvent ratio 1:10, isopropanol was most selective for UA, but acetone for overall yield; the temperature was 25±2°C.

The chromatographic analysis was performed using LC-20AD Prominence Shimadzu HPLC System (Japan).

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## **PREPARATION OF EFFECTIVE ADSORBENT FOR BINDING AFLATOXINS**

**I. Mikade\*, R. Uridia, N. Tserodze, N. Karkashadze, L. Tatiashvili**

Petre Melikishvili Institute of Physical and Organic Chemistry

5, A. Politkovskaya str., 0186, Tbilisi, Georgia

Iv. Javakhishvili Tbilisi State University, 3, Ilia Chavchavadze Ave., 0179 Tbilisi, Georgia

\*imikadze21@yahoo.com

Mycotoxins belong to one of the dominant groups of biogenic toxins that contaminate the nutritional products of animals and humans, deteriorate their nutritional value and quality. By means of a contaminated food materials mycotoxin get into organisms of people and animals causing different types of poisonings that results in the specific diseases called mycotoxicosis. Commonly, stored food products are poisoned by species of fungi - *Fusarium* and *Aspergillus* that are producing very aggressive mycotoxin T2 and aflatoxin B1. Aflatoxin B1 and other toxins of this group can link irreversibly to protein molecules in the liver and produce DNA adducts (eg, Aflatoxin B1 – lysine in the albumin molecule). Aflatoxins represent one of the most aggressive and dangerous groups of mycotoxins with strong carcinogenic properties. Aflatoxins are isolated from two strains of fungi: *Aspergillus flavus* Link and *Aspergillus parasiticus* Speare. These fungi belong to the mesophilic microscopic order with the ability of growth at a temperature of 26-28°C.

In recent years, major efforts are done to develop rapid methods of analysis that allow to make diagnosis immediately after the taking samples. Immune- and immuno - fermentation analysis of particles replies to these goals well, as they are giving an opportunity of visual interpretation of the results. In the most countries, the considerable content of high-toxic and carcinogenic aflatoxins is mainly discovered in nutrients. It has led to the necessity of development of detoxication methods of raw materials, foodstuffs and feeds. There are three

possible methods of detoxication of aflatoxins: mechanical, physical and chemical methods. The mechanical method of detoxication means removal of contaminated raw materials and stuff by means of hands or electronic-colorimetric sorters. During the application of the physical method the contaminated materials are processed thermally in the autoclave, or the ultra-violet radiation and ozonization are used. The chemical method means the treatment of materials by strong oxidizers.

It is necessary to note that each of the mentioned methods has a significant drawback, since the use of mechanical and physical methods does not give a high effect, and the chemical method causes breaking down of aflatoxins and useful nutrients as well. The use of various types of adsorbents in warehouses is highly effective to prevent contamination by aflatoxins of vegetables and wheat crops, consumer and fodder materials, various types of dried fruits, bread and confectionery. The advantage of the adsorption method is its availability and effectiveness. Adsorbents of aflatoxins are divided into several groups: mineral, carbon-containing, polysaccharide and mixed.

The samples of the filings were selected: sawdust of coniferous and deciduous wood, and their mixture as well. The technical lignin was obtained by two methods: 1. Hydrolysis of the sawdust samples, then treatment by 4-6% dilute NaOH solution and then by Na<sub>2</sub>S, and 2. Extraction of lignin by water solution acidified with sulfuric acid and then treatment by 4-6% dilute NaOH solution. The matter gained by both methods was concentrated, dried at 20-30°C and crushed up, brown matter of 7-8% humidity had been obtained.

Among the preparations used for the detoxication of aflatoxins, we have selected the adsorbent prepared on the basis of sawdust – technical lignin that is distinguished by low cost price and high efficiency. Dry sulfated lignin is brown powder. The size of such a lignin particle varies from 10 mm to 5 mm. Sulfated lignin belongs to non-toxic compounds, it is used as wet pastes, does not produce dust and is not fire-dangerous.

Therefore, considering urgency of the issue and the above-mentioned factors, elaboration of a simplified scheme of obtaining technical, sulfated lignin from mixed sawdust (deciduous and coniferous plants) and preparation of preparative forms for absorption of aflatoxins is one of the ways for resolving this problem. The development of effective and selective methods using various physicochemical and microbiological methods is required.

**ORGANIC-INORGANIC HYBRID MATERIAL - AEROGEL'S  
SYNTHESIS VIA SOL-GEL METHOD  
(Mixtures and Materials with specific features)**

**K. Merabishvili\*, G. Dalakishvili**

San Diego State University Georgia/ Chemistry/Biochemistry

\*merabishvili.kh@gmail.com

Organic compounds have been used for drug production and cosmetics; inorganic compounds utilized many materials for building production. Scientists started to get interested in more complex structures such as organic-inorganic hybrid materials. By definition, organic-inorganic hybrid materials include structures that have two moieties having a connection to each other at the molecular scale. These linkages can be regulated by different forces, especially with weak interactions such as electrostatic interactions, hydrogen bonding, van der Waals forces, or by covalent bonds. The interest in developing this topic of materials lies in the extending and improvement of the material's positive characteristics without cutting off the important existing ones.

According to IUPAC definition one of the best inventions -aerogels are mainly composed of a microporous material that is scattered phase in gas. Applied to aerogels, the coordination of organic features such as organic, metalorganic groups, or biochemical polymers may develop the mechanical steadiness of the solidified mesoporous structure with help of addition of some pliability to the matrix. Therefore, the two different parts of chemistry provide useful practical material. The soft features of polymeric aerogel can accumulate and then add some inorganic elements for solidity and rigidity of the material. For example, NASA uses them as insulation for Mars Rover, also for commercial purposes: "Aerogels have been combined with batting to create insulating "blankets," as well as filled in between panes of glass to create translucent panels for day-lighting applications".

There are other necessary features like hygroscopicity which should be improved by the incorporation of suitable organic groups into the inorganic complex, that results in changing the chemistry of the surface of prepared aerogel. A general method of integration of organic functional groups is a sol-gel process, which creates mixtures of organic polymers with or without specific bonding to inorganic moiety. Interfacing organic molecules into gels without chemical linkages can be achieved by dissolving the molecules in the precursor solution. Even though this process is effective, further processes may result in washing away the organic molecules such as the washing of the filigree gel or supercritical drying.

Useful mixtures can be created with organic polymers that are able to form hydrogen bonds or just covalent bonding. For example, there are silicate systems- compounds of the type  $R'Si(OR)_3$  that can be utilized where R is the organic functional group (radical). In this case, the functional organic group is linked through a hydrolytically steady Si-C linkage to the network.

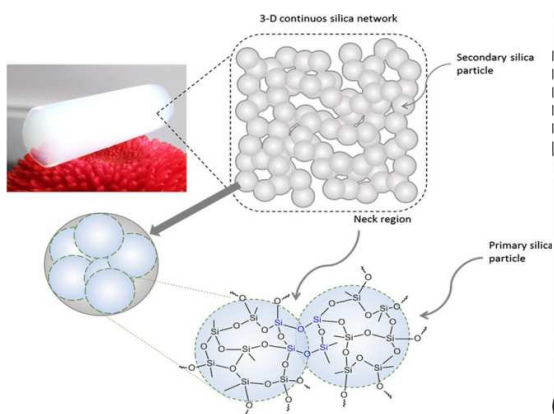
Picture II represents a scheme of the different possibilities (A and B) to get acquainted with a Si-C bond into the inorganic silica complex. This could be attained via using organo-silane with single-way functionality such as  $R'Si(OR)_3$  or with help of alkyl bridged bis-alkoxysilane  $Si(OR)_3 R'Si(OR)_3$ . Later procedures show that when the bridging component is formed as a long aliphatic hydrocarbon chain, the complex gains extra mechanical durability. This approach is exclusive only for siloxane-based materials as long as Si-C bonds have good stability compared to metal-carbon bonds. These specific bonds aren't perfect for metal alkoxide complexes because of the hydrolytic unsteadiness of M-C bonds. Another approach is that the organic groups can be represented with bidentate ligands too. Scientists indicate how organic functional groups are sitting sometimes on the inside or outside pore surfaces of mesoporous solids by utilizing different methods or by co-condensation. One of the researchers discovered novel multifunctional polymethylsilsesquioxane-silk fibroin aerogel hybrids for environmental and thermal insulation applications through simultaneous processing of silk fibroin proteins with organically substituted alkoxysilanes via a successive sol-gel approach to produce homogeneous interpenetrated IPN polymethylsilsesquioxane PMSQ-SF hybrid aerogels with significantly improved mechanical properties.

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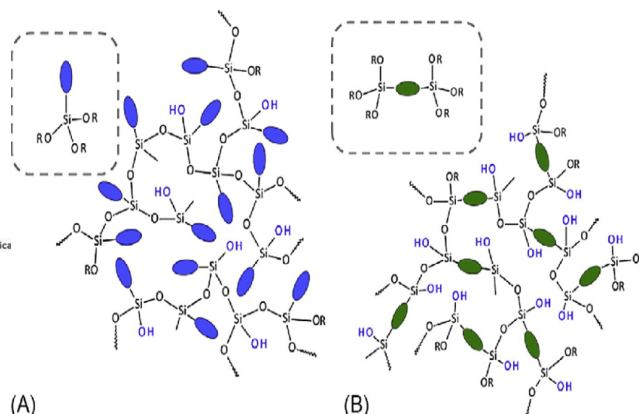
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### Appendix:

#### Picture I



#### Picture II





## SYNTHESIS AND CHARACTERIZATION OF HIGHLY SULFONATED POLY(PHENYLENE PHOSPHINE OXIDE SULFONE)

**N. Dumbadze**

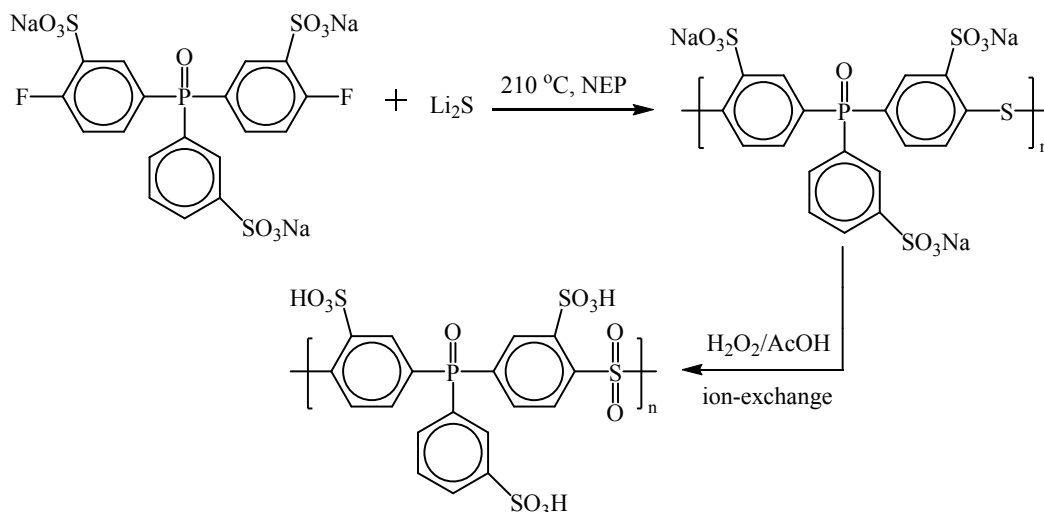
Agricultural University of Georgia, 240 David Aghmashenebeli Alley  
0159 Tbilisi, Georgia; ndumb2019@agruni.edu.ge

There is increasing demand for electricity production technologies relying on the electrochemical processes. In this respect, proton exchange membrane fuel cells (PEMFCs) have great potential due to the high energy-conversion efficiency and zero local pollution [1]. Special interest in PEMFCs is due to their application in electric vehicles [2, 3]. Proton exchange membrane (PEM) is the core component of the system and plays crucial role in fuel cell performance. Currently, in commercial PEMFCs perfluorinated sulfonic acid containing ionomers (PFSA), such as Nafion<sup>®</sup>, are typically used as PEM materials showing optimum performance at moderate operation temperatures (<80°C). However, PFSA ionomers suffer from several significant drawbacks such as limited operation temperature (<80°C) leading to CO poisoning of catalyst, negative environmental impact, deterioration of mechanical properties at high temperatures (>80°C), high gas permeability and a very high electro-osmotic drag of water [4, 5].

Sulfonated aromatic polymers are materials of choice to overcome these drawbacks. Among these materials sulfonated poly(arylene sulfone)s with a backbone consisting of merely phenyl rings connected with electron-accepting units deserve special interest. Their advantage over frequently reported sulfonated poly(arylene)s containing electron donating units in the main chain is higher thermal, thermooxidative and hydrolytic stability. The stabilization effect is caused by the presence of electron-withdrawing groups in the ortho-position to the sulfonic acid groups [6]. The ionomer with highest IEC (4.5 meq/g) of this class is fully sulfonated poly(phenylene sulfone) (sPSO<sub>2</sub>-220) revealing proton conductivity exceeding the one of Nafion by factor of 5-7 [7]. This polyelectrolyte due the pronounced ionic character has extremely bad mechanical properties and is water soluble. Therefore, sPSO<sub>2</sub>-220 in its pure form is not suitable as a separator material of PEMFC, but can be successfully used in an acid-base blend form or as a hydrophilic block of multiblock co-polymer [8]. Further increase of IEC of sulfonated poly(arylene)s may allow increase of the base polymer content in case of acid-base blends and the length of hydrophobic block in case of multiblock co-polymers, while keeping the same IEC as for sPSO<sub>2</sub>-220 systems and improving mechanical properties. In this respect we have synthesized novel sulfonated poly(phenylenephosphine oxide sulfone) having IEC=5.15 meq/g, which is the highest for the ionomers belonging the above described class. Polymer was obtained by nucleophilic aromatic substitution reaction of pre-synthesized tri-sulfonated bis(4-



fluorophenyl)phenylphosphine oxide with lithium sulfide. Synthesized polymer showed excellent proton conductivity.



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## SYNTHESIS AND RESEARCH OF 2-(1-ADAMANTYL-METHYL)BENZIMIDAZOLE'S SOME DERIVATIVES

**Aleksandre Vanishvili\* , Davit Zurabishvili, Shota Samsoniya**

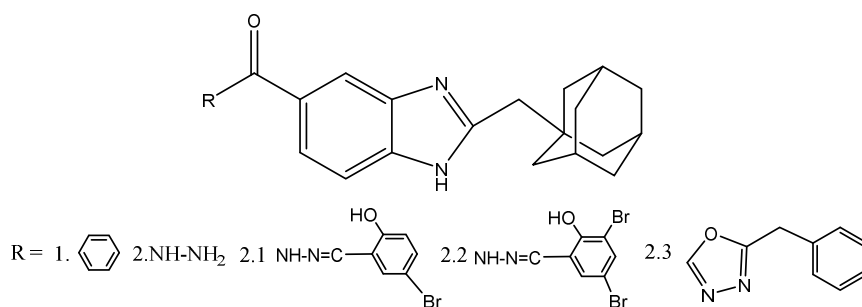
Ivane Javakhishvili Tbilisi State University  
3, Ilia Chavchavadze Ave., Tbilisi, Georgia

The Main topic in medicine is the resistance of microorganisms to drugs. Therefore, the synthesis of new substances that need to be characterized by higher activity becomes popular.

The aim of the study is to synthesize substances containing a new biologically active adamantane nucleus, which should be characterized by higher pharmacological action.

The discovery of Adamantan compounds from the 1960s, which were characterized by antiviral and anti-Parkinson's effects, has aroused great interest among scientists. This discovery laid the foundation for the synthesis of Adamantan compounds, the establishment of Adamantan products in medical chemistry, and the study of their biological activities.

Benzimidazoles are characterized by a wide range of biological activity. They are based on drugs that are widely used in medicine, veterinary medicine, agriculture. Characterized by fungicidal, antimicrobial, antiviral, antihelminthic and anti-cancer activity. The biologically active molecule of benzimidazole is effective in combating microorganisms, as evidenced by biochemical and pharmacological experiments.



Scheme 1

The study is about 2-(1-adamantylmethyl) synthesis of some benzimidazole derivatives (Scheme 1.) and their study. During the study, 2-(1-adamantylmethyl)-1H-benzimidazole-5(6H)-carboxylate and methyl-2-(1-adamantylmethyl)-1H-benzimidazole-5(6H)-carboxylate were synthesized. Relevant carbohydrazide was obtained by hydrazinolization of the latter, by interacting with various aromatic aldehydes and carbonic acid the corresponding Schiff bases and amide were obtained. The identities of the synthesized substances were checked by infrared and NMR spectroscopy.

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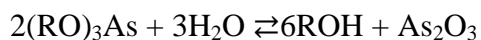
## COORDINATION COMPOUNDS OF SOME LANTANIDES

**D. Miminoshvili, M. Rusia\***

Ivane Javakhishvili Tbilisi State University, Faculty of Exact and Natural Sciences,  
Department of General, Inorganic and Organometallic Chemistry  
3, I. Chavchavadze Ave., 0179 Tbilisi, Georgia; \*maia.rusia@tsu.ge

Harm-neutralization of arsenic-containing waste is one of the global problems today. Such waste from the production of non-ferrous and precious metals accumulates millions of tons, leading to a sharp deterioration in the ecological condition of the environment. Residues of arsenic production in Georgia are mainly collected on the territory of Racha and Tsani mining and chemical plants. This waste is dumped in open ground near the plant and is still the leading cause of pollution in the entire valley.

From the residues of arsenic-containing products including arsenous acid anhydride, the action of amyl, iso-amyl, and n-hexyl alcohols yields trialkylarsenites (azeotropic drying method). As is already known, this reaction is selective. Alcohol reacts with arsenous acid existed in the residue, and the accompanying products are deposited in the form of sludge on the bottom of the reaction vessel. With this method it is possible to completely remove arsenic. Synthesized arsenous acid ethers are the starting materials to get various products:



Sodium monoselenosarnesate composed of  $\text{Na}_3\text{AsO}_3 \cdot 12\text{H}_2\text{O}$ , is easily obtained by the action of elemental selenium on the product of the interaction of sodium hydroxyde and white arsenic, without releasing the latter in the free state. "Technical white arsenic" from waste, high-purity sodium hydroxyde and similar high-purity elemental selenium were used for the reaction:



We used Holmium (III), Erbium (III), Telmium (III), Iterbium (III) and Luitecium (III) water-soluble salts to obtain lanthanide monoselenosarnesates. Synthesis was carried out by mixing the aqueous solutions of the starting substances at room temperature. As soon as the solution was mixed, small crystalline substances were released:  $\text{M}(\text{AsO}_3\text{Se}) \cdot n\text{H}_2\text{O}$ .

These compounds are solid compounds of different colors. None of them dissolve in water, alcohol, or other organic solvents, and when treated with acid ( $\text{HCl}$ ,  $\text{H}_2\text{SO}_4$ ) they undergo a transformation to produce selenide of arsenic (V). The composition and structure of the synthesized substances, in addition to the elementary analysis, are determined by spectroscopy, X-ray and thermographic examinations. Physico-chemical methods have shown that the obtained compounds are individual substances.

## BIO-BASED COMPOSITES MATERIALS

**E. Markkarashvili\*, L. Londaridze, T. Tatrishvili, I. Esartia, D. Otiashvili,  
J. Aneli, O. Mukbaniani**

<sup>1</sup>Iv. Javakhishvili Tbilisi State University, I. Chavchavadze Ave., 1, Tbilisi 0179, Georgia

<sup>2</sup>Institute of Macromolecular Chemistry and Polymeric Materials, Iv. Javakhishvili Tbilisi State University, I. Chavchavadze Ave., 13, Tbilisi 0179, Georgia

\*markkarashvili@yahoo.com

The utilization of biomass for processing novel composites has attracted growing interest because of this eco-friendly and renewable nature. Materials reinforced with wood flour and others natural fibers increased considerably in recent years. Wood flour is easily available, light and cheap, and it can be added to commodity matrices in large quantities thus offering economically advantageous solutions.

One of the main disadvantages of wood polymer composites is the low compatibility between the hydrophilic wood filler and hydrophobic polymer matrix. Thus, two ways of improvement of the interface properties are generally used surface treatment of the reinforced fibers in order to increase their compatibility with the surrounding polymer, or modification of the matrix. The introduction of functional groups inside the polymer chains of the matrix aims to create chemical or physical interactions with the reinforcing fibers, and is a solution which leads to excellent results in practice. Functionalized styrene introduced by radical copolymerization in styrene constitutes one of the most efficient modifications agents used to functionalize the styrenic polymers. Then, high molecular weight copolymers based on functionalized polystyrene and styrene may act as coupling agents in polystyrene composites reinforced by triethoxysilylated polystyrene.

On the basis of sawdust and silylated styrene the composite materials were obtained. The binders in the composites were included with amount 3 and 5 wt%. The composites were obtained via hot press method at various temperatures.

The used silylated styrene in situ polymerization reacted with sawdust, which contain functional groups in cellulose, hemicellulose, pentosanes, lignin and silicon dioxide with formation of three-dimensional systems.

**Acknowledgements.** The financial support of the Shota Rustaveli Georgian National Science Foundation Fundamental Grant №19-795 is gratefully acknowledged.

## **ADSORPTION OF IRON IONS ON CARBONACEOUS SORBENTS OBTAINED FROM CELLULOSE-CONTAINED SECONDARY RAW MATERIAL**

**T. Marsagishvili, N. Giorgadze\*, N. Ananiashvili, E. Tskhakaia, M. Machavariani**

Ivane Javakhishvili Tbilisi State University, R. Agladze Institute of Inorganic Chemistry and Electrochemistry; 11, Mindeli str., 0186, Tbilisi, Georgia

\*giorgadze-nino93@rambler.ru

The rapid development of chemistry and the intensive implementation of the achievements of the chemical industry led to a swift increase of environmental contamination. The rational use of water resources is one of the urgent ecological problems, in the solution of which purification of drinking and waste water is very important [1].

Chemical and biological agents existing in water cause various health problems; therefore, regulation of water quality is an important task of protecting public health [2]. Heavy metals are biologically hazardous components of natural waters. They enter the environment as a result of production processes. Monitoring the concentration of heavy metals in water becomes very important due to the complex environmental background created by these processes [1].

Water purification is connected with large financial resources, so, the creation of natural, renewable and inexpensive adsorbents is an urgent problem.

A technology was developed at the R. Agladze Institute of Inorganic Chemistry and Electrochemistry [3], with the help of which sorbents can be obtained from cellulose-containing secondary raw materials.

The aim of the work was to determine the adsorption capacity of sorbents, in particular, carbon materials obtained from nutshells, nutshells and nectarine stones (factory-made activated carbon of grade A was taken for comparison), with respect to iron ions (of two and three valence). The results are shown in Table 1.

As can be seen from the table, the best adsorption capacity is shown by the carbon material of the hazelnut shells, which is no worse than the adsorption capacity of factory activated carbon. The adsorption capacity of the carbon materials of nutshells and nectarine seeds relative to iron ions is lower, although the parameters of the adsorption process can be selected if necessary. The advantage of the mentioned adsorbents is their low cost and high adsorption ability in relation to heavy metals [4, 5].

**Table 1.** Adsorption of iron ions on various carbon materials

Metal	Carbonaceous material	Initial concentration of metal, g/L	Final concentration of metal, g/L	Adsorption, mg/g
Common Iron (Fe <sup>2+</sup> , Fe <sup>3+</sup> )	Nutshell	0.56	0.48	8
	Hazelnut shell		0.25	31
	Nectarine stone		0.43	13
	Activated carbon		0.25	31

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## STUDY OF NITROSATION REACTION IN FISHER-BASED BIS-ANALOGUES

**Marina Trapaidze\*, Sophiko Kvinikadze, Shota Samsoniya**

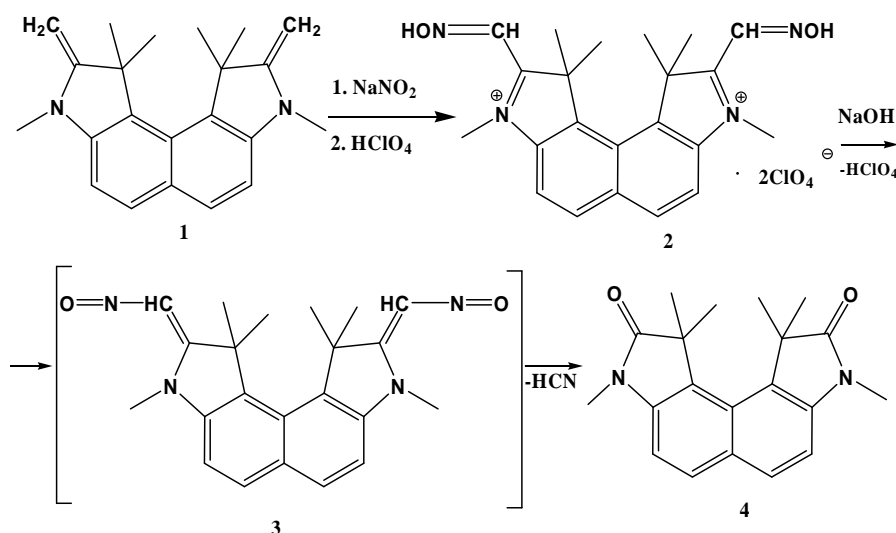
Iv. Javakhishvili Tbilisi State University  
3, Ilia Chavchavadze Ave., 0179 Tbilisi, Georgia  
\*marina.trapaidze@tsu.ge

2-methylenindoline bases, the so-called Fischer bases, are important reactive by-products in synthesis of several different organic compounds [1,2]. It should be noted, that it reacting with exogenous methylene bond in terms of elimination and electrophilic substitution reactions. In presented research is provided nitrosation reaction of new bis-analog of Fischer base, which are synthesise by us [1,2].

It is well known, that nitroso compounds are formed at a certain stage of oxidation of amino compounds in living organisms and perform an important biological function. Therefore, the synthesis of new heterocyclic nitroso compound is considered an interesting task in terms of studying their biological activity.

Earlier [3], in order to synthesize nitrosation of compound, we were carried out reaction of new bis-analog (hexamethyldimethylenindolo[4,5-e]indole) of Fischer base with nitric acid, by us. At the first stage of the reaction, dioxime is isolated in the form of chloric acid salt-perchlorate.

As a result of processing the obtained alcohol solution, instead of the expected dinitroso compound with the aqueous solution of sodium hydroxide, a symmetrical structure - 1,1,3,8,10,10-hexamethyl-2,9-dioxo-indolino[4,5-e]indoline was separated. Thus, in the case of indoloindole, unlike indole, the action of a strong base from the dioxime perchlorate with chloric acid (HClO<sub>4</sub>) also breaks down the HCN molecule. Accordingly, 2,9-dioxo-indoloindole of symmetrical structure is obtained (Fig. 1).

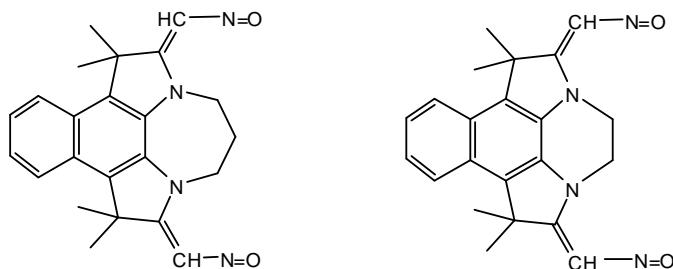


It is interesting nitrosation reaction with fisher base new isomeric bis-analogs. They were synthesized on a base of benzopyrrole[3,2-g]Indole [4,5] by us. It should be noted, that their molecules contain quinoxaline and diazepine nuclei interesting in terms of biological activity. Drugs based on them are used to treat diseases such as epilepsy, alcoholism, mental disorders.

Nitrosation reaction of base of fisher base bis-analogues dipyrrolonaphthodiazepine and dipyrrolobenzoquinoxaline via analogy of above mentioned methodology was carried out. Reaction process in acetic acid and hydrochloric acid with an aqueous solution of sodium nitrite was carried out. Nitrosation reaction consists of two steps of which the first synthesis dioxime. Its sodium hydroxide processing results in the formation of nitrosation of compound, such as 1,1,9,9-Tetramethyl-2,8-di(Nitrosomethylidene)4H-dipyrrole[1,2,3-e,f:3,2,1-n,o]naphtho[2,3-b][1,4]diazepine (yield is 45%) and 1,1,8,8-tetramethyl-2,7-di(Nitrosomethylidene)dipyrrole [1,2,3-d,e:3,2,1-i,j]benzo[g]quinoxaline (yield is 36%) (Fig. 2).



Synthesised bis-spiropyranes are highly soluble in polar solvents, such as in chloroform, diethyl ether, acetone, and ethanol. The color obtained is yellow. Spectrometric (IR) research of synthesized new compounds was carried out. Interpretation of characteristic IR absorptions of functional groups was carried out. Characteristic IR absorptions of functional groups were interpreted. The research of their structures continues.



**Figure 2**

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## TRANSITION METAL SALEN COMPLEXES: SYNTHESIS AND BIOLOGICAL ACTIVITY

**T. Khatisashvili**

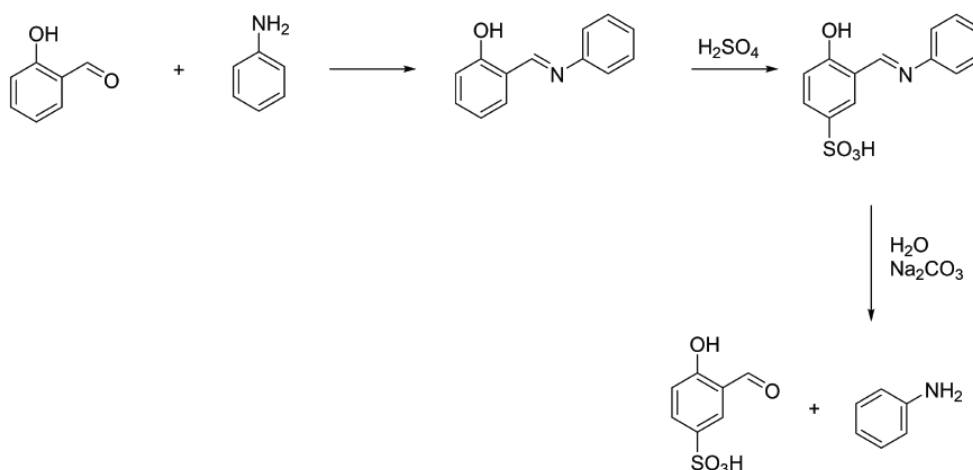
Agricultural University of Georgia  
tkhat2016@agruni.edu.ge

Transition metal Salen complexes have been extensively studied because of their wide range of physical and chemical properties. They are commonly used in industrial, pharmacological and biochemical applications. Furthermore, ease and flexibility of the synthetic procedure makes Salen complexes more commercially suitable.

Many reports have demonstrated that metal Salen complexes have various biological properties such as antitumor, antibacterial, antifungal and the most significant - “enzyme mimics”. Salen complexes can be active against several diseases or at least prevent them. Thus, our research objective was synthesis of biologically active metal complexes and detection of their biological activity.

We synthesized Nickel(II), Cobalt(II), Copper (II) and Iron(III) Salen type complexes. Potentially each and one of them has to have biological and enzymatic activity, based on their structural specifications.

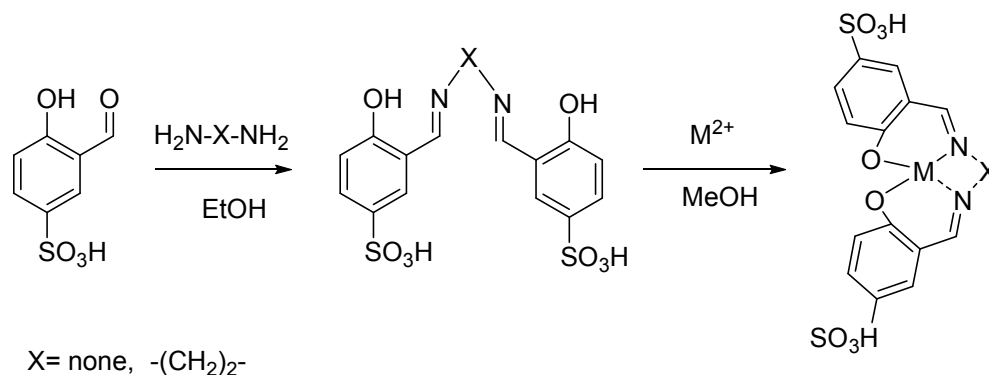
Results have shown that synthesized complexes have some kind of biological activity. However, results are unsure, because organic solvents negatively affect living cells and we can't distinguish direct effect of our compound. These kinds of manipulations on living organisms require water soluble compounds. So, on this next phase of research our objective is to synthesize water soluble salen complex. Thus, we decided to increase water solubility with changing origin compound (Salicylaldehyde) to 3-carboxyl, 4-benzenesulfonic acid, which was synthesized according to scheme 1.



**Scheme 1. Synthesis of water soluble Salen precursor**

Salen precursor was synthesized from salicylaldehyde. Aldehyde group was protected by reaction between salicylaldehyde and aniline. Protected product was further sulfonated by Sulfuric acid and further decomposed by basic hydrolysis. Salen precursor and aniline were easily separated by distillation.

Salen precursor will be used to synthesize water soluble Salen derivative, by reacting with diamine (hydrazine, ethylenediamine). This derivative further reacts with metal salt (chloride or acetate) and forms water soluble metal complex (scheme 2).



**Scheme 2. Synthesis of Metal Salen complexes**

## PHENOL CONTENTS IN QVEVRI WINES

**E. Sordia, G. Kvartskhava**

Georgian Technical University

Wine is becoming an increasingly sought-after product not only in Georgia but around the world too. It takes a significant role in the dining culture; therefore, its quality is important. Throughout centuries, Georgian people developed a particular way winemaking - holding concentrated grape juice in a large underground clay vessel- Qvevri.

Kakhetian wine has always been a favorite. Its uniqueness comes from the grape variety which has valuable bioenergetic, nutritional, and healthful characteristics. Phenolic compounds are one of the most revealing features when it comes to assessing wine quality. They affect the taste, flavor, color, and turbidity of wine, hence are relevant markers to measure.

The objective of our study was to investigate the phenolic compounds in wine and find the differences between the qvevri and European style wines.

Phenols found in grapes and their derivatives play an active role in the complex biochemical processes of winemaking and conservation. They directly affect the taste, bouquet, color, turbidity, and stability of wines.

Total phenol content was determined and compared in both qvevri and European style wines. The results were obtained spectrophotometrically, using a Folin-Ciocalteu reagent.

According to the research, total phenol content in traditional Kakhetian qvevri wines was found to be much higher than in wines made with the standard European winemaking methods.

## SYNTHESIS OF NOVEL AZO DYES BEARING NON-TOXIC MOIETIES

**K. Dzuliashvili**

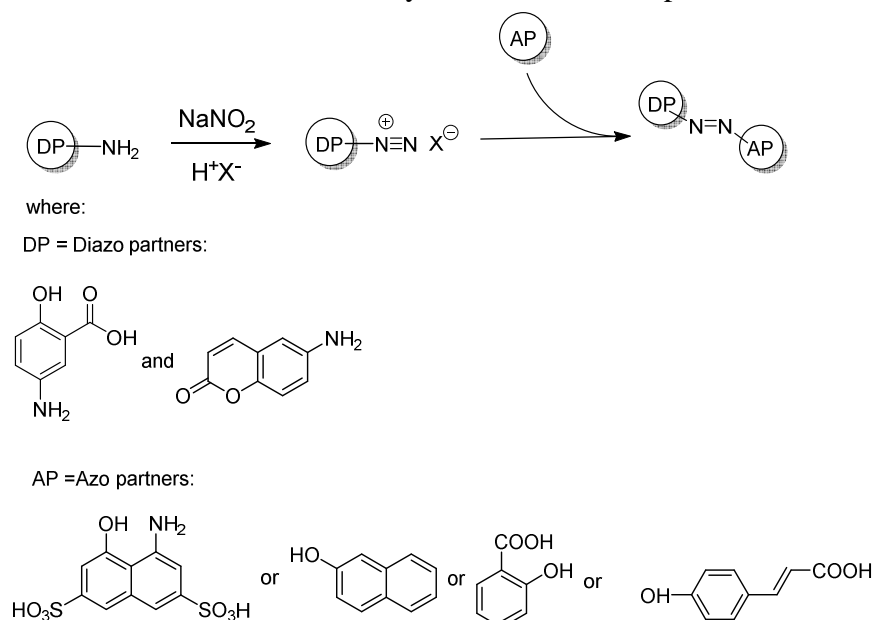
Agricultral university of Georgia  
kdzul2016@agrni.edu.ge

Nowadays the synthesis of non- or less toxic materials is extremely important, therefore there are several papers concerning the novel methods of the synthesis of new interesting materials or updated methodologies for obtaining already known compounds.

In the current research, we have studied the possibility of the synthesis of novel azo dyes bearing non-toxic moieties. The target azo dyes have been synthesized according to the scheme 1.

5-aminosalicylic acid (5-ASA) and 6-amino-2H-chromen-2-one have been chosen for the diazo partners. 4-amino-5-hydroxynaphthalene-2,7-disulfonic acid, naphthalen-2-ol, 2-hydroxybenzoic acid and (E)-3-(4-hydroxyphenyl)acrylic acid have been selected as azo partners.

We have developed the modified method of the synthesis of olsalazine, which comprises the diazotization of 5-aminosalicylic acid in the tetrafluoroboric acid, isolation of obtained diazonium salt in the solid state as 4-carboxy-3-hydroxybenzenediazonium tetrafluoroborate and azo coupling between salicylic acid and solid diazo partner in minimal quantity of water. The high solubility of 5-aminosalicylic acid in the tetrafluoroboric acid and the ability of isolation diazonium salt in the solid-state increases the yield of olsalazine up to 68%.



**Scheme 1. Synthesis of azo dyes**

In addition, it has been found that 6-amino-2H-chromen-2-one having multiple interesting biological activities, is an excellent diazo partner and easily reacts to nitrosyl chloride, giving diazonium salt with the ability of following azo coupling with 4-amino-5-hydroxynaphthalene-2,7-disulfonic acid and naphthalen-2-ol (modeling compounds) as well as with 2-hydroxybenzoic acid and (E)-3-(4-hydroxyphenyl)acrylic acid. The yield of azo dyes varies from moderate to good. Synthesized azo dyes have been used for dyeing wool and have excellent fastness against light and wet treatment.

## **THE SYNTHESIS OF *H. HALYS*'S PHEROMONE VIA HAGIWARA AND ALDOLE CONDENSATION REACTIONS AND DEVELOPMENT OF PILOT PLANT PRODUCTION METHOD OF THEREOF**

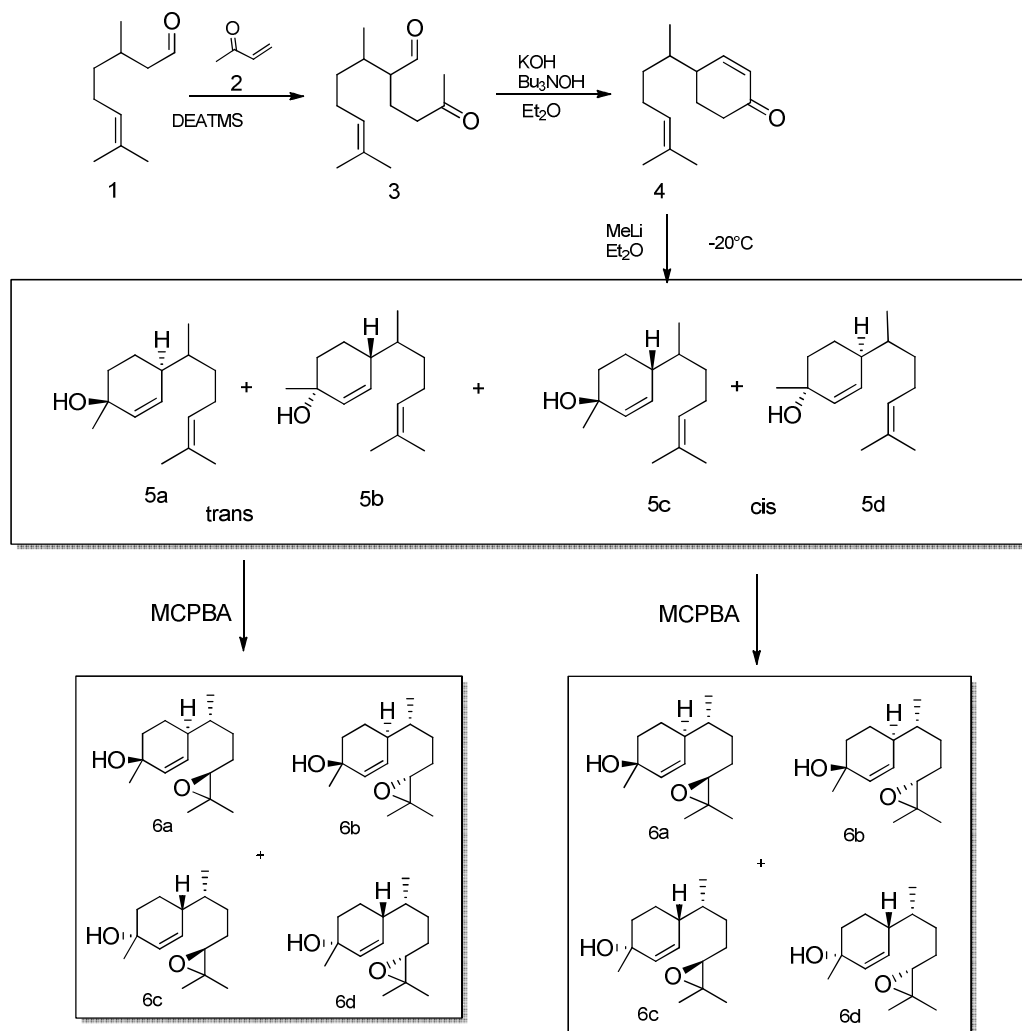
**N. Rusishvili**

Agricultural university of Georgia  
nrusi2016@agruni.edu.ge

The one interesting field of the current research comprises the chemistry of the biological active compounds, responsible for chemical communication in insects. These signal-carrying ones are known as pheromones. There are two main types of pheromones called as releasers and primers. The first is used for initiation of immediate behavioral responses in insects upon reception, while the second one is for causing physiological changes in an animal, i.e. the sex pheromones release the entire repertoire of insect's sexual behavior and this phenomenon can be used for artificial regulation of insects' replication.

In the current research the pheromone of *H. halys* has been synthesized according to Hagiwara and aldol condensation reactions for the aim of whole process optimization and development of pilot plant technological scheme.

The target compound has been synthesized according to the scheme given below. Citronellal (**1**) and methyl vinyl ketone (**2**) have been selected as a starting compound. The first step of the transformation is Hagiwara's 1,4-conjugated addition reaction catalyzed by diethylamino(trimethyl)silane (DEATMS). The obtained addition product **3** undergoes cyclization reaction in the presence of alkali and tributylammonium hydroxide or iodide with following formation of cyclic unsaturated ketone **4**. The methylation of the last one by methyl lithium under nitrogen at -20°C forms mixture of four stereoisomers **5**. **5** has been used for the next step as crude compound because of decreasing the casts. The last step of transformation is oxidation of side-chain double bond in the oxirane moiety. Meta-chlorobenzoic peroxide has been used as an oxidant and obtained final product has been used without further purification as a pheromone.

Scheme. The synthesis of *H. halys*'s pheromone

Pheromone has been used for the preparing of insect's attractant composition and put on the chromatographic silufol plates. The last one is placed in the insect's scavenger bottles and positioned in the fields near nuts gardens, which is under observation currently.

The research has been carried out by financial support of SRNSF under the grant project "Application of ecofriendly tools for control Brown marmorated stink bug (BMSB) *Halyomorpha halys* in Georgia".

## UTILIZATION OF WASTE WATERS PRACTICING IN GALVANIZING PLANTS, DEVELOPMENT OF WASTELESS TECHNOLOGICAL PROCESSES

**R. Gotsiridze\*, N. Mkheidze, L. Kontselidze, S. Mkheidze**

Batumi Shota Rustaveli State University Agrarian and Membrane Technologies Institute

\* niimt@bk.ru

The galvanizing plants practice coating of metals with such heavy metals as nickel, cobalt, chrome, etc. After completion of coating they are washed with running water. That is why, waste waters contain toxic heavy metals what causes pollution of the environment and endangers it. In the galvanic industry water consumption is great because of difficulty of washing of the parts ( $2\text{m}^3$  or more for each  $1\text{ m}^2$  of a part). Treatment and concentration of the industrial waste water and its return into the technological cycle will surely considerably reduce water and chemical agents' consumption and prevent pollution of the environment (as the scientist proved, heavy metals used in galvanizing plant are tens time more dangerous, then radiation).

Electromembrane method allows creation of closed technological systems and their local inclusion into the general technological scheme of production.

There are many methods of separation of heavy metals from such waters, namely, electromembrane method has some prospective for treatment of chrome-containing water. This method is based on transfer of electrolytes into ion-selective membranes under action of electric field. Ion-exchange membranes pass only the ions having the same charge as the moving ions.

Ionite membranes are used in a process due to their properties. Physicochemical properties of a membrane depend to a large extent on its content, nature and technologies of production.

Many kinds of heterogeneous and homogeneous ion-exchange membranes are known. But it is not enough for operation of membrane to have good initial properties, as it is also required to keep them stable during prolong period of operation.

We have researched stability of heterogeneous membranes (MK-40, MA-40, MA-41) to chrome ions in solutions.

The aim of our research included study of possibility of the processes of desalination and concentration of solutions containing chrome ions by electromembrane method.

Anionite membranes easily get "poisoned" in aggressive media, that is why, the first task included matching of membranes and running of the process with membrane package which gets "poisoned" to less extent; the second task was to determine efficiency of electro dialysis process; finally - possibility of return of the received products, i.e. water and concentrate into the technological cycle.

For this purpose, we provided demineralization process in the concentration chamber in the same conditions and various concentrations of the initial solutions. Besides, we have researched



possibility of maximum concentration of chromate ions in the concentration chamber without considerable reduction of desalination rate.

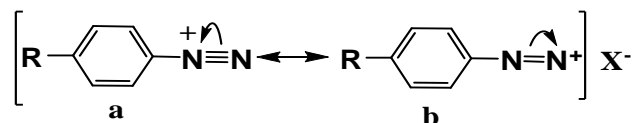
The results of our research showed that treatment of chrome containing waters in case of furnishing of the apparatus with MK-40 and MA-40 membranes is impossible due to “poisoning” of membrane MA-40 with chromate-ions. It is proved that the process may be provided only in case of furnishing of the apparatus with MK-40л and MA-41л membranes. Besides, deep desalination of chrome containing waters is ineffective. It is purposeful to provide the process in the dialyzates with 8-10 mg/l chromate-ions residual concentration; we have achieved maximum (200g/l) concentration of chromate-ions without considerable reduction of desalination rate. It is proved that the electro dialysis method allows treatment of chrome ions containing waters in galvanic industry and return of the received water and concentrate into the technological cycle.

## SOME INTERESTINGARYLDIAZONIUM SALTS

Sh. Samsoniya, N. Megrelishvili, N. Targamadze, I. Chikvaidze\*

Iv. Javakhishvili Tbilisi State University  
3, Ilia Chavchavadze Ave., 0179 Tbilisi, Georgia  
Kutaisi Akaki Tsereteli State University  
59, Tamar Mefe Ave., Kutaisi, Georgia  
\*iosebc@yahoo.com

The electron-acceptor substitutes boost the stability of the diazocompunds. In general, the temperature of azo-coupling reaction depends on the basic nature of an amine compound, the amines, with the strong basicity, easily convert into the diazonium salt. This process is supported by the positive inductive and mesomeric effects of substituents. In this case, the mesomeric equilibrium is deviated to the right.

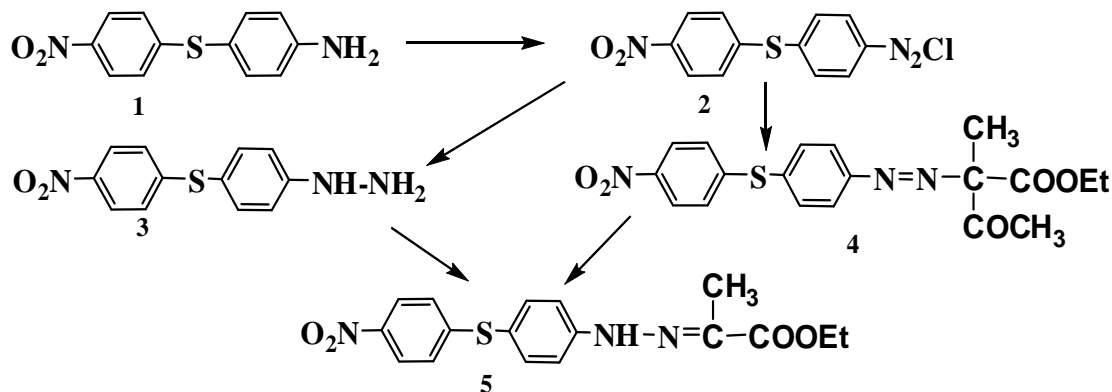


The nitrosation reaction of weak bases are difficult to proceed. The negative inductive and mesomeric effects of additional substituents have a negative impact in this direct process.

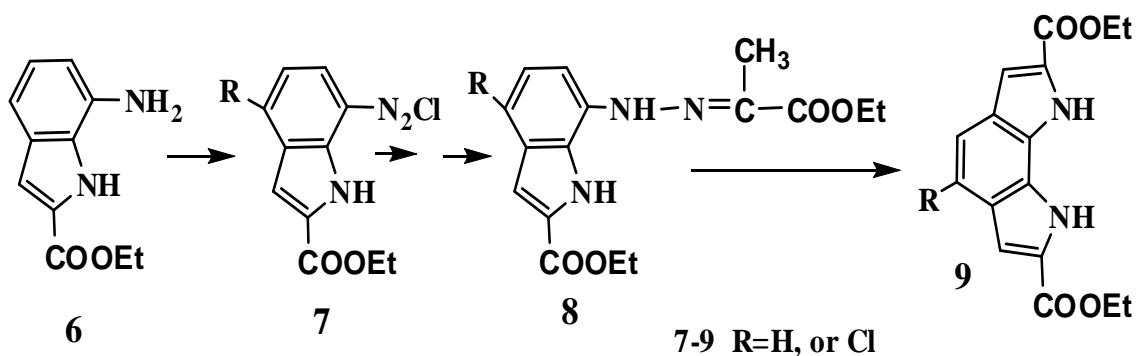
Essential arylhydrazones (5) for the Fisher indole-synthesis reaction, are obtained from the substituted anilines, by reducing of the diazonium salts resulted arylhydrazines (3) condense with oxo-compounds.

It is noticeable, that the diazotization of 4-nitro-4'-amino-diphenylsulphide is carried out at 35-40 °C temperature. We have obtained diazonium chloride as a colorless, needle-like crystals.

The reduction of this compound is a complicated process, but the azo-coniugation by japp-clingeman and subsequent hydrolysis of this azoesters (4) are proceeded with one stage.



Yields are respectively 66 and 58% from the initial amine. It should be noted, that the same process has happened during the synthesise of one of the isomeric pyrroloindoles on the stage of diazotization. The diazotization of this compounds are described by the Indian authors in anormal condition- 0-5°C; (conc.HCl.). But, we noticed, that the reaction mixture was always containing the initial amines even after 5 hours and the reaction could be completed only in 0.5 hour at 35-40°C. On the following stages we have produced hydrazones (8) and pyrroloindoles (9).



It was discovered, during the diazotization of amino groups in this condition, simultaneously carried out an unusual reaction of chlorination in the indole ring. (compound 7-9 R=Cl)

## SYNTHESIS OF THREE- AND MORE RINGED INDOLE HETEROCYCLES

**Sh. Samsoniya; N. Targamadze, D. Kadjrshvili, E. Mumladze, N. Narimanidze,  
A. Tsutskiridze, I. Chikvaidze\***

Iv. Javakhishvili Tbilisi State University  
3, Ilia Chavchavadze Ave., 0179 Tbilisi, Georgia  
\*iosebc@yahoo.com

The report discusses the development, stages, achievements, challenges, and outcomes of new of Indole heterocycles, which include two-and-more nitrogen atoms. A multi-year survey was done by the staff of the Organic Chemistry department and the institute of Organic Chemistry in this field and as a result, symmetrical and asymmetrical bi- and tri-indoles, aryl- and di-aryl-indoles; Condensed and isomeric pyrrolo-indoles, a new type of five-ringed pyrrolo-indolo-quinoxaline and Pyridazino-indoles, Isomeric bis-tricyclicpyridazino-indoles were obtained.

Principles of constructing these key systems and general preparatory methods for synthesis have been developed; their physical-chemical and chemical properties, quantum-chemical parameters were also studied. We have received compounds substituted by different functional groups, and they have been identified to have antiseptics, cytotoxic, biocidal, Curare-like, and other beneficial properties. Some of these compounds are florescent biomarkers, which have the ability to bind strongly to biomolecules.

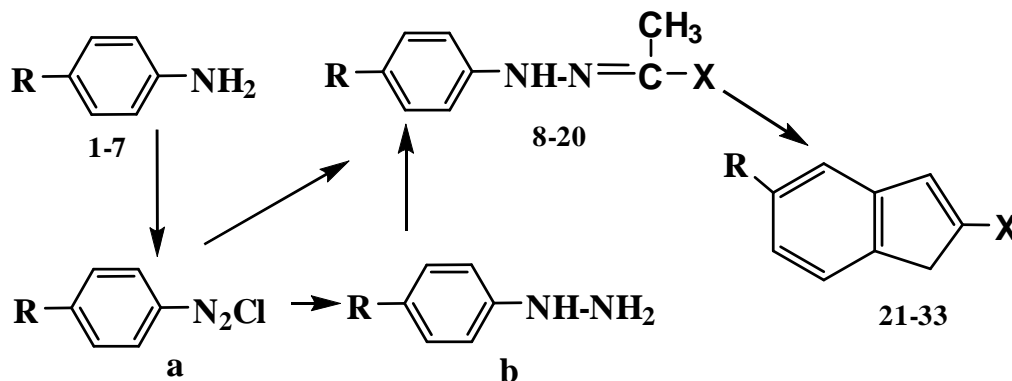
New reactions have also been found, for example: de-formylation of heterocyclic aldehydes, chlorination of the Indole nucleus and 1,7-shift of the benzyl group. The mechanisms of these reactions are provided; the influence of substitutional groups on the key stage of E. Fisher's reaction - the indole synthesis from arylhydrazones – is also explained.

## SYNTHESIS OF SOME NEW INDOLE DERIVATIVES

Sh. Samsoniya, N. Megrelishvili, T. Giorgadze, N. Esakia, M. Turiashvili,  
S. Zedginidze, I. Chikvaidze\*

Iv. Javakhishvili Tbilisi State University  
3, Ilia Chavchavadze Ave., 0179 Tbilisi, Georgia  
Kutaisi Akaki Tsereteli State University  
59, Tamar Mefe Ave., Kutaisi, Georgia  
\*iosebc@yahoo.com

Indole derivatives have a high physiological activity, at the same time their non-toxicity has been well known. Due to this reason, we aimed to obtain 2- and 5-substituted products of indoles 21-33, which are interesting because of their potential importance in numerous fields.



1,8-10,21-23R=CH<sub>3</sub>; 2,11-13,24-26 R=Br; 3,14-16, 27-29 R=Cl; 4,17,30=COOEt;  
5,18,31 R=CN; 6,19,32 R=C<sub>6</sub>H<sub>5</sub>; 7,20,33 R=S-C<sub>6</sub>H<sub>4</sub>-NO<sub>2</sub>(p); 8,11,14,17-20, 21,24,27,30-33X=COOEt; 9,12,15,22,25,28 X=C<sub>6</sub>H<sub>4</sub>-NO<sub>2</sub>(p); 10,13,16,23,26,29 X=C<sub>6</sub>H<sub>4</sub>-NH<sub>2</sub>(p);

The 8-20th phenylhydrazones were obtained by multistep reactions from aryl-diazonium cations (a) they were synthesized by diazotization of 1st-7th anilines. (1) In first general way, diazonium salts were hydrogenated by (SnCl<sub>2</sub>/HCl) and the resulting substituted phenylhydrazines condensed with ketones or (2) on the other hand, they were formed by azo-coupling reaction between diazonium salts and methyl-aceto-ethylester and subsequent hydrolysis.

Poly-phosphoric acid and its ethyl esters are used for the indolisation from 8-20 phenylhydrazones.

The report discusses effects of substituents in the reaction.

## SYNTHESIS AND STUDY OF BIMETALLIC COMPLEX COMPOUNDS OF COBALT (II) AND NICKEL (II)

D. Margievi<sup>1</sup>, T. Gogelishvili<sup>1</sup>, L. Ratiani<sup>1</sup>, N. Gegeshidze<sup>1,2</sup>

<sup>1</sup>Georgian Technical University

<sup>2</sup>R.Agladze Institute of Inorganic Chemistry and Electrochemistry

The subject of our study is the synthesis of bimetallic complex compounds of cobalt (II) thiocyanate and nickel (II) with N, N-dimethylformamide and 4,4'-dipyridyl.

Over the past 30 years, interest in studying the structure and properties of binary and bimetallic complex compounds has increased. New research methods have appeared to study the structural and magnetic properties of these types of compounds. We can also consider them as precursors for new polymetallic compounds. They are also of interest in terms of biological and analytical chemistry.

The biological role of nickel and cobalt is undeniable; therefore, it is interesting to synthesize complex compounds of this metal and study their properties.

The bimetallic complex compounds  $[\text{Ni}(\text{L})_n][\text{Co}(\text{NCS})_4]$  were synthesized, where L is N,N-dimethylformamide (DMF),  $n=6$  and 4,4'-dipyridyl (dipy),  $n=3$ . Some their physicochemical properties have been studied.

To identify donor atoms by the quantum chemical semi-empirical method AM1, the influence of a solvent on the ability of a 4,4'-dipyridyl complex to form was studied.

The composition of the bimetallic complex compound  $[\text{Ni}(\text{DMF})_6][\text{Co}(\text{NCS})_4]$  and some physicochemical properties are established. The synthesized compound was studied by the IR spectral method and a thermographic study was performed.

Studies have shown that an ion-type coordination compound is synthesized in which the synthesized complex  $[\text{Ni}(\text{DMF})_6]^{2+}$  cation has an octahedral structure and the  $[\text{Co}(\text{NCS})_4]^{2-}$  complex anion has a tetrahedral structure.

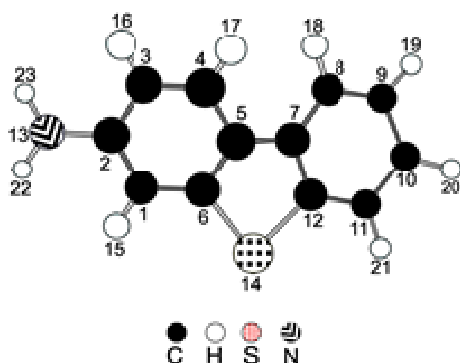
## THE EFFECT OF SOLVENTS ON AMINODIBENZOTHIOPHENE ON THE ABILITY TO CREATE COMPLEXES

Z. Gogberashvili, T. Giorgadze<sup>1</sup>, M. Tsintsadze<sup>1,2</sup>, D. Lochoshvili<sup>2</sup>

<sup>1</sup>Georgian Technical University, 77, M. Kostava St., 0175, Tbilisi, Georgia

<sup>2</sup>R. Agladze Institute of Inorganic Chemistry and Electrochemistry  
11, Mindeli Str., 0186, Tbilisi, Georgia; \*nino-kilas@mail.ru

In order to study the complex generation capacity of aminodibenzothiophene (Pict. 1), the semi-empirical quantum-chemical AM1 method calculates the energy, electronic and structural characteristics of the molecule both in the air phase and in different solvents.



**Picture 1.** Aminodibenzothiophene molecule

Analysis of the total settlement of atoms (electronic density) and their effective charges with a large deficit of electronic density in the aminodibenzothiophene molecule S (14) is on the sulfur atom ( $q = 0.434 \div 0.440$ ), which precludes the ability of the sulfur atom to participate in the formation of the donor-acceptor bond.

The different picture is for N (13) nitrogen atoms where the highest values of negative effective charges are ( $q = -0.338, -0.361$ ). The analysis of the bond angles C (2)-N (13)-H (22) and C (2)-N (13)-H (23) indicates the  $sp^3$  hybrid state of the nitrogen atom. C(2)-N(13) by the values of bond lengths and bond sequences, it can be concluded that nitrogen atom orbitals do not interact with the  $\pi$ -electron system of the benzene nucleus. The electron pair of N (13) nitrogen atom, by analyzing the settlement of orbitals, is concentrated on p<sub>z</sub>-orbital.

Therefore, according to the analysis of energy, electron and structural characteristics of the aminodibenzothiophene molecule, only one N (13) nitrogen atom has the ability to provide an electron pair and form a donor-acceptor bond with the metal.

## SYNTHESIS OF MIXED LIGAND COORDINATION COMPOUNDS OF BIOLOGICALLY ACTIVE METALS WITH N-N-DIMETHYLFORMAMIDE

**M. Abesadze<sup>1</sup>, M. Tsintsadze<sup>1,2</sup>, N. Gegeshidze<sup>1,2</sup>, N. Kilasonia<sup>1,2</sup>**

<sup>1</sup>Georgian Technical University, 77, M. Kostava St., 0175, Tbilisi, Georgia

<sup>2</sup>R. Agladze Institute of Inorganic Chemistry and Electrochemistry  
11, Mindeli Str., 0186, Tbilisi, Georgia; \*nino-kilas@mail.ru

By synthesized chloride and sulfate coordination compounds of cobalt (II), nickel (II), copper (II), manganese (II), cadmium (II) and zinc with N, N-dimethylformamide, as well as double thiocyanate coordination compounds of cobalt (II), nickel (II) and manganese (II), bimetallic coordination compounds of zinc, copper (II), cobalt (II), nickel (II), manganese (II), copper (II), iron (II), lead (II), cadmium (II) with N, N-dimethylformamide. We synthesized binary and bimetallic complex compounds in several stages in a solution of ethanol. The composition of the synthesized compounds and their specific physicochemical properties were established. The synthesized complex compounds were studied by the spectral method, thermographic studies were carried out.

Based on a study of the spectra of the synthesized complexes, it was found that in all types of synthesized complexes, the N, N-dimethylformamide molecule is coordinated with the metal atom by the oxygen atom of the carbonyl group, which is completely consistent with the results of quantum chemical calculations.

Considering the intrasphericity of N, N-dimethylformamide molecules, we can assume the octahedral structure for the chloride and sulfate complexes of cobalt (II), nickel (II) and manganese (II), as well as the tetrahedral structure for copper(II) chloride and sulfate and cadmium (II) chloride and sulfate.

In binary and bimetallic complex compounds, the coordination of the thiocyanate ion with the complexing metal is carried out through the nitrogen atom and the  $M \leftarrow NCS$  isocyanate structure is realized.

By synthesized double complex compounds of the type  $[Me(DMF)_6][Me(NCS)_4]$ , in which Me - Co (II), Ni (II), Cu (II), Mn (II), Cu (II). ) In the case of cobalt (II) and manganese (II), the compounds are of the ionic type, in which the synthesized  $[Me(DMF)_6]^{2+}$  cation has an octahedral structure and the  $[Me(NCS)_4]^{2-}$  anion has a tetrahedral structure. As for the double complex compounds of nickel (II) and copper (II), in their case in the complex anion, the medium of the metal ion  $Me^{2+}$  (Me = Ni (II), Cu (II)) consists of three monodentate ions of thiocyanates, which are coordinated with metal through the nitrogen atom, the fourth thiocyanate ion acts as a bridge.

By synthesized bimetal complex compounds  $[Me(DMF)_n][Ni(NCS)_4]$ , where Me represents Co (II), Cu (II), Cd (II), Fe (II), Pb (II), Zn, n = 5, 6. In the case of cobalt (II), iron (II), and lead (II), ionic type compounds are synthesized in which the synthesized complex cation



$[\text{Me}(\text{DMF})_6]^{2+}$  has a octahedral structure. While the complex anion  $[\text{Ni}(\text{NCS})_4]^{2-}$  has a tetrahedral structure and is coordinated with the thiocyanate group by an atom (the structure of the  $\text{M} \leftarrow \text{NCS}$  isocyanate is obtained).

For bimetallic coordination compounds  $[\text{Cu}(\text{DMF})_5][\text{Ni}(\text{NCS})_4]$ ,  $[\text{Zn}(\text{DMF})_5][\text{Ni}(\text{NCS})_4]$ ,  $[\text{Cd}(\text{DMF})_5][\text{Ni}(\text{NCS})_4]$  and  $[\text{Mn}(\text{DMF})_5][\text{Ni}(\text{NCS})_4]$  the structure of the complex cation is octahedral, and in the complex anion with nickel  $\text{Ni}^{2+}$ , three monodentate thiocyanate ions are coordinated by a nitrogen atom, and the fourth thiocyanate ion acts as a bridge.

## COORDINATE COMPOUNDS OF MANGANESE WITH HETEROCYCLIC LIGANDS

**M. Macharashvili, T. Tusiashvili, T. Tsintsadze, M. Matnadze**

<sup>1</sup>Georgian Technical University, 77, M. Kostava St., 0175, Tbilisi, Georgia

Synthesized manganese coordinating compounds with heterocyclic condensed nuclear ligands, in particular 3-aminodibenzofuran. The synthesis of this compound - ligand - was produced on the basis of known methodologies from dibenzofuran: oxidation of dibenzofuran and recovery of the obtained nitro product. We took the chloride and sulfate of manganese (II) as the starting substances, we choose for organic ligand - 3-aminodibenzophoran.

We cleaned the substances used for synthesis with crystallisation. Ethanol, dimethylformamide, and acetone were used as solvents. To synthesize the coordinating compounds, we heated 0.01 moles of the corresponding salts and dissolved them in 5 ml of ethyl alcohol. We also dissolved 0.004 moles of heterocyclic in conditions of constant stirring and heating in 10 ml of alcohol. After the hot solution of ligand (solutions should have the same temperature). Add the hot ethanol solution of salt in a ratio of 1: 4 (salt: 3-aminodibenzophoran).

We kept the solution until the separation of precipitation. The crystals that had been transferred to the filter paper were separated, washed with small amounts of cold ethanol and dried in an exsiccator with  $\text{CaCl}_2$ . Received air-resistant pink fine crystalline substances are stored in a closed container for a long time. Determine the melting temperature and solubility of the synthesized coordinate compounds in different organic solvents, also known metal content in synthesized complex compounds.

Compound	Solvent							Colour	$T_{\text{melt}} \text{ C}^\circ$
	acetone	DMP	DMSO	Benzole	Ethanole	Methanole	Water		
$\text{MnCl}_2 \cdot 4\text{L}$	Sl.sol	Sol.	sol.	X	X	X	Heat	light pink	122-124
$\text{MnSO}_4 \cdot 4\text{L}$	Sl.sol	Sol.	sol.	X	X	X	Heat	dark pink	114-116

## SYNTHESIS AND PROPERTIES OF MIXED LIGAND COMPLEX COMPOUNDS OF NICKEL (II)

**L. Arabuli<sup>1</sup>, N. Gegeshidze<sup>1,2</sup>, M. Kereselidze<sup>2</sup>, L. Skhirtladze<sup>2</sup>**

<sup>1</sup>Georgian Technical University, 77, M. Kostava St., 0175, Tbilisi, Georgia

<sup>2</sup>R. Agladze Institute of Inorganic Chemistry and Electrochemistry  
11, Mindeli Str., 0186, Tbilisi, Georgia; \*nino-kilas@mail.ru

The aim of our study was the synthesis and study of mixed coordination compounds of nickel (II). We chose nickel (II) chloride and potassium thiocyanate as starting materials and N, N-dimethylformamide and isonicotinamide as organic ligands.

The aim of our study is to study the complexing ability of the isonicotinamide molecule in various solvents, the donor properties of the molecule in the formation and synthesis of new coordinate compounds based on the results, study their physicochemical properties.

The semi-empirical quantum-chemical method AM1 calculated the energy, geometric, and structural features of the isonicotinamide molecule. In accordance with the electronic structure, the influence of a solvent on the ability of a molecule to form a complex with a metal is determined. As solvents, water, acetone, methanol, ethanol, dimethyl sulfoxide, chloroform and hexane were selected.

The heat release of a molecule, total energy, dipole moment, ionization potential, bond length, bond angles between atoms, effective charges on atoms, calculation of atomic orbitals, etc. are determined.

The electron density values (formal calculation) and analysis of the effective charge values show that the oxygen atom of the carbonyl group is characterized by a high electron density.

The oxygen atom has an  $\delta$ -type electron pair, that is, a  $sp^2$ -type hybrid orbital with an s-component. This, in turn, determines the basic properties of the oxygen atom O(8), is, its ability to form a donor-acceptor bond with a metal atom.

The high degree of deposition of s-orbitals of the pyridine nitrogen atom is high, which also determines its electron-donating properties.

As for the nitrogen atom of the amide group, the electron pair is located on the  $2p_z$  orbital, which cannot participate in the formation of a coordinate bond of the type with a complex metal.

Based on the processed results, new mixed coordination ligand compounds were synthesized and the physicochemical properties of the synthesized compounds were studied. We synthesized coordination compounds in ethanol solutions.

We synthesized nickel (II) complex compounds: the complex compound  $[Ni(L)_2(DMF)_2(SCN)_2]$  and the double complex compound  $[Ni(L)_6][Ni(SCN)_4]$ , where L is isonicotinamide, DMF - N, N-dimethylformamide.

The resulting coordination compounds are isolated in the solid state. Their composition is determined by elementary analysis, and individuality is determined by the melting point. Some physicochemical properties were studied: solubility in various inorganic and organic solvents. The synthesized compounds were studied by infrared spectroscopy.

The range of synthesized coordination compounds is fixed in the range of 400 - 4000 cm<sup>-1</sup>. In the synthesized compounds, rules for the coordination of N, N-dimethylformamide, isonicotinamide, and thiocyanate ion are determined. The results obtained made it possible to construct a synthesized coordinate relationship.

## **SYNTHESIS OF COORDINATION COMPOUNDS OF COBALT CONTAINING 2-AMINODIBENZOTHIOPHEN – HETEROCYCLE LIGAND**

**N. Margvelashvili, N. Bolkvadze, K. Tsikarishvili, N. Gakhokidze**

<sup>1</sup>Georgian Technical University, 77, M. Kostava St., 0175, Tbilisi, Georgia

One of the main directions of search for new medical products is the synthesis of biologically active compounds on the basis of heterocyclic compounds. It is for this purpose that the subject of our study is the synthesis of cobalt coordinating compounds with 2-aminodibenzothiophene. Both the complex generator and the ligand are characterized by high biological activity. Among the products of dibenzothiophene are substances with a wide spectre of physiological effects- Analgesic, antimicrobial, antibacterial, antidepressant, anti-inflammatory action. For organic ligands were selected - 2 aminodibenzothiophenes, which were synthesized based on known methods, 2 - Nitro dibenzothiophene is generated by the nitrification of dibenzothiophene and by restoring the nitro product produced from a mixture of dibenzothiophen (5) oxide. Cobalt (II) chloride and sulfate coordinate compounds with 2-aminodibenzothiophene have been synthesized. Heterocyclic and cobalt compounds were dissolved in ethanol under constant stirring and heating conditions in a ratio of 1: 4. Hot salted ethanol solution add drop by drop ethanol solution with same temperature of ligand. The reaction mixture was transferred to the porcelain sum and left for one day until the before separation of the precipitate. The pink crystals were separated, which we washed with a small amount of cold ethanol and dried in an exsiccator with CaCl<sub>2</sub>. The resulting compound is air-resistant. Store in closed containers for a long time. It dissolves well in DMPA, DMSO, Acetone, Ethanol; does not dissolve in benzene. In order to determine the individuality of the synthesized compounds, determine the melting temperature and solubility of the synthesized coordinate compounds in different organic solvents, also known metal content in synthesized complex compounds.

## **ANALYSIS OF PLANT RAW MATERIALS CONTAINING ANTHOCYANINS BY BORTREGER**

**I. Goderdzishvili, N. Gelovani, I. Gvelesiani, L. Targamadze**

Georgian Technical University, 77, M. Kostava St., 0175, Tbilisi, Georgia

From the flora of Georgia, we have selected the following plants: 1. Aloe vera (Áloë véra) - real aloe, as it is often called. It is a herbaceous, perennial plant with thin green leaves; 2. Rhamnaceae: a. Frangula alnus (grows in Abkhazia, Svaneti, Racha-Lechkhumi, Samegrelo, Imereti, Guria, Adjara, South Ossetia, Kartli, Mtiuleti, Kakheti, Meskhети); B. Kheshavi - Joster (Rhamnus cathartica) (common in Imereti, Kartli, Samachablo, Mtiuleti, Kiziki, Outside Kakheti, Trialeti, Meskhети); G. Paliurus (Paliurus spina-christi) (quite common in our country).

As it is experimentally proven, most of the anthracene substances are found in the form of glycosides, so we have selected several samples of plant raw materials. Their numerical indicators are as following: humidity not more than 10%; Total ash not more than 17%; 10% soluble ash in a solution of hydrochloric acid not more than 4%; Mineral impurities (dust, soil, sand) not more than 0.05%.

It is known that anthraglycosides in the bark of khechreli are up to 8%, the juice of kind of woody aloe leaves contains 2% of anthracene derivatives.

Anthracene are crystalline substances. Their color can be red, orange or yellow. Anthracene aglicones are well soluble in ethyl ether, chloroform, benzene, and other organic solvents; they do not dissolve in water, but in solutions of alkalis diluted with water, they dissolve easily with the formation of phenols.

Anticonvulsants in the form of glycosides are soluble in water, well soluble in stems, poorly soluble in methanol and ethanol. Insoluble in organic solvents - benzene, ethyl ether, chloroform, etc.

When heated to 210 ° C, they undergo sublimation.

In the selected plant raw materials, we separated the anthracene substances by the response of well known Bortreger's process. The essence of this reaction is as follows: during the fermentation of substances released from plant raw materials with alkali, hydroglycosides are hydrolyzed and free aglycones are formed. At the same time, anthrone and anthranol derivatives are oxidized to anthraquinones. Oxidantraxins are formed with the help of phenolic hydroxide, which gives us water-soluble phenols (anthraquinones). During the alkaline aqueous acid processing, the dissociation of phenolic hydroxyl is inhibited and the compounds become lipophilic, resulting in a mixture of chloroform with a solution of water passing from the water layer to the chlorophyll, and the last one gets yellow color of oxidantraxins. When chloroform is mixed with ammonia solution, phenolic colouring of the ammonia layer occurs again.

The ammonia layer of 1,8- takes cherry-red color, while the 1.2-dioxyantraquinone layers turns purple.

## SYNTHESIS OF SOME NEW 5H-PIRIDAZINO[4,5-B]INDOLE DERIVATIVES

**Sh.Samsoniya, V. Badalashvili, I.Chikvaidze\***

Ivane Javakhishvili Tbilisi State University  
3, Ilia Chavchavadze Ave., 0179 Tbilisi, Georgia  
\*iosebc@yahoo.com

The main objective of pharmaceutical chemistry is a synthesis of the medicaments, which are characterized by efficiency and less toxicity. Often the active components are heterocyclic fragments. One of their representatives, Nitrogen-containing heterocycles, are the most interesting compounds, because of their biological activity.

The systems which are obtained by the union of two or many of heterocycle fragments in one molecule are more active and give an opportunity of producing the new physiological active compounds.

The aim of our research is the synthesis of biologically active substances. 4-oxo compounds of 3H,5H-piridazino[4,5-b]indole were obtained to synthesize the other compounds containing indole and piridazine rings.

For these, the following steps were realized: the diazotization of 2-bromo-4-methylalanine, the azo conjugation of this product with ethyl 2-methylacetoacetate and the hydrolyze in one step without extraction of azoester by Japp-Klingeman. The indolization of ethyl 2-(2-(2-Bromo-4-methylphenyl)hydrazineylidene)propanoate was carried out by Fisher indolization in polyphosphoric acid. 7-bromo-3-formyl-2-ethoxycarbonyl-5-methylindole was obtained by formylation of 7-bromo-2-ethoxycarbonyl-5-methylindole. The reflux of 7-bromo-3-formyl-2-ethoxycarbonyl-5-methylindole with hydrazine hydrate in acetic acid allows the formation of a target product 6-bromo-5-methyl-4-oxo-3H,5H-piridazino[4,5-b]indole. In order to synthesize chloride containing compounds, 6-bromo-4-chloro-5methyl-5H-piridazino-[4,5-b]indole, the target product was refluxed with  $\text{POCl}_3$ . The presence of halogen atoms in these compounds makes the possibility of the substitution this group by the amino -, hydrazine -, ciano - and other groups.

It is noteworthy that the unusual deformylation reaction of 7-bromo-3-formyl-2-ethoxycarbonyl-5-methylindole does not proceed.

## **STUDY OF MIXED REVERSE MICROEMULSIONS ON THE BASIS OF SODIUM BIS(2-ETHYLHEXYL) SULFOSUCCINATE**

**M. Rukhadze**

Ivane Javakhishvili Tbilisi State University, Department of Chemistry, Faculty of Exact and Natural Sciences, 3, I. Chavchavadze ave, Tbilisi, 0179, Georgia

\* marina.rukhadze@tsu.ge

The doping of most widely used sodium bis (2-ethylhexyl) sulfosuccinate (AOT) reverse micelles interface by surfactants of different nature alters elastic rigidity of the interface, changes water solubilization capacity and microviscosity of the confined water, also affects percolation of conductance, etc. Such flexibility of microemulsions is very important for various biological and technological applications of these mixed aggregated systems.

The goal of the proposed work was to study the influence of additives of nonionic polyoxyethylene (4) lauryl ether (Brij-30), anionic sodium cholate (SC) and cationic promethazine hydrochloride (PMT) introduced in the AOT ionic reverse micelles on the: ratio of the bound, free and trapped water fractions, binding process of optical probe with reverse micelles, study of influence of amount of water additives on percolation of conductivity and sizes of water droplets of mixed reverse microemulsions with an infrared and UV-visible spectroscopy, as well as with dynamic light scattering method and conductivity measurements.

The O-H stretching vibrational absorption spectra in the region of 3100-3700  $\text{cm}^{-1}$  were fitted into three subpeaks with the help of a Gaussian curve fitting program. The microenvironment of (AOT+Brij-30; AOT+SC; AOT+PMT) mixed reverse micelles was investigated by UV-visible spectroscopy via o-nitroaniline as optical probe. Electrical conductivity of the reversed mixed micellar solutions was measured with conductivity meter Orion Star A215.

The revealed changes in: a) ratio of the free, bound and trapped water fractions; b) retardation or early occurrence of percolation; c) binding constants of molecular probe with mixed reverse micelles and d) sizes of water droplets under the influence of additives of surfactants of different nature may be useful to clarify the complex structure and properties of mixed reverse microemulsions as they widely are applied in mimicking of biomembranes, enzymatic catalysis, drug delivery, extraction processes, etc.

## **OBTAINING OF MULTIFUNCTIONAL CERAMIC COMPOSITION MATERIALS BASED ON SIC - SIALON AND AL<sub>2</sub>O<sub>3</sub> – SIALON SYSTEMS**

**N. Darakhvelidze\*, Z. Kovziridze\*, N. Nizharadze, M. Balakhashvili**

Department of Chemical and Biological Technologies of Georgian Technical University

69, Kostava str., 0175, Tbilisi, Georgia

\*darakhvelidzenino3@gmail.com; kowsiri@gtu.ge

Intense progress of science and technology demands perfection of various branches of industry, which in its turn is connected with the necessity of creation of new materials characterized by hetero modular properties. Taking into consideration practical experience in materials science an advantage of carbides, borides, nitrides and silicides over other type materials were proved, since hardly melted materials are distinguished by precious properties such as: high refraction, corrosion resistance to a number of aggressive media, high mechanical characteristics, specific electro and heat-physical properties and others [1-6].

Among the oxygen-free hardly melted materials silicon carbide- and silicon nitride-based materials are distinguished, which by their unique physical-technical and chemical properties are widely used in modern technology: machine-building, chemical, atomic energy, petroleum refining industries et al [7-14].

Intense work is in progress in recent years in the sphere of obtaining types of ceramics in which properties of oxygen-free substances and oxygen substances will be fused and SiALON are namely such materials [15-18].

Our work pursued to obtain SiALON-containing composites by reactive sintering, on the basis of silicon carbide and corundum. This method enables us to obtain desirable phase composition material and such materials possess properties of the hot-pressed objects. In the process of obtaining SiALONs by reaction sintering, sintering temperature is sharply decreased at the application of active materials, in our case we had to select materials which would enable us to use newly formed components obtained by the method of reactive sintering, since at the obtaining of solid solution of SiALON inculcation of  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> and AlN in  $\beta$ -Si<sub>3</sub>N<sub>4</sub>-Si is especially simplified when its crystalline lattice is still in the process of formation. Therefore, we gave preference to silica-alumina material – kaolin, aluminum powder and elemental silicon.

We have studied physical-chemical properties of specimens sintered at 1500<sup>0</sup>C (Table 1). As is seen from the Table 1, C<sub>7</sub>, then C<sub>6</sub> and C<sub>8</sub> are distinguished by high physical-technical properties. Open porosity, correspondingly equals to 15,2, 15,0 and 15,4 %. Hardness limit at compaction is 258, 256 and 254 MPa, which refers to the fact that 1500<sup>0</sup>C is not enough for complete hardening. Despite this, chemical resistance to water and acid (H<sub>2</sub>SO<sub>4</sub>  $\rho$ -1.84) is still high. Refractoriness of specimens equals to 1770<sup>0</sup>C.



Table 1. Physical-technical characteristics of specimens sintered at 1500°C

Composite index	Open porosity w, %	Hardness limit at compaction, MPa	Density, $\rho$ , g/sm <sup>3</sup>	Chemical resistance, %	
				Water	Sulfuric acid, $\rho$ 1.84
SN-1	16.2	230	2.28		
SN-2	15.0	245	2.8	99,41	99.16
SN-3	16.0	240	3.2	99.36	99.15
SN-6	15.0	256	2.25	99.82	99.20
SN-7	15.2	258	2.31	99.79	99.25
SN-8	15.4	254	2.78	99.80	99.30

At sintering of kaolin and aluminum powder blend in 800-1500°C interval temperatures of formation of aluminum and silicon nitrides and on their base mullite structure X-SiALONs was fixed and proved. While at sintering of SiC-aluminum powder, silicium and  $\alpha$ - $Al_2O_3$  - aluminum powder – silicon blends the SiC-SiAlON and  $Al_2O_3$ -SiAlON composites on  $\beta$ -SiALON lattice were obtained. The obtained results are confirmed by X-Ray diffraction and microscopic analyses.

**Acknowledgments:** This work has been supported by Shota Rustaveli National Science Foundation grant № YS-18-077.

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## SYNTHESIS AND ENANTIOSEPARATION OF NOVEL PHENOTHIAZINE DERIVATIVES IN HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY

**R. Kakava<sup>1\*</sup>, I. Matarashvili<sup>1</sup>, A. Volonterio<sup>2</sup>, B. Chankvetadze<sup>1</sup>**

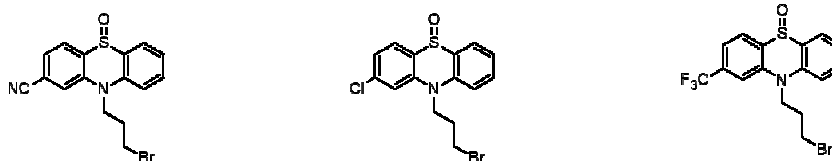
<sup>1</sup>Institute of Physical and Analytical Chemistry, School of Exact and Natural Sciences,  
Tbilisi State University, Chavchavadze Ave 3, 179 Tbilisi, Georgia

<sup>2</sup>Dipartimento di Chimica, Materiali ed Ingegneria Chimica "Giulio Natta",  
Politecnico di Milano, via Mancinelli 720131 Milano, Italy

\*rusudan.kakava@tsu.ge

Phenothiazine derivatives are valuable drug compounds with wide range of pharmaceutical activities, including antipsychotic, antiadrenergic, anticholinergic, insecticidal, antifungal, antibacterial and antihistaminic activity [1].

Chiral phenothiazine sulfoxide derivatives shown on Fig. 1 were synthesized using three step synthetic path [2].



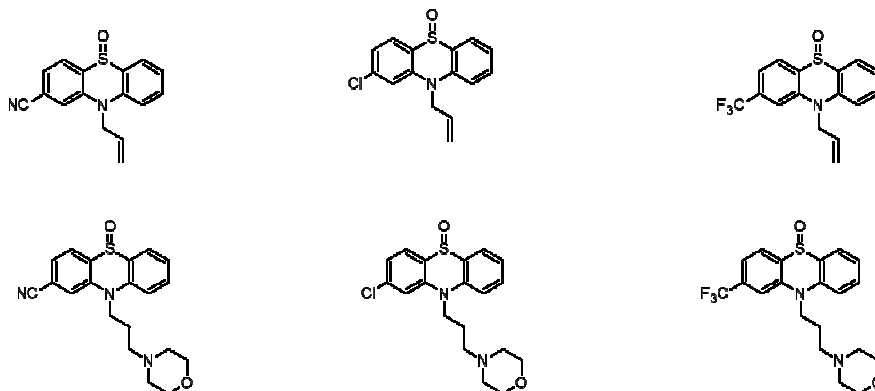
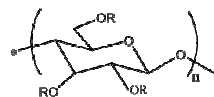


Fig.1. Structures of synthesized phenothiazine sulfoxide derivatives

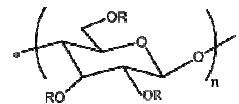
Synthesized compounds were isolated, purified and their structures were confirmed with IR, NMR spectroscopy and mass spectrometry techniques. The enantiomers of synthesized compounds were separated using high performance liquid chromatography in polar organic mobile phases such as methanol and acetonitrile. 10 polysaccharide-based chiral columns were used as stationary phases. Structures of chiral selectors are shown on Fig. 2.

Chromatographic analysis has revealed correlation between retention / separation factor of enantiomers on stationary phases and structural features of analyte molecules, as well as chiral selectors.

### Cellulose derivatives



N	Column	Name of chiral selector	Structure
1	Cellulose-1	Cellulose tris(3,5-dimethylphenylcarbamate)	
2	Cellulose-2	Cellulose tris(3-chloro, 4-methylphenylcarbamate)	
3	Cellulose-3	Cellulose tris(4-methylbenzoate)	
4	Cellulose-4	Cellulose tris(4-chloro, 3-methylphenylcarbamate)	
5	iCellulose-5	Cellulose tris(3,5-dichlorophenylcarbamate)	
6	ISP11	Cellulose tris(3-chloro, 5-methylphenylcarbamate)	
7	-	Cellulose tris(3,4-dimethylphenylcarbamate)	

**Amylose derivatives**

N	Column	Name of chiral selector	Structure
1	Amylose-1	Amylose tris(3,5-dimethylphenylcarbamate)	
2	Amylose-2	Amylose tris(3-chloro, 6-methylphenylcarbamate)	
3	iAmylose-	Amylose tris(3-chloro, 5-methylphenylcarbamate)	

Fig.2. Structures of chiral selectors

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## PREPARATION OF ALUMINA BASED ON POWDERY COMPOSITES BY BALL MILLING METHOD

**N. Jalagonia, T. Archuadze, L. Kalatozishvili, N. Darakhvelidze, M. Mumladze, G. Bokuchava, T. Kuchukhidze**

Ilia Vekua Sukhumi Institute of Physics and Technology  
7 Mindeli Str., 0186, Tbilisi, Georgia \*sipt@sipt.org

Alumina based on composites are one of the most known and widely used ceramics. *Due to its excellent characteristics, alumina is used for biomedical, electronic, automotive, industrial, defence and space applications.* To improve ceramic composites mechanical properties, doping of sintered powder composites with different compounds (Carbon nanostructures, fibers, MgO, ZrO<sub>2</sub>, SiC, etc.) is used; dopants represent grain size growth inhibitors, which facilitate the production of nanostructured ceramic materials [1-2].

*Components homogenization is important process to obtain improved ceramic composites.* For this purpose, powdery composites carried out in nanomill with different conditions (6, 12, 24

h). Optimal regime was developed to obtain uniformity pressing powdery composites. In this study following ceramic composites have been obtained,  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>-GO and  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>-RGO [3].

**Preparation of pressing powdery composite.** Pressing powdery composites obtained by grinding of 65 g  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> with graphene oxide (1.5% mas.) and in the other hand to reduced graphene oxide. Mass ration of balls and powdery was equal 4:1. Nano mills (FRITCH planetary mill Pulverisette 7 premium line and RETCH PM 100) were used for grinding. Grinding process depends on content of powdery composites and grains sizes of initial powdery (1-24 h). The suspension has dried at 130°C and further powders again dry grinding during 1 h in mill. Then the mixture dried and placed in press form.

During the work the following devices have been used: Electronic Scanning Microscopes JEOL JSM-6510LV, Planetary mill Pulverisette 7 *premium line*, XRD.

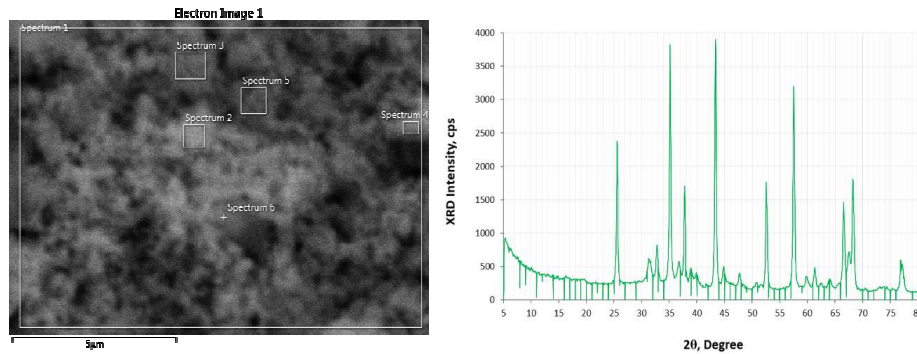


Fig. 1. SEM and XRD of  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>-GO

Table 1. EDS analysis of  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>-GO

Result Type	Atomic %					
Spectrum Label	Spectrum 1	Spectrum 2	Spectrum 3	Spectrum 4	Spectrum 5	Spectrum 6
C	6.41	6.09	6.29	6.24	8.12	6.26
O	60.39	61.49	63.96	62.86	59.73	62.68
Al	33.20	32.42	29.74	30.90	32.15	31.07
Total	100.00	100.00	100.00	100.00	100.00	100.00

EDS analyses confirmed that fillers distribution into alumina is almost equal. Average size of powdery particles is <50.

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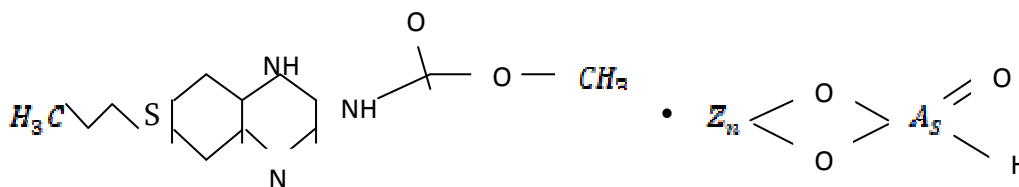
**USE OF SUPER-PURE COMPOUNDS WITH SPECIFIC PROPERTIES****Rus. Gigauri**

<sup>2</sup>R. Agladze Institute of Inorganic Chemistry and Electrochemistry, TSU  
11, Mindeli Str., 0186, Tbilisi, Georgia; \*gigaurirusudan@gmail.com

Arsenic super-pure compounds are characterized by physiological activity. Particularly non-toxic are As(V) compounds used in medicine and veterinary medicine - in homeopathic treatment. In the helminthic treatment of animals, helminthic disease of animals is highly unhealthy and causes great harm to animal industry. The veterinary service is trying to develop and research effective anti-helminthic agents worldwide, which will have a positive effect on all species of animals and birds. Metal arsenic has been found to be one of the most effective helminths among many other drugs. Such as tin(II) hydroarsenate and zinc(II) hydroarsenate. The structure of their particles has also been studied, which has been determined with an accuracy of seven zeros, which means that it is close to the nanoparticles.

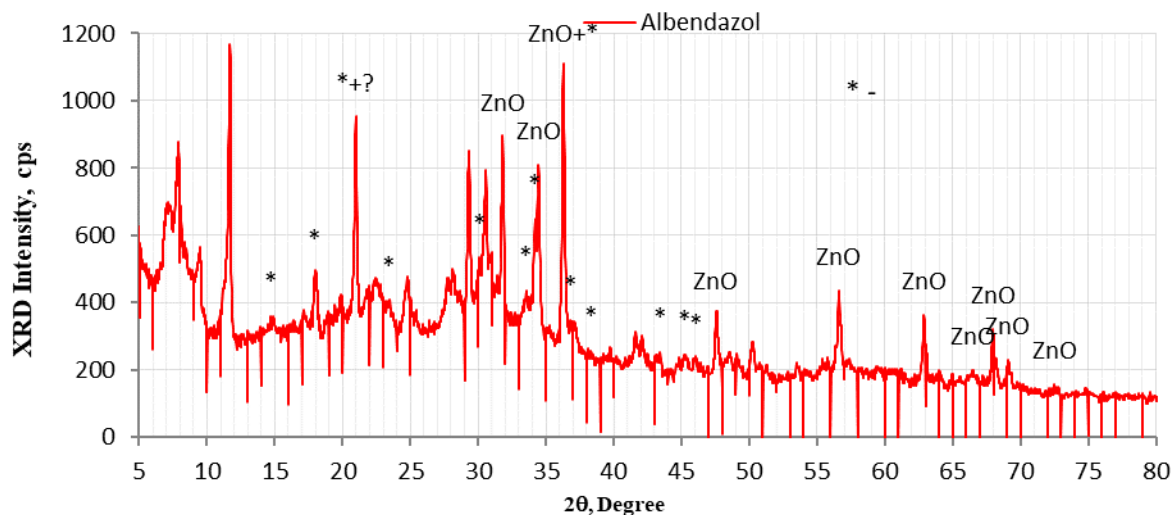
We have developed two new antihelminthic composites:

1. Tin(II) in combination with hydroarsenate and copper cypress. Optimal conditions were established. Pilot tests of their ratios have shown that the drug is the best way to dehelminate both sheep and cattle.
2. The second antihelminthic agent is an albendazole in presence of zinc(II) hydroarsenate. As it is well know, albendazole is a derivative of benzimidazole carbamate. The composite proved to be highly effective and active for dehelminthization.



Optimal operating conditions, ratios, maximum and minimum doses have been established. They are widely used in animal industry and poultry-farming for the treatment of roundworms, lungworms, flatworms, gastrointestinal invasions caused by liver butterflies, shellfish, and adult worms. It also has an ovulatory effect.

X-ray fluorescent examination of the drug was performed. We offer spectra where the behavior of the compound with a pronounced crystalline structure is clearly seen.



## PHYTOREMEDIATION OF CONTAMINATED SOILS IN BOLNISI MUNICIPALITY USING LOCAL PLANT

**G. Avkopashvili<sup>1,2\*</sup>, R. Gakhokidze<sup>1</sup>, Al. Gongadze<sup>1,2</sup>**

<sup>1</sup>Ivane Javakhishvili Tbilisi State University  
3, Chavchavadze Ave., Tbilisi, Georgia

<sup>2</sup>Elefter Andronikashvili Institute of Physics,  
6, Tamarashvili str., Tbilisi, Georgia

\*guranda.avkopashvili@tsu.ge

Modernization of the modern world, global development, maximum utilization of mineral resources and ruthless treatment of the environment by human have caused many ecological problems in many countries, and Georgia is no exception.

In this respect, among the ores in Georgia, one of the most important is the Kaztreti RMG (formerly “Madneuli”) ore, which is located in the Bolnisi municipality, on the right bank of the Mashavera River. The mentioned enterprise causes soil pollution. And contaminated soils often pose a threat to human health and ecosystems that require cleaning measures. Phytoremediation



is one of the best cleaning methods, when the plant is capable of high accumulation of heavy metals.

Within the research, the amaranth plant (*Amaranthusviridis*) has been investigated in the soils of Bolnisi municipality, and its accumulation ability has been studied. Within the research, the ability of absorption of heavy metals such as cadmium (Cd), copper (Cu) and zinc (Zn) has been studied. As a result of research the phytoremediation capabilities of the amaranth plant (*Amaranthusviridis*) have been identified.

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## HYDRO-CHEMICAL ANALYSIS OF MUASHI MINERAL WATERS

**M. Chikovani\*, A. Kvastiani**

Kutaisi Akaki Tsereteli State University

59, Tamar Mefe Ave., Kutaisi, Gergia

\*manucharchiqovani65@mail.ru

The object of our research was the mineral water of the village Muashi in Lentekhi district. We were first to make a hydro-chemical analysis of Muashi mineral water. The consistence of  $Ca^{2+}$ ,  $Mg^{2+}$ ,  $HCO_3^-$ ,  $Cl^-$ ,  $SO_4^{2-}$ , ions, oxidation, dissolved oxygen, dry remains and Carbon dioxide are studied with chemical methods.

Analysis were made in the laboratory of Analytical Chemistry at Akaki Tsereteli State University, appropriate methods have been used for the analysis.

The rate of acidity is measured with pH (673–M). Dry remain was determined by the gravimetric method, after drying the remain at  $110^{\circ}C$  as a result of evaporation.

Hydro carbonates were determined by acidometric method. We used 0,01 mole/equiv. Hydrochloric acid as Titrant. Methyl-red was used as an indicator.

Mercurometric method was used to determine chlorides. We used 0,01 mole/equiv.  $Hg_2(NO_3)_2$  as Titrant and diphenyl-carbazone as an indicator.

Sulfate ions in highly mineral waters are determined with classical gravimetric method; the divide form is  $BaSO_4$ .

The consistence of Calcium and Magnum and also the total hardness of the water in samples are determined with complex-geometric method. the influence of hard metals was important by adding  $Na_2S$  in parallel determinations. Biogenic substances were determined with photometric methods:  $NH_3$  –Nessler Reactive,  $NaNO_2$  – Grese Reactive.  $NO_3$  – Sodium  $NO_3$ Salicylate, and  $PO_4^{3-}$  – Ammonium Phosphor-molybdate (blue complex).

Dissolved oxygen is determined with Iodometric method, we used 0,02 mole/equiv. concentrate solution of  $Na_2S_2O_3$  as Titrant. Starch was used as an indicator. In order to define total concentrations of organ substances in the water, we used Permanganatometric and Bi-chromatic acidity methods.

The content of  $CO_2$  in the water is defined with alkalimeter method. We used 0,01 mole/equiv. solution of Sodium Alkaline and Phenophthalene as an indicator. The results of the analysis are shown in the Table 1.

Muashi mineral water of Lentekhi region is of medium mineralized, for what their reaction is slightly sour ( $pH = 5,22$ ).

Table 1. The result of Hydro-chemical Analysis of Muashi Mineral Waters in Lentekhi Region

Name of the source	<i>pH</i>	Dry remain	$SO_4^{2-}$	$Ca^{2+}$	$Mg^{+}$	$HCO_3$	$Cl^{-}$	Dissolved oxygen	Acidity	$CO_2$
	Mg/l									
Muashi	5,22	1.33	0,371	107,02	52,41	91,72	23,65	0,0095	4.856	41.23

The consistence of  $NO_3^{-}$ ,  $NO_2^{-}$ ,  $PO_4^{3-}$ ,  $NH_3$  is much lower than expected level. We also could not discover sulfide ion by sensitive methods. In studied mineral waters  $Ca^{2+}$ ,  $Mg^{2+}$ ,  $HCO_3^{-}$ ,  $Cl^{-}$ ,  $SO_4^{2-}$ ,  $CO_2$ ,  $NO_3^{-}$ ,  $NO_2^{-}$ ,  $PO_4^{3-}$ ,  $NH_3$ ,  $S^{2-}$  ions are in norm and using them for curing and personal consumption is quite reasonable.

## RELATIVE TRUE DEFORMATION OF GREENHOUSES FILM DEPENDING ON THE ORIENTATION

N.H. Benmiloud<sup>1\*</sup>, S.F. Chabira<sup>2</sup>, M. Sebaa<sup>3</sup>

<sup>1</sup>Amar Telidji University, Route de Ghardaïa BP 37 G Laghouat, 03000 Algérie.

<sup>2</sup>Engineering Process Department, Mechanics Laboratory (Ime)-RFME, Faculty of Technology, Amar Telidji University, Route de Ghardaïa BP 37 G Laghouat, 03000 Algérie.

<sup>3</sup>Mechanical Engineering Department, Mechanics Laboratory (Ime)-RFME, Faculty of Technology, Amar Telidji University, Route de Ghardaïa BP 37 G Laghouat, 03000 Algérie.

\*nh.benmiloud@lagh-univ.dz

Uniaxial tensile measurements on low-density polyethylene film samples have been realized by mean of a mechanical device. The optical measurement of ink lines drawn on the top surface of the film at respective distances between each other, has contributed in the understanding in the way of how the film deforms when subjected to a stress. The films are tested in three different directions ( $0^{\circ}$ ,  $45^{\circ}$  and  $90^{\circ}$ ). The results showed that relative elongation and true strain are greater in the  $45^{\circ}$  stretch followed by  $90^{\circ}$  then  $0^{\circ}$ . Also, it has been found that the deformation in the right side is more pronounced. However, it should be noticed that the planes delimited by the marks remain uniform during the whole deformation meaning that the lines of ink remain parallel during the total duration of the experiment

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