





Dear Colleagues,

On behalf of the Organizing Committee, I am pleased to extend a warm and cordial welcome to all participants of the "9th International Caucasian Symposium on Polymers and Advanced Materials," being held at Akaki Tsereteli State University in Kutaisi, Georgia.

First, in 2007, 16 years ago, this symposium took place at Tbilisi State University, Tbilisi, Georgia. We are now conducting the 9th meeting, which will also be hybrid. This will enable many scientists to join and attend the symposium remotely.

We are delighted to host you this year in our beautiful Georgia, in Tbilisi. These meetings led to the fact that we cooperate with the Max Planck Institute for Polymer Research (Mainz, Germany), Polish Universities in the Erasmus+ program, as well as with the Kaunas University of Technology.

We hope that this symposium will, in the future, lead to the strengthening of close scientific relations with other countries.

The conference's purpose is to encourage scientists working in polymer chemistry and advanced materials to present their investigations dedicated to problems and discoveries in the above-mentioned fields.

Also, "ICSP&AM 9" will help to introduce effectively innovative scientific research of Georgia in Caucasian and neighboring scientific teams, which are less known in the world scientific society.

We hope that this year's meeting, gathering many participants, shall provide a good platform for academic and industrial scientists to discuss recent advances in the area of polymers and advanced materials.

Dr. Tamar Tatrishvili

**Assistant Professor** 

T Tatrishvili

#### **Organizing Committee:**

Symposium Chair – Dr. Tamar Tatrishvili,

Assistant Professor.

Co. Chair – Prof. Marc J.M. Abadie

#### **Symposium Secretariat:**

Tamar Makharadze, PhD. - Executive Secretary of the Symposium.

Vladimir Chavchanidze Institute of Cybernetics.

Elene Tabeshadze- BA, Akaki Tsereteli State University.

Lana Gegechkori - BA, Akaki Tsereteli State University.

## **SYMPOSIUM SCHEDULE**

	OCTOBER 20	
	AKAKI TSERETELI STATE UNIVERSITY,	
	Address: Tamar Mepe Str. 59, Library bldg. 22, Room 22208	
	Kutaisi, Georgia	
1200-15.00	Registration	
15.00	Fourchette	
	OCTOBER 21	
	Address: Tamar Mephe Str. 59, Library bldg. 22, Room 22208	
09:00-09:30	Opening Ceremony	
(	Co-chairs: Prof. Helena Janik, Dr. Justyna Kozlowska,	
09:30-09:50	Marc J.M. Abadie- "The Development of Thermoplastic Composites: Is	1
	It a Lure or a Revolution in Structural Materials"	(Online)
	Institute Charles Gerhardt Montpellier ICGM, University of	
	Montpellier. France.	
09:50-10:10	Lela Mirtskhulava- "Harnessing Artificial Intelligence for Predictive	
	Design and Functional Optimization of Polymer Composites"	(Online)
	Ivane Javakhishvili Tbilisi State University, Department of Computer	
10.10.10.20	Sciences, Tbilisi, Georgia.	
10:10-10:30	<b>Dmitrii Roshchin-</b> "Deformation and Stability of Non-Newtonian	3
	Polymeric Droplets".	
10:30-11:10	N.N. Semenov Federal Research Center for Chemical Physics, Russia.	4
10:30-11:10	<b>Bagrat Godibadze</b> – "The Conductivity and Physical Characteristics of High Temperature Recovered Carbon";	4
	"Production of heat-resistant composite products by the SHS-electric	
	rolling method"	
	Ferdinand Tavadze Institute of Metallurgy and Materials Science,	
	Tbilisi, Georgia	
11:15-11:45	Coffee Break	
	Co-chairs: Prof. Serhiy Pyshyev, Dr. Nino Zavradashvili	
11:50-12:15	Vladimer Tsitsishvili- "Antimicrobial Activity of Metal-Containing	5
	Modified Zeolites".	
	Georgian National Academy of Sciences, Tbilisi, Georgia	
12:15-12:35	Justyna Kozlowska- Microcapsule-Based Waterless Cosmetic Systems	6
	with Tailored Polysaccharide Shells".	
	Nicolaus Copernicus University in Torun, Faculty of Chemistry.  Torun, Poland	
12:35-12:55	Helena Janik- "The Progress in Certification of Biodegradable and	7
12.33-12.33	Compostable Polymer Compositions"	/
	Gdansk University of Technology, Faculty of Chemistry, Gdansk, Poland	
12:55-13:15	Tinatin Bukia- "Synthesis of Adamantane-Scaffold-Containing	
-2.00 10.10	Derivatives Via the Ugi Four-Component Reaction".	(Online)
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	Ivane Javakhishvili Tbilisi State University; Institute of Macromolecular	
	Chemistry and Polymeric Materials. Tbilisi, Georgia	
13:15-13:35	<b>Armaz Tsutskiridze-</b> Synthesis of 1,2-Bis(2-Phenyl-1h-Indol-3-Yl)	9
	Ethene (Bpie) By McMurry Reaction."	(Online)
	Ivane Javakhishvili Tbilisi State University, Tbilisi, Georgia	
13:35-13:55	Mzia Tsitsagi- Eco-Friendly, one-pot synthesis of bis-4-	10
	hydroxycoumarins using different H-form of natural zeolite-	(Online)
	Clinoptilolite as a catalyst".	
	Tbilisi State Medical University, Tbilisi, Georgia	
14:00-15:00	Lunch Break	
Co-	chairs: Prof. Vladimer Tsitsishvili, Prof. Jozef Haponiuk	
15:05-15:25	Serhiy Pyshyev – "Development of Biodegradable Polymers with Good	11
	Antibacterial Properties Functionalized with Humic Acids".	
	Lviv Polytechnic National University, Lviv, Ukraine	
15:25-15:45	Zoia Haholkina-Chitosan Hybrid Nanocomposite Scaffolds for	12
	Diabetic Wound Therapy.	(Online)
	Universidade da Coruña, Campus Industrial de Ferrol, CITENI,	
	Grupo de Polímeros. Spain	
15:45-16:05	Nino Zavradashvili – "Pseudoprotein-Poly (Ethylene Glycol) Graft	13
	Copolymers for Biomedical Applications.	
	Institute of Chemistry and Molecular Engineering, Agricultural	
	University of Georgia. Tbilisi.	
16:05-16:50	Abdollah Esmaeili, Laura Garzon- "Nano Polymers and Their	14
	Applications for Enhanced Oil Recovery in Fractured Carbonated	(Online)
	Reservoirs"; "The Advantage of Using Nano Fluids (Smart Fluids) in	
	the Petroleum Industry"; Nanocatalysts and Their Applications in	
	Petroleum Industry". Universidade Federal do Pará (UFPA), Brazil	
16:50-17:15	Eldar Zeinalov- "Metal-carbon nanocatalysts in the aerobic peroxide	15
	oxidation of decahydronaphthalene "	(Online)
	Nagivev Institute of Catalysis and Inorganic Chemistry, Ministry of Science and Education of the Republic of Azerbaijan. Baku.	
17:30-18:00	Coffee Break	
18:00	Poster Presentation	
	OCTOBER 22	
	Address: Tamar Mepe Str. 59, Library bldg. 22, Room 22208	
	Co obsing Duck Congress Vertical Dr. Dr. Verti De 1 1	
	Co-chairs: Prof. Sergey Kostjuk, Dr. Dmitrii Roshchin	
09.00-09.20		1
09.00-09.20	Maia Merlani - "Synthesis and biological activity of analogues of	1
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	"Acrobic Oridation of A Diagol Danaffin Nambthania Fraction	
	"Aerobic Oxidation of A Diesel Paraffin-Naphthenic Fraction Catalysed with Transition Metal- Carbon Nanotubes";	
	Institute of Geotechnological Problems of Oil, Gas and Chemistry,	
	Azerbaijan State University of Oil and Industry, Ministry of Science and	
	Education of the Azerbaijan Republic, Baku, Azerbaijan.	
09:55-10:15	Narine Durgaryan - "Aniline Oligomers: Synthesis and Investigation",	3
	Yerevan State University, Yerevan, Armenia.	
10:15-10:35	Natela Dzebisashvili - "Zero Polymer Waste: Development of a	4
10.10 10.50	Method for Obtaining Carbon Materials";	(online)
	R. Agladze Institute of Inorganic Chemistry and Electrochemistry of	(01111110)
	Ivane Javakhishvili Tbilisi State University; Institute of	
	Hydrometeorology at Georgian Technical University; Tbilisi, Georgia.	
10:35-10:55	Giorgi Ananiashvili- "Simulation of Diesel Fuel Desulfurization	5
	Process Using Artificial Intelligence Models and Optimisation Study";	(online)
	TSU, Petre Melikishvili Institute of Physical and Organic Chemistry,	
	Tbilisi, Georgia.	
11:00-11:30	Coffee Break	
	Co-chairs: Prof. Narine Durgaryan, Dr. Maia Merlani	
11:35-11:55	<b>Elene Tabeshadze-</b> "Determination of Some Metal Ions in the Waters	6
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	of the Spring in Ukheshi Village, Ambrolauri Municipality''.	
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	Institute of Polymer Materials of the Ministry of Science and Education of the Republic of Azerbaijan, Az5004, Azerbaijan Republic.					
15:25-15:45	Nuraliyeva Gunay- "Structure and Properties of Basalt-Filled	13				
	Thermoplastic Elastomers Based on Polypropylene";	(Online)				
Institute of Polymer Materials of the Ministry of Science and Education of the Republic of Azerbaijan, Azerbaijan Republic.						
15:45:16:05	Vijaya Kittu Manda- "Recent Biomedical Advances with Piezoelectric	14				
	Materials"; Researcher, PBMEIT, Visakhapatnam, India	(Online)				
	Recording Presentations:					
Prof. Irina Savchenko, Prof. Efkan Catiker, Prof. Petro Linnik, Dr. Vladyslav Zhezherya,						
Dr. Rostyslav Linnik, Prof. Samad Khaksar.						
18:30	Gala Dinner					

## OCTOBER 23

08:30- Excursion

## THE DEVELOPMENT OF THERMOPLASTIC COMPOSITES TPCS: IS IT A LURE OR A REVOLUTION IN THE STRUCTURAL MATERIALS

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This is a compelling and timely question, especially as industries from aerospace to automotive seek materials that are lighter, stronger, and more sustainable. To assess whether thermoplastic composites are a mere *lure* or a true *revolution*, let's break it down across key aspects:

- 1. What Are Thermoplastic Composites (TPCs)? Thermoplastic composites consist of a thermoplastic polymer matrix (like PEEK, PPS, or PA) reinforced with fibers (usually carbon or glass). Unlike thermoset composites, which irreversibly cure, TPCs can be melted, reshaped, and recycled—a major differentiator.
- 2. Why They Seem Revolutionary
- **a.** Recyclability and Sustainability: i) Thermoplastics can be re-melted and reprocessed, unlike thermosets which are difficult to recycle. ii) This is a huge step forward for circular economy goals, especially in aerospace, wind, and automotive sectors.
- **b. Faster Processing: i) Out-of-autoclave manufacturing** and **shorter cycle times** reduce costs and increase throughput. **ii)** Technologies like **automated fiber placement (AFP)** and **additive manufacturing** integrate well with TPCs.
- **c. Mechanical Performance:** i) Comparable or superior **impact resistance**, **fracture toughness**, and **fatigue life** compared to thermosets. ii) Performance can be tailored via fiber architecture and hybrid materials.
- d. Weldability and Repair i) TPC parts can be welded instead of bonded, simplifying assembly and repair. ii) Enables modular design and reduced use of fasteners or adhesives.
- 3. The Catch (Is It a Lure?)
- **a. High Material Costs:** High-performance thermoplastics (e.g., PEEK, PEKK) are **expensive**, which can be a barrier to mass-market adoption.
- **b. Processing Challenges:** i) Requires **high-temperature tooling and equipment**. ii) Not all industries are ready or willing to invest in new infrastructure.
- c. Limited Design Maturity: i) Compared to thermosets, fewer design guidelines and standards exist. ii) Engineering culture still leans heavily on thermoset experience, especially in aerospace.
- **4. Current and Future Applications:** i) **Aerospace**: Airbus and Boeing are integrating TPCs into primary structures (e.g., clips, brackets, fuselage panels). ii) **Automotive**: BMW, Porsche, and others are exploring TPCs for **lightweighting and part consolidation**. iii) **Consumer goods & sports equipment**: Durable, lightweight, and recyclable solutions. iv) **Infrastructure**: Bridge decks, rebar, and modular construction elements.

#### **Conclusion: Lure or Revolution?**

- ◆ Verdict: A Revolution in Progress, Not a Gimmick: i) Thermoplastic composites are not just a lure—they offer fundamental advantages that can reshape material science and engineering practices. However, widespread revolution is gated by cost, process readiness, and industry conservatism.
- ii) As manufacturing methods mature and sustainability pressures increase, TPCs are likely to become central to next-generation structural design, particularly in high-performance and high- volume applications; (we will take the modern manufacturing of aircraft as an example).

# SYNTHESIS AND INVESTIGATION OF THE PROPERTIES OF COPOLYMERS OF ALLYL ESTER OF SALISYLIC ACID WITH STYRENE, METHYL METHACRYLATE, AND MALEIC

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Copolymers of unsaturated derivatives of salicylic acid are an important research area from both theoretical and practical perspectives. These derivatives are synthesized mainly in the form of allyl, vinyl, methacrylic and other unsaturated esters and amides and are copolymerized with various monomers to obtain new functional materials. Such copolymers exhibit high reactivity because they contain both aromatic hydroxyl and unsaturated groups in their structures, and as a result, they allow the obtain of materials with specific physicochemical, mechanical, and biological properties. Our main goal in this work is to synthesize copolymers of allyl ester of salicylic acid with styrene, methyl methacrylate, and maleic anhydride, to study their biological activity properties, and to study their industrial application.

We have studied the regularities of the radical copolymerization reaction of styrene with the monomer of the allyl ester of salicylic acid. For this purpose, the study of the preparation of the copolymer, the regularities of the process, the relative activity of the monomers, the composition, structure and properties of the obtained copolymer, including its antifungal activity, was planned. In the IR spectra of the copolymers, absorption bands related to the valence vibrations of the C=O bond in the ester group (1674 cm<sup>-1</sup>) and the valence vibrations of the C-O bond in the ester group (1156 cm<sup>-1</sup>) were observed [1].

Our other copolymer is a copolymer formed by allyl salicylate with methyl methacrylate. The main quality of polymethyl methacrylate, which is produced on an industrial scale and has a wide range of applications, is determined by its high transparency. However, the drawback of these polymers is that they are not resistant to bacteria and fungi. To overcome this feature, we obtained a copolymer of allyl salicylate with methyl methacrylate, studied all its regularities, and determined that this copolymer has antimicrobial properties. In the IR spectra of the copolymers, absorption bands (1480 cm<sup>-1</sup>) belonging to the ether group of methyl methacrylate units were observed [2].

As is known, polymers derived from maleic anhydride are widely used in antimicrobial surfaces, drug delivery, food packaging, etc. The main goal of the research work carried out was the synthesis of a new type of biologically active copolymer using allyl ester of salicylic acid and maleic anhydride, the study of some regularities of the copolymerization reaction, the composition, structure and properties of the obtained copolymer samples, including their biological activity. The obtained copolymer was subjected to IR spectrum analysis and UV analysis, and both analysis results were observed to be consistent with the new copolymer.

The main objective of the study was to investigate the biological activity and antimicrobial properties of the three synthesized copolymers. This research was carried out in the scientific laboratory of the Department of Medical Microbiology and Immunology, and the obtained results were confirmed by the conducted analyses. The findings indicate that the synthesized copolymers may serve as promising components for the development of new antimicrobial materials in the future.

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### POLYMERIZATION OF N-ALLYL- N-(β-CHLORO) ALLYLAMINOBUTANE-DICARBOXYLIC ACID

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Continuing the research on the synthesis of diallylaminocarboxylic acids and their polymerization[1], this work presents the radical polymerization of N-allyl-N-( $\beta$ -chloro)allylaminobutanedicarboxylic acid (ABA) in aqueous solutions using ammonium persulfate (AP) as an initiator. Conducting the polymerization reaction without radical initiators showed that the reaction practically does not proceed. The radical polymerization of ABA occurs according to the following scheme:

The results of polymerization are shown in the table.

Table. Results of the reaction of radical polymerization of ABA

Monomer,	Initiator,	Polymerization	Temperature, °C	Yield, %	Reduced
[M]=2 mol/l	$[I]=5x10^{-3} \text{ mol/l}$	medium			viscosity
					$(\eta_{red.}), dl/g$
ABA AP		Water	60	40	0.15
AP		Water	70	45	0.17
AP		Water-alcohol	60	30	0.05
	AP	Water-alcohol	70	35	0.07

As can be seen from the table, the highest values of the reduced viscosity were obtained in an aqueous solution as a AP initiator at a temperature of 70°C.

To establish the structure of the monomer (ABA) and polymer, they were investigated by physical and chemical metods.

By the bromide – bromated method (Knopp method), it was found that the resulting ABA – based polymer does not contain unsaturated allyl groups. Thus the polymerization of ABA proceeds according to the known cyclolinear mechanism via double bonds of diallyl grups with the formation of a polymer with a pyrrolidine structure. The synthesized polymer based on ABA was tested as a soil structure.

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## PREPARATION OF FIRE-RETARDANT RUBBER BASED ON HEXACHLOROCYCLOPENTADIENE AND BUTADIENE-STYRENE RUBBER

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This paper investigates a method for producing fire-resistant elastomeric materials obtained by combining flame retardant components synthesized on the basis of hexachlorocyclopentadiene with butadiene-styrene rubber, and their properties. The halogenated structure of hexachlorocyclopentadiene [1] has an effect that inhibits the combustion process and creates heat resistance. The technological stages of obtaining and areas of application of such composite materials are presented.

Butadiene styrene rubber [2, 3] has high technical characteristics and a wide range of applications among synthetic elastomers. However, styrene-butadiene rubber is structurally weak to high temperatures and open flames. Therefore, its modification with flame retardant properties is required.

Hexachlorocyclopentadiene is a cyclic compound enriched with a large number of chlorine atoms. This substance is widely used in the synthesis of halogenated flame retardants. Its main feature is the formation of reagents that decompose at high temperatures and stop the spread of flames. Substances synthesized on the basis of hexachlorocyclopentadiene provide a high flame retardant effect when used together with butadiene-styrene rubber.

Synthesis of flame retardant rubber based on hexachlorocyclopentadiene and butadiene-styrene rubber. Technological process: 1. Mechanical mixing — butadiene-styrene rubber and hexachlorocyclopentadiene additive are mixed to a homogeneous state in a twin-roll mill; 2. Vulcanization — the mixture is vulcanized under pressure at a temperature of 140–160 °C for 10–20 minutes; 3. Cooling and molding — the finished product is removed from the molds and prepared for testing.

The introduction of 10–20% hexachlorocyclopentadiene increases the limiting oxygen index (LOI) of the material from 18% to 24–26%. The decomposition temperature in thermogravimetric analysis exceeds 300°C. Elasticity and tensile strength may decrease slightly, but remain at a level acceptable for technical applications.

Butadiene-styrene rubbers modified with hexachlorocyclopentadiene and its derivatives enable the production of technical elastomeric materials with high fire-retardant properties. Such composites play an important role in the creation of fire-safe and safe products in industry.

Fire-resistant rubbers based on butadiene-styrene rubber modified with hexachlorocyclopentadiene can be used in cable sheaths and insulation layers, in the automotive industry, construction—in the production of fire-resistant sealing materials, as well as in the defense and security sectors—as floor coverings, protective clothing components, and technical elastic products.

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#### NEW AROMATIC POLYESTERSULFOIMIDE OF HIGHLY BRANCHED STRUCTURE

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It was known that the polyesterimides are heterocyclic polymers, in which the aromatic rings are alternated with ester and imide groups. The high solubility of polyesterimides favors the preparation of low-viscosity solutions with a high polymer content. Recently, the highly branched polyesterimides – class of high-molecular polymers possessing high thermal, chemical and mechanical resistance, easiness of processing, dielectric properties, and also controlled degree of branching have become of the greatest importance [1, 2]. Such polymers are branched or dendritic structures on the basis of polyesterimide fragments.

In connection with the above-mentioned one, on the basis of the previously synthesized triglyceride-1,2,3-tricarboxymethylimide of saccharin-6-carboxylic acid [3], the new highly branched polyestersulfoimide – polytriglyceride-1,2,3-tricarboxymethylimide of saccharin-6-carboxylic acid (PTG-1,2,3-TCMI C-6-CA) with the following composition has been obtained:

The yield of the purposeful product was 74%. The composition and structure of the obtained compound have been confirmed by data of elemental analysis and IR spectroscopy [4, 5].

It has been found as a result of the investigations that PTG-1,2,3-TCMI C-6-CA obtained by this method has a viscosity  $[\eta]$ =0.16 dl/g, which is characteristic for highly branched polymers.

It has been established on the data of differential-thermal analysis (DTA) that the synthesized polymer is thermally stable in the range of 235-272°C and is well soluble in polar aprotic and phenolic solvents [6].

On the physical-mechanical parameters, PTG-1,2,3-TCMI C-6-CA has the following data: relative elongation,  $\varepsilon$  – 5%, tensile strength,  $\sigma$ t – 110 MPa.

The synthesized PTG-1,2,3-TCMI C-6-CA can be used in the production of paint and lacquer products, glues, heat-resistant coatings, films, and also polymer composites.

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# EFFICIENT USE OF POLYMER WASTE — THE KEY TO ECOLOGICAL BALANCE <u>Alimirzaeva Nahida Amanulla</u>, Manafov Mubariz Arziman, Khalilova Sanam Musa, Jafarov Valeh Jabbar

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One of the priority areas of modern chemical science is the development and application of polymer composite materials with a range of performance properties, consisting of various matrix and filler compositions. However, conducting such scientific research has a direct negative impact on the environment. Therefore, the goal is to maintain maximum ecological balance when developing materials with complex performance properties. In this regard, scientific research was conducted based on the processing of polyolefins and waste of natural mineral rocks. As a result of the research, relatively environmentally friendly and safe polymeric materials were obtained. In recent years, world-famous scientists have seen the problem of cleaning the environment from waste as a way to prevent a serious global threat associated with the disruption of the ecological balance of planet Earth. This, in turn, requires both additional costs and excess labor. Pollution of the atmosphere, as well as the lithosphere and hydrosphere surrounding the Earth, directly harms nature and leads to the rapid death of the living world through the destruction of its gene pool. This process is also closely related to the gradual indifference of man to nature in many ways.

The Japanese Environmental Protection Agency conducted a survey and named the following reasons:

- environmental pollution with chemicals;
- deforestation and destruction of forests;
- oil pollution of various bodies of water;
- an increase in the amount of carbon dioxide in the atmosphere as a result of economic development;
- the destruction of wildlife:
- the soil is becoming increasingly unsuitable for use and subject to erosion;

There are several examples of measures taken to eliminate such problems.

- 1. Development of new waste-free technologies
- 2. Minimisation of the amount of harmful and toxic substances polluting the atmosphere.
- 3. Implementation of anthropogenic processes to destroy or reduce emissions of toxic substances into the environment.

Urgent implementation of all of the listed measures directly leads to the preservation of ecological balance.

There are many methods for solving the global problem.

- Use of heat released during thermal neutralization
- Obtaining the necessary products through thermal decomposition
- Waste recycling

Of all the listed methods, the most important is waste disposal. It is in this regard that the our laboratory has been developing various polymer composite materials for many years, using polyolefins and their waste as a polymer matrix. Various natural resources (rocks) found in the most beautiful corners of Azerbaijan are used as a modifying agent. To ensure compatibility of the polymer matrix and filler, as well as to obtain a higher quality product, gluing agents (binders) with the appropriate functionality, synthesized in laboratory conditions, were added to a relatively homogeneous complex system. To achieve high results, a number of factors are taken into account in scientific research processes, such as stereoregularity, structure, structural properties of polyolefin, dispersion of the filler, the space in which it is obtained, its shape, chemical and mineralogical composition, functionality of the coating, its reactivity, etc. Thus, polymer composite materials created with different mass fractions of components based on polymer processing and addition of fillers, which are used in various fields of technology and industry, such as construction products, household items, containers, pipes, agricultural implements, etc., can be used as raw materials in their manufacture. Obtaining materials that have both economic and quality criteria, as well as achieving ecological balance as a result of work carried out in this direction, indicate the prospects of targeted scientific work.

## EPOXY COMPOSITIONS BASED ON MODIFIED UNSATURATED HETEROCYCLIC EPOXYKETONES

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It is known that composite materials based on epoxy oligomers, along with their positive properties, face a number of problems in their cured state, resulting in these composites becoming less elastic and having low thermal and light stability, which do not meet the requirements of modern technology and limit their—use in various fields of engineering [1]. To eliminate these drawbacks and to obtain composite materials based on epoxy resins with high physicomechanical properties, active diluent-modifiers are usually introduced as modifiers into the ED-20 resin composition [1].

Earlier, we demonstrated that ED-20 epoxy resins modified with unsaturated monoepoxyketones [2], followed by curing with polyethylenepolyamine (PEPA) or maleic anhydride (MA), exhibit improved physicomechanical properties and enhance the technological characteristics of epoxy compounds. This work is devoted to the synthesis and study of the modifying properties of unsaturated monoepoxyketones of the furyl and dihydropyran series-6-furyl-2-methyl-2,3-epoxy-5-penten-4-one (I) and 6-(3,4-dihydropyranyl)-2-methyl-2,3-epoxy-5-penten-4-one (II)—in epoxy compositions. The synthesis of compounds (I, II) was carried out according to the method [3] by aldol-crotonic condensation of 2-methyl-2,3-epoxypentan-4-one with 2-furfuraldehyde or 3,4-dihydro-2H-pyran-2-carbaldehyde under interphase catalysis conditions (40% aqueous NaOH solution, TEBA) according to the scheme:

Compounds I and II were tested as modifiers for creating epoxy compositions based on ED-20 resin, aiming to achieve optimal physicochemical properties. The content of active diluents in the compositions varied from 10 to 30 wt.% per 100 wt.% of the ED-20 oligomer. After appropriate processing, the research data showed that during the modification process in the compositions, the tensile strength increased by 1.5 to 2.1 times, elasticity by 5 to 6 times, impact resistance by 1.3 to 2 times, heat resistance by 1.3 to 1.7 times, and dielectric strength increased by 1.5 to 2.6 times.

The study showed that the obtained compositions containing 20 wt.% of modifying additives (compounds I and II), when cured in the presence of 15 wt.% polyethylenepoliamin (PEPA) and maleic anhydride (MA), exhibit maximum values of physico-mechanical properties with unmodified resin.

It has been established that during the curing process, the epoxy ring of both the resin and the modifier opens, forming a secondary hydroxyl group, which apparently participates in additional cross-linking between epoxy rings. As a result, a network structure is formed, leading to an improvement in the physical and mechanical properties of the compositions. Thus, the identification of the modifying properties of the studied unsaturated epoxyketones during the curing of ED-20 resin allows obtaining epoxy compositions with improved physical and mechanical properties, making them suitable for various applications requiring enhanced mechanical and thermal characteristics.

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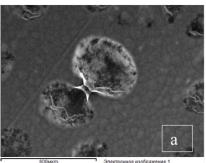
# INFLUENCE OF RADIATION DOSE ON THE SEGREGATION STRUCTURE AND PROPERTIES OF NANOCOMPOSITES BASED ON HIGH DENSITY POLYETHYLENE AND GRAPHITE

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One of the main requirements for polyolefin-based nanocomposites is their ability to operate for a long time under more severe extreme conditions [1,2]. To this end, the present study investigated the effect of gamma irradiation on the structure and properties of nanocomposites based on high-density polyethylene and graphite. Irradiation of samples with the Co<sup>60</sup> isotope was carried out using the MRX-γ-25M setup. The radiation dose varied within the range of 100–500 kGy. The main objective of the study was to investigate the effect of the specified radiation dose on the melting temperature and morphology of the samples. DTA analyses of the nanocomposites were performed under nitrogen atmosphere in the temperature range of 20–750 °C on a STA 6000 Synchronous Thermal Analyzer (Perkin Elmer), and SEM images were obtained on a JEOL JSM-6610 instrument (Nanolab, UCLA, Los Angeles) with an X-MAX-20 mm² energy analyzer.



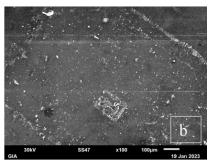


Figure 1. Initial (a) and 500 kGy irradiated nanocomposite

Studies have shown that at low doses of radiation, the melting temperature of nanocomposites changes insignificantly. However, at a radiation dose of 500 kGy, a decrease in the melting temperature of the sample by 19°C compared to the initial one is observed. SEM images also show that at high irradiation doses the surface of the sample becomes smooth. Studies have shown that irradiation (~500 kGy) causes destruction in the interphase region, which leads to a decrease in the melting temperature of the composite to 130°C.

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## SUSTAINABLE HYBRID POLYPROPYLENE COMPOSITES REINFORCED WITH NUTSHELL AND MINERAL FILLER

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The growing demand for sustainable materials has accelerated the development of hybrid polymer composites that incorporate agricultural waste and natural mineral fillers, delivering both environmental and performance advantages [1-3]. These eco-friendly materials not only improve mechanical properties but also minimize environmental impact. This study investigates the formulation of sustainable hybrid polypropylene composites, reinforced with a combination of nutshell and mineral fillers, with the goal of achieving an optimal balance between enhanced material performance and environmental responsibility.

The hazelnut nutshell, a readily available agricultural byproduct, serves as a biomass-based filler, providing a renewable and cost-effective alternative to conventional petroleum-derived fillers [4]. Clinoptilolite, a naturally occurring and widely available zeolite mineral, is characterized by its unique microporous structure, which enables it to adsorb and exchange ions effectively. As one of the most abundant and stable members of the zeolite family, clinoptilolite is found in various geological deposits worldwide. Its high surface area, selective adsorption capabilities, and ion-exchange properties make it a valuable addition to composite materials, enhancing their thermal stability, moisture resistance, and overall durability. These features make clinoptilolite particularly beneficial in applications where environmental sustainability and material performance are key considerations. The synergistic effect of these two fillers within a polypropylene matrix was investigated through melt blending, highlighting their potential to create a sustainable and high-performance composite material.

Hazelnut shells grown in the Khachmaz region of Azerbaijan were used as an environmentally friendly filler. These shells were milled and sieved to obtain a fine powder. The polymer matrix utilized in this study was a thermoplastic polypropylene random copolymer. The nut shell powder was incorporated into the polymer matrix at various weight fractions (1-30 wt%).

The synergistic effect between the hazelnut shell and clinoptilolite fillers in the polypropylene matrix was evident from the improved mechanical performance, especially in the optimal composite formulation. The results demonstrate the potential of combining agricultural waste and natural minerals to create high-performance, environmentally responsible composite materials. This study lays the groundwork for future research on optimizing filler content and exploring alternative sustainable materials for use in hybrid polymer composites. Furthermore, these findings contribute to the growing body of knowledge supporting the development of circular economy strategies in polymer materials.

In conclusion, the hybrid polypropylene composites reinforced with hazelnut nutshell and clinoptilolite fillers present a promising solution for applications that require a balance between performance and environmental sustainability. The use of agricultural and mineral waste as fillers offers a significant step toward reducing the reliance on petroleum-based materials and minimizing environmental impact. Further investigations into long-term durability, biodegradability, and potential industrial applications of these composites will provide a deeper understanding of their full potential and facilitate their adoption in various sustainable material technologies.

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## RADIATION PROTECTION MATERIALS ON THE BASIS OF LEAD-CONTAINING COMPOUNDS

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One of the perspective developing directions of the chemical and petrochemical technology sets the task for researchers to synthesize new radiation-protective materials for capture of the radiation rays formed around operating nuclear reactors. Considering the above-mentined one, we have synthesized the lead-containing oligomers (I-VI):

1) Pb 
$$\left[R_{3}Si(CH_{2})_{3}OCH_{2}CH-CH_{2}-\frac{NH(CH_{2}-NH_{2})_{4}-NH_{2}}{OCH_{2}CH_{2}CN}\right]^{+2Cl-}$$
2) Pb  $\left[CH_{2}-\frac{C}{-}\frac{COCH_{2}CH-CH_{2}-N_{2}-\frac{(CH_{2}-NH_{2})_{4}-NH_{2}}{OCH_{2}CH_{2}CN}\right]^{+2Cl-}$ 
3) Pb  $\left[CH_{2}-\frac{C}{-}\frac{COCH_{2}CH-CH_{2}-N_{2}-\frac{(CH_{2}-NH_{2})_{4}-NH_{2}}{OCH_{2}CH_{2}CN}\right]^{+2Cl-}$ 
4) Pb  $\left[R_{3}Si(CH_{2})_{3}-\frac{OCH_{2}-CHCH_{2}-N(CH_{2}-N(CH_{2})_{4}-NH_{2})}{OH_{2}-\frac{(CH_{2}-NH_{2})_{4}-NH_{2}}{OH_{2}-\frac{(CH_{2}-NH_{2})_{4}-NH_{2}}{OH_{2}-\frac{(CH_{2}-NH_{2})_{4}-NH_{2}}{OH_{2}-\frac{(CH_{2}-NH_{2})_{4}-NH_{2}}{OH_{2}-\frac{(CH_{2}-NH_{2})_{4}-NH_{2}}}\right]^{+2Cl-}$ 
6) Pb  $\left[\frac{CH_{2}OCH_{2}CH(OH)CH_{2}N(CH_{2})_{4}-NH_{2}}{CH_{2}CH_{2}CN}\right]^{+2Cl-}$ 

The above-mentioned oligomers (I-VI) have been submitted to the Closed-Joint Stock Company "National Center for Nuclear Research" as radiation protection material. It has been revealed by the investigation that there are no artificial radionuclides in the composition of oligomers, however, the individual radionuclide efficiency ( $A_{eff}$ ) is 370 BQ/kg. From the point of view of radiation safety, these oligomers can be used in all fields without restrictions. It has also been revealed that the lead-containing oligomers (I-VI) can be used for decrease of artificial  $\gamma$ - and X-ray irradiation.

## INORGANIC POLYMER – CONDENSED CYCLOOCTAPHOSPHATE OF GALLIUM WITH RUBIDIUM AND ITS POTENTIAL APPLICATIONS

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That's an undeniable fact: new inorganic polymers, notably condensed phosphates of rare earth and/or other polyvalent metals are destined to play an even greater role in our "technological" society in the XXI century than they have in the past. This judgement is based upon the trend of their increasing use consequential from the electronic structures of these composites [1-3]. It's just the structural composition that leads to their unusual chemical, and/or optical, magnetic, electrical and thermal properties, which are so valuable in today's material requirements. Conforming inorganic polymeric salts, for a long time called metaphosphates at present time are entitled and recognized such as cyclophosphates [2-4].

Several cyclooctaphosphates of rare earth and other trivalent metals with alkali metals were synthesized by us the last time, notably the double cyclooctaphosphate of Gallium-Rubidium  $Rb_2Ga_2P_8O_{24}$  throughout experiments, such as from solution - melts of polyphosphoric acids and/or by thermal condensation of provisionally synthesized acidic diphosphate  $RbGa(H_2P_2O_7)_2$ . The optimal temperature of synthesis of new cyclic inorganic polymer was strictly established within 310 ° C - 415° C. Initial molar ratios of oxides of phosphorus, gallium and rubidium was variable: from 18/1/4.5 to 18/1/8. Obtained cyclic compound was isostructural with studied  $K_2Ga_2P_8O_{24}$  and confirmed the existence of long empty channels (figure 1). As we have been mentioned about crystals of  $K_2Ga_2P_8O_{24}$  - they are monoclinic, space group A2/m, with a 5.138(3), b 12.290(5), c 16.802(13) Å, and  $101.04(5)^\circ$ ; density (exptl.) = 2.55 for Z=2. The structure was explained by the heavy-atom and Patterson methods and refined by least-squares to R=0.041. The structural arrangement contains  $P_8O_{24}$  cyclic rings of  $PO_4$  groups with inversion-centers and mirror plane symmetry elements. Atoms of Gallium are in octahedral coordination with six atoms of Oxygen. About Potassium-it is coordinated to six atoms of Oxygen in a distorted trigonal prism.

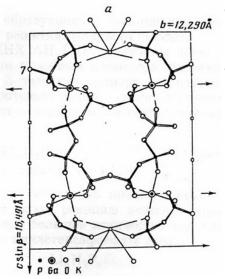
The structure contains open-worked octa-cycles by long cavities: diameters are about 5.2 Å. Based on the presence of empty hollow long channels, experiments were carried out to study their zeolitic and catalytic properties, by analogy with the one: K<sub>2</sub>Ga<sub>2</sub>P<sub>8</sub>O<sub>24</sub> already studied earlier.

It was established by experts of the Analytical Center "Geoanalitika" that above mentioned double cyclooctaphosphates there characterized by the best catalytic activity during dehydration of n-Butanol, and the total conversion percentage is approximately 55-65%. Rb<sub>2</sub>Ga<sub>2</sub>P<sub>8</sub>O<sub>24</sub> is active as well as normal boron phosphate, and as the recognized catalytic agent Bi(PO<sub>3</sub>)<sub>4</sub>, and catalyst NaZr-A.

The tests showed that the reaction products - C4 hydrocarbon olefins - were very well "captured"/retained by the catalyst.

It was also noted that the aforementioned double cyclooctaphosphate of Rb-Ga and its iso-structural analogue – cyclooctaphosphate of K-Ga are the best catalysts in organic synthesis reactions; in other words: the cyclooctaphosphate  $Rb_2Ga_2P_8O_{24}$  is an excellent catalytic agent for obtaining C2-C6 diolefins - this fact has been proven in the reaction of separation of gaseous products with relatively low molecular weight.

As a general assumption, we would like to note-by examining the spectrum of compounds and structures of  $M^IM^{III}(PO_3)_4$  type studied by us, where  $M^I$  is alkaline or any other monovalent metal, and  $M^{III}$  is any of trivalent metals such as gallium, indium, scandium, and others, including rare-earth elements, we can draw the following conclusions:



- As the radius of M<sup>3+</sup> decreases, the period of identity so to say the length of polyphosphate chain increases due to the complexity of its arrangements.
- The tendency for cycles to appear is slowly revealed, and the number of different structural types increases, due to the ratio of the average distances between the trivalent metal and the oxygen atom, as well as the atoms of the monovalent metal and oxygen.

Figure 1. The P<sub>8</sub>O<sub>24</sub> group observed in cyclooctaphosphate of Gallium

**Acknowledgement:** We would like to express our appreciation and deep respect to the memory of academician Ivan Tananaev and Professor André Durif (France) for their crucial contribution to the chemistry of condensed phosphates and their involvement in the classification & cataloguing of the condensed compounds we obtained.

We would also like to express our sincere appreciation and infinite gratitude for the examination and systematization of various inorganic compounds synthesized by us for the first time.

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#### PREPARATION OF REDUCED GRAPHENE OXIDE – MeOx COMPOSITES (Me= Mo, W)

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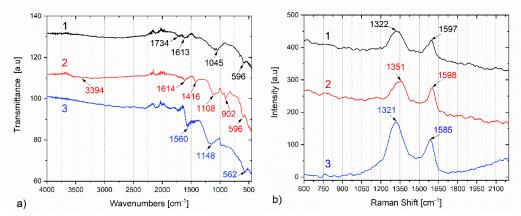
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Reduced Graphene Oxide (rGO)-MeOx Composites (Me=Mo, W) have a wide range of applications like catalysts, optoelectronics, energy storage, lithium-ion batteries, solar cells, phototherapy, sensors, etc. The presence of rGO in these composites enhances their electrical conductivity and contributes to their excellent performance in supercapacitors. We obtained the composites by interacting water-soluble molybdenum and tungsten compounds (which do not contain other metal cations) with a suspension of graphene oxide under ultrasonication. Graphene oxide was obtained from flake graphite powder by oxidation with KMnO<sub>4</sub>–H<sub>2</sub>SO<sub>4</sub> at 20–50°C. The hydrodynamic diameter of GO the particles size reaches 220-250 nm and  $\zeta$ -potential values - 47  $\div$  –50 mV. For the GO obtained from flake graphite, the atomic ratio of carbon to oxygen C:O = 1.7:1.



**Figure 1.** (a) FTIR spectra of GO foil (I), GO-H<sub>4</sub>Mo<sub>4</sub>O<sub>12</sub>(O<sub>2</sub>)<sub>2</sub> complexes and rGO-MoO<sub>3</sub> composite (300°C); (b) The Raman spectra of the samples GO foil(I), GO-H<sub>4</sub>Mo<sub>4</sub>O<sub>12</sub>(O<sub>2</sub>)<sub>2</sub> (100°C) complexes and rGO-MoO<sub>3</sub> composite (300°C)

It has been confirmed that GO- $H_4Mo_4O_{12}(O_2)_2$  and GO- $H_4W_4O_{12}(O_2)_2$  complexes undergo the following phase transformations when heated in argon: XRD analysis confirmed that GO phase characterized by the peaks located at  $2\theta$  = and  $10.41^{\circ}$ – $10.67^{\circ}$  was converted into rGO ( $2\theta = 22^{\circ}$ – $26^{\circ}$ ). Peroxy acids of Mo and W transforms into oxides of variable composition (MoOx or WOx). It has been established that the complex GO- $H_4W_4O_{12}(O_2)_2$ , when heated in the argon, forms rGO– $WO_{2.9}$  (>170°C), rGO– $WO_2$  (600°C), and under hydrogen, forms the rGO–W composite. The GO- $H_4Mo_4O_{12}(O_2)_2$  complex also undergoes similar phase transformations. Samples are studied using spectroscopic methods (UV–Vis, FTIR, Raman spectra). The morphology and microstructure of the powders were studied with SEM JEOL–JSM 6510 LV equipped with Dispersive Micro-X-ray Spectral Analyzer X-MaxN.

### SYNTHESIS AND UV-VIS SPECTROSCOPIC INVESTIGATION OF AZO-CONTAINING SPIROCHROMENE DERIVATIVES

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In this study, a novel photochromic hybrid compound containing both azo and spirochromene groups was synthesized and characterized. The target molecule, (E)-1-((1',3',3'-trimethyl-5,7-dinitrospiro[chromene-2,2'-indolin]-5'-yl)diazenyl)naphthalen-2-ol, was prepared via diazobeta-naphthol coupling at the 5'-position of the indolenine fragment. The structural design aimed to integrate the chromophoric features of both spiropyran and azo dyes within a single framework. The UV–Visible absorption spectra of the compound were investigated in various solvents before and after ultraviolet light irradiation. The azo moiety exhibited a stable trans configuration due to its linear geometry and coplanarity of the aromatic rings with the N=N bond, preventing trans—cis isomerization upon irradiation.

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

In contrast, the spirochromene unit demonstrated reversible photochromic behavior, undergoing light-induced ring opening to form a colored merocyanine species. The coexistence of azo and spiro functionalities within one molecule enabled a synergistic photoresponse, where illumination promoted the formation of both merocyanine and azo-based chromophores [1-3]. These findings highlight the potential of azo-spiro hybrids as multifunctional photochromic systems with tunable optical properties for applications in smart materials and molecular photonic devices.

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## PASSERINI-3CR AS AN EFFICIENT STRATEGY FOR THE CONSTRUCTION OF ADAMANTANE-CONTAINING COMPOUNDS

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Multicomponent reactions (MCRs) represent an efficient synthetic strategy for the construction of diverse and structurally complex molecules. Among them, the Passerini three-component reaction (Passerini-3CR) is a powerful isonitrile-based transformation that enables the one-pot assembly of polyfunctionalized compounds through the reaction of an aldehyde, an isonitrile, and a carboxylic acid. This approach is particularly valuable for the generation of multifunctional scaffolds with potential biological relevance [1-4].

In this study, novel adamantane-containing derivatives were synthesized via the Passerini-3CR using various carboxylic acids (including 1-adamantane carboxylic acid and adamantane acetic acid), phenylglyoxal, and isonitriles (including 1-adamantane nitrile). The reactions were carried out in DMF/dichloromethane, affording the desired products in good yields (60–80%). Furthermore, the obtained intermediates underwent cyclization in the presence of ammonium acetate or ammonium formate in acetic acid or acetic acid/water, leading to the formation of heterocyclic derivatives bearing imidazole and oxazole cores.

The synthesized compounds were characterized using IR, NMR, and mass spectral analysis, confirming the successful incorporation of adamantane moieties into the final heterocyclic frameworks.

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## SYNTHESIS OF ADAMANTANE-SCAFFOLD-CONTAINING DERIVATIVES VIA THE UGI FOUR-COMPONENT REACTION

### <u>Tinatini Bukia</u>, Tamar Tabatadze, Tamar Tatrishvili

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Adamantane-containing derivatives represent a privileged class of molecular scaffolds in medicinal chemistry, recognized for their broad spectrum of biological activities and distinctive physicochemical features. The rigid, lipophilic, cage-like architecture of adamantane not only enhances pharmacokinetic behavior by improving membrane permeability and metabolic stability but also strengthens drug-target interactions through increased binding affinity. Harnessing these advantages, the present study explores the synthesis of novel adamantane-functionalized peptidomimetics using the Ugi four-component reaction (U-4CR). This multicomponent transformation serves as a powerful synthetic strategy, enabling the rapid assembly of structurally diverse molecules in a single operational step.

Our approach integrates adamantane-based building blocks - including adamantane-1-carboxylic acid, and 1-aminoadamantane - together with aryl/alkyl isocyanides, aldehydes, and carboxylic acids to generate a library of structurally rich peptidomimetics [1-4].

The resulting compounds were thoroughly characterized, and selected derivatives were evaluated for antimicrobial potential against ten clinically relevant bacterial strains employing the disk diffusion method.

The outcomes highlight a strong synergistic effect between adamantane pharmacophores and multicomponent reaction chemistry, demonstrating that the Ugi protocol is not only an efficient synthetic route but also a versatile platform for creating multifunctional bioactive molecules. Collectively, this work underscores the potential of adamantane-based peptidomimetics as promising therapeutic candidates and provides a foundation for further exploration in drug discovery and chemical biology.

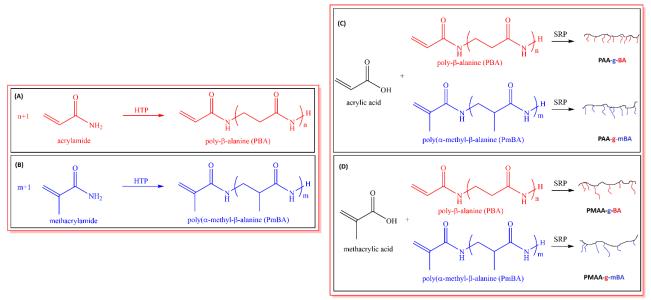
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## SYNTHESIS AND CHARACTERIZATION OF POLY(METH)ACRYLIC-BASED GRAFT COPOLYMERS, AND PRODUCTION OF THEIR NANO/MICROFIBERS

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Graft copolymers of poly(acrylic acid) (PAA) and poly(methacrylic acid) (PMA) were synthesized by using the corresponding monomers, and the macromonomers of poly-β-alanine (PBA) and poly(α-methyl-β-alanine) (PmBA). The macromonomers with vinyl end-group were introduced into the backbones of poly[(meth)acrylic acid] via "graft through" approach. The novel architecture of the graft copolymers resulting from the modification of chain structure was confirmed by FTIR spectroscopy, ¹H-NMR spectroscopy and elemental analysis. The quantitative/semi-quantitative results obtained from the FTIR spectra, ¹H-NMR spectra, elemental analyses, and EDX calculations show that the grafting yields of the PmBA macromonomer are at least two-times higher than those in the PBA macromonomers. Nano/microfiber mats of the copolymers based on PAA and PMA were prepared by a basic electrospinning process. They were characterized by scanning electron microscopy (SEM) and Energy Dispersive X-ray Spectroscopy (EDX) analysis. Not only the existence of nitrogen atoms on the fiber mats and the homogeneity of their distribution were revealed by (EDX) analysis, but also well-distributed nano-/microfibers of PAA-g-BA, PAA-g-mBA, PMAA-g-BA mats with a range of average diameters of 160–700 nm were shown to be received by SEM analysis.



**Figure 1.** Reaction outline: (A) HTP of acrylamide, (B) HTP of methacrylamide, (C) SRP of AA and PBA/PmBA, and (D) SRP of MA and PBA/PmBA.

**Acknowledgement:** The study has been supported by the Ordu University Scientific Research Project Coordination (ODUBAP) with project number B-2112.

# DETERMINATION OF DISSOLVED OXYGEN, BOD5, CARBON DIOXIDE, AND PERMANGANATE OXIDIZABILITY IN THE WATERS OF THE SPRING IN ZANATI VILLAGE, ABASHA MUNICIPALITY

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In the waters of the Zanati spring in Abasha municipality, the concentrations of dissolved oxygen, BOD<sub>5</sub>, free carbon dioxide, and permanganate oxidizability were determined. The analyses were conducted at the Hydrochemistry Laboratory named after Iason Moseshvili, Department of Chemistry, Faculty of Exact and Natural Sciences, Akaki Tsereteli State University.

Natural waters contain almost all chemical elements, but in varying concentrations. One of the primary objectives in the study of water composition is the determination of ion content. The analysis is based on the specific properties of each ion and determines its concentration in water. Natural waters always contain gases such as oxygen, nitrogen, and carbon dioxide[1]. Surface waters typically contain oxygen, nitrogen, inert gases, and carbon dioxide. Carbon dioxide has good solubility. The biochemical oxygen demand (BOD) indicates the amount of free molecular oxygen consumed by microorganisms during the transformation of organic substances in biochemical processes.

Permanganate oxidizability indicates the amount of oxygen (in mg/L) required to oxidize dissolved organic substances in one liter of water. According to regulatory standards, permanganate oxidizability should not exceed 3-5 mg/L. Based on the permanganate index, the total organic substance content in the water can be assessed. This method is simple and widely used in water supply and environmental monitoring[2]. For the analysis, sensitive methods were chosen: Free carbon dioxide was determined by the alkalimetric method, using 0.1-0.01N NaOH. titrants, and phenolphthalein as an indicator. Permanganate oxidizability was determined using the permanganatometric method (oxidant 0.01 N in acidic conditions). Dissolved oxygen and BOD<sub>5</sub> were determined using the iodometric method (titrant 0.01 N in alkaline conditions). Oxygen dissolved in the water reacts with iodine and converts into a divalent manganese compound, which is formed when the solution is acidified [3]. The results of the hydrochemical analysis of the waters of the spring in Zanati Village, Abasha Municipality, are presented in Table 1.

Table 1. hydrochemical analysis of the waters of the spring in Zanati Village, Abasha Municipality

N	Angular name of spring waters	Free CO <sub>2</sub>	Disso lved oxyg en	BO Ds	Perma nganat e oxidati on	
1	Saguno	0,62	1,86	25,92	0,47	
2	Gagma Zanata I	0,26	1,95	19,46	0,34	
3	Gagma Zanata II	0,70	1,82	24,90	0,40	
4	Uchaneishvili I	0,36	1,57	25,22	0,96	
5	Uchaneishvili II	0,42	1,86	27,46	1,28	
6	Makalatie	0.44	1,70	24.13	0.24	

The hydrochemical analysis of the spring waters in Zanati Village, Abasha Municipality shows that the permanganate oxidizability, dissolved oxygen, BOD5, and carbon dioxide levels meet the technical regulations for drinking water in Georgia. Therefore, the water is suitable for both drinking and household use.

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### QUANTITATIVE DETERMINATION OF CL<sup>-</sup>, BR<sup>-</sup>, HCO<sub>3</sub><sup>-</sup> IONS AND TOTAL SALINITY IN THE WATERS OF THE SPRING IN INCHKHURI VILLAGE, MARTVILI MUNICIPALITY

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In the waters of the Inchkhuri spring in Martvili Municipality, the concentrations of Cl-, Br-, HCO3-ions and total salinity were determined. The analyses were conducted at the Hydrochemistry Laboratory named after Iason Moseshvili, Department of Chemistry, Faculty of Exact and Natural Sciences, Akaki Tsereteli State University.

Water covers a large part of the Earth's surface and is present everywhere around us and within our bodies. Water is an essential substance for life. Much like carbon, water holds particular importance for living organisms. Its significance for life cannot be overestimated [1]. Biogenic elements include carbon, chlorine, bromine, salinity, and others. Microelements are widely distributed in natural waters and play a crucial role in the formation of their properties. Proven methods widely used in hydrochemical practice were applied for the analyses. To determine chlorides, the mercurometric method was used (titrant 0.01 N, indicator: diphenylcarbazole). Total salinity was determined using the iodometric method, with titrant 0.05 N iodine solution, and starch as the indicator. Free carbon dioxide was determined by the alkalimetric method, with titrants 0.1-0.01 N, adding small amounts of segment salt and phenolphthalein as the indicator [2].

Bromide ions were determined using the iodometric method. The sample water was treated with sodium hydrophosphate, sodium hypochlorite, and sodium formate, heated, and then cooled. Potassium iodide, sulfuric acid, and ammonium molybdate were added. Titrant 0.01 N and starch were used as the indicator. Bromide ions are oxidized to bromate ions by sodium hypochlorite [3]. The analysis results are presented in Table 1. The results of the analysis of the waters of the spring in Inchkhuri Village, Martvili Municipality, are shown in Table 1.

There is a final point of the waters of the spring in membran a mage							
N	Angular name of spring	L & m					
11	waters	C 1	Br -	Н С О <sub>3</sub>	— t t C C C C C C C C C C C C C C C C C		
1	Ferma	8,52	0,115	5,70	0,041		
2	Tobishi	9,23	0,141	2,98	0,015		
3	Gyuka	9,94	0,168	4,52	0,011		
4	Sakire	11,22	0,160	4,34	0,023		
5	Enveri	9,94	0,153	3,78	0,030		
6	Makhuzia	7,67	0,122	5.62	0,031		

Table 1. Analysis of the waters of the spring in Inchkhuri Village

The concentration of chloride, bromide, bicarbonate, and total salinity in the waters of the studied springs in Inchkhuri Village, Martvili Municipality, complies with the technical regulations for drinking water in Georgia. Therefore, the water is suitable for both drinking and household use.

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## DETERMINATION OF SOME METAL IONS IN THE WATERS OF THE SPRING IN UKHESHI VILLAGE, AMBROLAURI MUNICIPALITY

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We studied the chemical composition of the water from the spring in Ukheshi village, Ambrolauri Municipality. For this purpose, we determined the content of Mg2+, Ca2+, Cu2+ ions, and total iron in the studied spring waters. These elements play a significant role in the vital processes occurring in organisms.

Magnesium is abundant in plants as chlorophyll. It is also part of enzymes such as carboxypeptidase, adenosine triphosphatase, and cholinesterase [1].

Calcium plays a vital role in the functioning of the organism. It is present in every cell of the human body. Its absorption is regulated by vitamin D. The strength of bones, bone growth, and mineralization depend on calcium levels. Calcium ions are also involved in nerve impulse transmission, muscle contraction, and heart function regulation. Iron is an essential element for the vitality of living organisms. In organisms, iron is divided into functional, transport, and storage components. Functional iron includes hemoglobin and myoglobin; transport iron is represented by transferrin, while storage iron is stored as ferritin and hemosiderin[2]. Copper is present in almost all organs, with the highest concentrations found in the liver and brain. Copper-containing enzymes include hemocyanin, ceruloplasmin, and tyrosinase. Pure water does not exist in natur e. Water is an excellent solvent and dissolves substances encountered along its path.

The analyses were conducted at the Hydrochemistry Laboratory named after Iason Moseshvili, Department of Chemistry, Faculty of Exact and Natural Sciences, Akaki Tsereteli State University. Proven methods commonly used in hydrochemical practice were applied for the analyses. The concentrations of calcium and magnesium were determined by complexometric methods (titrant 0.01 N, complexon III). For determining magnesium ions, we used Eriochrome black T as an indicator and created an ammonia buffer solution. For calcium ion determination, Merexide was used as an indicator, and the titration was carried out in an alkaline medium using 2N sodium hydroxide[3].

Total iron and copper (II) were determined spectrophotometrically. Total iron was determined after preliminary oxidation in an alkaline medium (phosphosalicilic acid as a photometric reagent), while copper (II) was determined using sodium diethyldithiocarbamate as a reagent (UN-5100B UV/VIS Spectrophotometr). The analysis results are presented in Table 1.

Table 1. Analysis of the waters of the spring in Ukheshi Village, Ambrolauri Municipality, are shown

			0 /		<b>3</b> /	
N	Spring Waters Angular	mg/L				
14	Name	$\mathrm{Mg}^{2^{+}}$	Ca <sup>2+</sup>	Total Iron	C c + +	
1	Soso	14,15	53,60	0,029	0,001	
2	Agara	0,98	62,40	0,035	-	
3	Jobenauri	5,17	44,00	0,033	0.003	
4	Chenchkhia	8,30	68,80	0,040	0.002	
5	Momtsemlidzeebi	5,27	60,00	0,100	0.003	

The concentrations of calcium, magnesium, total iron, and copper (II) in the waters of the studied springs in Ukheshi Village, Ambrolauri Municipality, comply with the technical regulations for drinking water in Georgia. Therefore, the water is suitable for both drinking and household use.

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## INFLUENCE OF THE STRUCTURE OF DIOIE AND ISOCYANATE COMPONENTS ON THE PROPERTIES OF POLYURETHANES

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Among the numerous polymers synthesized to date, polyurethane is one of the most promising in terms of variety and scope of practical application. Polymers of this class are characterized by unique physicomechanical and dielectric properties and find universal application in various fields [1,2].

In the presented work, the synthesis of new types of linear homogeneous card-type polyurethanes was processed and implemented for the first time. Their properties and the basic patterns of the polymerization reaction have been studied. The influence of the structure of dipole and isocyanate components on the properties of the resulting polyurethane has been studied [3].

The study of the effect of the diisocyanate structure on the course of the reaction showed that in the case of aliphatic diisocyanate (1,6-hexamethylene diisocyanate), the reaction proceeds much slower than in the case of aromatic diisocyanates (2,4-toluylenediisocyanate and 4,4-diphenylmethanediisocyanate). Replacing aliphatic diisocyanate with aromatic significantly increases the thermal resistance of polyurethane. An increase in the volume of the cord group also affects the softening temperature of polyurethane. This is especially noticeable in the presence of an indane group in the polymer chain.

The influence of the nature of the diol component on the reactivity when interacting with diisocyanate has been studied. For this purpose, both aliphatic and diols containing bisphenol fragments were used, which in the bisphenol fragment contained card groups – phthalide, fluorene, norbornane, antrone, adamantine. It was found that the reaction with an aliphatic diol, in particular with 1,4-butanediol, slows down significantly compared with diols containing bisphenol fragments.

For example, if the softening temperature of polyurethane based on oxyethylated phenolphthalein and 2,4-toluene diisocyanate is 190-195°C, then the softening temperature of polyurethane that does not contain a card group is 115-140°C.

The presence of card groups is well demonstrated in the ability of polyurethanes to dissolve. For example, polyurethanes based on 1,4-butanediol and other oxalkylated diols, which do not contain card groups and have a crystalline structure, are poorly soluble in chlorinated aliphatic hydrocarbons and other common solvents, while polyurethanes containing card groups are highly soluble in these solvents and form concentrated solutions (>20%).

Thus, card polyurethanes are characterized by good solubility in chlorinated hydrocarbons, tetrachloromethane, cyclohexane and other organic solvents. Polyurethanes that contain card groups in the diol component, along with good thermal properties, are also characterized by high physico-mechanical and dielectric characteristics, which gives us reason to consider them as promising polymer materials for practical use.

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## EXTERNAL AND INTERNAL STIMULI-RESPONSIVE SMART DRUG DELIVERY SYSTEMS BASED ON LIQUID CRYSTAL MICROSPHERES

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Controlled drug delivery smart systems are becoming increasingly important compared to traditional drug delivery methods [1]. By delivering drugs at a controlled rate and targeting specific placement, therapeutic compounds can accumulate at the target site, thereby minimizing undesirable side effects. Colloidal drug carrier systems, such as micellar solutions, vesicles, and liquid crystal (LC) dispersions, show great promise in this field [2]. Liquid crystals possess unique optical, thermal, and photo-optical properties, making them ideal materials for delivering medicinal preparations to specific sites in the human body at designated times. We have developed LC spheres in micron and submicron sizes (Figure 1) that respond to environmental changes such as light, temperature, and pH. Experiments have demonstrated that substances loaded in the LC microspheres are released when exposed to specific stimuli. This release can be precisely controlled based on the timing and intensity of either an external or internal stimulus. Additionally, we have introduced a new concept for a multi-drug delivery system featuring sequential release based on LC microspheres as drug carriers. By utilizing these innovative LC microspheres, it is possible to create smart drug delivery systems that intelligently release therapeutic medications at the right place and suitable time.

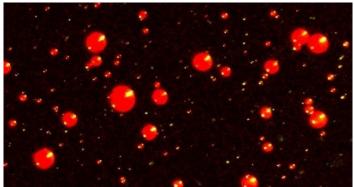


Figure 1. Liquid crystal microspheres filled with therapeutic drugs

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### PHOTOCHROMIC LIQUID CRYSTAL POLYMER FILMS FOR SENSORY **MATERIALS**

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New nanostructured polymer films, consisting of photochromic spiropyran (SP) doped to a nematicchiral liquid crystal (LC) matrix, were obtained by the authors using the technological process of the microencapsulation method [1]. The presented SPLC polymer films contain SP doped to such a nematic-chiral LC mixture whose helix pitch significantly depends on the temperature, hence the LC mixture is not only a matrix with improved photosensitivity, but also a thermal indicator, which is characterized by a significant temperature shift of the selective reflection of the light, especially in the long- wavelength region of the visible spectrum. Exposure to ultraviolet (UV) light causes a change of SP form to merocyanine colored form. The absorption band of the merocyanine in the short-wavelength region appears, and the color of the polymer film changes noticeably from the original yellow to blue and dark violet. The color change corresponds the level UV light radiation dose (Figure 1). The polymer films have high intensity of coloring in the long- wavelength region, which is distanced from the absorption band of SP in the short-wavelength region, and with the temperature chainges are visually reflected by a changes in the green, yellow, orange and red spectra (Figure 2).





Figure 1. Non-irradiated and irradiated parts of polymer films. Figure 2. Visualization of temperature distribution.

The studies showed that at all stages of the microencapsulation process, regulation of the technological characteristics of the polymer films affect their optical properties. Reducing the size of microcapsules and stretching of the film increases the photosensitivity and intensity of coloring. Increase in thickness of the film results in increase of photosensitivity [2]. Development of a smart rewritable nanomaterial based on SPLC polymer films [3,4] is promising for multiple use in thermo- and photo-optical devices as photosensitive sensory LC material that respond to UV rays with a reversible color change, capable of controlling the UV radiation dose, and as a thermal indicator for optical visualization of the temperature distribution.

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## SYNTHESIS AND INVESTIGATION OF THE COPOLYMER BASED ON OLIGOPROPYLENE MACROMONOMER AND STYRENE

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Functionalization and copolymerization of macromonomers represent effective strategies for the design and synthesis of advanced polymeric materials with enhanced performance characteristics. In some cases, macromonomers are utilized as reactive modifiers to tailor the properties of conventional polymers. A notable example involves the plasticization of polystyrene (PS), aimed at improving its processability and flexibility [1]. Although polystyrene is extensively employed across a broad range of industrial applications, its inherent brittleness and limited thermal stability significantly constrain its functional use. To mitigate these shortcomings, researchers have explored the development of PS-based copolymers or polymer blends incorporating more robust components [2].

To further explore the reactivity of the synthesized macromonomer, a radical copolymerization of oligopropylene macromonomer (OPMM) with styrene was carried out. The reaction kinetics and copolymer structure were systematically investigated. Based on the experimental data, the monomer reactivity ratios were calculated using the Fineman–Ross method, yielding values of  $r_1 = 0.02$  for OPMM and  $r_2 = 9.2$  for styrene, respectively.

The extremely low reactivity ratio of OPMM ( $r_1 \approx 0$ ) indicates its negligible tendency toward homopolymerization. Instead, OPMM participates solely in cross-propagation reactions with radicals derived from styrene. This behavior suggests a preference for alternating or block copolymer structures rather than random copolymers. The copolymerization results also demonstrate that OPMM fails to incorporate into the growing chain through self-propagation and only reacts via its interaction with styrene radicals. As a result, the reaction predominantly yields block copolymers with distinct microphase-separated domains. Additionally, increasing the molar fraction of OPMM in the monomer feed was found to significantly reduce both the copolymerization rate and the resulting polymer's molecular weight. This phenomenon is attributed to the enhanced chain transfer activity of OPMM, which facilitates premature termination events through monomer-mediated chain transfer mechanisms typical of radical polymerization systems. This is mainly due to the fact that St has a high activity, and on the other hand,  $\alpha$ -olefins with a high molecular mass are passive in radical polymerization.

The radical copolymerization of oligopropylene macromonomer with styrene was conducted in sealed glass ampoules using 0.2 wt% benzoyl peroxide as an initiator. The reaction was performed at 75 °C for 24 hours. Upon completion, the obtained copolymer appeared as a colorless solid and exhibited good solubility in aromatic hydrocarbons and in decane. The chemical composition and molecular structure of the synthesized copolymer were elucidated through elemental analysis and Fourier-transform infrared (FTIR) spectroscopy. The IR spectrum of the copolymer revealed characteristic absorption bands associated with the substituted benzene ring at 693 cm<sup>-1</sup>, confirming the presence of styrene units. Additionally, absorption bands at 2955, 2917, and 2844 cm<sup>-1</sup> were observed, which are attributable to the C–H stretching vibrations of the aliphatic chains derived from OPMM.

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## MAGNETICALLY-INDUCED POLYMERIZATION OF 2-HYDROXYETHYL METHACRYLATE IN THE PRESENCE OF POLYVINYLPYRROLIDONE

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The modern development of science and technology requires the creation of new materials and products, which is especially relevant for the pharmaceutical and biomedical fields. One promising approach to synthesizing new polymers and enhancing existing ones is polymerization involving polymer matrices, particularly such active substances as polyvinylpyrrolidone (PVP). PVP is non-toxic, hydrophilic, and capable of forming complexes with acrylic monomers. In the composition with 2-hydroxyethyl methacrylate (HEMA) it activates polymerization and enhances the properties of the copolymers. Such hydrophilic, biocompatible (co)polymers are used in the production of endoprostheses, contact lenses, membranes, dental materials, and implants [1]. Research conducted at the Department of Chemical Technology of Plastics Processing at Lviv Polytechnic National University showed that PVP activates the polymerization process, forming charge transfer complexes with the monomer, which enabled the development of a non-initiator method for synthesizing block polymers for soft contact lenses. However, these processes are sensitive to synthesis conditions, in particular, to the presence of oxygen. Previous studies have shown that the reactivity of the polymer matrix can increase under external energy fields, such as a magnetic field (MF). Although literature data on the influence of MF on polymerization are often contradictory, analysis indicates the possibility of targeted influence of MF on the initiation of matrix polymerization of vinyl monomers [2,3].

The study aim is to establish the effect of a permanent magnetic field (MF) on the polymerization of HEMA in the presence of PVP, as well as to examine the structure and properties of the synthesized copolymers. The patterns of copolymer formation under different synthesis conditions, in particular depending on the magnetic field strength, were investigated. It was found that MF accelerates the polymerization of HEMA–PVP compositions but has almost no effect on HEMA homopolymerization. The reaction rate increases proportionally to the increase in PVP content in the composition. MF affects the orientation, enhances complex formation, and promotes the development of a more ordered supramolecular structure. Copolymers synthesized in MF exhibit a higher degree of crystallinity and fewer structural defects compared to those made by traditional methods.

Since these copolymers are intended for biomedical use, key operational properties such as water content, swelling coefficient, hardness, and heat resistance were examined. Water content and swelling increase with PVP addition and polymerization in MF. These materials also show increased permeability to low-molecular-weight substances, which is important for medical applications. As PVP content rises, so do the hardness and heat resistance of the polymers, due to an increase in chemical and physical cross-links. Although polymers produced in MF have a lower mesh density, their hardness and heat resistance are higher. This indicates that a more ordered structure with fewer defects forms in MF. The impact of MF on physical and mechanical properties is most significant for homopolymers, likely due to the greater mobility of monomer molecules and their dipole-dipole interactions in MF.

The synthesized copolymers are recommended for manufacturing soft contact lenses, accommodative lenses, and implants, as they combine high hydrophilicity, mechanical strength, and biocompatibility.

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## METAL-, FULLERENE-CONTAINING NANOCOMPOSITES BASED ON ISOTACTIC POLYPROPYLENE

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Polypropylene (PP) is currently one of the most widely used synthetic polymers due to its advantageous properties and broad applicability across various sectors of human activity. In recent years, special attention has been paid to increasing the heat and fire resistance of PP by introducing various nanofillers into its composition [1].

Currently, significant attention is being devoted to the development of composite materials based on various polymer matrices modified with carbon-based nanostructures—such as fullerenes, carbon nanotubes and graphene—due to their potential to enhance the performance properties of polymers.

Nanocomposite polymer materials were prepared by mixing PP in the presence of nanofillers: a mixture of fullerenes  $C_{60/70}$  and NiO nanoparticles using laboratory rollers at a temperature of  $160-165^{\circ}$ C for 15 minutes. The obtained mixtures were then pressed into plates with a thickness of 1 mm at  $190^{\circ}$ C under a pressure of 10 MPa for 10 minutes.

The ratio of the initial components (wt.%): PP/NiO = 100/(0.5),  $PP/C_{60/70} = 100/(0.02)$ , and  $PP/C_{60/70}/NiO 100/0.02/0.5$ . SEM analysis of the obtained nanocomposite samples was carried out using a Scanning Electron Microscope (SEM EDX JSM-IT200LA, Jeol, Japan).

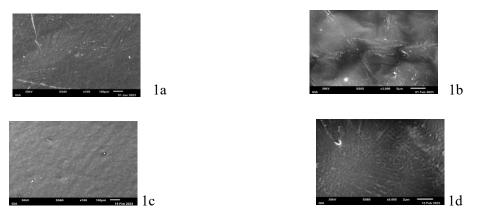


Fig. 1. Micrographs of the composites: 1a – isotactic PP; 1b- isotactic PP /  $C_{60/70}$ , 1c- PP/NiONPs = (100/0.5) % wt.; 1d-PP/ $C_{60/70}$ /NiONPs = (100/0.02/0.5) % wt.

The NiO nanoparticles used in this study, being located in the interfacial layer of the structural elements of polypropylene (PP), promote the formation of heterogeneous nucleation centers in the polymer melt. During the stepwise cooling of the nanocomposite, these centers contribute to an increased number of crystallization sites, which overall enhances the crystallization process and leads to the formation of a relatively fine spherulitic structure, thereby improving the material's properties.

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#### ANILINE OLIGOMERS: SYNTHESIS AND INVESTIGATION

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Aniline oligomers are commonly utilized as model compounds to investigate the structure and specific interactions within polyaniline (PANi). However, these oligomers can also exhibit properties superior to those of the parent polymer. Extensive research has focused on the synthesis of aniline oligomers with varying lengths and structures. Despite numerous established synthetic methods for phenyl-terminated (Ph/NH<sub>2</sub>) and phenyl-capped (Ph/Ph) tetramers, which serve as model compounds with structures similar to the repeating unit of PANi, amine-terminated (NH<sub>2</sub>/NH<sup>2</sup>) capped oligomers have received limited attention. These NH<sub>2</sub>/NH<sub>2</sub> capped oligomers are of particular interest as bifunctionalized monomers for the synthesis of other polymers. A novel, one-step condensation method has been developed for the synthesis of an NH<sub>2</sub>/NH<sub>2</sub> capped aniline tetramer in the emeraldine oxidation state. The optimization of the reaction conditions was successfully conducted. Structural investigations were performed using NMR, UV, and IR spectroscopic methods. The synthesized tetramer demonstrated a conductivity of 10<sup>-4</sup> S/cm.

## ZERO POLYMER WASTE: DEVELOPMENT OF A METHOD FOR OBTAINING CARBON MATERIALS

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The increasing amount of polymer waste in municipal solid waste poses a big environmental and technical problem, mainly in areas where the waste processing is not that good. This work is devoted to the development of a waste-free method to turn solid organic polymer waste into environmentally friendly carbon sorbents.

Polypropylene and some other polymer fractions of municipal solid waste were subjected to low-temperature thermochemical treatment (420-550°C) under anaerobic conditions using the laboratory/semi-industrial reactors. We used different analyses like thermogravimetric analysis (TGA), X-ray fluorescence analysis (XRF), scanning electron microscopy (SEM), and porosity studies to determine physical and chemical properties of the obtained carbon materials and improve the thermochemical treatment process and the final products.

The carbon materials we received were good at removing pollutants as biogenic substances, heavy metals, and microbiological contaminants from wastewater, ranging from 60 to 95%. Apart from being valuable in water/wastewater treatment, these materials could also be used as diverse industrial materials, which is a wide way to use them on a large scale. This research shows how using polymer waste to make functional carbon materials has sustainable advantages. It shows that we can use advanced processes in circular economy, which would cut down on pollution, make less waste, and promote green technologies in the Caucasus area and other places.

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## THE ADVANTAGE OF USING NANO FLUIDS (SMART FLUIDS) IN THE PETROLEUM INDUSTRY

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By adding nano particles to a fluid, the properties of the fluid such as density, viscosity, thermal conductivity and specific heat can be optimally adjusted. In low volume fractions, nano scale particles are suspended in the liquid phase [1], [4]. The liquid phase can be any liquid such as water, oil or conventional liquid mixtures. Nano particles that are used to design such fluids are preferably inorganic [2]. These fluids are designed in such a way that they are compatible with the fluids inside the reservoir and are also environmentally friendly [3], [5]. The emerging applications of nanotechnology in the petroleum industry are the use of nano fluids for many purposes, especially for the enhanced oil recovery [6], [7]. In this paper, The advantage of using Nano fluids (smart fluids) in the petroleum industry will be discussed.

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## NANO POLYMERS AND THEIR APPLICATIONS FOR ENHANCED OIL RECOVERY IN FRACTURED CARBONATED RESERVOIRS

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With the decrease in the price of oil, the global demand for fossil fuels has increased and has encouraged oil companies to look for new discoveries and develop new technologies in order to increase oil recovery from reservoirs with low permeability [2]. At the beginning of oil drilling, most of the wells drilled in oil reservoirs had a very high production capacity, but after hundred years of production, most of these reservoirs have suffered a pressure drop and as a result production has decreased [1], [6]. Studies and field tests have shown that the method of increasing oil recovery with the help of chemicals, including polymers, has had a significant effect on the process of increased recovery, and on the other hand, the use of nano particles has caused a change in the reservoir fluid composition and rock-fluid properties and lead to the movement of trapped oils [3], [5]. In such reservoirs, the use of ordinary polymers will be ineffective because these polymers lose their properties at high temperature and salinity and their viscosity decreases drastically [4], [7]. In this paper, nano polymers and their applications for enhanced oil recovery in fractured carbonated reservoirs will be discussed.

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#### NANOCATALYSTS AND THEIR APPLICATIONS IN PETROLEUM INDUSTRY

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A catalyst is something that increases the rate of a reaction. Chemists are very interested in producing a catalyst with high activity and efficiency, full selectivity, ability to be separated and recovered from the reaction mixture, low energy consumption and long life [1]. Catalyst performance can be determined by controlling variables such as size, structure, spatial and electronic distribution, surface composition, thermal and chemical stability [4]. High efficiency, economic efficiency, low wastage of chemicals, low heat and energy consumption, high safety and optimal use of primary chemicals are among the advantages of nanocatalyst. Research in the field of nanocatalyst has always been one of the fascinating discussions in nanochemistry and green chemistry [3]. Green chemistry deals with healthy chemical reactions with safe products and with maximum efficiency (minimum material and energy consumption) and nanocatalyst can lead us towards this ideal [2].

Catalysts with nanoparticles are called nanocatalysts. These catalysts must have at least one dimension in nano dimensions and in some cases their nanostructure has been corrected to improve the catalytic properties. Nanocatalysts provide a larger surface area for the reaction to take place. Catalysts are used to increase or decrease the rate of chemical reactions, without consuming or without permanent physical and chemical changes [5]. Nanocatalysts are used in oil and gas, refining and petrochemical industries. Nanoparticles are used as catalysts, or metals with high dispersing power to upgrade heavy crude oil and tar sands in petroleum industry.

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#### SYNTHESIS AND RESEARCH OF NANOCOMPOSITE MATERIAL

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Our goal is to create such nanocomposite anthelmintics that differ from existing ones by having fewer side effects, greater stability and improved environmental safety for both humans and animals [1]. We synthesized a nanocomposite material - albendazole with zinc phosphate, with the formula:  $C_{12}H_{15}N_3O_2S \times Zn_3$  (PO<sub>4</sub>)<sub>2</sub>. The resulting material forms a composite with advantegous properties, fewer side effects, and no resistance [2]. A visual representation of the synthesized nanomaterial is provided below.



Figure 1. Synthesized albendazole with zinc phosphate

The antimicrobial properties of composite anthelmintics were studied. On the one hand, their use is highly relevant in medicine, veterinary medicine, and other related fields; on the other hand, it is also important to examine their properties from the perspective of environmental safety. In particular, gram-positive and gramnegative microorganisms - Aspergillus niger F-119, Fusarium oxisporium F-137, Nocardiopsis dassonvillei G-89, Xantomonas campestris G-37, Bacillus subtilis G-39, Esherichia coli G-72 [3,4].

It is important to study the physiological activity of the anthelmintic composite using lab mice in a plusmaze test. A control group of mice matched by the age and weight was selected. Minimum, average, and maximum composite doses were chosen. The behavior of mice correlated with the state of their central nervous system. Research in this area is still ongoing, aiming to obtain conclusive results.

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### BIOLOGICALLY ACTIVE POLYETHYLENE GLYCOL (PEG)-BASED MULTIPLE-CATECHOL-CONTAINING BIOPOLYMER FROM *TRACHYSTEMON ORIENTALIS* (L.) G. DON (BORAGINACEAE)

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As part of our ongoing study on biologically active caffeic acid-derived polymers, specifically poly[3-(3,4-dihydroxyphenyl)glyceric acid] (**P-DGA**) (**Figure 1A**), from various genera of the Boraginaceae family, we have isolated a water-soluble, high-molecular-weight (Mr > 500 kDa) preparation from *Trachystemon orientalis* (**HMP-TO**). The structure elucidation of the main chemical constituent of **HMP-TO** was carried out using data from different techniques of NMR spectroscopy, including <sup>1</sup>H NMR, <sup>13</sup>C NMR, and 2D <sup>1</sup>H/<sup>13</sup>C gHSQCED (**Table 1**). It was found that the polyethylene glycol (**PEG**) chain forms the backbone of **P-DGA**, with a residue of 3-(3,4-dihydroxyphenyl)glyceric acid functioning as the repeating unit.

Table 1. Signal assignment of <sup>1</sup>H and <sup>13</sup>C NMR spectra of methylated carboxylic groups for P-DGA

The repeating unit of	C atom	<sup>13</sup> C chemical	<sup>1</sup> H chemical shift, δ <sub>H</sub> , ppm	
P-DGA; R=H, CH <sub>3</sub>	no.	shift, $\delta_C$ , ppm		
	1'	175.53(- <u>C</u> OOH)		
1'coor	1'	173.0(– <u>C</u> OOCH <sub>3</sub> )		
1 2		51.92(-O <u>C</u> H <sub>3</sub> )	3.83(–OC <u>H</u> <sub>3</sub> )	
—O-HC-CH-	1	79.79	5.67	
6" 1" 2" 3" 5" OH	2	81.85	5.0	
	1''	132.89		
	2''	118.91	7.61	
	3''	146.16		
	4''	145.24		
	5''	120.09	7.51	
	6''	123.78	7.51	

The 3,4-dihydroxyphenyl (catechol) and carboxyl groups consistently substitute for two carbon atoms in the **PEG** backbone chain (**Figure 1B**). A portion of the carboxylic acid is methylated (**Table 1**). Therefore, **P-DGA** represents a unique class of natural polyethers. Likely, the synergistic combination of catecholic groups with the **PEG** main chain of **P-DGA** highlights its diverse and fascinating biological activity. Each repeating structural unit of the regular biopolymer **P-DGA** is tri-functional, comprising two *vicinal* hydroxyl groups of catechol and one carboxyl group, which are likely responsible for its broad spectrum of biological activities. Incorporating catechol moieties into macromolecules and the multifunctionality of **P-DGA** probably explain its wide range of biological effects and enhance the exceptional therapeutic properties, including anticomplementary, antioxidant, anti-inflammatory, burn, and wound healing, antimicrobial, and anticancer effects.

**Figure 1. A -** Poly[3-(3,4-dihydroxyphenyl)glyceric acid] **(P-DGA); B -** Catechol moieties and carboxyl groups are regular substituents attached to two carbon atoms in the **PEG** backbone of **P-DGA**.

## THE IMPACT OF LOW AMINO-POSS LOADING ON THE FORMATION KINETICS AND VISCOELASTIC PROPERTIES OF POLYCYANURATE NANOCOMPOSITES

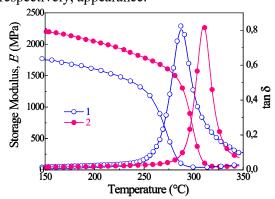
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Polyhedral oligomeric silsesquioxanes (POSS) are among the most effective inorganic nanofillers that are actively used for the modification of polymeric materials. Even at low loadings (<1 wt%) of POSS in the composition of organic-inorganic polymer nanocomposites, a significant non-additive improvement of the complex of thermophysical, thermomechanical, viscoelastic, dielectric properties, etc. is observed [1]. This work aimed to determine the effect of ultralow concentrations of aminopropylaminoethyl polyhedral oligomeric silsesquioxane (AEAPIB-POSS) containing one primary and one secondary amino groups, on the formation kinetics and viscoelastic properties of heat-resistant hybrid organo-inorganic nanocomposites based on a polycyanurate network (PCN).

The catalytic effect of AEAPIB-POSS (0.05–1.0 wt%) on the polycyclotrimerization of dicyanate ester of bisphenol E (DCBE) during the formation of a hybrid PCN was observed by dynamic DSC. A decrease in the temperature of the exothermic maximum (by 9–23°C), a shortening of the induction period and the total reaction time, as well as an increase in the maximum reaction rate (up to  $\sim$ 1.5 times) and a decrease in the apparent activation energy were detected.

The chemical incorporation of AEAPIB-POSS into the matrix at room temperature was fixed by FTIR and  $^1H$  NMR. In the FTIR spectrum of hybrid PCN/AEAPIB-POSS nanocomposite a new absorption band (absent in the spectra of the individual components) with a maximum at  $\Box\Box\Box$  1680 cm<sup>-1</sup>, caused by stretching vibrations of the C=NH group from intermediate isourea fragments, appeared. In the  $^1H$  NMR spectra new chemical shifts at  $\delta=7.54$  ppm and at  $\delta=5.73$  ppm corresponding to the Hydrogen atoms of the =NH groups of the formed isourea bonds and in the -C<sub>triazine</sub>-NH< fragments of the PCN/AEAPIB-POSS hybrid network, respectively, appearance.



**Figure 1**. Temperature dependencies of storage modulus E' and  $\tan \delta$  for (1) neat PCN and (2) PCN/AEAPIB-POSS nanocomposite

**References:** 

DMTA analysis revealed a significant improvement in viscoelastic properties and an increase in the glass transition temperature by ~23°C (by  $\tan \delta$ ), as well as an increase in the degree of structural disorder of the hybrid PCN with AEAPIB-POSS (0.025 wt%) (Fig.1). Additionally, the elastic modulus E' (at T=150 °C) of the nanocomposite sample increases by 25.5% compared to the value of E' for the individual PCN.

These results demonstrate that even ultralow loadings of AEAPIB-POSS effectively catalyze the formation of the polycyanurate network while simultaneously enhancing the viscoelastic and thermal performance of the resulting hybrid nanocomposites.

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#### OPTICALLY TRANSPARENT FUNCTIONAL POLYMER SYNTHESIS BASED ON P-CHLOROPHENYLOXYMETHYLCYCLOPROPYL METHACRYLATE

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P-chlorophenyloxymethylcyclopropylmethacrylate (CPOMCMA) was synthesized and polymerized via radical initiation in bulk and benzene solution. IR and NMR analyses confirmed polymerization through the vinyl group. The resulting polymer showed high optical transparency (nD<sup>20</sup> = 1.607). It also exhibited good thermal and mechanical stability. These findings demonstrate that CPOMCMA-based polymers are promising candidates for optically transparent and durable materials, offering superior optical clarity and stability compared to some conventional plastics. Polymers and copolymers derived from cyclopropane-based monomers exhibit a unique combination of valuable performance characteristics, making them well-suited for use in various fields of science and technology as photosensitive and optically transparent materials. This study focuses on the synthesis and polymerization processes, as well as the investigation of the optical transparency of the resulting polymer [1].

Radical polymerization of CPOMCMA was carried out both in bulk and in benzene solution using azobis (isobutyronitrile) as the initiator [2]. Under the studied conditions, the polymerization proceeds without an induction period and follows a constant initial rate, which is significantly higher than that observed for styrene polymerization. It was found that the introduction of a chlorine atom into the phenyl ring has a notable effect on the polymerization rate. As a result, the polymer was obtained as a white powder with a high yield of 85%. It was demonstrated that at 70 °C, the polymerization of CPOMCMA in benzene follows typical kinetic behavior: the polymerization rate is directly proportional to the monomer concentration (first order) and to the square root of the initiator concentration (order 0.5).

IR and NMR spectroscopic data confirm that the polymerization proceeds through the vinyl group, providing clear evidence of the selective vinyl radical polymerization mechanism of CPOMCMA.

The synthesis of CPPS and its subsequent polymerization follow the scheme below:

The obtained polymer was dissolved in benzene and precipitated using methanol, then dried under vacuum at room temperature until a constant weight was achieved. The intrinsic viscosity of the polymer solution was measured in benzene at 20 °C using an Ubbelohde viscometer, yielding  $\eta=1.0$  dL/g. It was found that the polymer exhibits excellent optical transparency with a refractive index of nD<sup>20</sup> = 1.607 and light transmittance of 88%. This cyclopropane-containing polymer surpasses certain conventional plastics in terms of optical clarity, demonstrating high transmittance across a broad spectral range, including the UV region. Moreover, the polymer retains a favorable combination of physical and mechanical properties over a wide temperature range from –50 °C to 80 °C. Shaped articles made from this material maintain their transparency even after being held at 200 °C for 3 hours. In addition, the polymer demonstrates good impact resistance and is suitable for standard processing methods.

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## SYNTHESIS AND POLYMERIZATION OF EPOXY AND THIOEPOXY-CONTAINING POLYMERS

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Studies on the synthesis and polymerization of new monomers containing functional substituents of different nature, usually possessing various specific properties [1, 2], are attracting increasing attention. Very promising in this regard are functionally substituted cyclopropylstyrene, which is a new class of compounds with a complex of various valuable specific properties - bactericidal activity and photosensitivity [3, 4].

The main problem in creating photosensitive polymeric materials is to obtain photoresists with a sufficiently high degree of photosensitivity and combined with a high capacity for thinning, resistance to aggressive media, good adhesion, heat resistance and other lithographic properties.

The aim of this work is to study the synthesis of a new epoxy and thioepoxy of substituted cyclopropylstyrene monomer. 2-epoxy-1-(p-vinylphenyl)cyclopropane 2-thioepoxy-1-(p-vinylphenyl)cyclopropane and the study of radical polymerization. A systematic study of the effect on photoresist of cyclopropane-containing polymers substituting for cyclophane in the side chain of macromolecules was also part of this work.

The synthesis of a new cyclopropane-containing styrene monomer was carried out as follows. In the beginning, 2-epoxycarboxyl-1-(p-vinylphenyl)cyclopropane was synthesized by the interaction of ethyldiazoacetate with divinylbenzene in the presence of a catalytic anhydrous CuSO<sub>4</sub>. The synthesis of monomers was carried out in the following reactions:

$$\begin{array}{c|c} & \text{LiAlH}_4 \\ \hline & \text{CH\_CH\_C} \\ & \text{OC}_2\text{H}_5 \\ \hline & \text{CH}_2 \\ \hline \end{array} \begin{array}{c} \text{EXH} \\ \hline & \text{Thiocarbamide} \\ \hline & \text{-CH}_2\text{OCH}_2\text{-CH\_CH}_2 \\ \hline & \text{(I)} \\ \hline \end{array} \begin{array}{c} \text{CH}_2\text{OCH}_2\text{-CH\_CH}_2 \\ \hline & \text{(II)} \\ \hline \end{array}$$

It was found that the reaction system remains homogeneous until high conversion ~94%. It was found that polymerization occurs without induction period. The structures of the obtained monomers I and II, as well as the polymer have been investigated by spectroscopic methods. The special structure of the synthesized polymer, namely the presence in the links of the cycloproane macrochain of the episolfide ring fragments, led to the study of their photochemical stripping with the aim of producing negative photoresist materials. Thus, the presence of a reactionary group in the macromolecules allowed to create negative photoresist materials with high photosensitivity of 52-56.7 cm<sup>2</sup>·J<sup>-1</sup> on the basis of these polymers.

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## METAL-CONTAINING THERMOELASTOPLAST NANOCOMPOSITES BASED ON ISOTACTIC POLYPROPYLENE AND ELASTOMERS

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Thermoplastic elastomers (TPE) based on thermoplastics - isotactic polypropylene (PP) and elastomers have gained considerable attention owing to a combination of rubbery properties, such as low compression set, high flexibility, resistance to fatigue, and heat resistance, along with their thermoplastic nature, including extrusion and injection molding as well as their simple preparation method [1]. TPE are widely used for various applications in the automotive, electrical, medical and packaging industries due to their high strength, low density and relatively low production cost. Innovative replacement of traditional polymer composites became possible due to the use of nanosized fillers (NF) (layered silicates, carbon nanotubes, fullerenes, metals, metal oxides) to improve the thermal, mechanical and physical properties of polymers. Combinations of nanosized materials and polymer matrices for the production of polymer nanocomposites with the required characteristics became possible due to interactions at the molecular level. Metal-containing nanofillers provide ample opportunities to control the properties of substances without a significant change in their composition due to the manifestation of size effects that affect the electronic, thermal, mechanical, electrical, and other properties of the filler and affect the properties of materials [2, 3]. In this regard, the use of metal oxide nanoparticles in the production of thermoplastic elastomers based on PP and rubbers in order to improve their physical, mechanical and operational properties is of particular interest. The objects of the study were thermoplastic elastomer composites based on PP and various elastomers: butadiene-nitrile rubber and butadiene-styrene rubber. Metal oxide nanoparticles (Cu<sub>2</sub>O, ZnO, NiO, CoO) stabilized by a polymer matrix of industrial polyethylene (PE) and high-density maleinized polyethylene (MPE) were used as NF. The ratio of the composition components (wt.%): PP/elastomer/NF=70/(30;50)/(0.5; 1.0; 2.0). Metal-containing TPE nanocomposites were obtained, the structure, physical-mechanical, thermal and thermal properties of the obtained nanocomposites were studied. It is shown that in case of using MPE as a stabilizing matrix, higher TPE indices are obtained than when using PE. In this case, zinc oxide nanoparticles show higher results. Thus, for ZnO nanoparticles, relative elongation increases by a factor of 2.5, melt flow index by a factor of 1.8, the activation energy of thermooxidative destruction (E<sub>a</sub>) increases from 124.48 to 204.77 kJ·mol<sup>-1</sup>; for Cu<sub>2</sub>O nanoparticles: the corresponding figures increase by factors of 1.5, 1.4, Ea from 124.48 to 176.49 kJ·mol<sup>-1</sup>. This is due to the fact that in the nanostructured composite, along with zinc oxide nanoparticles, there are structures of zinc maleate dihydrate, which, being located in the interfacial layer of the structural elements of polypropylene, elastomer, and maleinized highpressure polyethylene, form heterogeneous nucleation centers in the composition melt, which in the process of step cooling of the nanocomposite contributes to the creation of additional centers of crystallization, leading in general to an improvement in the crystallization process and the formation of a relatively fine spherulitic structure. The obtained TPE nanocomposites with improved properties can be recommended for use as a promising material in mechanical engineering, electrical engineering, medicine, food industry, petrochemistry, construction, etc.

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## SYNTHESIS AND RADICAL POLYMERIZATION OF 2-(p-VINYLPHENYL) CYCLOPROPYLNITROCINNAMATE WITH STYRENE

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Synthesis of (p-vinylphenyl) cyclopropylmethylnitrocinnamate was carried out, its radical homopolymerization and copolymerization with styrene were carried out. Electroacceptor functional group NO<sub>2</sub> was introduced into para position of macromolecule. Photosensitivity of materials obtained on the basis of synthesized polymer was studied. Composition and structure of synthesized copolymer were established, values of constants of relative activity of monomers were determined and parameters Q-e were calculated.

Functional polymeric materials are a broad class of substances that are used in a variety of areas of modern life and have certain physical and chemical properties. The importance of using functional polymeric materials is determined by the diversity of their properties - mechanical, electrical, optical, photosensitive.

As is known, negative photoresists based on polyvinyl cinnamates were one of the first polymeric materials studied as electron resists.

In the course of the study, the aim was to synthesize new cyclopropane-containing monomers and polymers based on them, in the macromolecule of which there are three-membered carbon rings, double bonds and a nitro group in combination with a carbonyl group located in the side chain. These groups, being light-sensitive, should impart high photosensitivity and other technological properties to the macromolecules, necessary for using it as a light-sensitive base in the creation of photoresist materials.

The objective of the present work was to systematically study the effect of a functional substituent on the photosensitivity of a cyclopropane-containing polymer. For this purpose, 2-(p-vinylphenyl) cyclopropylmethylparanitrosinnamate (FCPC) was synthesized, its radical polymerization was carried out, and the photosensitivity of the resulting polymer was studied. The compound was obtained by the interaction of 2-hydroxymethylparacyclopropylstyrene with paranitrocinnamic acid chloride.

$$O = C - CI$$

$$+ CH$$

$$CH$$

$$CH$$

$$CH_{2} - CH_{2} - CH_{3}$$

$$O$$

$$X = -CH_{2}OC - CH - C_{6}H_{4}NO_{2}$$

$$AIBN$$

$$AIBN$$

$$AIBN$$

$$X$$

Polymerization of FCPC was carried out in bulk and in benzene solution at a temperature of 70°C in the presence of AIBN. The composition and structure of FCPC and its polymer were established by elemental and spectral analysis methods.

It was found that polymerization of FCPC occurs without an induction period with a constant rate up to 86% conversion. The resulting polymer dissolves in benzene, chlorinated hydrocarbons, and polar solvents. Based on spectral analysis, it was shown that the polymerization process under the conditions under study occurs due to the opening of the double bond of the vinyl group with the preservation of the cyclopropane ring and the double bond of cinnamic acid.

The structural feature of the synthesized polymer, which has reactive groups of different chemical nature in the links of the macromolecule, makes it possible to study the photochemical structuring of this polymer due to the ease of breaking the C-C bond in the cyclopropane ring and the double bond of nitrocinnamic acid. Irradiation imparts high sensitivity to UV irradiation to these polymers (56 cm<sup>2</sup>/J).

The conducted studies have shown the possibility of creating a new type of negative photosensitive material with good film-forming ability, good adhesive properties, and is of interest for obtaining photoresistive materials for microelectronics.

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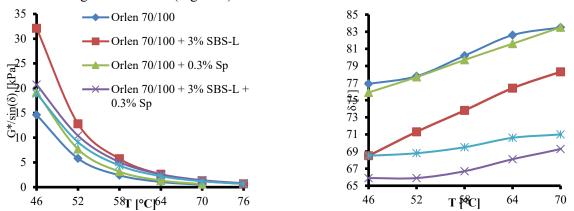
## RHEOLOGICAL PROPERTIES OF SBS/POLYMERIC SULFUR MODIFIED BITUMENS Volodymyr Gunka, Olena Astakhova

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This study investigates the rheological properties of bitumens modified with linear triblock styrene—butadiene—styrene (SBS–L) and polymeric sulfur, aimed at enhancing their mechanical and thermal performance for high-quality pavement applications.

For the modification, Orlen 70/100 bitumen (Lithuania) was used as the base binder. In addition to polymeric sulfur (Sp), rhomboid sulfur (Sr) was used for comparison. The modifier contents were: SBS -3.0 wt.% and S -0.3 wt.%. The modification was carried out at 180 °C under constant stirring (600 rpm) for 3 hours. The resulting modified binders were then characterized by DSR in accordance with ASTM D7175-23.

The temperature-dependent values of  $G^*/\sin(\delta)$  and phase angle ( $\delta$ ) were measured in the range of 46–76 °C for the investigated bitumens (Figure 1).



**Figure 1.** The  $G/\sin(\delta)$  (left)and phase angle  $\delta$  (right) in the temperature range of 46–76 °C for the investigated bitumens

In the  $G/\sin(\delta)$  plot\*, the base bitumen (Orlen 70/100) exhibits the lowest stiffness across the temperature range. Modification with 3 % SBS–L significantly increases the high-temperature stiffness, while 0.3 % polymeric sulfur also enhances stiffness, but to a lesser extent. The combination of SBS–L + Sp shows a synergistic effect, yielding higher  $G^*/\sin(\delta)$  values than the individual modifiers. When using rhomboid sulfur with SBS–L, the stiffness increase is slightly lower than with polymeric sulfur. Overall, all modified binders demonstrate higher  $G^*/\sin(\delta)$  compared to the unmodified bitumen, particularly at lower temperatures.

In the phase angle ( $\delta$ ) plot, the base bitumen shows the highest  $\delta$  values, indicating more viscous behavior. The addition of SBS-L reduces  $\delta$  significantly, reflecting increased elasticity. Polymeric sulfur (Sp) slightly lowers  $\delta$ , and the combination of SBS-L + Sp further decreases  $\delta$ , indicating improved elastic response. The SBS-L + Sr combination shows similar trends but with slightly higher  $\delta$  values than SBS-L + Sp. The decrease in phase angle across all modified binders indicates enhanced elastic behavior, especially at lower temperatures.

These results illustrate that combined SBS and polymeric sulfur modification improves both stiffness and elasticity of the bitumen, enhancing its performance at high service temperatures.

**Acknowledgement:** This work was supported by the National Research Foundation of Ukraine (Grant No. 2023.05/0026).

## PECULIARITIES OF CURING KINETICS FOR NANOCOMPOSITE SYNTACTIC FOAMS BASED ON THERMOSTABLE POLYCYANURATES

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Lightweight and thermally stable polymer composites combining low density, high mechanical strength and thermal insulation properties are in high demand for aerospace applications. Hollow glass microspheres (HGMs) are traditionally used to reduce weight and enhance stiffness of polymer composite materials, while carbon nanotubes (CNTs), even at very low contents, reinforce polymer matrices. Therefore, simultaneous incorporation of HGMs and CNTs into a polymer matrix appears to be a promising strategy for developing novel high performance syntactic nanocomposite foams. Since the structure and properties of the final materials strongly depend on the curing process, the present work focused on evaluating the influence of the introduced modifiers (HGMs, CNTs, and catalysts) on polymer network formation.

Cyanate ester resin (CER) under the trade name *Primaset*® *PT-15* (Lonza, Switzerland) was used as a base matrix. 30 wt.% of hollow glass microspheres K25 (3M<sup>TM</sup>) and 0.2 wt.% of commercial multiwalled carbon nanotubes with diameters of 10–20 nm, specific surface area of 200–500 m²/g, and bulk density of 10–43 dm³ were added in the matrix to produce the nanocomposite foam. To catalyze the CER polycyclotrimerization process 2 phr of nonylphenol and 200 ppm of cobalt acetylacetonate was also added.

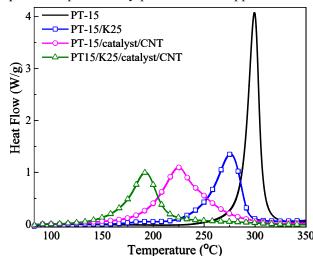


Figure 1. DSC kinetic profiles of the samples investigated.

DSC studies, performed from 40 to 350°C at 5°C/min, revealed pronounced differences in curing behavior of CER depending on the type of filler used (Fig.1). For the neat PT-15, the exothermic curing maximum was observed at  $T_{\rm exo}$  = 299 °C. The total enthalpy  $\Delta H_{\rm f}$  of CER network formation in this case was around 775 J/g.

The incorporation of HGMs (K25) reduced the induction period and caused broadening of the main DSC peak, shifting  $T_{\rm exo}$  to ~276 °C and decreasing  $\Delta H_{\rm f}$  to ~756 J/g, suggesting the formation of more heterogeneous network as well as a catalytic effect of HGMs on CER conversion.

The observed effect became even more pronounced in the PT-15/catalyst/CNT composition indicating enhanced formation of CER network at significantly lower temperatures with the lowest curing onset

 $(T_{\rm onset} \sim 113~{\rm ^{\circ}C},~T_{\rm exo} \sim 226~{\rm ^{\circ}C})$  and reduction of the induction period from  $\sim 42.5~{\rm min}$  for the neat CER to  $\sim 17.7~{\rm min}$  for PT-15/catalyst/CNT composition with  $\Delta H_{\rm f} \sim 708~{\rm J/g}$ . The combination of catalyst, HGMs, and CNT in CER provided a synergistic effect with the  $T_{\rm onset} \sim 118~{\rm ^{\circ}C},~T_{\rm exo} \sim 193~{\rm ^{\circ}C},~H_{\rm f} \sim 736~{\rm J/g}$  and the highest conversion degree at reduced temperatures.

Thus, one can conclude that the curing process in the presence of all fillers proceeded faster and reached

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higher conversions at earlier stages of the thermal cycle as compared to the neat PT-15. The most pronounced catalytic effect was observed for the PT-15/K25/catalyst/CNT foam, highlighting the potential of such hybrid fillers for the development of lightweight, thermally stable, and highly crosslinked CER nanocomposite syntactic foams.

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## CHITOSAN HYBRID NANOCOMPOSITE SCAFFOLDS FOR DIABETIC WOUND THERAPY

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Diabetic foot ulcers (DFUs) are a severe complication of diabetes, characterized by chronic, non-healing wounds that carry a high risk of amputation. Effective wound management is critical to improve patient outcomes, and the development of advanced biomaterials offers promising solutions for enhanced healing and tissue regeneration. Recent advancements in tissue engineering for DFU treatment have focused on designing biocompatible, multifunctional scaffolds to promote tissue regeneration.

Natural polymers, such as chitosan (CS) and cellulose nanocrystals (CNC), are increasingly utilized due to their ability to mimic the extracellular matrix, creating an optimal environment for cellular adhesion, proliferation, and differentiation [1]. Furthermore, integrating antimicrobial nanoparticles, particularly silver nanoparticles (AgNPs), into scaffold matrices plays a pivotal role in reducing infection risk and accelerating wound healing [2]. These combined strategies result in nanocomposite scaffolds that integrate biocompatibility, mechanical robustness, and antimicrobial properties, providing an effective platform for tissue regeneration in DFU treatment. CNCs act as a stabilizing carrier, preventing nanoparticle aggregation and enabling controlled, sustained silver release. Microwave-assisted synthesis enables rapid, uniform, and environmentally friendly incorporation of silver nanoparticles into cellulose nanocrystals with minimal aggregation [2].

Chitosan-based composites with AgNPs on CNCs were prepared by reducing silver nitrate on CNCs via microwave irradiation, followed by mixing the resulting AgNPs-CNC hybrid with a chitosan solution and crosslinked with genipin. The final porous scaffolds were obtained through lyophilization.

The method enables the green fabrication of porous chitosan scaffolds with silver-loaded CNCs, providing strong antibacterial properties. These biomaterials show great potential for wound healing, particularly in the treatment of chronic DFUs.

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#### POLYMER INOCULATED SILICA GELS FOR CHROMATOGRAPHIC COLUMNS

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High-performance liquid chromatography (HPLC) is a versatile analytical technique widely used for the analysis of pharmaceuticals, biomolecules, polymers, and many organic and ionic compounds. Inoculation (Modification) of porous silica by organic compounds with different functional groups occupies a special place in the design of HPLC columns. Silanol groups play a key role in the process of modification of the silica gel surface by a number of modifiers (in particular, alkyl chlorosilanes). The presence of silanol groups grafted to the surface of the resulting phases is mandatory. At the same time, this fact causes problems in the chromatography of compounds ("tailing" of peaks, limited pH stability range, etc.).

The problems of inoculation of the silica gel surface with polymer layers, as well as the effect of the type and amount of the polymer applied on the chromatographic properties of the resulting sorbents are considered. Modification of the silica gel surface by the polymer is described. The polymer layer itself is formed due to the copolymer of octadecyl methacrylate-methyl methacrylate. As a result, effective columns for reversed-phase high-performance chromatography (HPLC OF) were obtained.

The effect of polymer inoculation of silica gel on the chromatographic parameters of columns packed with polymer-mineral sorbents in the HPLC mode was investigated. A comparison was made between the usual widely used HPLC columns (in particular, Waters Symmetry C<sub>18</sub> columns) and the columns prepared by us, packed with a silica gel-based sorbent with a copolymer layer of poly-octadecyl methacrylate-butylacrylate-maleic anhydride (poly-ODMA-BA-MA). NMR <sup>1</sup>H shows that the above functional groups are indeed fixed on the surface of the silica gel carrier. In addition to the chromatographic indicators, Van Deemter curves were also compared. Despite the fact that after polymer inoculation, the working speed interval for efficient chromatographic studies is narrowed, such inoculation makes it possible to obtain sorbents could be successfully used at higher pH values.

Polymer-containing sorbents for HPLC have properties that differ from those of conventional  $C_{18}$  sorbents. Polymer inoculation has a number of advantages. The processes are significantly simplified. It is possible to deposit larger number of functional groups (in particular,  $C_{18}$ ) on the silica gel surface than in conventional silanization, when the number of  $C_{18}$  groups deposited is limited by the number of silanol groups on the silica gel surface, as well as steric problems associated with the mass transfer of inoculant with a long carbon chain.

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## NEW, SUSTAINABLE POLYURETHANE FOAMS CONTAINING POWDER FROM PET BOTTLES – PRODUCTION AND PROPERTIES

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Polyurethane foams are widely used polymeric materials in many applications thanks to their good properties, such as lightweight and low density. They are good thermal and sound insulators. Due to the fact that substrates used for the production of polyurethane foams are still largely dependent on petroleum, new solutions are being explored, such as the use of natural or waste-based monomers. Thanks to such solutions, we support green chemistry and sustainable development. The use of waste from PET bottles is one such example of the modification or synthesis of new materials. Waste PET can serve either as a filler or as a chain extender in the production of polyurethane foams. To obtain a chain extender from PET, a glycolysis process must first be performed.

Glycolysis is a form of the chemical recycling of polyethylene terephthalate (PET). It involves recovering monomers from the polymer, which can then be reused to synthesize PET or other materials such as polyurethane foams (PU). The aim of the study was to evaluate the impact of PET chemical and mechanical recycling products on the synthesis and properties of rigid polyurethane (PU) foams, including their chemical structure and physical and thermal properties.

In this study, a one-step synthesis of polyurethane materials was carried out using polyether polyol (RF 551), polymeric diphenylmethane diisocyanate (pMDI), PET glycolysate, catalysts such as potassium acetate (PC CAT®TKA30), 1,4-diazabicyclo[2.2.2]octane (DABCO) and dibutyltin dilaurate (DBTDL), surface active agent (SPC), flame retardant (TCPP) and blowing agent (n-pentane). The PET glycolysate was obtained in the glycolysis process, which was carried out using 1,4-butanediol (BDO). The ratio of PET to BDO was 1:4. The reaction was catalyzed by potassium acetate. PET, used as a filler, was obtained by grinding PET waste into powder and added at the stage of component mixing. Synthesized materials were analyzed to determine their thermal conductivity, compressive strength, acoustic performance, hardness, and density.

Results showed that using PET bottle waste can be used to produce new polyurethane foam materials. The materials obtained from waste PET were characterized by greater hardness and compressive strength.

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### S-[2(4)-GLYCIDYLOXY]ALKYL-N,N-DIETHYLDITHIOCARBAMATES – PLASTICIZERS, THERMAL STABILIZERS OF THE POLYVINYL CHLORIDE COMPOSITION

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It was known that the derivatives of dithiocarbamic acids consist of an extensive field of organic chemistry and are used as potentially biologically active substances, accelerators of rubber vulcanization in the rubber industry, protectors for radiation protection, multifunctional additives to lubricating oils, etc. The versatility of the area of application of dithiocarbamates is undoubtedly stipulated by the combination of heteroatoms of various natures (N, S, O) in their molecule and it is no coincidence that they are attracting increasing attention of researches of various scientific profiles. Nevertheless, the works devoted to the use of dithiocarbamates and, in particular, derivatives of diethyldithiocarbamic acid as a plasticizer-thermal-stabilizer for polymer compositions are extremely limited.

In this work information on the synthesis of s-[2(4)-glycidyloxy)alkyl-N,N-diethyldithiocarbamates (IV, V) by the interaction of the corresponding 1,2-epoxy-3-(2-chloro-alkoxy)propane (II, III) with trihydrate of N,N-diethyldithiocarbamate sodium, proposed as new plasticizers-thermostabilizers of PVC compositions are presented. The reaction has been carried out in an aqueous medium according to the scheme:

$$(C_{2}H_{5})_{2}N-C(=S)SNa + CH_{2} - CHCH_{2}O(CH_{2})nCl - \frac{H_{2}O}{NaCl} \rightarrow (C_{2}H_{5})_{2}N-C(=S)S(CH_{2})nOCH_{2}CH - CH_{2}$$

$$(I) \qquad (II, III) \qquad (IV, V)$$

$$n=2 (II, IV); n=4 (III, V).$$

The synthesized s-(2-glycidyloxy)ethyl-(IV), s-(4-glycidyloxy)butyl-N,N-diethyldithiocarbamates (V) are transparent liquids with almost no odor. They are insoluble in water, well soluble in organic solvents (ether, CCl<sub>4</sub>, CHCl<sub>3</sub>, DEC, etc).

It has been established that dithiocarbamates (IV, V) are well combined with PVC resin and, as a result,

the combination of glycidyloxy group with dithiocarbamate fragment SN-C(=S)S containing a tertiary nitrogen atom in their molecule, they simultaneously stipulate plasticization and thermal stabilization of PVC plasticat and, moreover, the availability of dithiocarbamate group can play an important role in protection of the materials from the effects of mold fungi and bio-damage. Thus, the tensile strength and relative elongation of the plates obtained with the participation of the tested compound (V) taken in the ranges of 20, 30, 40 mass p. per 100 mass p. of PVC and 2 mass p. of Zn-stearate are 1.3-1.4 times higher than the same values of plates made using a standard plasticizer (DOPh) at the same ratios. The thermal stability of the tested samples (250°C)\* is 1.4-1.5 times higher than the corresponding indicator of plates made from PVC with the participation of DOPh (150°C).

Thus, the obtained results allow to expand the range of effective chemical compositions for PVC plasticat, and the created materials can be recommended for practical use in various branches of industry. **Acknowledgement:** The authors express their gratitude Nurullayeva D. R. for the assistance in the preparation of this work.

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<sup>\*</sup>It was determined on the chromatograph of Paulik-Paulik-Erdei system (Hungary).

#### SYNTHESIS AND STUDY OF FIRE-RESISTANT EPOXY ACRYLATE OLIGOESTERS

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It is known that epoxy resins have great technical significance and are widely used in various industries. However, in the cured state, they have some disadvantages, in particular low heat resistance, brittleness, hardness and frost resistance. To improve these disadvantages, epoxy resins are modified with chemical compounds containing various functional groups.

The aim of the presented work is devoted to the synthesis of new low-viscosity modifiers containing epoxy acrylate oligoesters with a branched structure, from the reaction of propanetriol-polyoxychloropropylene triepoxy ether with acrylic acid and the study of optimal conditions for their production.

Epoxy acrylic compounds are widely used as binders for reinforced plastics, as well as modifiers for epoxy resins. Their use as reactive modifiers allows obtaining polymeric materials with increased elasticity, high adhesive and impact strength. Of interest from this point of view are chlorine-containing oligoester epoxy acrylates synthesized by ethrification of polyoxychloropropylene triepoxide with acrylic acid [1, 2]:

The presence of chlorine atoms in the composition of these compounds allows them to be used as fire retardants, and the presence of epoxy groups, along with acrylate fragments, leads to chemical bonding with the modified epoxy resin during curing of the resulting mixture with amine and anhydride hardeners.

The results of the study showed that the yield and composition of the resulting epoxy oligoesters depend mainly on the molar ratio of the initial reagents and the reaction temperature. The synthesized epoxy acrylates were tested as modifiers-fire retardants of ED-20 resin [3].

It is shown that the synthesized epoxy acrylates, actively participating as a fire retardant modifier in the process of forming a network structure in epoxy compositions, provide them with high physical-mechanical, thermal-physical and adhesive properties, imparting self-extinguishing properties to the compositions.

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## COMPOSITION ON THE BASIS OF LOW-DENSITY POLYETHYLENE FILLED WITH MINERAL ROCK

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Currently, the development of filled composite systems on the basis of industrial and household polymer waste and the creation of new composite materials based on them remains an actual problem. The solution of this problem from the point of view of creation of new composites with high operational properties, as well as from the point of view of maintenance of the ecological balance of the environment is one of the main requirements of materials science. In particular, the use of inexpensive natural resources as a filler in solution of the above-mentioned problem is of great economic importance.[1]

İn this work, the results of the physical-mechanical investiogation of the characteristics of the polymer composites based on low-density polyethylene filled with volcanic rock are presented (Ceramite, Ganja). For provision of higher physical-mechanical indices of the obtained composite materials, the copolymer of maleic anhydride with hexene-1 has been used as an apprete in the system. [2] A comparative analysis of the results obtained in the presence of apprete and without it showed that the composite materials obtained in the presence of apprete are characterized by comparatively high operational characteristics (Table 1). It has been established that the introduction of 5% of apprete into the composition of the composite system leads to an improvement in the strength properties of the compositions. So, a tensile strength is increased by 2-2.5 MPa and a relative elongation, as expected, is decreased by 5-10%.

**Table 1.** Physical-mechanical properties of compositions filled with volcanic rock filler without apprete (samples 1-4) and with apprete (samples 5-8)

№	Composition of composites	Tensile strength σ MPa	Relative elongation ε	MFI g/mol
1	PE:filler 70:30	12.62	30	4.7
2	PE:filler 60:40	13.35	30	4.5
3	PE:filler 40:60	16.22	16	2.8
4	PE:filler 30:70	16.4	16	2.6
5	PE:filler 70:30	13.02	38	3.6
6	PE:filler 60:40	15.8	27	3.4
7	PE:filler 40:60	18.24	12	2.4
8	PE:filler 30:70	18.5	8	1.2

It is seen from Table that the tensile strength without the apprete is 12.62 MPa, with the apprete – 18.5 MPa, and the relative elongation decreased from 30% to 8%. Since the preparation of compositions with various content of solid substances by recycling is inexpensive, then the preparation of compositions with high physical-mechanical properties is considered economically and ecologically beneficial.

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#### POLYMER COMPOSITES BASED ON FINISHED NATURAL MINERAL ROCK

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It is known from a number of literatures that obtaining more complex polymer systems by mixing two or more polymers and the dominance of a number of properties in these systems is considered a promising direction in the field of chemistry [1]. In general, in complex open systems of various compositions, the characteristic properties of the components that make up the system are of great importance.

Composite samples were obtained and their properties were studied at various mass % ratios corresponding to the filler size of 106 microns and the size of the finish 3 mass %. The samples corresponding to both the size of the filler dispersion were taken as corresponding to the mass % of the components PP/Filler/Appret-70/30/3, 50/50/3 and 30/70/3.

Table 1. Physico-mechanical properties of composite samples (Filler: dispersions - 106 mkm; Appret: [MA-Hepten-1]

No.	Compound compositions, %	Traction force, σ, MPa	Elongation, ε, %	MFR
1.	PP-100	36.3	20	5
2.	PP-70 Filler-30 Appret-3	22.8	23	4.4
4.	PP-50 Filler-50 Appret-3	28.6	4	3.6
6.	PP-30 Filler-70 Appret-3	33.5	4	0.5

Table 1. presents the physical and mechanical properties of composite samples with different mass ratios with the presence of polyacrylate, synthesized in the laboratory. The tensile strength of the composite sample corresponding to the mass ratio PP/Filler/Appret-30/70/3 is  $\sigma$ =22.8 MPa, taking the minimum value. In all cases, the coupling agent is 3% by weight. When the ratio of the components included in the composite is PP/Filler/Appret-30/70/3 wt.%, the tensile strength reaches its maximum value and takes the value  $\sigma$ =33.5 MPa. The tensile strength value decreases with further increase in filler.

Thus, depending on the filler dispersion, higher quality composite samples are observed in those corresponding to their 30/70/3% mass content. Such materials can be used as raw materials in a number of areas of technology and industry.

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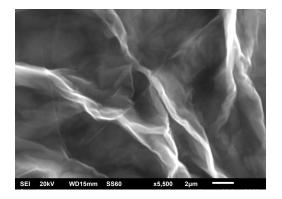
#### SYNTHESIS OF rGO/PDMS NANOCOMPOSITES FOR SIA PRINTER

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Stereolithography (SLA) employs a single beam laser to polymerize or crosslink a photopolymer resin. By drawing on the liquid photopolymer resin with a light beam, thin layers of polymer are stacked layer-by-layer [1]. Elastomers based on polydimethylsiloxanes (PDMS) are important materials due to the properties, such as chemical inertness, flexibility, optical transparence. In addition, they have a very low surface tension (20.4 mN/m) and glass transition temperatures (146 K) [2]. It is possible to print a support material that holds the PDMS prepolymer in place until it is cured with UV light using a photoactive cross-linking agent [3]. PDMS needs crosslinking to satisfy operating requirements. The traditional thermal treatment of PDMS takes much time and energy. Because of this UV, treated PDMSs have synthesized by different methods (Fig 1). In addition, reduced graphene oxide (rGO) used as filler in nanocomposites was obtained.

Liquid UV curable PDMS has produced with rGO for SLA printer. Lab homogenizer has used for good dispersion of filler into polymer. Nanocomposites were produced with different content of 0.5-0.8 wt% filler for further characterization of electrical, electromagnetic, thermal and mechanical properties. Materials structure and composition have identified by FT-IR, NMR, TEM, Raman, X-ray and DSC analyses in order to determine the filler dispersion, exfoliation, defects and thermal characteristics.



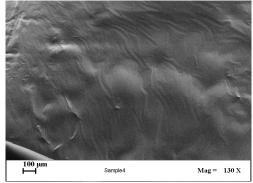


Fig. 1. Micrographs of rGO and rGO/PDMS nanocomposites

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## THE PROGRESS IN CERTIFICATION OF BIODEGRADABLE AND COMPOSTABLE POLYMER COMPOSITIONS

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The following topics will be covered in the lecture: an overview of the biodegradation definitions, biodegradability, tests used to assess them, current and future certification requirements, with particular emphasis on the environment and the lack of complete information on the composition of polymers considered biodegradable.

The broader interest in the subject of biodegradation can be observed at the end of the 20<sup>th</sup> century [1,2, ISO 9408:1991]. Firstly, it was considered a process of decomposition facilitated by biochemical mechanisms. Later, it was added that the products of biodegradation are carbon dioxide, water, mineral salts and biomass. Then, based on the above statements, the definition of biodegradable plastics was adopted. One approach to the current definition was given by Barenberg et al. [3]. According to him, biodegradable plastic means a plastic material that disintegrates under environmental conditions within a reasonable and demonstrable period of time, where the primary mechanisms are bacteria, yeast, fungi and algae. The ASTM D5488-94d definition was expanded to include the requirement that the process should be subjected to standardized tests within a specified timeframe. In 1992, an international workshop on biodegradability was held, attended by manufacturers, regulators, research laboratories, environmentalists, and standards organizations from Europe, the United States, and Japan. It was determined that several key points should be considered when assessing biodegradability. As a result, standard methodologies were incorporated and developed by standardization organizations such as CEN, ISO, and ASTM. To simplify measurements, environments are generally categorized as either aerobic or anaerobic.

The following types of observations were taken into account: microbial growth, substrate depletion, reaction products, changes in substrate properties, and others.

In addition to these factors, biological oxygen demand (BOD) and Sturm tests were also considered. Therefore, for a specific application of the plastic, appropriate tests should be applied to assess the biodegradability of the material. Based on the results, relevant certification labels are assigned, e.g. OK water degradable (ISO 14851), OK soil degradable (ISO 17556, ASTM D5988), OK marine degradable (ASTM D6691).

In addition to the term "biodegradability of plastics", the concept of compostable plastics is very important. Polymer composting is a process in which polymer waste is transformed into soil-like products. It is a biological process that involves breaking down plastic waste by bacteria or algae into useful materials by partial biodegradation within a specific environment. Composting certificates are marked differently than those used to assess the biodegradability of polymers. The following labels are used to certify the compostability of polymers in specific environments: OK Industrial Compost (EN 13432 or Australian Standard AS 4736), OK Home Compost, and Compostable (ASTM D6400). The issue of determining how polymer biodegradation products affect living organisms is still a subject of debate in the literature.

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## THE EFFECT OF MICRO- AND NANOFILLERS ON THE COMPATIBILITY OF THERMOPLASTIC/GROUND TIRE RUBBER SYSTEMS

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The growing problem of waste tires, which are difficult to recycle and degrade very slowly in the natural environment, drives researchers to seek alternative methods to reuse them. One of the promising solution is the incorporation of ground tire rubber (GTR) into thermoplastic matrices. This approach not only reduces the volume of rubber waste but also lowers production costs and provides opportunities for developing innovative polymer composites.

The requirement for combining thermoplastics with GTR lies in the poor compatibility between the two phases, which results in reduced mechanical strength and limited processing properties [1]. To improve compatibility, micro- and nanofillers such as silica, carbon black, montmorillonite nanoclay, graphene nanoplatelets or carbon nanotubes can be introduced into the systems. These additives enhance interfacial adhesion, facilitate the dispersion of rubber particles, and contribute to improved microstructure and mechanical properties of the composites.

One of the most common methods for producing polymer/GTR systems is melt-blending. This technology provides materials with a wide range of applications - from thermoplastic composites to thermoplastic elastomers - using standard processing equipment such as extruders or internal mixers.

As a result, it is possible to easier scale up the results from laboratory research to industrial production. Thermoplastic/GTR systems offer good processability and recyclability, with potential applications spanning construction, automotive, and innovative areas such as 3D printing or specialty materials (e.g., electromagnetic shielding). However, they still face limitations such as poor compatibility and the characteristic odor associated with processing of waste rubbers [2].

Research on the use of micro- and nanofillers opens new opportunities for tire recycling and the production of durable, functional polymeric materials. The application of such additives improves processability and mechanical performance, which is crucial for industrial implementation.

In the context of the circular economy, these composites may become valuable high-performance products, ranging from asphalt modifiers and automotive components to material dedicated for additive manufacturing technologies. The combination of economic and environmental benefits highlights the strong development potential of this approach in the near future.

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# CORRELATING THE SLIPPERY BEHAVIOR OF NANOSCALE POLY(DIMETHYLSILOXANE) LAYERS TO THEIR LIQUID LIKE MOLECULAR MOBILITY

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Nanoscale poly(dimethylsiloxane) (PDMS) layers prepared by grafting the polymer chains on smooth solid surfaces are typical example for the so called slippery covalently-attached liquid surfaces (SCALS). Such surfaces exhibit very low contact angle hysteresis (CAH) and low friction for sliding water drops [1-2]. These properties are commonly attributed to the liquid-like mobility of the tethered, low glass transition temperature, polymer chains. However, to date there is still no clear, molecular level understanding of the involved physical phenomena. Here, we used fluorescence correlation spectroscopy (FCS) to measure the diffusion coefficients of small fluorescent tracers dispersed in the PDMS layers as probes for the local nanoviscosity. Our results show a clear correlation between the molecular mobility in the polymer layers and their slippery behavior.

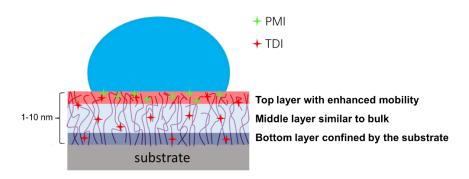


Figure 1. Molecular mobility of PDMS brushes probed by fluorescent tracers

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## ECO-FRIENDLY, ONE POT SUNTHESIS OF BIS-4-HUDROXYCOUMARINS USING DIFFERENT H-FORM OF NATURAL ZEOLITE-CLINOPTILOLITE AS A CATALYST

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Biscoumarins, derived from 4-hydroxycoumarin, have attracted considerable interest due to their wide pharmaceutical biological applications. of and range Given their diverse chemical and biological properties, there has been substantial focus on developing efficient methods for synthesizing biscoumarins. Numerous synthetic strategies have been documented in the literature. Despite their usefulness, many of these methods face limitations such as low product yields, prolonged reaction times, the use of large quantities of catalysts or reagents, non-recyclable catalysts, and environmentally hazardous solvents. As a result, designing straightforward, high-yielding, eco-friendly synthetic routes remains objective key chemists. The objective of this study was to develop a synthesis method based on natural zeolite, employing the H-

The objective of this study was to develop a synthesis method based on natural zeolite, employing the H-form of Clinoptilolite (zeolite was treated with 1M HCl) as a catalyst, in order to assess its efficacy in the production of biscoumarin compounds. In this method, aromatic aldehydes (such as benzaldehyde, p-nitrobenzaldehyde, and dimethylaminobenzaldehyde) were reacted with 4-hydroxycoumarin in the presence of H-form of clinoptilolite using ultrasonic irradiation for 30–60 minutes, resulting in high yields (90–97%) of biscoumarins. The use of ultrasound irradiation reduces the temperature and time required for the reaction.

Both electron-donating and electron-withdrawing substituted aldehydes smoothly converted to their corresponding biscoumarins with no detectable side products. The H-form of Clinoptilolite catalyst proved to be cost-effective, eco-friendly, readily available, and reusable across multiple cycles. This method is notable for its simplicity, avoidance of toxic solvents and hazardous agents, and several advantages, including excellent catalytic efficiency, straightforward procedure, minimal catalyst requirement, and easy workup.

## PROPERTIES OF BASALT-FILLED THERMOPLASTIC ELASTOMERS BASED ON HIGH-DENSITY POLYETHYLENE AND STYRENE-BUTADIENE ELASTOMER

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In recent years, much attention has been paid to the development and research of thermoplastic elastomers in world literature. This circumstance is due to the fact that as various branches of industry developed, high operational requirements began to be imposed on the quality of products made from polymeric materials. Polyolefins produced in industry cannot always meet the increasingly stringent quality requirements of modern technology and equipment. In this regard, special attention is paid to the development and research of thermoplastic elastomers (TPE), which have the properties of rubber, but are processed by standard thermoplastic processing methods - injection molding and extrusion. The advantage of these processing methods is the high productivity of the plant, environmental friendliness and technological efficiency of the process of obtaining products. Taking into account that the literature provides very scant information in the direction of obtaining filled TPE, it seemed interesting to use fibrous basalt (FBS) as a filler.

In this case, high-density polyethylene (HDPE) was used as the polyolefin, and styrene butadiene rubber (SKS) as the elastomer. It was important to identify the optimal ratio of mixture components, which would maximally demonstrate the highly elastic properties characteristic of rubber. The content of the rubber component varied in the HDPE+SKS composition within the range of 10-70 wt. %. It was found that for this composition, phase inversion occurred at 30% SKS content. This fact was established based on the strength characteristics of polymer mixtures, i.e., when the yield strength at tension was equal to the tensile strength at break. One of the key points is to achieve maximum compatibility and strength of the mixed components of the mixture. This is due to the fact that HDPE is a non-polar polymer, while SKS is a polar polymer. To ensure compatibility of the polymer components of the mixture, a HDPE graft copolymer with maleic anhydride was used as a compatibilizer, which was introduced into the mixture in an amount of 2.0 wt. %. To give the composition additional strength, FBS was introduced into its composition in an amount of 5.0-30 wt. %; the presence of SKS with a high content of double bonds in the TPE composition allowed us to carry out their sulfur vulcanization. In this case, cross-linking will occur predominantly between the elastomer macrochains, since HDPE is characterized by a relatively low content of vinyl groups. In this regard, the use of the process of dynamic vulcanization of the composite HDPE + SKS + FBS + compatibilizer is of particular interest. The advantage of dynamic vulcanization is that the mixing of components in melt mode and their vulcanization occur simultaneously in the extruder. In addition, this method of mixing and vulcanization allows to obtain extrusion products or granules for their further use in casting units and to obtain structural products with durable and highly elastic properties. It was found that the method of dynamic vulcanization of thermoplastic elastomers filled with FBS allows increasing the strength of samples by 2 times, and the relative elongation by 120%.

## STRUCTURE AND PROPERTIES OF BASALT-FILLED THERMOPLASTIC ELASTOMERS BASED ON POLYPROPYLENE

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With the expansion of industrial production in such industries as aircraft manufacturing, mechanical engineering, automobile manufacturing, shipbuilding, space and military technology, etc., interest in the development and use of polymer composite materials based on polyolefins and mineral fillers has increased significantly. One of the developing directions of modification is the mixing of polymer with polymer, as a result of which it is possible to obtain composite materials that combine the useful properties of the components of the mixture. In this regard, it is worth noting the development and production of thermoplastic elastomers (TPE), which exhibit properties characteristic of rubber, but are processed into products as thermoplastics using injection molding and extrusion methods. Therefore, the main goal of the study was to replace the labor-intensive process of obtaining rubber products with more productive, technological and environmentally friendly methods of obtaining TPE. Research based on TPE becomes promising and relevant when there is a need to use relatively cheap mineral fillers, which include fibrous basalt (FBS).

The regularity of changes in the tensile yield strength and tensile strength of polymer mixtures based on polypropylene and styrene-butadiene elastomer (SKS) was investigated. To improve the technological compatibility of the polymer components of the mixture, a compatibilizer was used, which was a graft copolymer of polypropylene with maleic anhydride in an amount of 3.0 wt. %. The objects of the study were PP+SKS mixtures in which the elastomer content varied within the range of 10, 20, 30, 40, 50, 60, 70 wt. %. During the conducted research it was established that as the content of SKS increased, a natural decrease in strength indicators was observed. It has been shown that when the content of SKS in the mixture is equal to 30 wt. % or higher, the value of the tensile yield strength becomes equal to the tensile strength. This moment indicates phase inversion, i.e. when the crystalline dispersed medium of the PP turns into a dispersed phase, and the dispersed phase of the SKS turns into a dispersed medium. In other words, plastic deformation is transformed into highly elastic deformation, characteristic of rubber. In this regard, all further studies were carried out in such a way that in the initial polymer matrix, consisting of a mixture of PP + SKS, the content of the elastomer component was 30 and 40 wt. %. Based on these mixtures, composites were obtained by introducing fibrous basalt (FBS) into their composition in melt mode. The content of FBS varied within the range of 5.0 - 30 wt. %. During the studies, it was found that when the content of FBS was over 20 wt. %, a decrease in the tensile strength of the composites was observed.

In order to obtain highly elastic composites based on PP+SKS+compatibilizer+ FBS, the samples were subjected to sulfur vulcanization. It was found that as a result of crosslinking the composites with 5.0% sulfur, an increase in the strength of the sample by 80-90% and elongation at break by 50-60% was observed.

## REMOVAL OF ZINC IONS FROM AQUEOUS SOLUTIONS UNDER STATIC AND DYNAMIC CONDITIONS USING GEORGIAN MINERALS

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With the rapid growth of industry, water pollution by heavy metals has become a global environmental concern. The contamination of water by heavy metals poses serious risks to both the environment and public health. Once inside the body, these metals can disrupt normal cellular functions and fundamental biological processes. Among heavy metals, zinc demonstrates significant acute toxicity when the concentration of  $Zn^{2+}$  in water exceeds the permissible limit of 3 mg/L. Among various water treatment methods, adsorption stands out due to its economic efficiency and environmental safety.

In this study, for the first time, natural Georgian minerals—travertine and limestone—were used as adsorbents for the removal of zinc ions from aqueous solutions. The work presents a comparative investigation of travertine and limestone under both static and dynamic adsorption conditions. In static experiments, the effects of adsorbent dosage, contact time, solution pH, and initial Zn<sup>2+</sup> concentration on adsorption efficiency were evaluated [1].

Dynamic experiments were conducted in glass columns filled with the minerals, through which zinc solution was passed at a flow rate of 0.1–0.8 L/h. Samples were taken every 15 minutes and analyzed. The travertine and limestone samples were collected from mountainous regions of Georgia and used without prior chemical treatment [2].

Analytical methods: Atomic Absorption Spectrometry (AAS) and X-ray Fluorescence (XRF) analysis of mineral composition.

Indicator	Travertine (static)	Limestone (static)	Travertine	Limestone
			(dynamic)	(dynamic)
Maximum adsorption	89.8	82.0	70.0	82.0
efficiency (%)				
Adsorption capacity (mg/g)	29.0	28.0	_	_
Solution pH	5–8	5–8	5	5
Optimal contact time (h)	1	1	3	5
Flow rate (L/h)	_	_	0.3	0.3

Table 1. Key results of Zn<sup>2+</sup> adsorption under static and dynamic conditions

The results demonstrate that Georgian minerals effectively adsorb Zn<sup>2+</sup> without prior activation, making them promising candidates for environmentally friendly and cost-effective wastewater treatment technologies, and laying the scientific foundation for the development of industrial-scale applications.

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## THERMALLY ACTIVATED DELAYED FLUORESCENCE FROM CYANOPYRIDINE EMITTERS FOR OPTOELECTRONIC AND SENSING APPLICATION

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The technology of organic light emitting diodes (OLEDs) is rapidly growing. The main option to increase the efficiency of the device is to effectively utilize triplet excitons in electroluminescence. Conventional phosphorescent OLEDs require the use of earth-rare metal complexes such as those of Ir, Pt, Au, etc. incorporated in the organic matrixes (hosts) [1]. The phenomenon of thermally activated delayed fluorescence (TADF) emerged as a cost-effective alternative to phosphorescent emitters [2]. TADF is a long-lived fluorescence of upconverted triplet excitons. Here, we report on the series of cyanopyridine derivatives as TADF emitters. The ionization potentials estimated from the photoelectron emission spectra are in the range of 5.37-5.86 eV. Drift mobility of the charge carriers of the compounds measured by the techniques of time-of-flight and charge extraction by linear increase of voltage were evaluated to be up to 10<sup>-3</sup> cm<sup>2</sup>/V·s at electric field of ca. 2.5×10<sup>5</sup> V/cm. TADF was detected for the toluene solutions of the compounds. The solutions were prior deoxygenated by purging with argon as oxygen intercepts triplet electronic excitation energy. Picric acid was added to the deoxygenated toluene solution of one of the compounds to test the sensitivity of its emission to the nitroaromatic explosive. The Stern-Volmer plot showed a linear correlation with the photoluminescence lifetime of the sample decreased by the factor of three when the concentration of picric acid in the solution of the studied compound increased to 20%. The optical sensitivity is due to the interception of triplet excitation energy. The emission peaks shifted from blue to green/yellow spectral regions for most of the compounds when molecularly dispersed in well-reported host 1,3-Bis(N-carbazolyl)benzene. The photoluminescence and electroluminescence lifetimes of up to 0.5 ms were recorded. The thermal activation of TADF was confirmed from the analysis of photoluminescence decay curves recorded at the different temperatures. The fabricated OLEDs showed the external quantum efficiency of up to 20.7%.

#### Acknowledgement:

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#### CHEMICAL CONSTITUENTS AND BIOLOGICAL ACTIVITY OF YUCCA GLORIOSA L.

Ether Kemertelidze<sup>a</sup>, Mariam Benidze<sup>a</sup>, Alexander Skhirtladze<sup>b</sup>, Vazha Nebieridze<sup>a</sup>

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The steroidal sapogenin tigogenin – (25R)- $5\alpha$ -spirostan- $3\beta$ -ol obtained from the leaves of *Yucca gloriosa* L. (fam. Agavaceae) introduced on an industrial scale in Georgia, is recognized as an economical raw material for the synthesis of  $5\alpha$ -steroidal hormonal preparations. Plantations of *Yucca gloriosa* were cultivated in eastern Georgia on an area of 150 ha to ensure a supply of tigogenin from plant raw material.

The leaves of the lower tier of *Yucca gloriosa* dry at 3-4 years of age. Our observations showed that leaves drying on the living plants contain only spirostanol glycosides. In all probability, the furostanols are converted to the corresponding spiro-forms during drying and they consist tetra-, penta- and hexaosides of tigogenin. Antifungal activity of the total and individual glycosides was studied *in vitro* tests against human pathogenic, yeast, dermatophyte and filamentous fungi. High activity was shown by individual yuccaloesides B and C in the concentration range of  $0.39 - 6.25 \mu g/ml$ , for dermatophyte fungi – in the range of  $0.78 - 12.5 \mu g/ml$  and were similar to those of reference agents – amphotericin B and ketoconazole.

Polyphenolic compounds of stilbene nature with a rare spiro-structure are obtained from the roots and bark of stem and rhizomes. They have been shown to have antioxidant, specific antiproliferative and proapoptotic effects on MCF-7, HepG2 and U937 cancer cells.

From the flowers of *Yucca gloriosa* there were isolated 8 individual substances. There chemical structures were established by physical - chemical data and modern spectral methods of analysis such as one-and two-dimensional NMR (<sup>1</sup>H, <sup>13</sup>C, HSQC, HMBC, COSY) and mass – spectrometry (ESI-MS). Spectral data of 1-7 substances were indicative to sesquiterpene glycosides of nerolidol type and 8 – triterpene glycoside derivative of soyasapogenol B with the structures:

- 1. (1E,3S,5R,6E,9E)-5-O- $\beta$ -D-Glcp $(1\rightarrow 6)$ -O- $\beta$ -D-Glcp-3,5,11-trihydroxy-3,7,11-trimethyldodeca-1,6,9-trien:
- 2. (1E,3S,5R,6E,9E)-5-O- $\beta$ -D-Glcp $(1\rightarrow 6)$ -O- $\beta$ -D-Glcp-3,5,11,12-tetrahydroxy-3,7,11-trimethyldodeca-1,6,9-trien;
- 3. (1E,3S,5R,6E,10E)-(12-O-β-D-Glcp)-5-O-β-D-Glcp-(1→6)-O-β-D-Glcp-3,5,12-trihydroxy-3,7,11-trimethyldodeca-1,6,10-trien;
- 4. (1E,3S,5R,6E,10E)-5-O-β-D-Glcp-3,5,12,13-tetrahydroxy-3,7-dimethyldodeca 1,6,10-trien;
- 5. (1E,3S,5R,6E,10E)-5-O-β-D-Glcp-3,5,12-trihydroxy-3,7,13-trimethyldodeca-1,6,10- trien;
- 6. (1E,3S,5R,6E,10E)-5-O-β-D-Glcp-3,5-dihidroxy-3,7,12,13-tetramethyldodeca-1,6,10-trien;
- 7. (1E,3S,5R,6E,10E)-5-O-β-D-Glcp-3,5-dihydroxy-12-carbonyl-3,7,13-trimethyldodeca-1,6,10-trien;
- 8. Soyasapogenol B 3-O- $\alpha$ -L-Rhap-(1 $\rightarrow$ 2)-O- $\alpha$ -L-Arabp. Sesquiterpene and triterpene glycosides is new class for the genus of Yucca.

In this way, our studies have determined that *Yucca gloriosa* L. cultivated in Georgia in an industrial scale is rich with substances of different chemical classes, they exhibit various biological activities, which gives a great opportunity to use them in practice.

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## SIMULATION OF DIESEL FUEL DESULFURIZATION PROCESS USING ARTIFICIAL INTELLIGENCE MODELS AND OPTIMIZATION STUDY

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The tightening of environmental requirements for fuels demands the development of efficient methods for the desulfurization of diesel fuel [1]. This study investigates the extraction of sulfur-containing compounds from diesel fuel obtained after desulfurization using *N-methyl pyrrolidone* (NMP). A theoretical analysis of the properties of NMP is presented, along with the extraction mechanism of thiophenic compounds and a review of existing experimental research [2, 3].

An experimental study was conducted on the removal of sulfur compounds from diesel fuel samples using NMP. Mixtures of *hydrogen peroxide* and *acetic acid* in various ratios were applied. The sulfur content was determined using a T-100 fluorescence analyzer. The results obtained confirm the promise of the method and provide essential data for selecting optimal process conditions.

To visualize the results, a simulation mesh grid was used, which included the systematic variation of reagent volumes within a defined range, generating a uniformly distributed dataset. The resulting data are displayed in a 3D map.

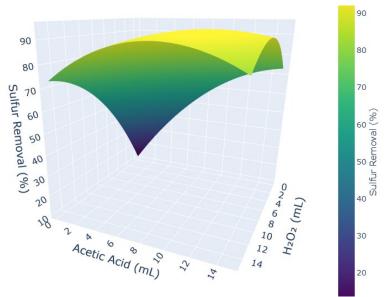


Figure 1. 3D Map of Diesel Fuel Desulfurization.

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## MICROCAPSULE-BASED WATERLESS COSMETIC SYSTEMS WITH TAILORED POLYSACCHARIDE SHELLS

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Microcapsule-based waterless cosmetic formulations represent an emerging strategy in response to the growing demand for sustainable and high-performance personal care products. Conventional cosmetics are predominantly water-based, with water content often exceeding 70–80% of the formulation. This approach, although technologically convenient, increases the need for preservatives, raises transport costs, and contributes to the environmental footprint of the cosmetic industry. The waterless concept addresses these challenges by eliminating or drastically reducing water, thus enabling higher concentrations of active ingredients, extending product stability, and reducing the need for synthetic preservatives [1]. At the same time, waterless formulations require careful design of delivery systems to ensure proper incorporation and release of bioactive compounds.

One promising strategy to overcome these limitations is microencapsulation, a technique that allows the physical entrapment of an active substance (core) within a protective polymeric shell. Such carriers can be designed to ensure controlled release, shielding of sensitive ingredients from environmental stressors, and improved sensory and functional properties of the final product [2]. Among the available encapsulation methods, coaxial extrusion combined with ionic gelation is particularly attractive for cosmetics due to its mild processing conditions, scalability, and ability to generate monodisperse, spherical capsules with tunable wall properties [3].

In this work, microcapsules were prepared using sodium alginate (SA) crosslinked with calcium ions and modified with maltodextrin containing postbiotic metabolites (Lactobacillus ferment) to enhance the flexibility and functional performance of the capsule wall. Various compositions of SA and maltodextrin were tested to optimize the mechanical integrity, elasticity, and ease of rupture during topical application. The encapsulation process was carried out with a Büchi Encapsulator B-395 Pro, employing coaxial nozzles and electrostatic droplet breakup to ensure uniform particle size distribution. The resulting capsules successfully entrapped selected lipophilic active substances, including lupine seed oil, goji berry macerate, marshmallow macerate, and vitamin E in a blend with forest fruit oils.

The microcapsules were subsequently dispersed in a carefully optimized anhydrous serum base composed of sunflower seed oil and dimethicone, stabilized rheologically by an organoclay thickener. This system provided favorable texture, spreadability, and stability over a 30-day accelerated storage test at 40 °C. Mechanical testing (texture analysis, viscosity profiling) confirmed that the optimized hybrid alginate—maltodextrin walls exhibited sufficient robustness during storage but remained breakable under gentle shear, enabling controlled release of actives during application.

The presented study demonstrates that natural polysaccharide matrices, such as alginate reinforced with maltodextrin-based postbiotics, are promising materials for the encapsulation of bioactive lipids in waterless cosmetics. The combination of coaxial extrusion and ionic gelation enables the production of microcapsules with tailored wall properties and stable dispersion in oil-based formulations. This approach aligns with the current shift toward sustainable, water-free, and functionally enhanced personal care products, while exploiting the versatility and biocompatibility of polysaccharide-based delivery systems.

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#### BAMBOO-BASED NANOCOMPOSITES REINFORCED WITH GRAPHENE AND NANO-SILICA

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Growing demand for sustainable materials has intensified interest in nanocomposites that combine natural fillers with advanced nanostructures. This study focuses on bamboo as a renewable reinforcing material in composites bound with tetraethyl orthosilicate (TEOS), further enhanced by the incorporation of graphene and nano-silica. Previous research has shown that bamboo fibers, when properly treated and combined with nanoscale additives, significantly improve the strength, durability, and thermal stability of composites, making them suitable for demanding industrial applications<sup>1,2</sup>.

In our approach, TEOS binder content and bamboo flour loading are systematically varied, with additional nanofillers and functional additives introduced to optimize material performance. Fabrication involves hot pressing under controlled temperature and pressure conditions, enabling uniform dispersion and strong interfacial bonding. The resulting composites are characterized using Fourier transform infrared spectroscopy (FTIR), mechanical and water absorption testing, optical microscopy, and thermogravimetric analysis (TGA)<sup>3,4</sup>.

Preliminary insights indicate that bamboo, combined with graphene and nano-silica, provides a strong basis for developing nanocomposites with superior mechanical integrity, lower moisture sensitivity, and improved thermal resistance. This work highlights the potential of bamboo as a versatile, sustainable filler in creating durable, eco-friendly nanocomposites for applications in construction, transportation, and packaging industries<sup>5</sup>.

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### PHOTORESPONSIVE HOMO- AND COPOLYMERS BEARING AZONAPHTHOL-PYRIDINE SIDE CHAINS FOR HOLOGRAPHIC APPLICATIONS

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The azobenzene derivatives and azo-based polymeric materials are the prominent candidates for application in photonics, photoelectronics, nonlinear optics etc. These are A- $\pi$ -D type chromophores which contain a donor and an acceptor moiety, as well as an azo group as a  $\pi$ -linkage. Their useful properties are related to reversible photoinduced  $trans \leftrightarrow cis$  isomerization, which makes possible the relaxation of the relevant material after exposure during its application. Because of the planar or near planar structure of azo chromophore, such materials are polarization-sensitive. This fact explains their applicability in polarization holography. When designing new photoactive materials, careful planning of the chromophore architecture is essential, since even the replacement of a benzene ring with a pyridine ring - by introducing a single nitrogen atom instead of CH - can dramatically alter key properties such as isomerization rate and the sign or magnitude of the nonlinear optical and holographic response [1], [2].

Scheme 1. Chemical structure of azobenzenefunctionalized poly(methyl methacrylate) polymers

The covalent bonding of azobenzene to a polymer chain can greatly increase the chromophore concentration in the material without causing aggregation of photosensitive molecules. It can make the photomaterials more sensitive to light irradiation and enhances a response efficiency of material. Thus, a new methacrylic monomer was synthesized by diazotization of 3-aminopyridine followed by coupling with 1-naphthol, and subsequent acylation of the resulting dye with methacryloyl chloride under standard conditions. The monomer was then copolymerized with methyl methacrylate *via* thermally initiated radical polymerization in the presence of AIBN in DMF solution at 80°C. The aim of this work was to determine the influence of the polymer composition (different ratios of MMA units) on the magnitude of the diffraction response.

Plane-wavefront holography was investigated using a DPSS laser with a wavelength of 532 nm (falling within the absorption tail of the polymers), and the diffraction efficiency was measured in the "-1" order.

Measurements of three "record-relaxation" cycles with a periodicity of "2 minutes-1 minute" respectively showed that, when moving from the homopolymer to the copolymer with a 1:1 comonomer ratio, and further to 1:3, a gradual but slight increase in the diffraction efficiency during the first cycle was observed, along with a progressive decrease in the difference between the values of the first and second, and the second and third cycles. At the same time, the value of the residual diffraction efficiency at the end of the 1-minute relaxation interval between recording cycles decreases when moving from the homopolymer to the copolymers. This effect may be attributed both to the greater "softness" of the polymer matrix in the copolymers and to the stronger intermolecular interactions of azobenzene chromophores in the homopolymer, which hinder rapid  $cis \rightarrow trans$  isomerization. For the copolymer with a 1:3 monomer ratio, the material appears promising for use as a dynamic holographic medium, whereas the homopolymer may be considered in the future as a recording medium for long-term information storage.

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## DEVELOPMENT OF BIODEGRADABLE POLYMERS WITH GOOD ANTIBACTERIAL PROPERTIES FUNCTIONALIZED WITH HUMIC ACIDS

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A prevailing trend in polymer science and technology involves the substitution of conventional polymers with biodegradable alternatives and developing materials derived from them. Contemporary biodegradable polymer materials (BPMs) can be synthesized from natural biomass (such as polysaccharides, proteins, lipids, and nucleic acids), renewable bio-based monomers (e.g., polylactic acid, PLA), or by means of microbial processes (e.g., polyhydroxyalkanoates, PHAs; polyhydroxybutyrate, PHB; bacterial cellulose; xanthan; pullulan, etc.). Nevertheless, despite their ecological advantages, existing BPMs frequently demonstrate inferior performance compared with synthetic polymers, particularly in aspects such as vapor permeability and gas barrier properties. Hybrid modification is one of the most promising approaches to overcoming these limitations. In this context, hybrid BPM composites are formed by combining organic and inorganic constituents that are chemically and structurally distinct, resulting in spatial and crystalline architectures that differ from the parent materials yet frequently retain or enhance their properties.

The authors explore the complex utilization of low-grade, high-ash, and high-sulfur coals (HASC) and their by-products as feedstock for the production of bitumen modifiers [1, 2] and environmentally benign energy carriers [3, 4]. Within this framework, an attempt has been made to apply HASC as a source for BPM modifiers. Ukrainian lignite deposits, currently underutilized due to their low quality, were selected as a potential raw material.

The study proposes synthesizing hybrid biodegradable polymers (HBPs) using humic acids (HAs) and their derivatives extracted from lignite. Due to their diverse functional groups and complex physicochemical nature, HAs significantly influence polymer structuring processes [5]. Previous investigations demonstrated both the feasibility of obtaining BPMs with HA incorporation and the antimicrobial effects of these substances on polymer matrices. Thus, elucidating the mechanisms of HA-driven hybrid modification and assessing their impact on the operational performance of polymers represents a novel and relevant research direction with considerable scientific and practical implications.

This work integrates and complements previous studies of hybrid modification of biodegradable polymers using HA in three polymer systems: gelatin, polyvinyl alcohol (PVA), and hydroxypropylmethylcellulose (HPMC). The mechanisms and results of such modification regarding structural organization and characteristics of the obtained materials are established.

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## THERMOMECHANICAL PROPERTIES AND THERMOOXIDATIVE STABILITY OF OPTICALLY TRANSPARENT CARBOCHAIN CO-POLYMERS

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The optically transparent carbochain co-polymers of the perfluoroalkyl- and siliconorganic (meth)acrylates by radical co-polymerization with dimethylvinylacetylenylcarbinol have been synthesized. Using the data of IR, UV and <sup>1</sup>H-NMR spectra and CLC methods the structure and the composition of the co-polymers have been determined. Based on the obtained data it has been also shown, that in the case of perfluoro(meth)acrylates the macrochains of the co-polymers are enriched with the links of the more reactive fluorocontaining monomers. In the case of siliconorganic methacrylates the main chain of the co-polymers contains the cyclic links of carbinol, which could be formed via interacting the primary radicals of dimethylvinylacetylenylcarbinol with its "own" monomers.

The thermomechanical properties and the thermooxidative stability of obtained optical adhesives have been studied. The dependence of the thermomechanical properties and thermooxidative stability'y on the structure of the hydroxy radicals of the methacrylates, on composition of the initial mixture of the monomers and on conditions of co-polymerization was established.

The thermomechanical curves of the obtained co-polymers are typical to the thermoplastic polymers. It has been shown, that the temperature of vitrification depends on the structure of methacrylates and the ratio of the molar concentration of the monomers in the initial mixture. By increasing the chain length of the fluorocontaining fragment and quantity of fluoroatoms,  $T_{vit}$  of the co-polymers decreases. The opposite effect takes place in the case of co-polymers of a fluoroperfluoroalkylacrylates with dimethylvinylacetylenylcarbinol. The largest shift of  $T_{vit}$  towards low temperatures in comparison with homopolymer is observed with the co-polymers obtained by radical co-polymerization of siliconorganic methacrylates with dimethylvinylacetylenylcarbinol. By increasing the ratio and the length of siliconorganic fragments in co-polymers,  $T_{vit}$  decreases.

The investigation of the thermooxidative stability of the co-polymers indicated the dependence of this property on the nature of hydroxy radical of the methacrylates. By increasing the length of the fluorocontaining fragment and the quantity of the fluoroatoms of the alcoholic radical of methacrylate, the temperature of the beginning of the thermooxidative destruction (comparing with the according temperature of the homopolymer) increases and the essential process of the thermooxidative destruction is shifted towards a higher temperature range.

The possibility of application of the obtained co-polymers for production of the optical adhesives has beeb determined.

## SYNTHESIS OF FUNCTIONAL POLYMERS VIA ELECTRON DONOR-ACCEPTOR COMPLEX-DRIVEN PHOTOINIFERTER RAFT POLYMERIZATION

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Polymer-biomolecule (drug) conjugates represent a promising avenue in drug development, constituting a rapidly expanding field. Such conjugates offer enhanced precision in biological targeting and treatment surpassing the capabilities of traditional drugs. The vast majority of bioconjugates are prepared by reversible addition-fragmentation chain-transfer (RAFT) and atom transfer radical polymerization (ATRP). However, these methods require laborious multistep synthesis of the corresponding ATRP / RAFT initiators and exhibit a lack of versatility. A breakthrough in this field was made by Fors et al. who reported controlled radical polymerization from hydridic C-H bonds and Hooper et al. demonstrated photomediated decarboxylation of unactivated carboxylic acids for initiation of controlled radical polymerization. However, the high oxidation potential of photocatalysts used and utilization of disulfides as chain-transfer agents significantly limit the range of tolerated substrates and functional groups as well as functionality at the  $\alpha$ -end (typically 60 - 90%).

In this work, a unified approach for photoiniferter RAFT polymerization technique allowing the utilization of organic molecules with the most ubiquitous functional groups (amines, carboxylic acids and alcohols) as initiators without significant limitations in substrate complexity providing close to complete  $\alpha$ -end functionalization of synthesized polymers will be presented. This approach consists in a combination of visible light-induced electron donor-acceptor (EDA) complex -driven initiation mechanism and photocontrolled radical polymerization to provide polymers with controlled molar mass, low dispersity and targeted α-end functionality. As an example, the Katritzky salt derived from benzyl amine in combined with sodium ethyl carbonotrithioate trithiocarbonate generated the corresponding EDA complex, which upon irradiation by blue light in results in initiation of RAFT polymerization of butyl acrylate affording well-defined polymers with controlled molecular weight, low dispersity ( $\mathfrak{D}=1.20$ ) and close to complete functionality at the  $\alpha$ -end ( $\sim 100\%$ ). To involve in similar reaction carboxylic acids, the corresponding N-hydroxyphtalimide (NHPI) esters were prepared as acceptor component of EDA complex. Through this method, a wide range of diverse amines and carboxylic acids including biorelevant and drug-like substrates were effectively attached to polyacrylates backbone. In addition to that, we have developed a universal reagent for effective initiation from complex amines and alcohols, which also provides a new dimension for the construction of conjugates with potentially biocleavable bridge between  $\alpha$ -end and polymer chain.

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# DOPA-BASED POLY(ESTER AMIDE)S: A TUNABLE BIOMIMETIC APPROACH FOR SURGICAL ADHESIVE DESIGN

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Surgical adhesives (SAs) are materials that upon in situ polymerization/crosslinking can bind biological surfaces together, having both haemostatic and sealant properties. Nature has developed high-performing protein-based adhesives in underwater environments, where the  $\alpha$ -amino acid (AAA) 3,4-dihydroxy-L-phenylalanine (DOPA) controls several key adhesive and cohesive mechanisms. Mimicking the biochemical richness of adhesive proteins in polymeric structures *via* straightforward methodologies is of utmost importance in SA design.[1]

Poly(ester amide)s based on AAA (AAA-PEAs) allow the direct incorporation of key AAA directly onto the polymeric backbone through simple methods, such as solution polycondensation (SPC). PEAs' properties and functionalities can be easily fine-tuned by the incorporation of different AAAs, diols and carboxylic acids.[2]

A library of AAA-PEAs was prepared *via* SPC.[3], [4] DOPA and L-arginine (Arg) were selected as key AAA, due to their known role in high-performing protein-based adhesive systems; L-phenylalanine (Phe) was selected as AAA with a supportive role.[5] This allowed tuning of the functionality and hydrophilicity of the PEA. PEAs were successfully prepared without compromising the integrity of the catechol group. The influence on adhesive performance was studied by tensile tests (Scheme 1). The PEA-based glues displayed comparable or superior adhesive strength to the commercial reference Dermabond® in two vastly different *ex vivo* tissues, dermis and liver, without any surface treatment or oxidizing agent.

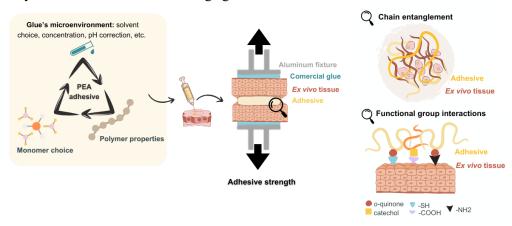


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# DISSOLVED CARBOHYDRATES IN THE UKRAINE'S SURFACE WATER BODIES OF DIFFERENT TYPES

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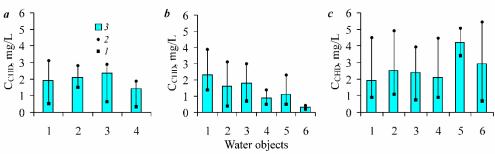
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Carbohydrates as an important class of biopolymers are always part of the dissolved organic matter (DOM) of surface waters and sediments. They are synthesized in living organisms such as plants, animals, and microorganisms, and excreted by them as exometabolites in the process of their vital activity. Carbohydrates include free reducing sugars (mixture of mono-, di-, and trisaccharides and their derivatives), as well as more complex carbohydrates, in particular oligosaccharides, polysaccharides, and carbohydrate-like compounds, where are registered in the composition of complexes with the other classes of substances [1]. Oligosaccharides include 3–20 monosaccharide residues connected by glycoside bounds. Polysaccharides can contain to 10,000 saccharide residues bound to each other and represented as widely branched structures. They contain residues of various monosaccharides, such as glucose, fructose, mannose, galactose, xylose, etc. Polysaccharides make up the bulk of algae carbohydrates. Almost all polysaccharides, despite the difference in structure and origin, have such specific features as an affinity for water, i.e., they are hydrophilic polymers [2].

Carbohydrates are excreted by aquatic organisms into surface water bodies and rivers. Dead organisms' decomposition and microbiological hydrolysis of mucus polysaccharides are also responsible for their release into the water. Significant amounts of dissolved carbohydrates flow into water bodies with surface runoff, atmospheric precipitation, and sewage. Algae are often considered a powerful source of carbohydrates [3].

The ion-exchange chromatography was used to separate carbohydrates other organic substances, including humic substances. Natural water filtrates were passed through the glass columns. The first column contained DEAE-cellulose, whereas the second column – CM-cellulose. DOM of the natural water was separated into three groups: acidic – containing mainly humic substances, basic – with a predominance of protein-like compounds, and neutral – containing mainly carbohydrates. Carbohydrate concentration was determined by the photometric method in an acidic medium using an anthrone reagent. The gel-chromatography method (glass column filled by the HW-55F gel, Japan) was used for investigation of carbohydrate molecular-weight distribution.

Carbohydrate concentration in Ukrainian water objects of different type are shown in Figure 1. It varies widely – from 0.19 to 5.43 mg/L depending on the season and the characteristic features of the water body. Maximum concentrations are characteristic for summer and autumn, when there is intensive development of phytoplankton. In the water bodies of the urbanized territory as highly eutrophic, the carbohydrate content is much higher than in the Dnipro reservoirs and rivers (see Figure 1, c).



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**Figure 1**. Limit (1, 2) and averaged (3) concentrations of dissolved carbohydrates (C<sub>CHD</sub>) in the different type water bodies of Ukraine:  $\boldsymbol{a}$  – the reservoirs of Dnipro cascade (1 – Kyivs'ke, 2 – Kanivs'ke, 3 – Kremenchuts'ke, 4 – Kakhovs'ke),  $\boldsymbol{b}$  – rivers (1 – Pripyat', 2 – Desna, 3 – Ros', 4 – Pivdennyi Bug, 5 – Seret),  $\boldsymbol{c}$  – water bodies of the urbanized territory (1 – Ternopils'ke reservoir, Ternopil City, 2–6 – small water bodies of Kyiv City (2 – Kytaivs'kyi pond, 3 – Tel'bin lake, 4 – Verbne lake, 5 – Almazne lake, 6 – lakes of the Opechen system).

The molecular weight of carbohydrates in surface water bodies of Ukraine varies over a wide range – from < 1.0 to > 70.0 kDa. Usually, high molecular weight compounds (polysaccharides) are dominated.

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# DISSOLVED CARBOHYDRATES AS IMPORTANT LIGANDS IN METAL COMPLEXATION IN THE UKRAINE'S SURFACE WATERS

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It is known that humic substances, as the most common group of dissolved organic matter (DOM), play a primary role in binding metal ions into complexes in surface waters. However, there is evidence that other DOM groups, such as carbohydrates, are also involved in complexation. This is especially noticeable for those water bodies with high carbohydrate concentrations and usually low humic substances content. First of all, these include high-trophic water bodies that often suffer from urbanization and experience increased algae blooms. Metal complexes with natural carbohydrates are of considerable interest because they are involved in various vital processes. A significant number of studies have been devoted to this problem, the results of which highlight various aspects of metal complexation with natural carbohydrates [1]. It is noted that the excretion of these organic macromolecules by phytoplankton has a noticeable effect on the metals bioavailability and toxicity in the aquatic environment [2]. The structure of exopolysaccharides contains ionizable functional groups such as carboxyl, acetate, hydroxyl, amine, phosphate or sulfate groups which may act as active sites for complexation. The conditional stability constants of metal complexes with algae exometabolites characterize them as quite strong (for example, log K\*1 of Cu(II) complexes with such ligands is 8.6–9.5, and Cd(II) – 6.8–7.5) [3].

We established the existence of neutral metal complexes in water bodies of different types in our long-term monitoring of the concentration and share of metals in such complexes. The average relative contents of the listed metals in the neutral complexes also varies in wide ranges: 23.8-66.1% Fe<sub>diss</sub>; 4.6-53.4% Al<sub>diss</sub>; 9.2-56.9% Cu<sub>diss</sub>; 12.3-53.5% Cr<sub>diss</sub>; 11.7-47.6% Zn<sub>diss</sub>; 14.5-33.3% Pb<sub>diss</sub>; 17.5-53.3% Cd<sub>diss</sub>; 5.6-36.5% Co<sub>diss</sub>; and 30.5-34.6% V<sub>diss</sub>.

The average relative content of carbohydrates in the composition of DOM does not exceed 10% C<sub>org</sub> in the water of Dnieper cascade's reservoirs, however, this group of organic compounds binds from 10 to 30% of metals in dissolved form (see Figure 1, *a*, *c*). The highest relative metal contents of the neutral complexes are observed in small water bodies which are characterized by a high bioproductivity and relatively low HS concentrations. These include, first of all, small reservoirs of Kyiv City (see Figure 1, *b*, *d*). They are characterized by intensive algae development, which contributes to an increase in the carbohydrates concentration in summer and autumn. For example, in the lakes of the Opechen system (Kyiv City), the share of carbohydrates in the total balance of DOM in summer reaches maximum values 11.4–19.4% C<sub>org</sub>, which is almost twice as much as in the Dnieper cascade's reservoirs. Due to this, the share of neutral metal complexes with carbohydrates increases noticeably at the same time of year.

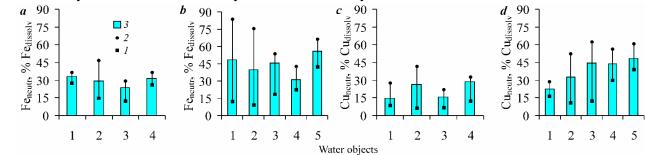


Figure 1. Limit (1, 2) and averaged (3) relative content (%  $M_{dissolv}$ ) of Fe<sub>neutr</sub> (a, b) and Cu<sub>neutr</sub> (c, d) in the composition of neutral complexes: a, c – the reservoirs of Dnipro cascade (1 – Kyivs'ke, 2 – Kanivs'ke, 3 – Dniprovs'ke, 4 – Kakhovs'ke), b, d – water bodies of the urbanized territory (1 – Ternopils'ke reservoir, Ternopil City, 2–5 – small water bodies of Kyiv City (2 – Kytaivs'ki ponds, 3 – Verbne lake, 4 – Tel'bin lake, 5 – lakes of the Opechen system).

The molecular weights of the neutral metal complexes like carbohydrates varies over a wide range: from <1.0 to >70.0 kDa. This finding provides evidence for the involvement of different molecular weight fractions of carbohydrates (both high and low molecular) in complexation with metals.

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# THE IMPACT OF ARSENIC TRIOXIDE ON CHEMICAL AND SUPERCONDUCTING PROPERTIES OF TI-2212 HTS

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The Tl-2212 phase is of particular interest for practical applications due to its enhanced phase stability. As it is well known, Group V elements play a significant role in semiconductor technology and are known to improve the properties of superconducting materials. Therefore, the present study investigates the effects of multivalent arsenic (As) substitution on the Tl-2212 high-temperature superconductor. To conduct this study, we employed the *in-situ* polymerisation method to synthesise high-purity, reactive precursors, which are essential for the controlled formation of the Tl-2212 phase and for achieving consistent doping efficiency.

In the present study, we successfully synthesized the  $Tl_2Ba_2CaCu_2O_{8+\delta}$  (Tl-2212) superconducting phase using a two-step method. In the first step, Tl-free precursors were prepared using the *in-situ* polymerization method. In the second step,  $Tl_2O_3$  and  $As_2O_3$  (x = 0.5 - 2.0 wt.%) were simultaneously introduced, and the final synthesis was carried out under an oxygen pressure of 2 atm. The influence of As-substitution on the structural and superconducting properties of the material was systematically investigated.

X-ray diffraction (XRD) analysis revealed that the undoped sample contained minor traces of the BaCuO<sub>2</sub> precursor phase. In contrast, the sample doped with 0.5 wt.% As<sub>2</sub>O<sub>3</sub> exhibited a nearly single-phase tetragonal structure. The temperature dependence of the nonlinear magnetic susceptibility  $\chi_3(T)$  indicated that the onset critical temperature  $T_{c(onset)}$  for the undoped sample was approximately 107 K, and increased to 112 K upon doping with 0.5 wt.% As<sub>2</sub>O<sub>3</sub>. In addition, T<sub>c</sub> monotonically continued to rise, reaching 114.5 K at 1.5 wt.%, before decreasing to 111 K at 2.0 wt.%, suggesting an overdoping effect. Moreover, the 0.5 wt.% As-doped sample exhibited a significant enhancement in transport critical current density ( $J_c$ ) compared to the undoped sample. However, further increase in arsenic concentration resulted in a gradual decrease in  $J_c$ , which can be attributed to a transition from optimal to overdoped regimes. In conclusion, the optimal doping level of arsenic trioxide (As<sub>2</sub>O<sub>3</sub>) notably enhances the superconducting properties of the Tl-2212 phase, with the best performance observed at 0.5wt.% As.

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# ELEMENTAL COMPOSITION AND DISSOCIATION CONSTANTS OF SUPRAMOLECULES (FULVIC ACIDS), ISOLATED FROM NATURAL WATERS

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Supramolecules, fulvic acids (FA) are major organic substances, dissolved in natural waters (70-80%). According to the literature, data concerning fulvic acids (FA) isolated from natural waters are not uniform. The carbon content varies within the range of 28.1–59.7%, hydrogen 2.7–8.9%, oxygen 36.3–58.1%, nitrogen 0.3–7.1% and sulfur 0.2–4.4%. The causes of such variations include the hygroscopic nature of FA, the high ash content of samples, and, most importantly, the application of different isolation techniques.

For the isolation of FA, we did not consider it appropriate to employ non-ionic polymeric resins of the XAD type, since the use of this adsorbent results, during alkaline desorption of the FA fraction, in the concurrent release of polyphenols and surface-active substances, adsorbed on XAD.

In our study, after the removal of humic acids from the investigated samples (rivers Paravani and Mtkvari; lakes: Paravani, Saghamo, Paliastomi and the Sioni reservoir), fulvic acids were isolated using an adsorption—chromatographic method (adsorbent-activated charcoal). Desorption of amino acids and carbohydrates was performed by means of 0.1 M HCl. For desorption of polyphenols was used 90% acetone water solution. The elution of the fraction of FA was performed with 0.1 N NaOH solution. Obtained alkalic solution of FA, for the purification was passed through a cation-exchanger (KU-2-8). The elemental composition of fulvic acids were determined using an C,H, N, S elementary analyzer (Elementar, Germany). The percentage contents of carbon, hydrogen, nitrogen, and sulfur were directly obtained by measurement and the percentage of oxygen was calculated by subtracting the percentages of carbon, hydrogen, nitrogen, and sulfur from 100. For the determination of dissociation constants of fulvic acids was used potentiometric titration (direct and back titration).

The obtained data indicate that FA samples isolated from natural waters of different classes, groups, and types do not differ significantly from one another in terms of elemental composition and dissociation constants. C 48,7  $\div$  54,2%; H 3,8  $\div$  5,2 %; N 1,5  $\div$  2,4 %; O 38,8  $\div$  45,1 % . H/C 0.88 $\div$ 1.23, pK<sub>H,COOH</sub> changes from 3.8 to 4.4.0 and pK<sub>H,Ph-OH</sub> -from 9.8 to 10.6.

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#### RECENT BIOMEDICAL ADVANCES WITH PIEZOELECTRIC MATERIALS

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Recent advances in material science are expanding the use of piezoelectric materials in the biomedical field. This 2025 literature review identifies key research trends in the biomedical field. It helps synthesize existing research literature and identify key field research dimensions. Emerging ultrasound-based neuromodulation techniques leveraging piezoelectric effects offer non-invasive strategies for targeted brain stimulation and therapeutic intervention [1]. Recent insights into the topological organization of biological piezoelectric materials reveal how intrinsic structural hierarchies govern electromechanical functionality in native tissues [2]. Five key dimensions are identified and discussed: tissue engineering and regeneration, neural applications [3], bone regeneration [4], cancer treatment/tumor therapy, and other medical applications. Innovations include ultrasound-mediated cartilage regeneration, corneal endothelialization, and innovative wound dressings that integrate photothermal, biochemical, and piezoelectric cues [5]. The literature review approach helps identify and point out future research directions. These research directions can set the agenda for future research and shape the future of piezoelectric research. Clinical translation, for example, still faces hurdles in biosafety validation, scalable manufacturing, standardization, and the absence of human trials [4,5]. The review concludes by outlining these challenges and highlights the need for interdisciplinary roadmaps to set the agenda for future research and shape the future of piezoelectric biomedicine. The study will help anyone involved in designing, regulating, prescribing, or receiving next-generation, minimally invasive electroactive therapies who stands to gain from the insights presented. The list includes healthcare and medicine sector stakeholders such as patients, clinicians and surgeons, biomedical-device and biomaterial companies, academic & translational researchers, and regulators & funding agencies.

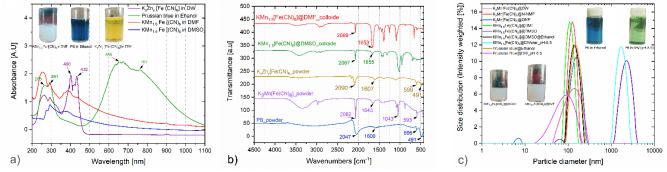
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# SONOCHEMICAL SYNTHESIS AND CHARACTERIZATION OF NANOSCALE METAL HEXACYANOFERRATES FOR ENHANCED CATHODE PERFORMANCE IN AQUEOUS ZINC-ION BATTERIES

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Aqueous zinc-ion batteries (AZIBs) are safe and cost-effective, yet require nanoscale cathodes with stable frameworks and high dispersibility [1,2]. We synthesized metal hexacyanoferrates (MHCFs)—Prussian blue (PB, Fe<sub>4</sub>[Fe(CN)<sub>6</sub>]<sub>3</sub>) and its analogues ( $K_xZn_y[Fe(CN)_6]$ , KMn<sub>1.5</sub>[Fe(CN)<sub>6</sub>])—by sonochemical coprecipitation under 20 kHz ultrasound, using FeCl<sub>3</sub>, K<sub>3</sub>[Fe(CN)<sub>6</sub>], H<sub>2</sub>O<sub>2</sub>, ZnSO<sub>4</sub>, or KMnO<sub>4</sub> in deionized water (DW), followed by dispersion of the products in organic solvents (DMF, DMSO, NMP, ethanol) for colloidal stabilization. Dynamic light scattering revealed hydrodynamic particle sizes of ~50–300 nm, with DMF/NMP yielding narrower distributions (PDI < 0.2) and reduced aggregation compared to water or DMSO (>100 nm). Notably, adding ethanol to KMn<sub>1.5</sub>[Fe(CN)<sub>6</sub>] colloids in DMSO, which initially showed severe aggregation (>1000 nm), reduced the size to ~100 nm, demonstrating a strong stabilizing/de-aggregating effect of ethanol.



**Figure 1.** Spectroscopic and size characterization of PB and PBAs: a) UV-Vis charge-transfer bands; b) FTIR spectra (CN and solvent peaks); c) DLS size distributions.

UV-Vis spectra identified charge-transfer features: PB at ~650–761 nm (IVCT), Zn-PBA at 285–432 nm (LMCT), and Mn-PBA with weak absorption, consistent with their characteristic colors. FTIR confirmed the hexacyanoferrate framework with CN stretching at 2047–2090 cm<sup>-1</sup>, shifted in Zn/Mn analogues, and low-frequency M–CN modes at ~491–599 cm<sup>-1</sup>; solvent-related peaks (C=O, S=O) were observed in colloids. Raman (785 nm) further supported structural assignments: PB showed weak CN intensity due to fluorescence, Mn-PBA exhibited a clear v(CN) band at ~2116 cm<sup>-1</sup> and lattice modes at ~200–400 cm<sup>-1</sup>, while Zn-PBA displayed multiple v(CN) bands (~2074–2150 cm<sup>-1</sup>) and low-frequency modes (~194–511 cm<sup>-1</sup>), indicating mixed Fe valence, high crystallinity, and enhanced lattice rigidity [3,4].

These findings demonstrate that sonochemistry enables tunable, nanoscale MHCFs with improved colloidal stability, highly suitable as cathode materials to promote efficient Zn<sup>2+</sup> intercalation in AZIBs. Ongoing electrochemical tests are expected to validate their performance.

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### RODUCTION OF HEAT-RESISTANT COMPOSITE PRODUCTS BY THE SHS-ELECTRIC ROLLING METHOD

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The process of SHS-electric rolling is considered with the purpose of obtaining heat-resistant sheets based on the composition of Ta-Al and Ti-Al-B. In particular, the electrical conductivity of the compacted and synthesized mass will be analyzed and based on the results obtained, the technological modes of the process will be established.

It was established that to produce a product of increased length and width and with a uniform structure, the combustion front must be spaced a specified distance from the deformation zone. Uneven deformation towards of the deformation line leads to uneven density in the obtained billets. Therefore, it is necessary to optimize the feed rate of the workpiece to such a value that the synthesized mass of the product is constantly fed to the deformation center in a homogeneous Visco-plastic state.

Structural studies have confirmed that with the correct selection of technological parameters for electric rolling, it is possible to obtain high-density plates with a perfect structure and specified properties. It was found that the combination of SHS and hot electric rolling processes allows consolidation and synthesis of high-density parts from Ta-Al-B(B<sub>4</sub>C) composite powders and obtaining material in the form of sheets. The structure and density of the obtained samples depend on the phase composition and the process temperature. Increasing the boron content to 10% allows obtaining high-density samples with uniformly distributed phases with a hardness value of up to 900 kg/mm2.

The above mentioned and other features of structure-property relationship in hot rolled Ta-Al-B(B<sub>4</sub>C) composites will be presented and discussed too.

# INVESTIGATION OF THE REGULARITIESD OF GENERATION AND DEATH OF COPOLYMERS 1-4 OF NAPHTHOOUINONE WITH 4-VINYLPYRIDINE

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The copolymerization reaction of 1,4-naphthoquinone (1,4-NQ) with 4-vinylpyridine (4-VP) in a medium of various solvents (ethanol, benzene, etc.) in the presence of various initiators (BP and triethylamine, etc.) has been carried out. It has been revealed that ethanol is an effective solvent, and triethylamine (TEA) is a catalyst. It has been established on the basis of chemical, IR spectral and GLC analyses that the synthesized copolymers are cooligomers consisting of naphthohydroquinone vinylpyridine links with molecular mass of  $\overline{M}_w = 870 \div 235$ ,  $\overline{M}_n = 690 \div 2110$ .

Since the copolymers contain hydroquinone groups, it was of interest to carry out oxidation and investigate the kinetic regularities of generation and death of radical centers formed during oxidation. It has been revealed that the oxidation process is a complex multistage process and proceeds with the participation of intermediate radicals. It should be noted that in neutral media, the synthesized cooligomers of 1.4-NQ with 4-VP (COONHQVP) are not oxidized by molecular oxygen, while their alkaline solutions intensively interact with molecular oxygen. In an alkaline medium, the acid-base equilibrium is instantly established: (formula):

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\text{OH} \\
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\text{CH-CH}_{2} \\
\text{OH}
\end{array}$$

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Next, an oxidation of the anions of naphthahydroquinone links occurs:

The formed intermediate radical centers undergo the further oxidation reaction into the quinone form, into a disproportionation reaction, and into a recombination reaction. Since the radical centers in alkaline media are relatively stable and can be fixed by the EPR method, then using this method, the kinetic regularities of generation of the radical centers during the oxidation of COONHQVP have been investigated.

For taking off of the EPR, the oxidation of the cooligomers has been carried out directly in the resonator of the spectrometer. It has been detected that EPR signals are fixed immediately after addition of KOH solution to the cooligomer solution. The radical centers are generated with very high rate and quickly reach a maximum value, followed by its sharp decrease. With growth of the concentration of anions of naphthohydroquinone links, the concentration values of the radical centers are increased. For example, at initial concentrations of naphthohydroquine links equal to 0,02, 0,035 and 0,58 mol/l, the maximum concentration values of the radical centers are  $1.6 \cdot 10^{-4}$ ,  $2.1 \cdot 10^{-4}$  and  $2.7 \cdot 10^{-4}$  mol/l and the radical death rate is  $4.35 \cdot 10^{-6}$ ,  $7.48 \cdot 10^{-6}$  and  $12.3 \cdot 10^{-6}$  mol/l·s. Both the values of the initial rate and the rate constants values (k) of the radical death are noticeably high and increased with temperature rise:  $k=(170 \div 254)$  l/mol·s. As expected, the stage of death of radical during the oxidation of cooligomers has a low activation energy (E=15.0 kJ/mol), which is characteristic for the death of radicals of phenoxyl and semiquinone type.

# HARNESSING ARTIFICIAL INTELLIGENCE FOR PREDICTIVE DESIGN AND FUNCTIONAL OPTIMIZATION OF POLYMER COMPOSITES

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In this study, we will explore the integration of machine learning techniques, especially deep learning, to accelerate the design and optimization of polymer composites. These materials are crucial for their tunable mechanical, thermal, and electrical properties, yet their performance remains challenging to predict given the vast combinatorial space of polymer matrices, fillers, and processing conditions. Building on previous studies (Mirtskhulava, 2023; Mirtskhulava, 2024; Mirtskhulava, 2025), this work presents a framework that combines high-throughput data collection, feature engineering, and multi-task neural networks (MT-NN) to efficiently predict composite properties. The approach allows for rapid screening of material formulations, identification of key structure-property relationships, and prediction of behavior under operating conditions. Case studies demonstrate machine learning-driven optimization to improve mechanical strength, thermal stability, and electrical conductivity. Integrating deep learning with polymer chemistry not only reduces experimental costs but also facilitates rational composite design, paving the way for a new generation of functional materials and their applications in both engineering and environmental monitoring.

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# THE EFFECT OF INTEGRATED NICKEL NANOPARTICLES AND CARBON NANOTUBES ON THE THERMAL PROPERTIES OF POLYETHYLENE COMPOSITES

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Nanocomposites offer new opportunities at entirely new scales to solve challenges ranging from the medical, pharmaceutical, food packaging to electronics and energy industries. Today's polymeric materials are multi-component systems, alloyed and mixed with various types of additives. The content of additives in polymer composites can vary widely [1]. By combining the volume content of the components, it is possible to obtain composite materials with the required values of physical-mechanical properties, heat resistance, and abrasion resistance, as well as to create compositions with the necessary magnetic, dielectric, radio-absorbing, and other special properties. Such nanostructured materials are obtained by introducing nanoparticles into various polymer matrices [2, 3].

The presented work is devoted to the preparation and study of the properties of nanocomposites based on low pressure polyethylene (LPPE) and high-pressure high-pressure polyethylene (HPPE) using nikel oxide nanoparticles (NPNiO) stabilized by a polymer matrix and multi-walled carbon nanotubes (MWCNTs) as nanofillers. Nanocomposite polymer materials were obtained by mixing LPPE (HPPE) with a nikel-containing nanofiller and MWCNT on laboratory rollers at a temperature of 145-150°C for 15 minutes. To carry out mechanical tests, the resulting mixtures were pressed into plates 1 mm thick at 170°C and a pressure of 10 MPa for 10 min. The physicomechanical, thermophysical and thermal properties of the resulting nanocomposites were studied. SEM analyzes of samples of the resulting nanocomposites were carried out, too.

The optimal ratio of components for obtaining improved physical, mechanical and thermal properties of the studied nanocomposites (wt.%) was found: LPPE(HPPE)/NHNiO/MWCNT (100/1.0/0.05). An improvement in the strength and deformation properties, as well as the thermal-oxidative stability of the obtained nanocomposites was revealed, which can be attributed to the effects of structural and chemical stabilization of the polymer matrix. The the activation energy of the thermo-oxidative destruction (Ea) of thermal-oxidative destruction of LPPE / NHNiO / MWCNT increases from 153.64 to 225.00 kJ / mol (HPPE/NHNiO/ MWCNT increases from 129.45 to 267.91 kJ/mol). Numerous experimental data on mechanical, strength, relaxation and other properties of polymer-polymer and polymer-filler mixtures are explained within the framework of the concept of the presence of an interphase layer. A necessary condition for obtaining the best properties of carbon nanomaterials in a polymer composite is achieving the maximum degree of dispersion of the filler and its optimal orientation in the polymer matrix.

The results of physical-mechanical and thermal properties are confirmed by SEM data. SEM analysis of the obtained nanocomposites showed that the combined use of metal-carbon nanoparticles leads to improved dispersion of nanofillers in the polyethylene matrix and the formation of a new three-dimensional fine-crystalline supramolecular structure, which has a positive effect on the physical-mechanical and thermal properties of the nanocomposites.

The results obtained indicate that small amounts of nanofillers introduced into the polymer obviously play the role of structure formers - artificial crystallization nuclei, which contributes to the appearance of a three-dimensional fine spherulite structure in the polymer, characterized by improved physical-mechanical and thermal properties of the resulting nanocomposite.

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# POROUS MATERIAL CONTAINING PERLITE FOR OIL-CONTAMINATED ENVIRONMENTS

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The development of modern and effective methods for removing oil and oil products from the surface of water and soil is currently very relevant. Numerous studies have shown that the most environmentally friendly, effective and cost-effective cleaning method is the use of sorbents. More than 200 different types of sorbents are produced and used to sorb spilled oil and oil products. At the same time, sorbents must have a number of specific indicators: hydrophobicity, regeneration ability, significant adsorption capacity, buoyancy, chemical and thermal stability.

We believe that the use of perlite in polymer compositions is promising. Oligomers of phenolic aldehydes, polyurethanes, polyethylene, polyamides and polymers of other classes are used as a polymer matrix in the compositions.

In order to activate the sorbents, they were subjected to thermal and chemical modification. Optimum conditions for thermal modification of natural sorbents have been determined: for perlite - heating at 420-660°C for 3.5 hours. In order to expand the pores of perlite and activate it, its chemical modification was carried out. Optimal conditions for chemical modification of perlite were determined: temperature, time, concentration of solutions and the ratio of components.

Optimal conditions for perlite hydrophobization were studied - 260°C for 5.5 hours in the silicon zone. Thermomodified perlite after hydrophobization does not get wet or sink, effectively absorbs oil and its products from the surface of contaminated water.

Perlite heated at 420-660°C is used when the oil concentration does not exceed 6·103 mg / L. At high concentrations of oil products, perlite modified at 700°C is used.

To obtain polymer compositions based on perlite, the second main component was synthesized - urea-formaldehyde, melamine-formaldehyde and urea-melamine-formaldehyde complex oligomers.

#### HYBRID, ELASTIC, POROUS POLYMER MATERIAL

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Very actual is protection of the environment from pollution with petroleum and petroleum products. At present, a huge number of industrial enterprises using various petroleum products discharge tons of untreated or insufficiently treated waste waters into lakes, rivers and seas. Therefore, this problem is becoming more and more urgent.

Decontamination of oceans, rivers, water basins and other surfaces polluted with petroleum and its products by way of development and use of new effective methods, usage of plastic foam materials and especially of polyurethane foams as insulation (heat-, vibration-, electric-, hydro- and soundproof) materials and for other constructional purposes contributes to partial solution of this global problem.

Our goal is to provide obtaining of new type of ecologically friendly, cheap, ultra light, flexible, hybrid polymer compositions on the base of homogenous olygoesthers, aromatic polyisocyanates and local natural sorbents with high sorption activity, enhanced physical and chemical properties. Instead of expensive silicone and paraffin oils the waste oils will be used in the polymer composition.

The natural sorbent – perlite – was selected to obtain organomineral elastic hybrid porous polymer compositions characterized by high sorption capacity and floatability, as well as high thermal, electrical, vibration, sound and heat-insulating properties. Thermal and chemical modification and then hydrophobization of the sorbent were carried out. The optimum conditions of thermal modification of perlite – heating at 480-700°C for 2.5 hours were determined. Porous materials based on perlite, aromatic polyisocyanate and polyester have been synthesized, which are characterized by high sorption activity and the ability to float on the surface of water together with the absorbed compounds. They can be removed from the surface of water mechanically.

# EFFECT OF BENTONITE CONTENT ON MELT FLOW INDEX OF POLYPROPYLENE RANDOM COPOLYMER / COMPATIBILIZER / ALUMINUM HYDROXIDE BASED COMPOSITES

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Mineral fillers are low cost additives which are added to thermoplastics to reduce cost and enhance performance [1]. The presence of mineral fillers such as aluminum hydroxide increases the melt processing difficulty in terms of viscosity of the composite [2]. The aim of the presented work was to study the effect of bentonite/aluminum hydroxide content on the melt flow index (MFI) of the composites based on polypropylene random copolymer / compatibilizer / aluminum hydroxide / bentonite. Industrial samples of polypropylene random copolymer (Topilene® R200P) were used as research object. Polypropylene copolymer grafted with maleic anhydride PPC-g-MAH (DuPont<sup>TM</sup> Fusabond® P353) were used as compatibilizer. Concentration of fillers (aluminum hydroxide, bentonite) was fixed at 50 wt. % of total amount of composite. To determine the melt flow index, a capillary rheometer CEAST MF50 (Instron, Italy) shown in Figure 1 was used. The studies were conducted at a temperature of 190 °C under a load of 5 kg.

One of the important indicators characterizing a polymer during the molding process is MFI. MFI is an indicator of the flowability of the thermoplastic materials. MFI characterizes the rate of flow of molten thermoplastic through a capillary of standard dimensions at a given temperature and pressure. As can be seen from the Figure 1, as the amount of bentonite in the composite increased (5, 10, 15, 20 and 25 wt. %), that is, as the amount of aluminum hydroxide decreased, a significant increase in the MFI was observed. We have previously shown in a number of studies that the use of natural fillers such as montmorillonite, bentonite, vesuvianite and clinoptilolite in the composition of polyolefins is accompanied by some increase in the melt flow of the composites [3, 4]. This is interpreted by the fact that bentonite has a layered structure. It is possible that during the process of thermomechanical mixing of compositions on hot rollers, intercalation of macrochains into the corridors of the interlayer space of clay occurs, followed by the exfoliation of the layers into smaller particles.

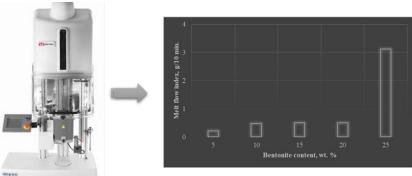


Figure 1. MFI of PP-R/PPC-g-MAH/Al(OH)<sub>3</sub>/bentonite based polymer composites

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#### TUDY OF THE STABILITY OF A NEW POLYMER-BASED ENZYME GEL

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The proteolytic enzyme of plant origin - papain is increasingly used in the compositions of various pharmaceutical and cosmetic products. At the Institute of Pharmacochemistry, a papain-containing medicinal product "Caripazim" was developed from the latex of the fruit of the melon tree (*Carica papaya*) for the treatment of burn and purulent wounds, keloid scars, chronic pulpitis and other dental diseases, as well as for the treatment of inflammatory and degenerative processes in craniocerebral and spinal injuries. The drug is produced in the form of a lyophilized powder and is introduced into the human body by the electrophoresis. Taking into account the ability of papain to gently but effectively exfoliate dead skin cells, improving the texture and appearance of the skin, the Institute is conducting the development of a new dermatological agent in the form of a polymer-based gel. Polyethylene glycol (PEG) with molecular weights of 4000 and 1500 were used as the basis, as well as a cross-linked polymer of acrylic acid - Carbomer 940.

Enzyme gels were prepared in three different dosages (0.5%; 1%; 2%) for foot skin care. The resulting gels were whitish-yellow in color and had a characteristic odor. Visually, all gels were homogeneous. Some physicochemical parameters and structural-mechanical characteristics of model gel samples were studied. Microscopic examination of the gels confirmed the homogeneity of the samples and the absence of large inclusions in all the obtained models. A study of thermal and colloidal stability showed that gels based on PEG and Carbomer 940 are thermally stable at a temperature of 40-42°C for 3 days, do not delaminate or disperse. The proteolytic activity of some models changes slightly compared to the original.

Considering the advantages of Carbomers, safety during long-term use, ease of technology of the desired consistency and viscosity of the gel, ensuring the stability of the formula and a long shelf life, samples based on Carbomer 940 were selected for further research. Stability was studied for samples of carbomer-based gels under various storage conditions - at a temperature of +5 to +7°C in the refrigerator and in a thermostat at +40°C (accelerated aging method).

A study of the stability of papain gel samples on a Carbomer 940 base at different temperatures showed that at room temperature ( $+20^{\circ}$ C) for 2 months the activity is retained by approximately 95-97%, and at  $+40^{\circ}$ C – up to 80-85% (which corresponds to 2 years of storage under natural conditions), when stored in a refrigerator ( $+5-+7^{\circ}$ C) the activity of the gel is completely retained for 2 months (observation time) (Table 1.).

Table 1. Proteolytic activity changes of the gel depending on storage conditions and time

Samples	Initial proteolytic activity of	Proteolytic activity of gel depending on storage time,			
	the gel, PE/g	PE/g			
		2 weeks	1 month	1.5 months	2 months
Gel sample at +20°C	222,91	228,2	225,8	220,8	216,23
Gel sample at +4 <sup>0</sup> C	222,91	226,06	225,2	222,37	220,35
Gel sample at +40°C	222,91	202,35	193,2	190,7	188,77

# SELECTED PROPERTIES OF SUSTAINABLE BIO-POLYURETHANE MATERIALS CONTAINING R-PET

### <u>Lena Naruniec</u>, Zuzanna Hinc, Joanna Smorawska, Krzysztof Formela, Paulina Kosmela, Ewa Głowińska

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Polyurethane (PU) materials rank among the most widely used polymers. As such, it is crucial to adapt their manufacturing methods and properties to enhance environmental friendliness and enable suitability for a circular economy, all while preserving their desirable performance characteristics. The subject of the presented research is the synthesis of cast polyurethanes made from bio-polyols and containing chemically recycled PET (polyethylene terephthalate) waste bottles as a chain extender (PET-PDO glycolysate) and powdered PET as a filler.

As part of the experimental work, PET bottles were collected, cleaned, and shredded, and then subjected to glycolysis. Bio-1,3-propanediol was used in glycolysis in the presence of a catalyst, which was potassium acetate at a concentration of 0.5% m/m. The mass ratio of PET waste to glycol was 1:4. The glycolysis product was then used to synthesize new cast polyurethane materials. PU synthesis was carried out using a two-step (prepolymer) method. Prepolymer was synthesized by the reaction between bio-based polyether polyol (Velvetol H2000) and diphenylmethane diisocyanate (MDI). For the preparation of the reference PU, bio-based 1,3-propanediol was used as a chain extender, while modified samples were obtained with the use of PET-PDO glycolysate. Polyurethanes were obtained at an NCO to OH molar ratio of 1.0. Powdered PET was used as a filler in an amount of 20 wt.% and added to the prepolymer, prior to chain extension.

The obtained materials were examined using various instrumental analysis methods and techniques e.g. Fourier Transform Infrared spectroscopy (FTIR), thermogravimetric analysis (TGA), uniaxial tensile tests, Shore A hardness and density measurements. The obtained results revealed that the use of chemically and mechanically recycled PET products affects the properties of PUs. FTIR analysis confirmed a complete polymerization reaction and revealed the presence of functional groups characteristic of PU. TGA results showed that the use of PET-PDO glycolysate slightly affected the thermal stability of the obtained polyurethane materials. Comparing the use of PET-PDO glycolysate as a chain extender, an improvement in the tensile strength and hardness was observed. The application of powdered PET as a filler resulted in higher density and hardness of the samples of PUs. In summary, the use of recycled PET products and bio-based monomers supports sustainable development and the principles of green chemistry.

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### 4-(N,N-DIETHYLTHIOCARBOMOYLTHIO)ALKYL-1,3-DIOXOLANES – PLASTICIZERS OF POLYVINYLCHLORIDE COMPOSITION

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It was known that the combination of dithiocarbamates, heteroatoms of various nature (N,S,O) with an unstrained five-membered cycle with two heteroatoms in a molecule considerably expands the areas of their application as potentially biologically active substances, accelerators of rubber vulcanization, protectors for radiation protection, multifunctional additives to lubricating oils and it is no coincidence that this area is increasingly attracting the attention of researchers of various scientific profiles. Nevertheless, the works devoted to the synthesis and application of N,N-disubstituted derivatives of dithiocarbamic acids and, in particular, diethyldiocarbamic acid as a plasticizer polymer composition materials are extremely limited.

In this work the information on the synthesis of 4-(N,N-diethylthiocarbamoylthio)alkyl-1,3-dioxolanes (VII-XI) by the interaction of the corresponding 4-chloromethyl-2-alkyl-1,3-dioxolanes (II,VI) with trihydrate of N,N-diethyldithiocarbamate sodium (I) in an aqueous medium proposed as new plasticizers of polyvinyl chloride (PVC)plasticate is presented.

The composition of compounds(VII-XI) has been confirmed by elemental analysis, and the structure – by data of IR and <sup>1</sup>H NMR spectra. The synthesized 4-(N,N-diethylthiocarbamoylthio)methyl- (VII), 4-(N,Ndiethylthiocarbamoylthio)methyl-2-ethyl- (VIII), 4-(N,N-diethylthiocarbamoylthio)methyl-2-propyl- (IX), 4-(N,N-diethylthiocarbamoylthio)methyl-2-butyl-1,3-dioxolanes (X) and 4-(N,N-diethylthiocarbamoylthio) ethoxymethyl-1,3-dioxolane (XI) are transparent liquids with almost no odor. They are insoluble in water and well soluble in organic compounds (ether, CHCl<sub>3</sub>, CCl<sub>4</sub>, DEG, etc.).

It has been established that the inclination of the sodium cation in a molecule (I) to solvation and the unique solvating (hydrating) ability of the used solvent (H2O) together facilitate the penetration of the anion

into the organic phase of the reaction system and stipulate the substitution of the chlorine atom in a molecule of the corresponding alkylating agent (II-VI) under comparatively soft conditions and high selectivity of the process.

It has been shown that the dithiocarbamates (VII-XI) are well combined with PVC-resin and, due to the combination of five-membered heterocycle with dithiocarbamate fragment containing tertiary nitrogen atom in their molecules, they simultaneously provide plasticization of PVC-plasticate; in addition, the presence of dithiocarbamate group can play an important role in protection of materials from the effects of mold fungi and bio-damages. So, the ultimate strength and relative elongation of the plates obtained with the participation of the tested compound (VII), taken in the ranges of 20, 30, 40 mass p. per 100 mass p. of PVC and 2 mass p. Znstearate, are at the level (with a slight increase) of the same indices of plates made of PVC and well-known plasticizer (DOPh) at the same ratios.

The obtained results allow to expand the assortment of the chemical compositions providing simultaneously the plasticization of PVC-plasticate. Therefore, these materials can be recommended for practical use in various branches of industries.

# MODIFICATION OF CARBAMIDE BY A CHEMICAL METHOD TO OBTAIN A NITROGEN FERTILIZER OPERATING BY A PROLONGED MECHANISM

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Intensive population growth requires a constant increase in food production – cereals, meat, milk and other products. Agricultural land is rapidly shrinking as a result of increasing urbanization and industrial intensification. One of the ways to solve the problem is the use of intensive technologies in agriculture, such as the use of nitrogen-containing chemical fertilizers in high doses. Due to the particularly good solubility of nitrogen fertilizers in water, a significant part of them is lost as a result of evaporation and leaching, which leads to huge economic losses. At the same time, the environment is being poisoned, especially fresh water. In recent years, interest in urea-formaldehyde polymers has increased [1,2]. It turned out that they can be used as nitrogen fertilizers that are difficult to dissolve in water [3].

The work is devoted to this problem - modeling and optimizing the synthesis of urea-formaldehyde fertilizers and analyzing the factors influencing these processes. We have studied the process of polycondensation of urea with formaldehyde in order to develop a technology for producing a biodegradable polymerized nitrogen fertilizer with prolonged action. The influence of various factors on the course of the reaction has been studied: the duration of the process, temperature, molar ratios of the initial components, structure and composition of the amide component, concentration.

The main kinetic parameters of the process were determined during the reaction in the temperature range of 50- $70^{\circ}$ C, before the deep conversion of formaldehyde. The reaction rate constants during the reaction retain a constant value if they are calculated using a second-order equation. The values of the activation energy of the reaction (E) and the probability coefficient (A) are calculated. E average = 7.94 kcal/mol.; A =  $0.0223 \times 102$  l/mol.sec.

The molar ratio of urea and formaldehyde largely determines the chemical structure of the resulting product. At a ratio of 1:1.5 - 3.5, when the pH decreases even to 4-4.5, the formation of a polymer with a spatial structure is possible, which is extremely undesirable, since the adaptation period for degrading microorganisms is greatly prolonged and the period of biodegradation is also prolonged. The optimal reaction conditions for the production of a biodegradable polymer acting by a prolonged mechanism can be considered the molar ratio of urea and formaldehyde 1:1.

To determine the urease activity of microorganisms isolated from the soil, the analysis showed that urease activity was found in the following genera of microorganisms: clostridium, actinomycetes and Aspergillus. Polymerized urea does not evaporate and does not cause destruction of the ozone layer, does not wash out and does not poison fresh water, thereby protecting the population and fauna from various serious diseases.

**Acknowledgement:** The abstract was prepared within the framework of the project № FR-23-29704 - "A method for obtaining polymer nitrogen fertilizers of prolonged action containing a functional group", funded by the Shota Rustaveli National Science Foundation of Georgia.

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#### TARGETED SYNTHESIS OF BIODEGRAABLE LINEAR HOMO-AND COPOLYMERS

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The widespread use of fertilizers, including nitrogen fertilizers, is a prerequisite for increasing crop yields and obtaining high-quality products. But the use of nitrogen fertilizers at the same time creates serious environmental problems [1, 2]. The solution to this problem is extremely urgent and requires the development of new technologies that will significantly reduce the application rates of nitrogen fertilizers and make nitrogen fertilizers difficult to dissolve[3].

We have developed fundamentally new nitrogen fertilizers and a technology for their preparation that eliminates their leaching and peeling, as well as environmental pollution. The most important thing is that the gradual, slow transition of these fertilizers to a soluble state under the action of microorganisms in the soil provides the plant with nitrogen throughout the growing season, resulting in an increased nitrogen absorption coefficient, quantitative and qualitative yield indicators.

A method has been developed for the targeted synthesis of biodegradable linear homo- and copolymers containing peptide and functional (-NH<sub>2</sub>) groups of the amide type by polycondensation reaction based on melamine and carbamide.

The influence of various factors on the reaction of melamine, carbamide and formaldehyde has been studied: the duration of the process, temperature, molar ratio of the initial components, structure and composition of the amide component, and concentration.

The study of the influence of various factors on the degree of conversion during the synthesis of carbamide-formaldehyde and melamine-formaldehyde homopolymers has shown that the optimal conditions for the reaction are: temperature 60°C, ratio of melamine and formaldehyde 1:1 mol, ratio of carbamide and formaldehyde 1:1 mol, respectively. The reaction time is 1 hour, the initial concentrations of melamine and carbamide are 0.1 mol/l.

Studies have shown that, depending on the chemical structure, the amide components differ in their reactivity when interacting with formaldehyde. Depending on the increase in reactivity, they can be arranged in the following order: carbamide > melamine > thiocarbamide.

The combined condensation of amide components with different reactivity results in the formation of mixed oligomers. In the first stage of the reaction, formaldehyde interacts with the more active amide component. Therefore, it should be assumed that in the early stages of the process, when all the initial components are simultaneously introduced into the reaction zone, methyl derivatives of the more active component are formed, which subsequently form oligomers, the chains of which will be mainly enriched with more active components. Then, as the process progresses, the molecules of the second, less active amide component enter into the reaction.

**Acknowledgement:** The abstract was prepared within the framework of the project № FR-23-29704 - "A method for obtaining polymer nitrogen fertilizers of prolonged action containing a functional group", funded by the Shota Rustaveli National Science Foundation of Georgia.

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# THE CONDUCTIVITY AND PHYSICAL CHARACTERISTICS OF HIGH TEMPERATURE RECOVERED CARBON

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The electrical conductivity and fine structure of different type of recovered carbon after high temperature processing in vapor environment (flesh pyrolysis) were investigated. The low temperature pyrolysis products of shredded tire and plastics, as well as brown coal were investigated depending on its processing parameters and surface area characteristics. The processing temperature was near to 900°C.

As investigation showed the application of high temperature, near to 900°C during the process of flash pyrolysis allows essentially to increase the surface characteristics of recovered carbon, its purity and electrical conductivity too.

As study of conductivity of recovered carbon black (CB) and amorphous carbon (AC) showed that the recovered carbons with same surface characteristics but with different porosities differ from each other and with increase of porosity the conductivity of CB & AC increases too. The further chemical purification or annealing in vacuum at 1300°C showed positive effect on the conductivity which were essentially increased especially for recovered AC and the resistance at 1300g. loading is equal to 0.4 omm.cm.

The fine structure of Recovered CB and AC after flesh pyrolysis processing shows for AC the formation an amorphous-nano structure without any impurities. As for CB it was established that samples not contain carbonaceous residue ("coke"). No 'necking' between particles nor coke particles are seen, indicating a good quality of recovered carbon.

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# TUNING THE OPTICAL AND THERMO-OPTICAL PARAMETERS IN PLASMONIC NANOPARTICLES DOPED CHOLESTERIC LIQUID CRYSTAL NANOCOMPOSITE

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Research on plasmonic nanoparticle-based nanocomposites with tunable optical and thermo-optical properties is of significant current interest due to numerous potential applications [1,2]. Metal nanostructures exhibit strong plasmon resonance, while liquid crystals possess both order and fluidity. These materials can respond to external fields that influence their structure and properties, creating an attractive combination. Gold nanoparticles (GNPs) hold a unique position among metal nanoparticles due to their fascinating properties. These attributes include a well-organized distribution across various structures, as well as distinct electrical, magnetic, thermal, and optical characteristics that vary with size, shape, and concentration. In our work, we have developed a nanocomposite made of graphene nanoplatelets (GNPs) embedded in a chiral liquid crystal (CLC) matrix. We successfully demonstrated that a large quantity of GNPs can be incorporated into the CLCs without compromising their structural integrity (Figure 1). Additionally, by utilizing the CLC doped with GNPs and a luminescent dye, we achieved a non-intrusive and controlled tuning of the selective reflection bandwidth (SRB) of the CLC. This process enables us to enhance and fine-tune the laser emissions from the GNPs/CLC nanocomposite, stimulated by the GNPs. The results obtained can have various applications, including in solar cells and concentrators, as well as in luminescent and flexible displays. In the field of medicine, these findings can lead to the development of new drug delivery systems and improve the visualization and monitoring of biological cells, particularly in detecting cancerous cells, where the use of less toxic GNPs is preferred over silver nanoparticles. Additionally, these advancements can be utilized in photodynamic therapy to target and eliminate tumor cells, bacteria, and viruses.

Figure 1. GNPs dispersed in CLC

**Acknowledgement**: This work was supported by the Shota Rustaveli National Science Foundation of Georgia—project number FR-22-2543.

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#### SYNTHESIS OF POLYAMIDOIMIDES FROM ROSIN BIS-IMIDES

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The polymers with imide bonds in macromolecules are of great practical importance in the production of plastics. Such polymers are characterized by high thermal stability and are widely used in the manufacture of constructive materials for electrical insulating and technical purposes [1]. For preparation of thermostable polymers using natural raw materials – rosin, in this work the bis-imides have been synthesized, from which the adducts of levopimaric acid have been subsequently obtained. N,N'-R-bis-imides 1a-3a have been obtained by the reaction of hexamethylenediamine with maleic anhydride (compound 1), anhydride of 4-cyclohexene-1,2-dicarboxylic acid (compound 2) and anhydride of bicyclo-[2.2.1]-hept-5-ene-2,3-dicarboxylic acid (compound 3) on the scheme shown below:

$$\begin{array}{c|c} CO & OC \\ \hline N_-R_-N' \\ CO & OC \\ \hline 1a & 2a \\ \hline \end{array}$$

The reaction was carried out by addition of a solution of hexamethylenediamine in dimethylformamide to a solution of anhydride of the corresponding unsaturated cyclic dicarboxylic acid. The ratio of diamine to anhydride was 1:2. The reaction was initially carried out at room temperature, then the mixture was heated to 140°C for 4 h. After that, the diene condensation of bis-imides 1-3 with levopimaric acid was carried out, as a result of which diacids with bis-imide fragment –, compounds 1b-3b were obtained [2]:

The similar reaction was carried out with other bis-imides. There were found the optimal conditions for their obtaining: the process temperature  $-140^{\circ}$ C, the molar ratio of the initial components  $-2.5\div3.5:1$  and the reaction duration  $-12\div16$  h. It has been experimentally established that the reaction proceeds with the formation of both mono- and bis-amido acids at the initial stage, followed by their conversion into mono- and bis-imides. The diacids containing bis-imide fragments are converted into corresponding dichloroanhydrides by interaction with thionyl chloride. By their polycondensation with diamines, the polyamidoimides (PAI-1÷PAI-3) of the structure shown below have been obtained:

The composition, a number of physical-chemical indices and thermal stability of the obtained polyamidoimides have been determined. The polymers have low MW, but form good and durable films, thermally stable up to 350°C. Higher this temperature, these polymers begin to decompose. Their complete destruction occurs at temperatures higher 550°C.

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# SYNTHESIS AND QUANTUM-CHEMICAL ASPECTS OF THE HYDRIDE ADDITION REACTION OF A, $\Omega$ - BIS(TRIMETHYLSILOXY)METHYLHYDRIDOSILOXANE WITH TRIETHOXYACRYLOXYSILANE

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The addition reaction of  $\alpha, \omega$ -bis(trimethylsiloxy)methylhydridosiloxane with triethoxyacryloxysilane was studied using density functional theory (DFT). Two possible variants of the bimolecular reaction were considered: according to Farmer's and Markovnikov's rules[1,2].

For the first time, we discussed a variant of the Farmer's rule.

$$H_2C$$
  $CH$   $C$   $H$   $Si$   $Si$   $CH_2$   $CH_2$   $C$   $O$   $Si(OEt)_3$ 

The dependence of the system energy change ( $\Delta H$ ) on the distance between atoms is shown in Figure 1.

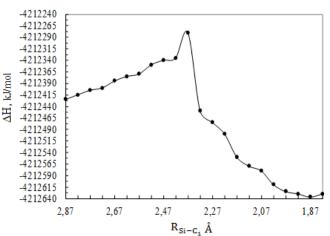


Figure 1. Dependence of system energy change ( $\Delta H$ ) on distance between silicon and carbon atoms  $R_{Si-C_1}$ 

Activation energy  $\Delta E^*=145$  kJ/mol, and reaction heat effect  $\Delta E=-212$ . As we can see, the reaction is exothermic.

The second time we discussed the variant of Markovnikov's rule.

The dependence of the system energy change ( $\Delta H$ ) on the distance between atoms is shown in Figure 2.

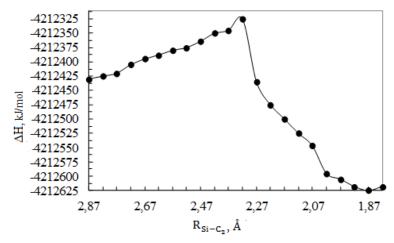


Figure 2. Dependence of system energy change ( $\Delta H$ ) on distance between silicon and carbon atoms  $R_{Si-C_2}$ 

Activation energy  $\Delta E^*=105$  kJ/mol, and reaction heat effect  $\Delta E=-195$  kJ/mol. As we can see, the reaction is exothermic.

Based on the comparison of the activation energies and heat effects of the reaction, the experiment between  $\alpha,\omega$ -bis(trimethylsiloxy)methylhydridsiloxane and triethoxyacryloxysilane is energetically more favorable with the second scheme[3,4]. The structure of the synthesized oligomer was confirmed by with functional and elemental analysis IR,  $^1H$  and  $^{13}C$  NMR spectral data. The order of hydrosilylation reaction, rate constants and activation energy are determined. Synthesized oligomer were studied by DSC, HPLC and wide-angle X-ray methods, which showed that the synthesized oligomers are single-phase amorphous systems with a chain spacing value of  $d_1 \approx 8.63$ -8.65 Å. The obtained oligomer are transparent products that are well soluble in common organic solvents  $\eta_{sp} \approx 0,05$ . To establish the truth, it is necessary to conduct a simple experiment and use more complete non-empirical methods of quantum-chemical calculations.

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#### BIO-BASED ADHESION ADDITIVES FOR BITUMINOUS BINDERS

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The growing focus on sustainable road construction has increased interest in environmentally friendly bitumen modifiers. This study presents the development of biodegradable adhesion additives obtained via the amidation of renewable raw materials – rapeseed oil (RO) and higher fatty acids (FA) – with polyethylene polyamine (PEPA). The aim of the research was to enhance the adhesion of bitumen to mineral aggregates while preserving the key physico-mechanical and rheological properties of the binder.

The amidation reaction with polyethylene polyamine was carried out under the following conditions: reaction temperature of 140 °C and duration of 4 hours and continuous mixing.

As the raw material for the modification process, 70/100 grade bitumen, sourced from PJSC "Ukrtatnafta" (Kremenchuk, Ukraine), was used. Bitumen modification was carried out with an adhesion promoter (AP) content of 0.4 wt.%. A dosage of 0.4 wt.% was selected as representative of the typical industrial range (0.3–0.6 wt.%). Mixing was carried out at a speed of 1000 rpm for 30 min, with the temperature maintained at  $150 \pm 2$  °C throughout the process.

The physical and mechanical properties of virgin bitumen and bitumens modified with adhesion promoters based on rapeseed oil (RO-AP) and higher fatty acids (FA-AP) are presented in Table 1. The results demonstrated that the incorporation of these modifiers, synthesized from renewable plant-based raw materials, at a concentration of 0.4 wt.% into oxidized road bitumen 70/100 did not lead to significant changes in the key physical and mechanical parameters, such as penetration, softening point, and ductility. This indicates that the developed additives do not compromise the fundamental performance characteristics of the bitumen, which is an essential requirement for industrial application.

Index	Virgin bitumen	RO-AP	FA-AP
Penetration at 25 °C, 0.1 mm	70	65	69
Softening point (SP), °C	48.5	49.5	48.9
Fraass breaking point (FBP), °C	-17.5	-16	-17
Ductility at 25 °C, cm	99.8	101.4	99.2
Penetration index calculated by SP	-0.78	-0.70	-0.71
Plasticity interval (PI = SP-FBP), °C	66.0	65.5	65.9
Adhesion to glass at 85 °C, %	38.8	97.4	95.8

Table 1 – Physical and mechanical properties of virgin and adhesion-promoter-modified bitumens

The conducted tests demonstrated a substantial improvement in bitumen–glass adhesion upon the introduction of the developed bio-based adhesion promoters. For the virgin bitumen, the adhesion value was 38.8%, whereas the incorporation of RO-AP and FA-AP at a concentration of 0.4 wt.% increased adhesion to 97.4% and 95.8%, respectively. This represents an enhancement of more than 2.5 times compared to the unmodified binder, confirming the high efficiency of the synthesized additives in promoting bitumen–aggregate bonding.

These findings suggest that biodegradable modifiers derived from renewable resources can serve as an effective alternative to conventional chemical additives, enhancing the bond between bitumen and mineral aggregates without adversely affecting other critical properties of the binder.

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### SYNTHESIS OF THE ANALOGS OF THE KNOWN SQUARINE DYES IN THE ANTI-CANCER PHOTODYNAMIC THERAPY USING 2-PHENYLINDOLES

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In the photochemical experiments using the common light source in the laboratory, as well as in nature, through the irradiation by natural sunlight, usually indoles exhibit single-photon absorption. If the intensity of the light increases, some compounds, usually referred to as photosensitizers have the capacity to exhibit two-photon absorption (TPA). Upon TPA, the photosensitizer is activated and emits energy that can ionize other molecules (e.g., DNA), which is similar to the ionization process caused by  $\gamma$ -rays [1].

Currently such photosensitive compounds are widely used for photodynamic therapy, upon which only cancerous cells are damaged. It is known from the scientific literature that some dyes that include an indole core have the capacity of two-photon absorption.

The purpose of our work is to synthesize the analogs of the photosensitive compounds used in photodynamic therapy based on 2-phenylindoles.

The target product was obtained by a two-step reaction according to the following scheme 1.

Scheme 1. Synthesis of the goal squarine dyes

In the first step, the reaction of 2-phenylindole and with benzyl bromide gave the intermediate 1-Benzyl-2-phenyl-1H-indole (3), and in the second step, the reaction of compounds 3 and 4 in n-butanol gave the goal product 5. Intermediary and final products were studied with TLC, IR and NMR spectroscopy.

**Acknowledgement:** This project was supported financially by the Shota Rustaveli National Science Foundation of Georgia (grant № FR- 21-1456).

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# DEFINITION PROCESS OF SORPTION OF LOW MOLECULAR SUBSTANCES BY POLYMERS

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For polymers that have an ideal, ineffective structure O.V. Olkhovic [1] classified types of tree volume:

- 1) Geometric free volume;
- 2) Thermal expansion capacity;
- 3) Fluctuating free volume.

In the works, there is an opinion that, in reality, the polymer of defects – The extent of defects-there is also a free volume, the role of which can be determined from the compression isotherm. Polymethylmethacrylate and polytetrafluoroethylene were investigated and shown that the volume of defects increases several times during the transition from the glassy state to the highly elastic state.

Consider the modern definition of the process of sorption of low molecular weight substances by polymers is a complex process and polymer, its porous structure, chemical structure, chain elongation, intermolecular interactions and polymer thermodynamic craving for sorbate. Depending on the size of the latter, the polymer may be excited to different degrees and the sorption mechanism will be different.

With different polymers about different substances' sorption existed big mess analyses gives possibility to separate the some mechanism that is characteristic for polymer's sorption.

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# LIGNIN AS A BIOPOLYMERIC COMPONENT OF ROAD PETROLEUM BITUMEN Yuriy Prysiazhnyi<sup>a</sup>, Myroslava Donchenko<sup>a</sup>, Taras Chipko<sup>a</sup>, Roman Serkiz<sup>b</sup>

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Despite efforts toward rational consumption, along with the continuous advancement and optimization of technological processes for the extraction, processing, and utilization of non-renewable energy sources, their global reserves are rapidly diminishing. Consequently, an increasing number of industrial sectors are prioritizing energy efficiency and resource conservation. Over the past 10–20 years, a notable trend has emerged toward incorporating various waste materials as modifiers for road petroleum bitumens. These include post-consumer products (such as plastic packaging, used vegetable oils, and end-of-life tires), off-spec materials from diverse industries (including agriculture, hydrocarbon resource processing, and wood processing), as well as products derived from the treatment of low-grade minerals (such as sulfur-rich and high-sulfur coals). Such additives are employed to enhance bitumen properties or to partially substitute virgin material with secondary raw resources, thereby contributing to the advancement of the circular economy and promoting sustainable development.

Considering its characteristics, availability, and safety for human health, lignin occupies a leading position among such materials. At present, it remains a relatively undervalued yet widely distributed resource, notable for its substantial (and renewable) reserves, as well as for its broad applicability across numerous industrial sectors. Lignin, the second most abundant organic polymer on Earth, plays a key role in imparting viscoelastic properties to plant structures. The optimal utilization of lignin as a component, specifically, as a partial substitute for bitumen, can be achieved only after a comprehensive investigation of the interaction mechanisms between this biopolymer and road bitumen.

The materials employed in the experimental investigations included road petroleum bitumen (grade BND 70/100, obtained via oxidation of petroleum residues) and technical hydrolytic lignin (a by-product of fodder yeast production, sourced from Zaporizhzhia region, Ukraine).

Lignin was added to petroleum bitumen in amounts ranging from 2.0 to 12.0 wt.% under the following conditions: temperature – 120 °C; duration – 60 min; and mixing intensity (using a Daihan Scientific HT-50 DX mixer) – 1000 rpm.

Based on comprehensive thermal analysis (DTA/DTG), it was established that the lignin-modified bitumen sample, in contrast to the unmodified bitumen, exhibits higher heat resistance and thermal stability. Thermo-oxidative processes in the lignin-modified bitumen begin to develop at higher temperatures (222 °C) compared to the unmodified bitumen sample (214 °C). In the modified bitumen, these processes are accompanied by a less pronounced mass loss than in the unmodified bitumen. The maximum mass loss rate for the modified bitumen sample is 1.8 %/min, whereas for the unmodified bitumen it reaches 2.5 %/min.

FTIR analysis revealed that, after mixing lignin with bitumen, certain characteristic lignin peaks associated with reactive methoxyl groups and organometallic compounds disappear (1510, 463 cm<sup>-1</sup>).

SEM micrographs of the examined samples demonstrated that lignin-modified bitumen is characterized by a less ordered structure compared to unmodified bitumen. At the same time, the modified bitumen exhibits the formation of a denser and more homogeneous structure with fewer branched pores relative to the original bitumen.

The applied analytical methods (complex thermal analysis, Fourier-transform infrared spectroscopy, and scanning electron microscopy) indicate that, under the selected conditions, the modification of road petroleum bitumen with lignin is of a chemical nature. In particular, it can be assumed that strong chemical bonds are formed between the reactive groups of lignin (e.g., methoxyl groups) and the functional groups of bitumen.

# ENANTIOSELECTIVE ANALYSES OF PENCONAZOLE IN AGRICULTURAL PRODUCTS USING LIQUID CHROMATOGRAPHY COUPLED WITH TANDEM MASS SPECTROMETRY (HPLC-MS/MS)

Ana Rakviashvili<sup>a</sup>, Natia Tchanturia<sup>a</sup>, Nino Takaishvili<sup>a</sup>, <u>Antonina Mskhiladze<sup>b</sup></u>, Marina Karchkhadze<sup>a</sup>, Bezhan Chankvetadze<sup>a</sup>

Penconazole is a widely used fungicide in agriculture for controlling fungal diseases across various crops [1]. Accurate quantification and enantiomeric separation are critical for understanding its behavior, efficacy and potential environmental impact [2].

The primary objective of this study was to develop a method for the enantiomeric separation of penconazole using high-performance liquid chromatography (HPLC) with polysaccharide-based chiral columns. The separation was optimized with mass spectrometry-compatible mobile phases to ensure broader applicability in pesticide residue analysis. Additionally, liquid chromatography coupled with tandem mass spectrometry (LC-MS/MS) was employed to identify and quantify penconazole enantiomers in various agricultural samples. Calibration curves were constructed to enable precise quantification.

The results highlighted the influence of mobile phase composition on the retention and enantiomeric separation of penconazole on polysaccharide-based chiral selectors. These findings provide valuable insights into optimizing chromatographic conditions for enantiomeric analysis of chiral pesticides.

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#### DEFORMATION AND STABILITY OF NON-NEWTONIAN POLYMERIC DROPLETS

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The deformation behavior and stability of droplets in flows through channels of various geometries are crucial for the development of various technological processes, such as the formation and processing of emulsions, and the creation of microcapsules and microparticles, including for targeted drug delivery. For the successful design and implementation of all these applications, a deep understanding of the mechanisms of droplet deformation and breakup is essential, both in simple model flows—such as simple shear or elongation—and in their combinations that arise in flows through channels with variable cross-sections. Most of these applications also involve non-Newtonian fluids with diverse rheological properties, examples of which include polymer solutions and melts, or biological fluids. Existing research to date has primarily focused either on Newtonian systems or on studying the effect of non-Newtonian behavior of the continuous phase on droplet deformation and stability, leaving aside the influence of non-Newtonian behavior of the dispersed phase. This work aims to fill this gap.

The deformation and stability of shear-thinning Carreau droplets and viscoelastic Oldroyd-B droplets in simple shear flow and in flow through channels with abrupt contraction and expansion are considered. For shear-thinning droplets in shear flow, computational results obtained through numerical integration of the Navier-Stokes equations, supplemented by the Volume of Fluid (VOF) method equations, are presented. For shear-thinning and viscoelastic droplets in channels with contraction and expansion, both experimental and computational results on droplet deformation and stability are provided.

For shear-thinning droplets in simple shear flow, it was found that the deformation curves change significantly with variation of the parameter in the Carreau model that controls the rate of viscosity change with increasing shear rate. For fluids whose viscosity is strongly dependent on shear rate, self-oscillatory deformation regimes were identified, and a connection was shown between the periodic change in droplet length and the periodic change in the average viscosity inside the droplet. Particular attention is paid to the heterogeneity of the viscosity distribution and the relationship between the viscosity distribution and deformation behavior in simple shear flow. For droplets in a channel with an abrupt contraction and expansion, a stability diagram is presented, and conditions for droplet breakup with the formation of one or two satellite droplets are identified. The dependence of droplet elongation upon entering the contraction on the capillary number and the confinement parameter is analyzed. The behavior of the viscosity field inside the droplet during its passage through the contraction region is analyzed, and it is found that droplet breakup corresponds to a sharp jump in the average viscosity. For a viscoelastic polymer droplet in a channel with an abrupt contraction, various deformation regimes were found for different polymer concentrations, and their stability was analyzed.

Acknowledgement: This research was supported by the Russian Science Foundation (Grant No. 24-29-00411).

# DEVELOPMENT OF A DUAL-REAKTOR CVD SETUP FOR ENVIRONMENTALLY FRIENDLY SYNTHESIS OF CARBON NANOTUBES

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Carbon nanotubes are the basic material in the research and application of carbon nanotechnology. The Chemical Vapour Deposition method is the most commonly used method for the synthesis of carbon nanotubes. The CVD method has great advantages over other synthesis methods. However, when using it, as a rule, depending on the type of raw material and catalyst, quite large quantities of by-products are formed. It is a mixture of polycyclic aromatic hydrocarbons such as naphthalene, anthracene, phenanthrene and others, which are highly toxic and can harm the environment. In this regard, our research group is developing a type of CVD installation that would not only allow the synthesis of high-quality carbon nanotubes, but also solve the problem of disposal of toxic by-products. The first reactor is designed for the synthesis of carbon nanotubes using conventional standard types of liquid raw materials, such as acetonitrile, toluene, and xylene. The second reactor will also be used for the synthesis of carbon nanotubes, but the by-products formed in the first reactor, i.e. polycyclic aromatic compounds, will be used as raw materials.

This paper presents the results of optimization of carbon nanotubes synthesis from acetonitrile. Research and development of synthesis from aromatic polycyclic compounds is our goal in the near future. The CVD synthesis setup for carbon nanotubes that we developed is shown in Figure 1.



Figure 1. CVD installation for environmentally friendly synthesis of carbon nanotubes.

In the synthesis of carbon nanomaterial, two different technological designs of the process were used. In the first case, ferrocene was used as a catalyst precursor, which was preliminarily dissolved in the used liquid raw material to a concentration of 20 mg per ml. In the second case, a Fe/Al<sub>2</sub>O<sub>3</sub> catalyst was specially prepared and then carbon nanotubes were synthesized with its participation. And although the first version of the synthesis is technologically simpler, the number of carbon nanotubes formed in it was almost 10 times less than when using a deposited iron/aluminum oxide catalyst.

This is, respectively, 1 gram of carbon nanotubes when using ferrocene and almost 10 grams of synthesized carbon nanotubes per experiment in the case of using a supported Fe/Al<sub>2</sub>O<sub>3</sub> catalyst. We associate this result with the large specific surface area of Al oxide, which provides a large contact area of the reactants with the catalyst. In the case of ferrocene, the contact surface is limited by the area of the inner surface of the quartz reactor, which does not exceed  $0.1 \text{ m}^2$  per 1 gram. The specific surface area of aluminum oxide is in the range from several m<sup>2</sup> per 1 gram of Al<sub>2</sub>O<sub>3</sub> to tens of m<sup>2</sup> per 1 gram, which ensures greater process productivity and such a difference in the amount of nanomaterial obtained.

The synthesized carbon nanotubes were characterized by SEM analysis, which confirmed their high quality and purity.

# PREPARATION OF NEW HYBRID COMPOSITES BASED ON CLAY MINERALS MODIFIED WITH OXYQUINOLINE POLYMER RESIN

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One of the most significant environmental problems today is environmental pollution by toxic substances, in particular industrial waste. Heavy metals, which enter the aquatic environment from various anthropogenic sources, are of particular danger, reducing the reserves of high-quality drinking water. In this regard, today the development of effective methods and materials for water purification from heavy metal ions is an extremely urgent task. Due to their unique properties, natural clays are considered as promising materials for the removal of heavy metals from wastewater [1]. Clays have several advantages over other adsorbents: they are available, inexpensive, non-toxic, have a large specific surface area, exhibit excellent adsorption properties and are capable of ion exchange, and are also suitable for recovery and reuse. The processes of heavy metal adsorption by clay minerals include various mechanisms, including direct binding of metal cations to the mineral surface, ion exchange, and formation of surface complexes. At the same time, the efficiency of natural clays as adsorbents of heavy metals can be significantly increased by modifying their surface with polymers, which significantly increases both the number of centers for adsorption of metal ions and expands the list of heavy metal ions that can be bound by such an adsorbent (fig.1).

This paper presents a study on the creation of new polymer-mineral composites based on natural clays, on the surface of which poly[8-hydroxyquinoline formaldehyde resorcinol] was immobilized. These polymers were synthesized by polycondensation of 8-hydroxyquinoline, formaldehyde and resorcinol in acidic and alkaline media. The structure of the synthesized polymers was confirmed by NMR and IR spectroscopy. Based on three natural clays (bentonite, saponite, clinoptilolite), new polymer-inorganic composites were obtained by physical adsorption of a polymer synthesized in an acidic environment on the surface of natural clays, and a polymer-inorganic composite based on clinoptilolite was obtained by in situ polycondensation of the starting monomers. The structure of the synthesized polymer-inorganic composites and the effectiveness of immobilization of the polymer poly[8-hydroxyquinoline formaldehyde resorcinol] on inorganic carriers were investigated by IR spectroscopy and thermogravimetric analysis.

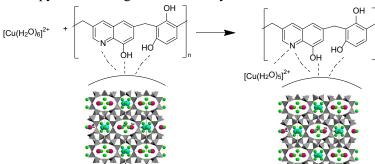


Figure 1. Scheme of adsorption of heavy metal ions on the surface of composites

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# USE OF ULTRASOUND IN THE SYNTHESIS OF POLYVINYLPYRROLIDONE COPOLYMERS AND THEIR (NANO)COMPOSITES

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Polyvinylpyrrolidone (PVP) copolymers with (meth)acrylic esters can be effectively used as osteoplastic composites for replacing damaged bone tissue. Such polymer composites are obtained by block polymerization with simultaneous Polyvinylpyrrolidone (PVP) copolymers with (meth)acrylic esters can be effectively used as osteoplastic composites for replacing damaged bone tissue. Such polymer composites are obtained by block polymerization with simultaneous foaming of the composition.foaming of the composition. The application of ultrasonic vibrations makes it possible not only to intensify polymerization but also to modify the structure and properties of polymers.

The influence of ultrasound (US) on the course of polymerization of homogeneous and heterogeneous compositions of (meth)acrylic esters with PVP has been studied, and the possibility of using it for the formation of (nano)composites based on them has been confirmed.

For the research, PVP with molecular weights of 300·10³, 44·10³, 28·10³, and 12·10³ was used, as well as monomers: 2-hydroxyethyl methacrylate, methyl acrylate, butyl acrylate, and styrene. As fillers for composites wollastonite, hydroxyapatite with particle sizes of 0.05–1.25 mm, and montmorillonite were used. The polymerization rate was determined by the change in the amount of unreacted monomer using a chemical method. The degradation of polymer matrices under the action of US was studied by changes in their molecular weight using the viscometry method.

Polymerization of vinyl monomers in the presence of PVP under US was carried out both for initial homogeneous systems, where PVP was dissolved in a monomer or its solution, and for monomers that formed a phase boundary with PVP solutions. The influence of US on the components of the reaction mixture, primarily on polymer matrices that can undergo degradation accompanied by a decrease in molecular weight and the formation of radicals and macroradicals, was studied. As comparative polymer matrices, polyvinyl alcohol with a molecular weight of 90·10³ and polyethylene glycol with a molecular weight of 7·10³ were used. It is assumed that the formed (macro)radicals can be used as active centers for further graft or block copolymerization.

A general pattern was revealed for the studied monomers – all of them polymerize in the presence of PVP under US without an induction period, and the polymerization rate increases in the series: butyl acrylate – methyl acrylate – styrene. The activating effect of US on the initiation of polymerization of 2-hydroxyethyl methacrylate compositions with PVP was established. In the case of homogeneous compositions, polymerization in a US field occurs only in the presence of polymerization initiators. Monomers that form a phase boundary with aqueous solutions of PVP polymerize in a US field without initiators under mild conditions.

The use of US significantly intensifies the process of obtaining porous composites based on polymer—monomer compositions and calcium-containing mineral fillers, including nanosized ones. The nature of the calcium-containing filler actively influences the polymerization rate of HEMA–PVP compositions. Compositions with montmorillonite and wollastonite exhibit higher reactivity compared to those containing hydroxyapatite as a mineral filler. The use of ultrasound enables polymerization at room temperature even in the presence of silver salts in the reaction medium, which are known to somewhat slow down polymerization. At the same time, the polymerization rate is significantly higher compared to polymerization without US, even at a temperature of 338 K.

The presence of silver salts in the initial composition makes it possible to obtain silver nanoparticles within the structure of composites and impart fungibactericidal properties to them.

The developed (nano)composites containing silver nanoparticles demonstrate high fungibactericidal properties and can be used in osteogenesis processes.

# DEVELOPMENT OF ANTIBACTERIAL NANOCOMPOSITIONS BASED ON POLYPROPYLENE AND PARA-DI-(2-ETHOXYCARBONYLCYCLOPROPYL)

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In introduction of the solid inorganic particles (including nanoparticles) into the composition of thermoplastic polymers, the filled compositions, characterized by increased strength are obtained. Such indices of compositions as heat-resistance, electrical-conductivity, magnetic properties, crack-resistance, fire-resistance and antimicrobial properties are simultaneously improved. In this case, it is advisable to choose the inexpensive and ecologically pure fillers [1]. The compositions with use of dispersed fillers are a continuous phase consisting of polymer matrix, filler particles and other ingredients. Under the influence of various microorganisms, such multicomponent compositions can be subjected to destruction, which considerably reduces their service life. For prevention of this process, various compounds with an antimicrobial effect are introduced into the composition of composites [2]. The compound – *para*-di-(2-ethoxycarbonylcyclopropyl)benzene (*para*-di-(2-ECCPB) synthesized by us, is obtained by the interaction of *para*-divinylbenzene (*para*-DVB) and ethyldiazoacetate at a ratio of 1:2 in the presence of the catalyst – anhydrous CuSO<sub>4</sub>, and possesses an antimicrobial effect [3]. Its introduction into the composition of the composites increases their elasticity and gives them antimicrobial properties:

In this work, we have developed and investigated the properties of the filled compositions based on polypropylene (PP) with use of the synthesized compound and a new mineral from the gypsum class detected in Absheron (Azerbaijan. Republic). The mineral nanoparticles, crushed to the size of 35-100 nm (determined on a Linseiz Start-1600 device (Germany)) were pre-impregnated (*para*-di-(2-ECCPB), then introduced into the composition of composite in a quantity of 5-20 mass% and mixed with PP on rollers at 160°C for 4 h.

The study of the physical-mechanical properties of compositions filled with impregnated (*para*-di-(2-ECCPB) mineral particles showed that in comparison with pure PP, they have improved indices of tensile strength, but slightly lower elongation values. Along with this, the antimicrobial properties of the obtained compositions have been also revealed (Table 1). The study of the antimicrobial properties was carried out using suspensions of *Aspergillus niger* and *Candida albicans* fungi according to GOST 9.049-91. The antifungal activity was estimated on a six-point scale.

ruote 1. Composition una physicur mechanicur maices of nanocomposites.										
Composition of composites (PP + nanofiller +	Tensile strength,	Relative elongation,	MFI, 10 g/min.	Heat- resistance, °C	Degree of fungus growth, points					
					Aspergillus	Candida				
para-di-(2-ECCPB)),%		90		-0	niger	albicans				
PP (neat)	32.60	32	1.2	170	2	1				
PP + 5 + 1	33.25	12	1.76	174	1	1				
PP + 10 + 1	34.10	12	1.7	173	1	0				
PP + 15 + 1	34.90	11	1.83	182	0	0				
PP + 20 + 1	36.10	10.7	1.90	185	0	0				

Table 1. Composition and physical-mechanical indices of nanocomposites.

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### SYNTHESIS AND STUDY OF BIOLOGICAL ACTIVITY OF BIS- AND SPIRO-CYCLOPROPANE-CONTAINING COMPOUNDS

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The cyclopropane fragments are present in the structure of many biologically active substances. Some anticancer and antifungal drugs, antibiotics, insecticides, plant growth regulators and fruit ripening contain a cyclopropane group. Many cyclopropane derivatives have antifungal, insecticidal and fungicidal activity, which allows them to be used for antimicrobial protection [1-3]. Being one of the intense cycles, it attracts special attention of researchers due to its high reactivity. The cyclopropane compounds are also used in organic synthesis for preparation of more complex cyclopropane derivatives [4, 5].

In this work, it is reported on the synthesis and study of the antimicrobial activity of a number of compounds with cyclopropane fragments containing various substituents:

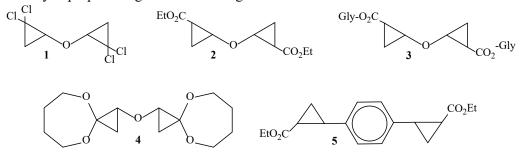


Figure 1. Structure of the synthesized cyclopropane-containing compounds

The synthesized compounds are structurally similar to *trans*- chrysanthemum acid and its derivatives and contain two cyclopropane groups with various substituents: *gem*-dichlorine (1), ester (2 and 5), glycidyl (3) and spirocyclic (4), which gives them expressed biological activity.

A number of potential biological activities of the synthesized compounds have been revealed using the PASS Online web resource. The primary screening of the fungicidal activity of these compounds in relation to mold and yeast fungi, as well as their activity in relation to gram-positive and gram-negative bacteria has been carried out. The synthesized compounds have been used as biocidal plasticizers in PVC-compositions, antimicrobial modifiers of epoxide resins, and also antibacterial additives in polyolefin compositions.

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# POLYMER COMPOSITES CONTAINING ELECTRICALLY CONDUCTIVE AND MAGNETICMICROPARTICLES THAT ABSORB RADIO WAVES

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Effect of different technological factors on the electromagnetic wave (EMW) with frequencies (3-10 GHz) absorbing properties of polymer composites based on epoxy resin with electric conducting (carbon black, graphene) and magnetic (ferrite) nanofillers have been investigated.

It is experimentally shown that absorbing properties of these materials essentially depend on concentration of the filler Relatively high absorption is manifested for composites containing 40 -50 wt% filler.

On the device created especially there are provided the investigation of the electromagnetic wave (EMW) absorbing properties of composites based on epoxy glue, which contain different carbon-graphite fillers. The effect of the EMW absorption increases wen the sandwiches composed from polymer films with different fillers. Improve of the absorption properties of polymer composites increases at using of the coatings with different profile of their cross sections.

It is established that the level of the EMW absorption may be regulated by change of cross section profile of the absorber and with collection of the sandwich type absorber contained several absorbing films with different distribution in the sandwich and content of these films.

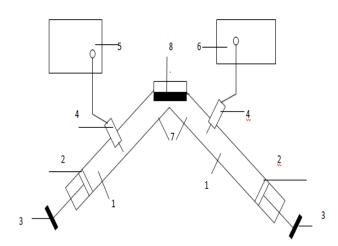


Fig.1. Scheme of registration of the EMW reflected from samples. 1- waveguide made from brass list;

- 2 plunger coordinator; 3 its handle; 4 –the transmitting and reciving antennas (left contains the detector);
- 5 generator of super high frequency; 6 coordinator of the reflected EMW intensity 7 substrate of waveguide;
- 8 reflecting plate with sample (attached from below)

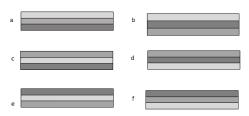


Fig.2. Schema of sandviches with variation of dislocation of the absorber films. Rectangle with light color corresponds to films with relatively low filler concentration, semi dark to middle and dark - high concentration of filler

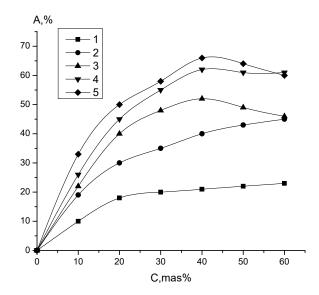


Fig.3. Dependence of the EMW absorption of composite containing carbon black of type P803(1), carbon black of type P357 (2), graphene synth.(3) graphene nat.(4), blend of graphite + carbon black P803(5)

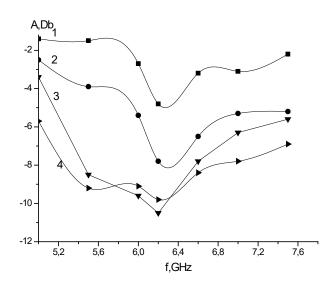


Fig. 4. EMW absorption ability of the composites based on epoxy resin and graphene for following concentrations of the filler (in wt%): 20 (1), 30 (2), 40 (3), 50 (4)

**Table 1.** EMW absorption by sandwiches designed from films on the basis of epoxy resin and graphene with different con centration of latter  $(f = 8.0 \text{ GHz})^{1)}$ 

#	Position of	Absorption of
	films	EMW, %

1	1-2-3	84.4
2	1-3-2	67.7
3	2-1-3	53.3
4	2-3-1	55.2
5	3-1-2	65.6
6	3-2-1	61.3

Film1: Epoxy resin (80 Wt.%):+ graphene (20 Wt.%)

Film 2: Epoxy resin (70 Wt.%) + graphene (30 Wt.%)

Film 3: Epoxy resin (60 Wt.%) + graphene (40 Wt.%)

Table 2. EMW absorption ability of the sandwich type absorbers (f = 5.6 GHz). The sequence of the plates in the package (concentration of graphene in the plates) (the wave falls on the package from left side -plate with less content of the filler)

Packing	Position of	Absorption
index	films	of EMW, %
A	30 - 40 -50	54.6
В	30 - 50 - 40	49.3
С	40 - 30 - 50	44.5
D	40 - 50 - 30	41.8
Е	50 - 30 - 40	38.4
F	50 - 40 - 30	37.5

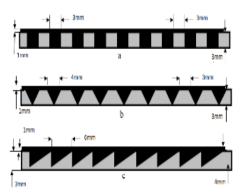


Fig.5. Vertical sections of the forms with different shapes: cylindrical; b) conical; c) ladder like. Black area -absorbent material, light color area - dielectric substrate

# DEVELOPMENT OF FLY ASH ACTIVATION METHODS FOR THE PRODUCTION OF GEOPOLYMER MATERIALS

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Fly ash (FA) is an aluminosilicate material: a waste product resulting from the combustion of coal in thermal power plants, consisting of fine particles emitted from the boiler with the flue gases.

FA is one of the precursors for the production of geopolymer materials (GPM), along with metakaolin and granulated blast furnace slag. Various studies have been devoted to the possibility of using FA in the production of GPM and it has been proven that mainly low-calcium FA (Class F) can be successfully used for this purpose [1].

The disadvantage of FA is its low reactivity compared to metakaolin and granulated blast furnace slag. To increase the reactivity of FA with respect to the alkaline agent and, consequently, to improve the strength and other physical and mechanical properties of geopolymers, various methods have been used, such as mechanical (grinding in various types of mills) [2], chemical (inclusion of various additives into FA, such as alkaline earth metal oxides) [3] and thermal treatment [4].

Previously, we conducted preliminary studies on the use of FA from the Kutaisi Thermal Power Plant (Georgia) to obtain GPM [5].

The aim of this work is to develop methods for activating FA and obtaining GPM with high physical and mechanical properties based on FA of Kutaisi TPP.

It should be noted that the amount of FA from Kutaisi TPP reaches several million tons, polluting the environment.

In laboratory conditions, the grinding and heat treatment regime of FA, as well as the composition and quantity of chemical activators, were established. GPM with optimal physical and mechanical parameters were obtained.

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# DERIVATIVES OF PROPARGYL ALCOHOL AS ACTIVE DILUENTS OF THE POLYMER COMPOSITION ON THE BASIS OF ED-20

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Propargyl alcohol is highly-reactive monomer, it is a semi-product and a building block for multipurpose organic synthesis. The perspectivity of practical use of these synthetic products, i.e. possibility of preparation of physiologically active substances, metal corrosion inhibitors, polymer modifiers, etc. based on them is of particular interest [1, 2].

In connection with the above-mentioned one, the results of the synthesis and use of propargyl alcohol derivatives as a modifier of epoxy diane resin are presented in the work. It has been revealed that bromohydrine and glycidyl ether of propargyl alcohol undergo the reaction of diene synthesis with cyclopentadiene at 175-180°C, and with hexachlorocyclopentadiene and 5,5-dimethoxytetrachlorocyclopentadiene at 145-150°C on a triple bond with the formation of the corresponding bicyclic adducts of the norbornadiene series (Figure 1):

Figure 1. Synthesis of propargyl alcohol derivatives

The structure of the synthesized adduct has been confirmed by IR and <sup>1</sup>H NMR spectra. In the IR spectrum of epoxides there are not the bands characteristic for acetylene and O-H bonds, but in this case, the absorption bands at 3065, 1260, 1180, 950, and 730-840 cm<sup>-1</sup> characteristic for the epoxy group, C=C, C-O-C, and C-Cl bonds have been detected.

For modification of the synthesized compounds, three compositions with the participation of the following component ratios: ED-20 – 90, 80, 70 compound 10, 20, 30 and the hardener PEPA-20 were respectively prepared. Each composition was cured separately in standard forms at room temperature for 24 h, after which the samples were subjected to thermal treatment at temperatures 800°C and 100°C for 2 h and the corresponding physical-mechanical properties of the obtained compositions were determined. It has been established that the test esters have both plasticizing and modifying properties in relation to the cured resin. The content of halogen atoms in the molecule also leads to effect of self-extinction. In introduction of bicyclic adducts of the norbornadiene series into the composition in the range of 10-30 mass p, in comparison with samples obtained by curing ED-20 without modifier, the tensile strength of the sample increases 2-3 times, heat resistance – 1,5 times, elasticity – 10-12 times, and dielectric strength increases 2-3 times. Thus, the obtained data indicate that the tested compounds participate in the crosslinking process during curing, essentially exceed the unmodified composition on all indices and can be used in various industries as highly effective diluents of the polymer composition based on ED-20.

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### FUNCTIONALLY SUBSTITUTTED PYRAZOLES AS MODIFIER ED-20

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Epoxy diane resin ED-20 being low molecular linear polymer, is one of the widespread industrial polymer products and is used as a stabilizer of halogen-containing polymers, chlorohydrocarbons and oils, an accelerator of vulcanization of rubbers, etc. [1-3]. Therefore, the creation of high-strength composition materials meeting the requirements, by modification of the cured ED-20, by introduction of low-molecular polyfunctional compounds and active diluents into the composition of compound is perspective and is becoming increasingly important with technological progress.

In this work, the results of the investigation of the synthesis reaction of functionally substituted pyrazoles on the basis of the interaction reaction of 3-alkyl-5-(diethylaminomethyl)-pyrazoles with chloroanhydrides of acrylic and methacrylic acids, forming pyrazoles containing unsaturated bond and keto groups in the side chain are presented (Ia-c-VIa-c) (Figure 1).

Figure 1. Synthesis of functionally substituted pyrazoles

The composition and structure of the synthesized compounds has been confirmed by data of the elemental analysis, IR and PMR spectra. The synthesized compounds have been tested as a composition modifier based on ED-20, cured by PEPA. Each composition was separately approved in standard forms at room temperature for 24 h, then the samples were subjected to thermal treatment for 2 h at 80°C and 120°C, after which the physical-mechanical characteristics of the samples were determined. It should be noted that the strength properties and electrical characteristics of the composition materials essentially depend on the nature of the modifier introduced into their composition. The obtained results also indicate that the created materials can be recommended for practical use as highly effective sealing compositions (Table 1).

Table 1	1. Physical-chemical	and dielectric pro	nerties of enc	vide compositions
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Modifier	Content. mass p.	Tensile strength, MPa	Relative elongation at break, %	Vicat heat- resistance, °C	Electrical strength, kV/mm-1	Dielectric permeability at 50 Hz
	10	81.3	17	136	40.7	8.7
Ia	20	84.6	20	150	42.1	8.1
	30	79.8	18	129	36.7	7.6
IIIa	10	81.8	20	112	39.1	3.8

	20	84.7	22	131	42.3	4.9
	30	77.3	20	100	40.8	4.4
	10	69.4	18	166	36.7	4.5
Va	20	73.6	20	170	42.4	4.3
	30	71.0	19	159	38.6	4.5
ED-20+PEPA		36.1	1.5	100	15-20	3.8
(without modifier)	_	30.1	1.3	100	13-20	3.6

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# THE EFFECT OF STARCH ADDITION TO PLA ON SELECTED PROPERTIES, BIODEGRADABILITY, AND IMPACT ON THE AQUATIC ENVIRONMENT

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The use of certain polymer products is currently under a huge discussion. Most of these products are obtained from non-biodegradable polymers of petrochemical origin. Furthermore, there are still no universal recycling procedures applicable to all plastic products on the market. To address the growing problem of plastic waste, one of the most promising solutions is the development of new biodegradable materials made from biobased polymers. Interest in bio-based polymeric materials is estimated to be growing annually by approx. 20-25 %. Currently, the most popular bio-based polymer from technical and processing point of view is polylactide (PLA) which is an aliphatic polyester that is biodegradable under certain conditions. PLA is synthesized from lactic acid, which is a product of bacterial fermentation of carbohydrates such as sugarcane, corn, and potatoes [1].

This work focuses on the study of selected properties, such as crystallinity, degradability, and the behavioral response of *Lymnaea stagnalis* in the presence of different PLA composites. Two fork-shaped samples from PLA blends were tested: the first was produced from commercial Bio-Flex granulate (containing 70 % PLA and unknown additives), and the second one from a newly developed composition (referred as KPG). The KPG samples were obtained from granulate prepared by authors, consisting of 75 % PLA (NatureWorks, Ingeo 3251D, Minnesota, USA) and 25 % thermoplastic starch modified with 1 % arabic gum. These samples were produced according to Patent EP 3064542 [2].

Standard analyses like DSC, IR spectroscopy, and biodegradability tests were conducted to compare the properties of obtained PLA-based compositions. Moreover, a novel test was performed to evaluate the behavior of *L. stagnalis* in the presence of studied samples. *L. stagnalis* snails were selected to assess the potential ecological response to the bio-based polymers in aquatic environment. These snails have been widely used since the 1970s to study fundamental mechanisms in ecotoxicology and neurobiology [3]. The test results indicated that the KPG forks may constitute food for *L. stagnalis*, in contrast to Bio-Flex samples. Notably, the snails remained alive after consuming the KPG samples, suggesting that the addition of starch to PLA may have a beneficial environmental impact.

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### COMPOSITE POLYMERS AS MODIFIERS FOR ROAD BITUMENS

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The most common bitumen modifiers are polymers – high-molecular-weight compounds whose macromolecules consist of a large number of repeatedly and structurally diverse repeating units of the same monomer or different monomers. Polymers may exist in the form of powders, crumbs, granules, or liquids, and they are classified into specific types for bitumen modification: thermoelastoplastics, thermoplastics, latexes, terpolymers, and composite polymers. Recently, composite polymers have gained particular popularity, as they reduce the cost and/or increase the effectiveness of the modifiers. Composite polymers are mixtures or blends of various types of polymers that may include plasticizers. Typically, such bitumen modifiers contain recycled polymeric materials that have already been used once.

For the modification of bitumen 70/100 produced by PJSC "Ukrtatnafta", Ukraine (penetration at 25 °C - 75 dm, softening point - 48.8 °C, ductility at 25 °C - >150 cm, strain recovery at 25 °C - not available) with composite polymer additives the following polymers were selected: PCD-20 (a mixture of stretch film and thermoelastoplast), PCCF (composite polyethylene with cellulose filler), Polyplast (a mixture of stretch film and natural bitumen Selenizza SLN 120). The modification parameters were as follows:

- additive content -1.0; 2.0; 3.0; 4.0 and 5.0 wt.% relative to bitumen;
- blending temperature of bitumen with polymers -180 °C;
- modification time 3.0 h with constant mixing using a mechanical stirrer at 1000 rpm.

Under these parameters, all modifiers were well dispersed in the bitumen. The main physical and mechanical properties of the modified bitumen are presented in Figure 1.

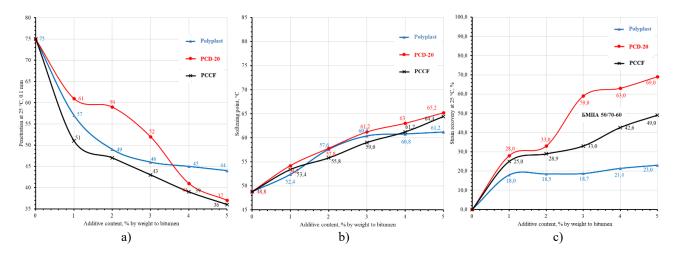


Figure 1. Main physical and mechanical properties of the modified bitumens : a) Penetration at 25 °C, b) Softening point, c) Strain recovery at 25 °C.

Among the studied composite polymer modifiers, the most effective is the composite PCD-20, since regardless of dosage it enhances the softening point and strain recovery of the base bitumen more intensively compared to PCCF and Polyplast additives. Moreover, these additives do not provide the bitumen with the required strain recovery. This is explained by the fact that the composite additives PCCF and Polyplast do not contain a thermoelastomer, while PCD-20 does.

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# THE SYNTHESIS OF A SERIES OF BIOLOGICALLY ACTIVE BENZENESULFONAMIDE DERIVATIVES

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Carbonic anhydrases (CAs) are ubiquitous metallo-enzymes performing important roles in a variety of physiological processes[1]. Abnormal levels and/or activities of human CAs (hCAs) have been often associated with different diseases. For these reasons, in recent years there has been a growing interest in hCAs as targets for the design of inhibitors with biomedical applications. In particular, the isoforms IX and XII, have been recently recognized as valuable targets for cancer treatment and diagnosis, since they have been shown to be overexpressed in many hypoxic cancers [2]. In this context the design of molecules able to regulate CA IX and XII catalytic activity could open new scenarios for cancer biomedicine.

In this scenario, the aim of the work was the development of organic molecules with high affinity and selectivity for the tumor-related hCA IX and XII, for biomedical applications in the treatment of hypoxic tumors. To this purpose, the design and synthesis of novel benzenesulfonamide inhibitors was performed. For the best result, were synthesized benzenesulfonamides introducing in para position of the benzene ring a veriety of functional groups consisting of liphopilic, hydrophilic, flexible or rigid tails, to establish favorable interactions with specific residues in both hydrophilic and hydrophobic halves of the enzyme active sites, and therefore, enhancing the selectivity towards hCA IX and hCA XII.

The synthesis was performed using multicomponent reactions involving the interaction of three or more components in a single reaction flask where condensation, refunctionalization, or cyclization occurred simultaneously. The reactants include various aromatic and aliphatic isocyanides, carboxylic acids, amines, and oxo compounds for obtaining multifunctionalized compounds and heterocycles through a one-pot process. These reactions were carried out in different reaction conditions using protic or aprotic solvents under various reaction temperature.

The structural analysis of the synthesized products was conducted using infrared spectroscopy (IR), proton nuclear magnetic resonance (<sup>1</sup>H-NMR), carbon-13 nuclear magnetic resonance (<sup>13</sup>C-NMR), and mass spectrometry (MS) techniques.

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# STEREOSELECTIVE ANALYZES OF DIFENOCONAZOLE USING LIQUID CHROMATOGRAPHY COUPLED WITH TANDEM MASS SPECTROMETRY (HPLC-MS/MS)

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Difenoconazole is a fungicide used in agriculture to control various fungal diseases in fruit, vegetables, cereals and other field crops [1]. Difenoconazole works by inhibiting demethylation during ergosterol synthesis.

Figure 1. Difenoconazole

Difenoconazole has two chiral carbon centers and therefore 4 stereoisomers. The aim of the present study was to investigate the separation of stereoisomers of difenoconazole by high-performance liquid chromatography using polysaccharide-based chiral columns. In this study we investigated the separation of stereoisomers of difenoconazole using mass spectrometer-compatible mobile phases.

Based on the results obtained, we made some conclusions about the influence of the mobile phase on the retention and separation of difenoconazole stereoisomers on chiral columns of polysaccharide nature.

The developed separation method was then used to generate calibration curves for difenoconazole and its stereoisomers in agricultural commodities. These calibration curves were used to assess the differences in residue levels of difenoconazole in agricultural products. The calibration lines allowed accurate quantification of difenoconazole content, providing a reliable tool for evaluating pesticide residue levels in these crops.

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# MATHEMATICAL MODELING FOR 8-OXOGUANINE SENSING ON POLYPYRROLE/VO(OH) COMPOSITE

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8-oxoguanine is one of the main products of reactive oxygen species (ROS) reaction with DNA, which is used as a marker of genomic alteration. Its formation results in a mismatched pairing with adenine resulting in G to T and C to A substitutions in the genome. Therefore, 8-oxoguanine determination is highly recommended to detect possible mutations.

Although 8-oxoguanine is guanine oxidized form, both cathodic and anodic determination may be applied to it. The electrode modifiers for both of the scenarios may be suggested from the reaction mechanism. By anodic way, 8-oxoguanine will be oxidized analogously to caffeine and other uric acid derivatives. Yet on cathode it will be reduced via 8-oxogroup or its carbamide moiety, resulting in the methanol formation.

In this work, the theoretical description for 8-oxoguanine determination by polypyrrole composite with vanadium oxyhydroxide. Two different behaviors are possible, being dependent on how the composite is obtained.

Either two-step or one-step syntheses may be applied to it, but the resulting composites will have nearly opposed properties. Moreover, in these cases, different models describe the 8-oxoguanine cathodic reduction.

Analyzing the correspondent mathematical model, we confirm that the steady-state stability range is wider than in the case of cathodic oxidation. Moreover, the oscillatory behavior is less probable, if the solution pH is maintained within the working interval (3<pH<14), correspondent to the stability of VO(OH) modifier.

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# CP-BASED ELECTROCHEMICAL REMOVAL OF HEAVY METALS. A CHEMICAL AND CIRCULAR ECONOMY APPROACH

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The term "heavy metals" has been introduced by german chemist Leopold Gmelin in 1817. This term became so popular that has given its name to the musical style, known as "heavy metal rock".

As for now, more then forty definitions for the term "heavy metals" are commonly accepted, but generally all the metals beginning with vanadium are considered as "heavy". Most of them are transition metals, capable to form stable complex compounds.

The heavy metal cations are among of the most aggressive pollutants in the environment. They may occur even in food and drinks (including those of traditional recipes). These cations are highly toxic, provoking different intoxication symptoms. For this and other reasons, the heavy metals concentration determination and removal is really actual, and the electrochemical methods may be a good solution for this problem.

Besides of the cathodic deposition, yet used in different systems of the wastewater treatment, anodic extraction may also be used. Generally, it is based on electrooxidation of a metallic cation or of a surface material in the presence of this cation, yielding thereby a more oxidized form and(or) a stable complex.

In order to implement this function, the anode will be modified by a conjugated dye, its polymer or another conducting polymer, possessing complex-forming functional groups. Those monomers and polymers are generally synthetic, but they may be substituted by natural analogous compounds.

In this work, a theoretical evaluation for heavy metal cations galvanostatic electrochemical determination and removal from wastewater, by means of their oxidation in the presence of a conducting polymer based on phenolic plant and mushroom toxins. As their main toxins are phenolic, it makes possible their possible electro(co)polymerization, and the complex formation of the phenolic toxins in the polymer phase with the heavy metal cations. The mathematical modeling of the system's behavior confirms its efficiency for the electrochemical determination and removal of heavy metals from natural waters and wastewaters. The procedure is foreseen to be realized by economical and green manner, according to the principles of the recycling approach.

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# POLYPYRROLE-BASED CARPROFEN ELECTROCHEMICAL DETERMINATION IN MILK. A THEORETICAL INSIGHT

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Carprofen (Fig. 1) is a veterinary NSAID, analogous to ibuprofen, but based on carbazolic moiety. Firstly developed by Pfizer for both human and veterinary medicine, nowadays it is used for treatment of post-operative pains in cattle and horses. On the other hand, the presence of vet drugs in meat and milk products is very important from the point of view of food safety, reason why the development of an efficient technique for carprofen rapid and precise quantification is really current.

Fig. 1. Carprofen

Considering the carprofen structure, both cathodic and anodic electrochemical determination may be applied to it. In the case of polypyrrole-based anode, carprofen will be doped in the polymer backbone and then oxidized by incorporation (with covalend bonding), phenolization and electropolymerization. For this reason, the same process could be used for carprofen removal from animal-based food.

Analysis of the correspondent mathematical model for galvanostatic mode, based on trivariant equationset (1):

$$\begin{cases} \frac{dc}{dt} = \frac{2}{\delta} \left( \frac{\Delta}{\delta} (c_0 - c) - r_d \right) \\ \frac{dp}{dt} = \frac{1}{p} \left( r_d - r_i - r_{ph} - r_p \right) \\ \frac{dq}{dt} = i - i_F \end{cases}$$
 (1)

Confirms the efficiency of polypyrrole as electrode modifier for carprofen detection and removal, despite of less stable behavior in galvanostatic mode comparing to potentiostatic.

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# DIBENZOXAZEPINE ELECTROCHEMICAL REMOVAL BY INDIRECT ELECTROPOLYMERIZATION. A THEORETICAL INSIGHT

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Dibenzoxazepine (Fig. 1 – code name CR) – i.e., according to the Hanch-Widman nomenclature, a heterocyclic compound with a seven-membered ring and heteroatoms of Nitrogen and Oxygen, condensed with two benzene rings – is a combat poison obtained in 1962 by the Swiss chemists Higginbot and Sushitsky. It belongs to the chemical warfare class of complex action stimulators.

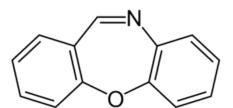


Fig 1. Dibenzoxazepine

By its effect, dibenzoxazepine is similar to BZ-gas, but twice as strong. From skin contact as little as 2 mg of dibenzoxazepine within 10 minutes will cause redness. 5 mg cause erythema, and 20 mg - excruciating pain, which increases when in contact with water. Therefore, the development of a circular economy approach for its removal from the environment is really actual, and the synthesis of a conducting polymer on its base

In this case, the strong oxidants, like peroxides, pentavalent bismuth compounds in pair with trivalent bismuth may be used for indirect dibenzoxazepine removal towards the polymer phase. As for dibenzoxazepine, it may be oxidized by either nitrogen atom or conjugated systems (electropolymerization).

For the first time, the electroanalytical system for the electrochemical determination and removal of dibenzoxazepine chemical warfare by electropolymerization, assisted by BiO<sub>3</sub>-/Bi<sup>3+</sup> redox pair. Two oxidation scenarios, including the electropolymerization and N-oxidation are possible for dibenzoxazepine. Either way, both dibenzoxazepine and its N-oxide will be removed from the environment towards the polymer phase. The analysis of the electroanalytical process by linear stability theory and bifurcation analysis confirms that the steady-state stability behavior lets use this process for both electroanalytical and electrocatalytical purposes.

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# MATHEMATICAL MODELING FOR INVOLUTIN AND ORELLANIN SENSING ON CONDUCTING POLYMER ELECTRODE

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Polyphenolic compounds are well known for their antioxidant, anti-inflammatory, pigment and organoleptic properties. They make important part of the human and animal nutrition, but if one of those compounds are necessary, other of them are toxic. Other toxic compounds mimic being polyphenolic, but aren't so. Involutin (Fig. 1 to the left), a mycotoxin from *P. involutus* mushroom is a phenolic compound, such as and yellow stainer (*A. Xanthodermus*) toxins, which include the proper phenol. Psilocin, a main toxin from *Ps. mexicana* and *Ps. cubensis* is also a phenolic compound. Orellanin (Fig. 1 to the right), a mycotoxin from *C. orellani* is a compound, analogous to a phenol, but bears N-oxide groups instead of CH group, being heterocyclic pyridinic derivative. For this reason, the development of an efficient methods for their quantification is really actual.

Fig. 1. Involutin and orellanin.

Moreover, both of the compounds may be seen as monomers for electropolymerization conducting polymers and, considering the rapid reproduction of mushroom organisms, they may be used as a font of the green conducting polymers.

In this work the electrochemical determination of involutin and orellanin on conducting polymers are described theoretically. For both compounds, either low-molecular (for example, hydroquinone to quinone) or high-molecular (electropolymerization, yielding a conducting polymer) oxidation mechanisms may be realized, being efficient from either electroanalytical or electrosynthetical points of view.

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# THE THEORETICAL DESCRIPTION FOR SUCRALOSE CATHODIC REMOVAL ON CONDUCTING POLYMER-MODIFIED CATHODE

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Sucralose is one of the most used sugar substitutes in the world. It is three times as sweeter as aspartame, twice as sweeter as saccharin and 800 to 1000 times sweeter than the sucrose.

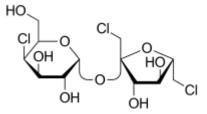


Fig. 1. Sucralose

It has been approved for use in the USA, in Canada, in Australia and in the European Union. Its chemical composition is related to that of the carbohydrates. But, containing three chlorine atoms, it may present different toxic effects, including environmental, oxidative and genomic stress, reason why the development of an efficient method for sucralose detection is really actual.

In this work, a cathodic sucralose removal on conducting polymer, containing pyridinic nitrogen atom, has been described theoretically. The process consists on use of the membrane electrolysis, in which the polymer electrode, based on:

- Overoxidized polypyrrole;
- Polymer of heterocyclic dye;
- Polymer with active basic groups.

The sweetener becomes thereby immobilized on the polymer surface and the polymer is cathodically reduced, yielding inorganic chloride. The membrane, at its turn, impedes the chloride ion, which appears in cathodic electrolyte from diffusion towards the anodic surface. The anodic reaction becomes water electrolysis and oxygen evolution. Therefore, the sucralose environmental impact will be diminished and concentration will be reduced.

Analyzing the correspondent mathematical model, we confirm that the steady-state stability range is wide, indicating the process efficiency. Moreover, the oscillatory behavior is less probable. The similar process may be also applied for carrelame supersweetener electrochemical removal.

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# THIABENDAZOL ELECTROCHEMICAL DETERMINATION ON POLYPYRROLE/VOOH COMPOSITE

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Thiabendazole is a widely used antihelmintic, antifungal and larvicide drug, used in treatment of different types of parasitoses in humans and pets. Moreover, it is one of few antihelmintic drugs, registered as a conservant food additive (E239), usually added to protect fruits and vegetables from helmints, larvae and some fungi. It may also be used as an antidot for heavy metal poisoning, due to the presence of complex-forming imidazole ring. Its pharmacological properties are due to fact of combining the benzimidazolic ring with the thiazolic.

Possessing both donor and acceptor functional groups, thiabendazole may be detected either cathodically or anodically. In the case of cathodic reduction, it will be realized by pyridinic nitrogen atom. In this case, bivalent vanadium or chromium compounds, including those generated *in situ* may be easily used in strongly acidic medium. In order to stabilize those inorganic forms in nanoparticles, conducting polymers may be used as a matrix, capable to host them.

In this work, the electrochemical determination of thiabendazole in pharmaceutical formulations biological liquids and food in galvanostatic mode has been described by a mathematical model, which was thereby analyzed by linear stability theory and bifurcation analysis. In this case the model is trivariant:

$$\begin{cases} \frac{ds}{dt} = \frac{2}{\delta} \left( \frac{\Delta}{\delta} (s_0 - s) - r_{r1} - r_{r2} \right) \\ \frac{dc}{dt} = \frac{1}{c} (r_{r1} + r_{r2} - r_{r1}) \\ \frac{dq}{dt} = i - i_F \end{cases}$$
 (1)

The model analysis shows that despite of the more expressed stability than in the case of the anodic process, the galvanostatic determination is less stable than potentiostatic. Nevertheless, this method is still efficient for thiabendazol determination in different media.

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# PREDICTION OF THE AGING OF POLYMER COMPOSITE MATERIALS

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To determine the possibility of using promising polymer composite materials as elements of aerospace engineering, it is necessary, taking into account operational requirements, to know the real terms of their reliable operation and storage. Only long-term full-scale tests give reliable results for assessing the aging of polymer composite materials, but they often become obsolete by the time they are obtained.

One of the ways to reduce the duration of the study of aging of polymer compositions is the intensification of the impact of climatic factors and the creation of accelerated laboratory procedures that simulate various climatic conditions.

For scientifically based accelerated studies, it is necessary to quantify the correlation relationship between the influence of climatic factors on changes in the physicochemical and, therefore, operational characteristics of a polymer composite material.

On the basis of experimental data, the possibility of studying the processes of accelerated aging to predict the performance and shelf life of polymer compositions of aviation technology elements by changing the thermogravimetric analysis constants of the corresponding polymer compositions is shown.

The relationship between the performance and shelf life of polymer composite materials and the change in the constants of derivatograph analysis has been established. By changing the effective activation energy of the thermo-oxidative degradation of polymer compositions during accelerated aging, it is possible to predict the retention time of the operational characteristics of structural elements of aerospace engineering.

### ANTIMICROBIAL ACTIVITY OF METAL-CONTAINING MODIFIED ZEOLITES

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Zeolites are inorganic polymers built from alternating SiO<sub>4</sub> and AlO<sub>4</sub><sup>-</sup> tetrahedrons forming open framework uniform structures with cages and channels. Natural and synthetic zeolites in which the ions that compensate for the negative charge of the framework are partially replaced by cations of such biocide metals as silver (Ag<sup>+</sup>), copper (Cu<sup>2+</sup>), zinc (Zn<sup>2+</sup>), etc., are recognized as promising among the materials that are advanced for the creation of new antimicrobial and antibacterial substances. Within the framework of the project GE-2506 "Scientific substantiation of the possibility of creating new bactericidal zeolite filter materials for purification-decontamination of water from various sources" financed by the International Science and Technology Center (ISTC), natural zeolites from the Dzegvi-Tedzami (Georgia), Chankanay (Kazakhstan) and Nor-Kokhb (Armenia) deposits [1] were studied; the samples were pre-calcined to temperatures preserving the zeolite structure [2] or pre-treated with hydrochloric acid with a concentration of up to 2 mol/L [3], and then subjected to ion exchange reactions in solutions of silver nitrate, copper and zinc chlorides [4].

Testing of bacteriostatic activity was carried out by the Kirby-Bauer disk diffusion method using cultures of Gram-negative bacteria *Escherichia coli* and *Salmonella typhimurium*, Gram-positive bacteria *Staphylococcus aureus* and *Bacillus subtilis*, fungal pathogenic yeast *Candida albicans*, and a fungus *Aspergilus niger*. For Georgian zeolite it was found that preliminary heat treatment, despite the increase in copper content, does not improve the disinfectant properties of metal-containing samples.

Preliminary acid treatment as a result of dealumination reduces the content of bioactive metals compared to the untreated sample, while the activity of silver-containing heulandite in relation to staphylococci slightly increases, and the copper-containing form, while maintaining slightly lower activity in relation to E. coli and hay bacilli, as well as staphylococci, loses activity against salmonella.

Preliminary acid treatment has the greatest effect on the properties of the zinc-containing form: the activity against staphylococci and salmonella inherent in the untreated sample is preserved, and the activity against E. coli and hay bacilli, as well as fungal microorganisms, which is absent in the untreated sample, is initiated [5].

For Kazakhstani zeolite only the silver forms are effective against Gram-negative bacteria, staphylococcus and fungal microorganisms; the Zn form, obtained by preheating at 600 °C, is most active against *Bacillus subtilis*. For Armenian zeolite activity of silver forms against *Salmonella* increases after preheating the zeolite, and against black fungus the activity increases after calcination and acid treatment, in other cases the activity remains at the same level of the untreated sample or slightly decreases; neither acid nor heat treatments enhance the activity of copper forms, and in relation to *Salmonella* and black fungus, treatment deprives the untreated sample of activity; preliminary acid treatment imparts zinc forms with activity against Gram-negative bacteria, *Staphylococcus aureus* and *Candida albicans*, and also increases activity against *Bacillus subtilis*. Overall, the results obtained indicate a significant role of the zeolite matrix in the process of

inhibiting the growth of microorganisms.

Testing the antimicrobial activity of zinc-enriched samples using Colony Forming Unit assays of E. coli, staphylococcus and salmonella showed that the most effective against all three bacteria were the Georgian and Armenian samples, pre-treated with a 1 mol/L hydrochloric acid solution.

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### SUPRAMOLECULAR CONSTRUCTS OF LIDOCAINE COMPLEXES

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The structure of the local anesthetic and peripheral analgesic lidocaine (2-(diethylamino)-N-(2,6-dimethylphenyl)acetamide, C<sub>14</sub>H<sub>22</sub>N<sub>2</sub>O, Lid) includes a planar aromatic ring of 2,6-dimethylaniline and a flexible chain of N,N-diethylglycine. Using low-temperature single crystal X-ray analysis, we studied the structure of lidocaine-containing complex compounds of zinc(II) ((LidH)<sub>2</sub>[ZnCl<sub>4</sub>]), copper(II) ((LidH)<sub>2</sub>[ZnCl<sub>4</sub>]), iron(III) ((LidH)<sub>2</sub>[FeCl<sub>4</sub>]Cl), and cobalt(II) ((LidH)<sub>2</sub>[Co(NCS)<sub>4</sub>]H<sub>2</sub>O) [1-5], and found that in the crystalline state, the chain from the aromatic ring to the diethylamino group –C1–N11–C12(=O12)–C13–N14 in the protonated LidH<sup>+</sup> cations adopts a stable conformation. In general, the arrangement of atoms in the lidocaine cation chains of all studied complexes has the same character, although the values of the torsion angles differ. The aromatic ring and the oxygen atom O12 adopt a synperiplanar (C) conformation relative to the carboxamide N11–C12 bond, and the nitrogen atoms of the amido and amino groups N11 and N14 adopt a staggered antiperiplanar (T) conformation; the T conformation excludes the formation of the intramolecular N11–H···N14 hydrogen bond that exists in crystalline lidocaine, in which the nitrogen atoms adopt a C conformation.

Despite the fact that the torsion angle O12–C12–C13–N14 does not always satisfy the criterion of not exceeding  $\pm 30^{\circ}$ , in all cases an intramolecular hydrogen bond of N14–H14···O12 type is realized. At the same time, the hydrogen atom H14 and oxygen atom O12 participate in bifurcated intermolecular hydrogen bonds with the formation of a 10-membered ring ···O12–C12–C13–N14–H14···O12<sup>i</sup>–C12<sup>i</sup>–C13<sup>i</sup>–N14<sup>i</sup>–H14<sup>i</sup>···, where the superscript i denotes the atom's belonging to the LidH<sup>+</sup> cation of the neighbouring complex. This 10-ring contains two donors and two acceptors, and according to the Etter-MacDonald-Bernstein classification, such a supramolecular construct represents a zero-dimensional  $R_2^2(10)$  motif. The geometric center of the ring coincides with the middle of the straight line connecting two adjacent metal atoms and is the center of inversion.

The 10-membered  $R_2^2(10)$  ring is not the only zero-dimensional supramolecular construct in the studied lidocaine complexes. For example, in  $(LidH)_2[ZnCl_4]$  the supramolecular constructs of zero dimension are also  $R_{16}^{16}(70)$  rings, which include two  $R_2^2(10)$  motifs and six zinc atoms, while the chains  $C_4^4(16)R_2^2(10)$ , formed by intermolecular hydrogen bonds of the N–H···Cl type and including one  $R_2^2(10)$  ring and two zinc atoms, are considered to be one-dimensional supramolecular constructs. The combination of  $R_{16}^{16}(70)$  rings into honeycomb-like spatial structures forms two-dimensional supramolecular constructs lying in planes making a dihedral angle of  $40.3^\circ$  with the **bc** plane and located at a distance of 6.25 Å from each other.

In the cobalt thiocyanate-N complex, along with the  $R_2^2(10)^{i \leftrightarrow j}$  rings (the second superscript  $i \leftrightarrow j$  denotes the connection between the complexes i and j), 10-membered rings are formed with the participation of water molecules forming hydrogen bonds with sulfur atoms. Such ring (-O1W-H1A···S4-C4-N4-Co1-N2-C2-S2···H1B-) contain one donor (oxygen atom O1W) and two acceptors (S2 and S4) and can be designated as the  $R_1^2(10)^1$ , where the second superscript 1 denotes the inclusion of a "central" cobalt atom Co1 in this ring. Zero-dimensional ring motifs are included in chains connecting neighboring complexes:  $\mathbf{C}^{1 \leftrightarrow ii} = R_1^2(10)^{1 \dots H111-N111-R_2^2(10)^{1 \leftrightarrow ii}-N111^{ii}-H111^{ii}\dots R_1^2(10)^{ii}$  (symmetry code ii: -x+2, -y+1, -z; (iv) -x+1, -y+2, -z+1),  $\mathbf{C}^{1 \leftrightarrow iv} = R_1^2(10)^1-N1-C1-S1\cdot··H211-N211-R_2^2(10)^{1 \leftrightarrow iv}-N211^{iv}-H211^{iv}\dots S1^{iv}-C1^{iv}-N11^{iv}$ 

 $R_1^2(10)^{iv}$  (iv: x+1, y, z); chains form endless tapes and layers, one- and two-dimensional supramolecular constructs, respectively.

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# SYNTHESIS OF 1,2-BIS(2-PHENYL-1H-INDOL-3-YL)ETHENE (BPIE) BY McMURRY REACTION

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Multiple derivatives of indole are characterized with high values of Stokes shift and consequently, the potential of luminescence. Therefore, their use is promising in sensors of electronic devices. Besides, some of the derivatives of 2-Arylindoles have high triplet energy that makes them promising in terms of their use as host materials in phosphorescent organic light-emitting diodes due to achieved high quantum efficiencies. The goal of our work was to synthesize luminophore systems containing 2-phenylindole ring, to determine the optical conditions for the olefination reaction, the physicochemical characterization of the attained products. The synthetic routes for the synthesis of the twin derivatives of 2-phenylindole are shown in Scheme 1.

the formylation of the 2-phenyl-indole systems were conducted, according to the Vilsmeier-Haack reaction in dimethylformamide in the presence of phosphorus oxychloride. Formyl products (2a-c) were olefination by McMurray reaction.

In order to study the luminescent *properties* of the synthesized compound 3a, its electronic spectra were investigated for a freshly prepared solution (c=0.01 mg/ml, chloroform), before and after the irradiation with UV rays, at 30 and 60 minutes intervals. The absorption maximum of the sample taken before the irradiation appeared at 375 nm. After 30 minutes UV irradiation, the absorption maximum shifted towards the short-wave region at 296 nm, and after 60 minutes – at 293 nm. These changes recorded in the electronic spectra confirmed the luminophore properties of the compound 3a.

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# RESEARCH OF BIOINKS FOR 3D-BIOPRINTING TECHNOLOGY BASED ON BIOLOGICALLY ACTIVE HUMIN-BIOPOLYMER HYDROGELS MODIFIED WITH LUMINOUS COAL DERIVATIVES

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Over the past decade, 3D bioprinting technologies have developed rapidly, representing a promising direction in obtaining artificial biological organs and regenerative and restorative medicine. 3D bioprinting can solve many serious transplantation problems and, compared to traditional medical technologies, makes it possible to produce individual, personalized tissue constructs, artificial joints, cartilage, and organs.

This work studied creating bioinks for 3D bioprinting technology based on biocompatible, environmentally safe humic-biopolymer materials [1]. As a hydrogel base for obtaining bioinks for 3D bioprinting, alginate-gelatin biopolymer systems modified with calcium salts of humic acids of brown coal (humates) were investigated.

The work studied the gelation processes and features of the rheological properties of biologically active hydrogel humin-biopolymer materials for 3D bioprinting technology. It was proven that using the polysaccharide-alginate-protein-gelatin system to create bioinks for 3D bioprinting technology allows optimizing one's own complex of biologically active hydrogel humin-biopolymer materials. With the help of rheological, microscopic, and thermodynamic studies, the strengthening of the humin-biopolymer hydrogel was revealed when it was modified with calcium salts of humic acids of brown coal due to crosslinking of polymer molecules with calcium ions, expansion of nanocrystalline areas, and an increase in the size of nanocrystals. It is shown that partial replacement of the polysaccharide sodium alginate with the protein gelatin allows creating a hydrogel system characterized by a significantly lower ability to ionotropic gelation by calcium ions or a complete absence of this ability, can cause a significant change in the porous structure of hydrogels, and the complex of structurally dependent properties of mixed hydrogels will be determined by their polymer composition.

It has been proven that biologically active biopolymer hydrogels modified with calcium humates for 3D bioprinting technology are viscous and thermostable (have a gel-sol transition temperature in the range of 55-60 °C), therefore, they are promising materials for creating bioinks for 3D bioprinting technology.

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# RUBBER COMPOUNDING BY PERIODIC AND CONTINOUS METHODS – PRELIMINARY INVESTIGATION

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Modern rubber industry is increasingly faced with the challenge of finding new methods of rubber compounding, which combine high quality of obtained products with production efficiency and limited impact on the environment. Generally, production of rubber compounds can be carried out periodically and continuously. The periodic methods involve the entire mixing and production process taking place in separate, closed cycles – each task is performed individually, and after it is completed, the device prepares for the next cycle. This allows for precise control of composition and quality, but it requires more human labor and longer production time. On the other hand, the continuous methods of rubber compounds based on the continuous supply of raw materials and the collection of the finished mixture. This approach is relatively new field of research, which gaining more and more attention [1-3].

Comparison of advantages and disadvantages of rubber compounding via periodic and continuous methods is presented in Figure 1.

Rubber compounding via continuous methods supports automation of process and as a consequence its higher efficiency and repeatability. Therefore, considering current trends, rubber compounding by continuous methods is a promising approach for further studies towards sustainable development of rubber processing technologies and circular economy. In this work, preliminary results obtained in this field of research will be presented.

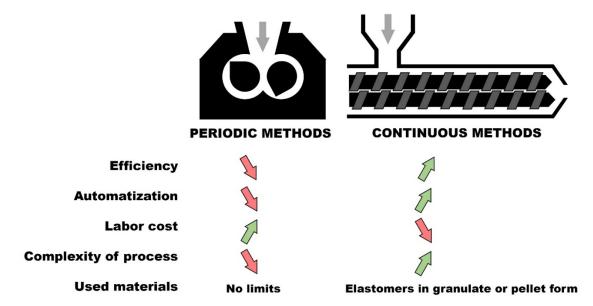


Figure 1. Pros and cons of rubber compounding by periodic and continuous method

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# PSEUDOPROTEIN-POLY(ETHYLENE GLYCOL) GRAFT COPOLYMERS FOR BIOMEDICAL APPLICATIONS

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Pseudoproteins (PPs) [1,2] are synthetic α-amino acid (AA) based polymers that mimic natural proteins [3]. Their backbones contain ester bonds together with other chemical linkages, including amide, urea, and urethane. The ester groups enable hydrolytic degradation (either nonspecific or enzyme-mediated), while the other linkages provide desirable mechanical and thermal properties [1,2]. Recent studies show that PPs can promote cell proliferation [4], underlining their promise in diverse biomedical applications [1-3]. However, most PPs are hydrophobic and poorly soluble in water. Introducing hydrophilicity can substantially broaden their functionality, enabling use as micellar drug delivery systems, surface-active agents, or stealth coatings for nanoparticles (NPs). A proven strategy to impart hydrophilicity is grafting poly(ethylene glycol) (PEG) onto the PP backbone, yielding amphiphilic copolymers [5, 6].

In this work, we synthesized biodegradable amphiphilic PEG-grafted PPs (PEG-PPs) via the cost-effective Michael addition of methoxy-PEG-thiol and methoxy-PEG-amine to leucine-based unsaturated copoly(ester amide) (FuL6)<sub>0.5n</sub>-(8L6)<sub>0.5n</sub>. The resulting PEG-PPs readily formed micelles (20.4 to 51.6 nm), and stabilized NPs (132.2 to 176.0 nm) prepared from poly(ester amide) 8L6 using the nanoprecipitation method, simultaneously coating the NPs with a protective PEG cloud. These findings demonstrate that PEG-PPs are versatile materials with potential applications as micellar drug carriers, surfactants, and protective nanoparticle coatings.

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Scheme 1. PEG-PP graft copolymers

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# DEVELOPMENT OF A NEW MODEL OXIDATION REACTION FOR KINETIC ANALYSIS OF POLYMERIC STABILIZERS-ANTIOXIDANTS

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The thermal and oxidative degradation of polymeric materials usually proceed according to the free-radical chain mechanism, which making enable to use the radical protectors- stabilizers and antioxidants to retard or even stop these disruptive reactions. These additives often operate either by deactivating the active radicals in the chain process or by decomposing intermediate products that provide a source of active radicals. In view of the continuous growth in the manufacture of various polymeric materials and substances for their stabilization, the testing of chemical compounds as stabilizers is actual and urgent problem to elucidate their potential activity and applicability. On the basis of last achievements in the field of chain oxidation processes a set of kinetic methods for the rapid and reliable quantitative assessment of various chemical compounds as potential stabilizers for polymers should be proposed.

The present work reports on elaboration of model liquid-phase aerobic oxidation reaction of cumene initiated by benzoyl peroxide (PBO) for determination of kinetic constants of potential stabilizers-antioxidants. PBO undergoes unimolecular and induced thermal decomposition to form free radicals. The rate constants for PBO decomposition in cumene were determined by measuring oxidation rate of initiated chain reaction (ORICR). The rate of oxidation was quantified by amount of absorbed oxygen using a laboratory gas-metric setup. The oxidation rate was determined by the tangent of the slope of the graphic curves (or straight lines) of oxygen absorption, which is represented by the equation  $dO_2/dt = W_{O2}$ . The model reaction of cumene aerobic oxidation initiated by PBO was launched at the rate of initiation  $W_i = 6.8 \cdot 10^{-8} \text{ Ms}^{-1}$ , T=333K,  $Po_2 = 0.2 \text{ Bar} (10^{-3} \text{ mol } O_2 \text{ I}^{-1})$ ]. It was established by the experiments that the reaction proceeds with a steady rate and may be represented by the following scheme:

### Scheme 1

Chain nucleation: generation of **R** radicals (**W**<sub>i</sub> is initiation rate)

rH (BPO)  $\rightarrow$  radicals of initiator  $r^{\bullet}$  and  $rO_2 \bullet (k_i) \rightarrow$  cumylalkyl radicals  $R^{\bullet}(k_1)$  [1]

Chain propagation:  $\mathbf{R}^{\bullet} + \mathbf{O}_2 \to \mathbf{RO}_2^{\bullet}$  (rate constant  $\mathbf{k}_2$ ) [2]

 $RH + RO_2 \bullet \rightarrow ROOH + R \bullet \text{ (rate constant } k_3\text{)}$  [3]

Chain termination:  $2 \text{ RO}_2 \bullet \rightarrow \text{ inactive products (rate constant } \mathbf{k}_6)$  [6]

with RH: cumene,  $R^{\bullet}$ : cumylalkyl radical,  $RO_2^{\bullet}$ : cumylperoxy radical, ROOH: cumylhydroperoxide, rH: initiator

For the scheme 1 the reaction rate is described as:

$$W_{02} = W_i^{\frac{1}{2}} k_3 k_6^{-\frac{1}{2}} [RH] = \{k_i [rH]\}^{\frac{1}{2}} k_3 k_6^{-\frac{1}{2}} [RH] = \{ek_d [rH]\}^{\frac{1}{2}} k_3 k_6^{-\frac{1}{2}} [RH]$$
 /1/

with:  $W_{02}$  – rate of initiated oxidation,  $W_i$  - initiation rate,  $k_3$  and  $k_6$  - the rate constants,

[RH] - concentration of cumene,  $\mathbf{k_i}$ - rate constant of initiation,  $\mathbf{e}$  -yield of radicals,  $\mathbf{k_d}$  -rate constant of initiator decomposition. From Equation /1/ the generated rate of initiation  $\mathbf{W_i}$  and rate constant  $\mathbf{k_d}$  for PBO decomposition at 333K can be calculated according to the measured oxidation rate and known rates for the cumene oxidation reaction:

$$W_{02} = W_i^{1/2} k_3 [RH] / k_6^{1/2} = W_i^{1/2} 1.75 \times 6.9 / (1.84 \cdot 10^5)^{1/2} = W_i^{1/2} 12.075 / 429$$

 $W_i^{\frac{1}{2}} = 3.16 \cdot 10^{-3} / 12.075 = 2.61 \cdot 10^{-4}$  $W_i = k_i \ [rH] = ek_d \ [PBO] = 6.8 \cdot 10^{-8} \ Ms^{-1}$ 

Using yield of the PBO radicals e = 1.2 at 333K and  $[PBO] = 1.65 \cdot 10^{-2}$  M, the following value for the PBO decomposition rate constant can be calculated  $k_{d(333K)} = 6.8 \cdot 10^{-8}/1.2 \times 1.65 \cdot 10^{-2} = 3.4 \cdot 10^{-6}$  s<sup>-1</sup>

The kinetic constants obtained for the oxidation of cumene initiated by PBO allow to use this reaction as a model for quantitative determining the parameters of antioxidant activity of basic stabilizers of thermo-oxidative degradation of polymers.

# METAL-CARBON NANOCATALYSTS IN THE AEROBIC PEROXIDE OXIDATION OF DECAHYDRONAPHTHALENE

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The peroxide oxidation of hydrocarbons is considered as process of the present day exemplified by a number of advantages in terms of modelling nature-like technologies and industrial ecology.

Followed this framework the liquid-phase noncatalytic and catalytic aerobic-peroxide oxidation of decahydronaphthalene (decalin) was undertaken. The reactions were carried out in a barbotage flow glass oxidation reactor at the temperature range of 120-140°C for 3 hours. Decalin 98% (h.p.) and 33% hydrogen peroxide (H2O2) solution were used in the work. The amount of hydrogen peroxide introduced into the reaction was 20wt % to the initial amount of decalin. In the case of the catalytic reaction, iron-containing multi-walled carbon nanotubes (Fe@MWCNT) synthesized by pyrolysis of hydrocarbon feedstock (cyclohexane) in the presence of ferrocene (precursor-catalyst) followed by chemical vapour deposition (CVD method) were used as a catalyst. As a result of the CVD synthesis process, Fe atoms in  $\alpha$  and  $\gamma$  crystal modifications and Fe carbides seem to be encapsulated by the hollow cylindrical carbon structures, so that they are located in the internal cavities of the final formed finished nanotubes.

The sequence of formation of oxidation products was traced and it was found that the maximum formation of carboxylic acids at a fixed reaction time falls at 130 degrees Celsius. Characteristic parameters of oxidation products - acid number (AN) and active oxygen (AO) content in oxidate and condensate were determined. IR spectrum of the oxidate, an absorption band of the valence vibrations of the C=O bond is observed in the region of 1710 cm<sup>-1</sup>. The asymmetric valence vibrational absorption bands of C-O bonds in carboxylate anions (COO-) are observed in the region of 1567 and 1447.7 cm<sup>-1</sup>, while the symmetric valence vibrational absorption bands of C-O bonds in carboxylate anions in the region of 1407, 1346 and 1306 cm<sup>-1</sup>. The oxidate also exhibited absorption bands of non-planar deformation vibrations of O-H bonds: δOH= 971-853cm<sup>-1</sup>. vOH = 3408 cm<sup>-1</sup> is a broad intense absorption band of valence vibrations of dimer or associative states of O-H bonds in carboxyl groups. Characteristic absorption bands of aromatic nuclei at 1570.51 cm<sup>-1</sup>, 1450 cm<sup>-1</sup> and 1405 cm<sup>-1</sup> and valence vibrations of C-H bonds of alkanes and cycloalkanes in the region of 2919cm<sup>-1</sup>, 2851cm<sup>-1</sup> are also observed.

The results of chromatography-mass spectroscopic analysis showed the formation of a number of a wide range of different oxygen-containing compounds. It was found that chain reactions of oxidation proceed with the destruction of the framework of naphthenic cycles and are accompanied by processes of oxidative dehydrogenation, functionalization and alkylation of intermediate molecular fragments. Despite hydrogen peroxide is a hydroxylating agent, the influence of air oxygen as a co-oxidizer allows to bring the reaction to the stage of acids formation. Total conversion of initial hydrocarbons is about 70-80%. As a result of the peroxide oxidation, unsubstituted and alkyl-substituted saturated (C<sub>6</sub>.C<sub>18</sub>), cyclic (C<sub>6</sub>-C<sub>14</sub>), unsaturated linear (C<sub>7</sub>-C<sub>12</sub>), aromatic (C<sub>12</sub>) hydrocarbons; primary aliphatic (C<sub>3</sub>-C<sub>12</sub>), alicyclic (C<sub>6</sub>) and aromatic (C<sub>10</sub>) alcohols; aliphatic (C<sub>10</sub>) and alicyclic (C<sub>4</sub>-C<sub>10</sub>) ketones, aliphatic (C<sub>4</sub>-C<sub>12</sub>) and alicyclic (C<sub>6</sub>) aldehydes; aromatic acids (C<sub>6</sub>) and oxyacids (C<sub>8</sub>-C<sub>9</sub>), fatty acids (C<sub>5</sub>) and oxyacids (C<sub>8</sub>), and alicyclic (C<sub>11</sub>-C<sub>12</sub>) acids have been formed.

From existing experience - Fe@MWCNT as oxidation catalyst was applied for the system, containing water solution of hydrogen peroxide [1]. It was expected the active behavior of the heterogenous catalysts at condition of intensive stirring. Results obtained have confirmed the applicability of the carbon nanocatalyst as

a phase transfer moiety – the formation of carboxylic acid occurs at early stage of the peroxide oxidation. Moreover, the experiments to learn a turnover capacity of the Fe@MWCNT give also positive results.

Despite the autoxidative nature of the reaction, the yield of monocarboxylic acids is significantly high  $(\sim 20\%)$ , which can be used for targeted processing of complex hydrocarbon feedstock.

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# AEROBIC OXIDATION OF A DIESEL PARAFFIN-NAPHTHENIC FRACTION CATALIYSED WITH TRANSITION METAL- CARBON NANOTUBES

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Carbon nanotubes (CNT) have been the subject of intense research due to their unique properties since their discovery. One of the valuable applications of CNT is nano-catalysis of oxidative transformations of organic substances. This field embraces also aerobic oxidation of petroleum hydrocarbons, which promise to solve the problem of selective output of targeted oxygen-containing products. However, these explorations are at the initial stage of study and require thorough development. The present work is focused on the determination of catalytic activity of multi-walled (MW) CNT in aerobic oxidation reaction of a diesel fuel paraffin-naphthenic fraction. Chromium clusters were deposited on the surface of Fe@MWCNT produced by CVD-synthesis. The nanotube samples were identified using TEM and X-ray diffraction technique and then applied for the aerobic oxidation of diesel paraffinic-naththenic fraction hydrocarbons. The mentioned fraction was isolated from diesel fuel and analyzed by GC-MS technique. It has been found that the fraction contains 60.782% aliphatic, 3.311% olefinic, 22.855% naphthenic hydrocarbons and 8.294% partial oxidation products. To determine the rate of the aerobic oxidation of paraffin-naphthenic fraction the gas-volume-metric setup was employed and kinetics of oxygen uptake at 80° and 130°C was studied. It was shown that the presence of a transition metal in the CNT's surface and channels play a key role to accelerate the oxidation (Figure 1)`

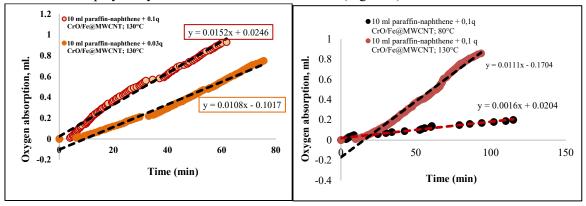


Figure 1. Kinetic dependences of oxygen consumption for a diesel paraffinic-naphthenic fraction aerobic oxidation in the presence of CrOFe@MWCNT(Cat.) admixtures.

The maximum catalytic activity of Cr-Fe@MWCNT is due to the direct, unimpeded contact between the Cr and the hydrocarbon substrate while use of Fe@MWCNT proceeds the oxidation in the diffusion field. A free radical mechanism scheme of the aerobic oxidation of hydrocarbons in the presence of Cr-Fe-containing carbon nanocatalysts is proposed.

These results may contribute to the nanodimensional catalysts dataabase for complete designing of industrial profile of chain oxidation processes.

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# CYCLOALIPHATIC EPOXY RESINS - MONOMERS OF HEAT- RESISTANT POLIMERS Budagova Rahila Nazim. Zevnalov Eldar Bahadur Oglu

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Previously, studies on the synthesis of alicyclic epoxyethers by interaction of alcohols, acids, amines, amino acids and epichlorohydrin followed by dehydrochlorination of chlorohydrins to epoxyethers have been carried out (1-4).

The reaction of 2,2,5,5-tetramethylolcyclopentanol and 2,2,6,6-tetramethylolcyclohexanol with ECH in the presence of alkali was investigated in order to obtain epoxy compounds containing a large number of epoxy groups and possessing increased heat resistance. In the course of the study it was found that the interaction of polyatomic alcohols with ECH in alkaline medium leads to polymerization reaction due to the large number of epoxy groups formed. To prevent the polymerization process, the polyatomic alcohols were first treated with acetic anhydride or acetic acid and then with ECH.

Depending on the epoxide and hydroxyl number content, a mixture of di- and tri-epoxy compounds is obtained. Synthesis of epoxy resins based on polyatomic alcohols was carried out at a molar ratio of alcohol: ECH = 1:5 in the presence of BF<sub>3</sub>O(C<sub>2</sub>H<sub>5</sub>)<sub>2</sub> in dioxane solvent at 80-90° C. After blocking with acetic anhydride, ECH was added dropwise and the reaction proceeded for 5-6 hours. Dehydrochlorination of the obtained chlorohydrins was carried out in the presence of powdered caustic KOH for 3 h. After washing, filtration and solvent removal, a viscous yellow colored cycloaliphatic resin was obtained. Similarly, a cycloaliphatic resin based on 2,2,5,5-tetramethylolcyclopentanol was synthesized according to the above methodology. After washing, filtration and solvent removal, viscous cycloaliphatic resins of yellow color were obtained, physicochemical parameters of which are given in table 1.

Name of epoxy resin	Exit,%	Epoxynumbe	Hydroxylnum	Hydrolyzedchl	Martensheat
		r, %	ber, %	orine,%	resistance
Epoxyresinof 2,2,5,5- tetramethylolcyclopentanol	95.4	18.5	1.28	0.42	310° C
Epoxyresinof 2,2,6,6- tetramethylolcyclohexanol	98.6	18.9	1.35	0.38	330° C

The synthesized viscous cycloaliphatic resins were subjected to curing with hexahydroftalic anhydride in the presence of accelerator-dimethylaminomethylphenol. After curing, the epoxy resins had a Martens heat resistance of 310-330°C. Synthesized epoxy resins can be used as monomers in the production of heat-resistant epoxy polymeric materials.

### **Acknowledgement:**

The author expresses his deep appreciation and gratitude to his scientific supervisor, Doctor of Chemical Sciences, Professor S.B. Zeynalov and the Institute of Catalysis and Inorganic Chemistry under the Ministry of Science and Education of the Republic Azerbaijan, for support and assistance in conducting this research.

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### SYNTHESIS AND STUDY OF A NANOCOMPOSITE ANTHELMINTIC

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Albendazole combined with copper sulfate ( $C_{12}H_{15}N_3O_2S \times CuSO_4$ ) represents an anthelmintic composite material that differs from standalone Albendazole (ABZ) by exhibiting higher stability, fewer side effects, and improved environmental compatibility. Based on theoretical calculations, suspensions of both components were prepared. The mixing process was carried out under constant stirring using a steam bath. The obtained composite was transferred, with a constant weight, into an airtight container. Below is a visual image of the synthesized anthelmintic sample.



Fig. 1. Synthesized Anthelmintic (ABZ × CuSO<sub>4</sub>)

The physiological activity of the composite anthelmintic against microorganisms was studied. It was determined that the anthelmintic exhibits selective antibacterial and stimulating effects. Using a scanning transmission electron microscope (NSX-100), the nanoscale dimensions of the sample were measured and found to be approximately 340 nm. The composite was also studied using X-ray fluorescence (XRF) analysis to determine the copper content and the purity with respect to possible impurities. Further research on the sample is ongoing using the CH Instruments, model CHI 660 F series potentiostat/galvanostat. The working electrode is platinum, the counter electrode is carbon, and the reference electrode is silver chloride, the solvent used is dimethyl sulfoxide - (DMSO).

### PLANETARY EXTRUDER IN RUBBER COMPOUNDING AND RECYCLING: POTENTIAL AND PERSPECTIVES

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The recycling of waste tire rubber (WTR) is a pressing environmental and technological challenge. Each year, millions of tons of used tires are generated worldwide, but current methods for their reuse remain insufficient. Due to the cross-linked structure of vulcanized rubber, conventional recycling routes are limited. Devulcanization, which partially breaks sulfur cross-links, has therefore emerged as a key strategy. It improves the compatibility of ground tire rubber (GTR) with virgin polymers, enabling the preparation of polymer-rubber blends with recycled GTR (rGTR). Thermomechanical devulcanization is particularly attractive, as it avoids chemical agents and can be scaled up for industrial applications [1].

The planetary roller extruder represents a promising alternative. Its unique screw geometry provides high shear, long residence time, precise temperature control, and effective degassing [2]. These features are advantageous when processing viscous compounds or materials containing fillers. Recent studies suggest that PRE can achieve comparable or even superior performance to conventional mixers with lower energy consumption [3].

This work is focused to develop an energy-efficient, scalable, and sustainable route for rubber recycling, supporting the principles of the circular economy.

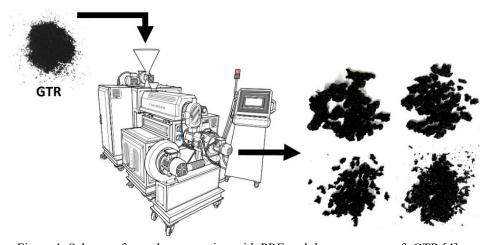


Figure 1. Scheme of sample preparation with PRE and the appearance of rGTR [4]

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# ZINC-CONTAINING NANOCOMPOSITES BASED ON A MIXTURE OF HIGH AND LOW PRESSURE POLYETHYLENE

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Among the priority strategic directions for the development of technologies and the creation of new generation materials, a significant role is given to the creation of composite materials for structural purposes on a polymer basis, including those containing nanosized fillers [1,2]. Currently, nanoscale layered silicate or metal-containing fillers are of great interest among developers of polymer materials, which, even with small amounts in the polymer matrix, lead to an increase in the modulus of elasticity, strength, increased thermal-, heat resistance and fire resistance, reduced gas permeability of the material. Due to their unique properties, metal oxide nanoparticles based on metal polymers are widely used in radio and optoelectronics as magnetic, electrically conductive and optical media.

The presented work is devoted to the obtaining and study of the properties of nanocomposites based on a mixture of high-pressure polyethylene (LDPE) and low-pressure polyethylene (HDPE) using zinc-containing nanoparticles stabilized by polymer matrices of high-pressure polyethylene (LDPE) and maleinized LDPE (M-LDPE) as nanofillers (NF). Nanocomposite polymer materials were obtained by mixing LDPE and HDPE with zinc-containing nanofillers on laboratory rollers at a temperature of 150 ° C for 15 minutes. For mechanical testing, the obtained mixtures were pressed in the form of plates with a thickness of 1 mm at 190 ° C and a pressure of 10 MPa for 10 minutes. The ratio of the components of the composition (wt%): LDPE/HDPE/NF=50/50/(0;0.3;0.5;1.0).

The physical- mechanical, thermophysical, thermal, and optical properties of the obtained nanocomposites were studied. The strength and deformation characteristics, as well as the thermal-oxidative stability of the composites based on a mixture of high- and low-pressure polyethylene with the addition of fillers containing zinc oxide nanoparticles stabilized by a polymer matrix of LDPE or M-LDPE, were improved; this is apparently due to the interphase interaction of zinc-containing nanoparticles with the components of the polymer composition.

Small amounts of the given nanofillers introduced into the polymer play the role of structure formers - artificial crystallization nuclei, which contributes to the emergence of a fine-spherolitic structure in the polymer, characterized by improved physical- mechanical and thermal properties of the resulting nanocomposite.

One of the main characteristics of wide-bandgap semiconductors such as ZnO is the bandgap width (E=3.37 eV). To determine the bandgap width, UV-Vis absorption spectra of the obtained nanocomposite samples were recorded and reconstructed in Tauc plot. The obtained data show that the introduction of ZnO nanoparticles into the composition of the studied nanocomposite samples leads to a shift in the absorption band edge to the visible region and demonstrates optical absorption in the UV-visible range E<3 eV (2.1-2.3) eV.

Additional scattering may occur when zinc nanoparticles are added, which can also be used to control the light properties of the material. Zinc nanoparticles can exhibit optical activity or fluorescence, which opens up opportunities for the creation of new optoelectronic devices. These properties are useful for creating sensors, lasers, and other high-tech devices.

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# RATIONAL DESIGN AND MECHANISTIC INSIGHTS INTO NOVEL METALLODRUGS FOR CANCER THERAPY

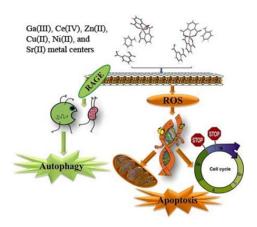
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### Text of abstract:

The development of metal-based anticancer agents represents a promising frontier in pharmaceutical research, offering alternatives to traditional platinum-based chemotherapeutics. This review presents recent advances in the design, synthesis, and mechanistic characterization of novel metallodrugs containing pyridine-2,6-dicarboxylate derivatives and various extra-nuclear cations. Through systematic investigation of complexes incorporating Ga(III), Ce(IV), Zn(II), Cu(II), Ni(II), and Sr(II) metal centers, we demonstrate how structural modifications significantly impact cytotoxicity profiles and cellular uptake mechanisms. Our comprehensive studies across multiple cancer cell lines (A431, SW480, BEL-7404, A375, HT29, MCF7, PC3, HCT-116) reveal IC<sub>50</sub> values ranging from 0.56 μM to 17.94 μM for the most potent compounds, with remarkable selectivity indices favoring cancer cells over normal cell lines. Mechanistic investigations employing flow cytometry, western blotting, and fluorescence microscopy reveal that these metallodrugs induce cancer cell death through multiple pathways including intrinsic and extrinsic apoptosis, autophagy, cell cycle arrest, and reactive oxygen species (ROS) generation. Notably, the choice of central metal ion and extra-nuclear cations critically determines the predominant cell death pathway, with some complexes inducing bimodal cell death mechanisms. The distorted octahedral geometry observed in most active complexes, combined with enhanced cellular uptake compared to metal salts alone, supports their therapeutic potential. These findings contribute significantly to the rational design of next-generation metallodrugs with improved efficacy and reduced side effects for cancer treatment.



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# SYNTHESIS AND BIOLOGICAL ACTIVITY OF ANALOGUES OF BIOPOLYMERS FROM PLANTS OF BORAGINACEAE FAMILY

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Oligomeric analogues of natural poly[2-methoxycarbonyl-3-(3,4-dihydroxyphenyl)oxirane] (PMDHPO), isolated from plants *Anchuza Italica* (AI), *Symphytum Grandiflorum* (SG) and *Borago officinalis* (BO) (Boraginaceae family) were synthesized by chemoenzymatic synthesis using lipase *Candida rugosa*. Ring opening polymerization of 2-methoxycarbonyl-3-(3,4-dibenzyloxyphenyl)oxirane (1) by lipase leads to the benzylated oligomeric analogue (2), deprotection of which gives true analogue of natural polymer - PMDHPO [1]. Antibacterial assessment of natural polyether from different species of Boraginaceae family AI, SG, BO and synthetic polymers, PMDBPO (2), PMDHPO (3) and fully methylated analogue of PMDHPO - poly[2-methoxycarbonyl-3-(3,4-methoxyphenyl)oxirane] PMDMPO (4), synthesized by us early [2] revealed, that only PMDHPO showed antimicrobial activity against pathogenic strains *S.aureus* ATCC 25923 and *E.coli* ATCC 25922 at the concentrations used (Table 1). PMDHPO would be an interesting target for diverse biological tests.

Scheme 1. synthesis of PMDHPO: a) C. rugosa lipase, toluene, 80°C, 7 days b) Pd/C, H<sub>2</sub>, THF/EtOH

**Table 1.** Antibacterial activity reported in terms of MIC against bacterial strains grown as planktonic cell cultivation on MHB.

Strains	PMDHPO MIC (μg/mL)
S. aureus ATCC 25923	100
E. coli ATCC 25922	100
P. aeruginosa ATCC 15442	No Activity.
E. faecalis ATCC 29212	No Activity

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