Dedicated to the 70th Anniversary of

Academician, Professor Gheorghe DUCA

The 7th International Conference

ECOLOGICAL AND ENVIRONMENTAL CHEMISTRY-2022

March 3-4, 2022, *Chisinau, Republic of* ***Moldova***

ABSTRACT BOOK

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Dedicated to the 70th Anniversary of Academician, Professor Gheorghe DUCA.

Editorial Production:
Dr. Viorica GLADCHI, Moldova State University
Dr. Lidia ROMANCIUC, Institute of Chemistry

Note!
The Authors of Abstracts submitted to the EEC-2022 Conference take full responsibility for their content/originality and for English language!

The Abstract Book covers the short resumes of the latest research results presented by local and international scientific community to the 7th International Conference: "Ecological and Environmental Chemistry", which is continuation of a series of successful conferences organized in 1995, 2002, 2005, 2008, 2012 and 2017, being supported by UNESCO, MFGS, CRDF/MRDA, ONRG, as well as Moldovan R&D organizations: Institute of Chemistry, Chemical Society of the Republic of Moldova, Department of Ecological and Industrial Chemistry of Moldova State University, Moldovan Research and Development Association, etc.

The EEC-2022 Conference is organized within the Moldova's State Program (2020-2022), Research Project ”RedoxPro”, Nr. 20.80009.5007.27, “Physico-chemical mechanisms of redox reactions with electron transfer involved in the vital, technological and environmental systems”.

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EEC-2022 PARTICIPANTS WELCOME

Dear EEC-2022 Conference Participants,

It is my honor to welcome you at the 7th International Conference on Ecological & Environmental Chemistry-2022, which became the good tradition, ensuring continuation of series of successful events in this field organized in 1985, 1995, 2002, 2005, 2008, 2010, 2012 and in 2017 in Chisinau, Republic of Moldova.

Ecological and Environmental Chemistry is progressively developing both in the Republic of Moldova and the other countries worldwide attracting the experienced and young scientists, specialists and experts to exchange the novel ideas and present the latest achievements and establish the partnerships in this field. Considering various approaches and development perspectives in Ecological and Environmental Chemistry, which appear in different countries, the EEC 2022 Conference will serve an arena for discussions and interconnections related to scientific approach in research of ecological, physical-chemical and biochemical processes in natural ecosystems and their impacts on human health and environment.

Due to the permanently increasing relevance and importance of theoretical and practical issues presented at the EEC-2022 Conference, this Abstract Book has gathered the scientific results presented by over 250 scientists from **Armenia, Algeria, Azerbaijan, Belarus, Brazil, Canada, China, Czech Republic, Finland, France, Georgia, Germany, Hungary, Israel, Italy, Jordan, Kazakhstan, Korea, Kuwait, Moldova, Montenegro, Morocco, Poland, Romania, Russia, Switzerland, Turkey, Ukraine, USA, Uzbekistan, Vietnam**, etc. and will represent the valorous scientific input in this field for our followers for many years afterwards.

I would like to express the profound acknowledgement to the Institute of Chemistry, Chemical Society of the Republic of Moldova, Moldova State University, Technical University of Moldova, Moldovan Research and Development Association and other organizations which offered the substantial support and ensured the combination of real and virtual participation at the EEC-2022 Conference.

Academician, Professor Gheorghe DUCA,

President of the Chemical Society of the Republic of Moldova,

Head of the Research Centre of Physical and Inorganic Chemistry, Institute of Chemistry

Academician, Professor Gheorghe DUCA

Biography Resume

Academician, Professor Gheorghe DUCA is author of 455 research papers, 143 co-edited books, 166 patents, 51 monographs, 13 manuals, 549 articles on science popularization and over 490 conference presentation materials.

Research interests: chemical kinetics and catalysis; physical-chemical mechanisms of redox processes with electron transfer; ecological and environmental chemistry; kinetics, thermodynamics and mathematical modeling of ecological systems; natural water self-purification; water treatment technologies; chemical risk assessment.

During 50 years of scientific, pedagogical and administrative activity, Acad. Gh. DUCA has been dealing with the following activities:

- developed and delivered the courses of lectures on physical chemistry, chemical technology, ecological chemistry, physical-chemical research methods, chemical risk assessment, kinetics and thermodynamics of ecological systems at the universities of Moldova (*Chisinau, Balti, Comrat, Cahul*), Italy (*Rome, Torino*), USA (*Austin TX, Riverside CA*), UK (*Newcastle),* China (*Chengdu*), Switzerland (*Zurich*), Hungary (*Budapest*), Czech Republic (*Prague*), Romania (*Iași, Timișoara, Cluj, Bucharest*).

- supervised the research activity of 31 doctors and habilitated doctors in sciences, including in cooperation with the National Institute of Applied Sciences, Lyon, France (1998), “Gh.Asachi” University of Iași, Romania (1998). Currently, under his supervision are 2 Postdocs and 8 PhD students.

- during 1992-2006 he was the President of the Scientific Council for the theses of doctor and habilitated doctor in chemical sciences, in 2019-2021 - President of the Scientific Council of doctoral schools of the "D. Cantemir" State University. Currently he is a member of Expert Commission of the National Agency for Quality Assurance in Education and Research (ANACEC), has been several times appointed as a referent and member of the Councils for the defense of doctoral theses in science in Moldova, Romania, France and Russia.

- within the 14-years period, he has headed the Academy of Sciences of Moldova, being responsible for the science and innovation sector administration and management in accordance with the Code of Science and Innovation of the Republic of Moldova.

- participated in the Central Authority governance, in a quality of Minister of Environment and Regional Development of the Republic of Moldova (for 3 years) and a Member of Parliament of the Republic of Moldova and Head of the Parliamentary Commission for Science, Education, Culture, Youth, Mass-media and Sport (for 3 years).

- founded the Department of Industrial and Ecological Chemistry (1992) and Research Center of Ecological and Applied Chemistry, (1992) within the State University of Moldova, Faculty of Ecology, Free International University of Moldova (1992), Research Center for Physical and Inorganic Chemistry, Institute of Chemistry (2006), Lyceum for Gifted Children (2007), University of the Academy of Sciences of Moldova (2007), "Terra Nostra" Non-Governmental Organization for Environmental Protection (1992), "MRDA" Moldovan Research and Development Association (2000), etc.

- founded the journals: "Environment" (2002), "Chemical Journal of Moldova" (2006), "Academos" Journal of Science, Innovation, Culture and Arts (2005).

- held the position of Editor-in-Chief of “Chemical Journal of Moldova” and Editorial Advisory Board Member of “Ecological Chemistry Journal”, Russia; “Environmental Engineering and Management Journal”, Romania; “Chemistry and Technology of Water” Journal, Ukraine.

- supervised the numerous governmental programmes, national projects, international projects awarded by NATO, SOROS Foundation, “FP7 and Horizon 2020” EU Framework Programmes, etc.

- on behalf of the Government of the Republic of Moldova conducted the preparatory negotiations and signed the International Cooperation Agreement with the American Civilian Research and Development Foundation U.S.CRDF (2000), Memorandum of Understanding between the European Commission and the Republic of Moldova for association to the Seventh Framework Programme of the European Union for Research, Technology Development and Demonstration Activities (2011), Association Agreement of the Republic of Moldova to the “Horizon 2020” European Union Framework Programme for Research and Innovation (2014), as well as signed over 45 bilateral Agreements between the Moldovan Academy of Sciences and relevant scientific academies and organizations from over 25 countries around the world.

- organized numerous international scientific conferences on Ecological and Environmental Chemistry (1985, 1995, 2002, 2005, 2008, 2010, 2012, 2017, 2022), as well as international events on science, education and innovation management (1995-2020).

The memberships of Acad. Gh. Duca are the following:

- *National Delegate to the European Academy of Sciences and Arts (2021-2024,*
- *Board of Directors Member of the European Academy ALLEA (2018-2020),*
- *Bulgarian Academy of Sciences and Arts (2018),*
- *Academy of Sciences of Kazakhstan (2016),*
- *Honorary Member of the Balkan Academy of Sciences (2013),*
- *Board of Directors Member of the Joint Research Center - JRC of the European Commission (2013),*
- *Doctor Honoris Causa of the Academy of Sciences of the Russian Federation (2012),*
- *Foreign Member of the National Academy of Sciences of Ukraine (2009),*
- *Romanian Academy (2007),*
- *Romanian Academy of Agricultural and Forestry Sciences (2006),*
- *Academy of Sciences and Arts of Montenegro (2006),*
- *Board of Directors Member of the International Fund for Cooperation and Partnership of the Black Sea and Caspian Sea - BSCSF (2004).*

Acad. Gh. Duca was awarded with numerous distinctions, diplomas, and medals, such as:

- *Knight of the Order of Inventions, Belgium Kingdom (2003),*
- *Cross of the Commander of the Honour Order, Poland (2004),*
- *Gold Medal for Progress and Distinctive Activity, Brussels (2005),*
- *Order of Cultural Merit, Romania (2006),*
- *Gold Medal "N.S. Kurnakov", Russian Federation (2007),*
- *Socrates International Award, Oxford, United Kingdom (2009),*
- *Silver Medal of the Chinese Innovators Association (2010),*
- *Gold Medal of "EUROINVENT", Brussels (2011),*
- *Order of the Republic of Moldova (2011),*
- *Award for outstanding achievements in the field of European integration of the Organization for Economic Cooperation in the Black Sea Countries (2013),*
- *UNESCO Medal (2014),*
- *Knight Order of the Romanian Crown (2015),*
- *International Organization for Science and Engineering Management ICMSEM, Japan (2017),*
- *European Innovation Award and Diploma of Commander of the European Commission, Belgium (2018),*
- *Advanced Grand Prize for Management of Science and Engineering Management, China (2020),*
- *Prize of the Academy of Sciences of Moldova in Chemistry –“N.Garabalau” (2021), etc.*

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- *Chemical Society of the Republic of Moldova*
- *Institute of Chemistry*
- *State University of Moldova, Faculty of Chemistry and Chemical Technology, Department of Industrial and Ecological Chemistry*
- *Technical University of Moldova, Department of Oenology and Chemistry, Faculty of Food Technologies*
- *Institute of Ecology and Geography*
- *Academy of Sciences of Moldova*
- *Moldovan Research and Development Association*
- *"Constantin Stere"University of European Political and Economic Studies*

RESPONSIBLE FOR TOPICS

	Sections	Name	Affiliation
A	*Fundamental Aspects of Ecological and Environmental Chemistry*	Dr. Hab. **Olga COVALIOVA,** Dr. **Iolanta BALAN,** Dr. **Lilia ANGEL, Crina VICOL**	*Insitute of Chemistry*
B	*Water Science and Society*	Acad., Prof. **Tudor LUPASCU**, Dr. Hab. **Maria GONTA**, Dr. **Raisa NASTAS,** **Elena CULIGHIN**	*Institute of Chemistry,* *Moldova State University*
C	*Climate Change and Atmospheric Chemistry*	Dr. **Vasile STEGARESCU,** Dr. **Ana DONICA,** Dr. **Inga ZINICOVSCAIA**	*Institue of Ecology and Geography ,* *Institute of Chemistry*
D	*Food, Soil and Waste Chemistry*	Prof., Dr. Hab. **Rodica STURZA**, Dr. **Iurie SUBOTIN,** Dr. **Ecaterina COVACI**	*Technical University of Moldova*
E	*Ecological and Environmental Chemistry within the Knowledge Triangle: Research-Education-Innovation*	Dr. **Viorica GLADCHI,** Dr. **Elena BUNDUCHI,** Dr. **Vladislav BLONSCHI,** **Angela LIS**	*Moldova State University*

The Ecological and Environmental Conferences Topics Overview 1995-2022

Year	Conference Topics
1995 – The first International Conference on Ecological Chemistry *(Moldova)*	*Natural Self-Purification Processes* *Transport and Fate of Pollutants in Ecosystems* *Remedial Measures to Degrade or Immobilize Pollutants Chemically or Biologically* *Impact of Chemical Pollutants and Risk Assessment* *Ecological Policy, Law, Education and Training* *Environmental Engineering* *Environmental Control and Monitoring*
2002 - 2nd International Conference on Ecological Chemistry *(Moldova)*	*Ecological Chemistry of Water/ Electochemistry and Ecological Chemistry* *Ecological Chemistry of Atmospheric Air* *Soil Contamination and Waste Management* *Environmentally Friendly Agricultural Technologies* *Chemical Risk Assessment and Health* *Pollution Prevention*
2005 - 3rd International Conference on Ecological Chemistry *(Moldova)*	*Ecological Chemistry of Water* *Ecological Chemistry of Air* *Ecological Chemistry of Soil, Waste Management and Cleaner Production* *Chemical Risk Assessment* *Ecological Policy and legislation* *Electrochemistry and Ecology*
2008 - 4th International Conference and NATO ARW: The Role of Ecological Chemistry in Pollution Research and Sustainable Development *(Moldova-Germany)*	*Organic Pollutants and POPs in the Environment: Occurrence, Fate and Prevention Measures* *Water Pollution and Wastewater Treatment* *Soil Pollution and Prevention* *Risk Assessment, Mitigation Measures and Environmental Awareness*
2010 – International Conference “Water: History, Resources, Perspectives *(Moldova-Austria)*	*Physics, Chemistry and Evolution of Water* *The Cultural Role of Water* *Water and Technology* *Environmental Aspects of Water* *Water and Watercourses of Moldova*
2012 - 5th International Conference on Ecological Chemistry *(Moldova)*	*Ecological Chemistry of Water* *Ecological Chemistry of Atmosphere* *Ecological Chemistry of Soil* *Ecological Chemistry and Healthy Lifestyle* *Ecological Chemistry and Sustainable Development*
2017 - 6th International Conference on Ecological and Environmental Chemistry *(Moldova)*	*Ecological Chemistry* *Environmental Chemistry and Engineering* *Green Chemistry* *Ecological and Environmental Aspects in Chemical Research and Education* *Young Scientists Research in Ecological and Environmental Chemistry*
2022 - 7th International Conference on Ecological and Environmental Chemistry *(Moldova)*	*Fundamental Aspects of Ecological and Environmental Chemistry* *Water Science and Society* *Climate Change and Atmospheric Chemistry* *Food, Soil and Waste Chemistry* *Ecological and Environmental Chemistry within the Knowledge Triangle: Research-Education-Innovation*

EEC-2022 Background

The 7th International Conference **ECOLOGICAL & ENVIRONMENTAL CHEMISTRY 2022** (EEC-2022) provides opportunities to exchange with the latest ideas, to present and discuss the recent results on physical-chemical and biochemical aspects of processes occurring in the environmental compartments – soil, air and water, and promising approaches of sustainable development including engineering and modeling, as well as social and educational implications. The aim of the conference is to encourage and facilitate the interdisciplinary communication among the scientists, engineers, economists, teachers and professionals working on environmental issues and sustainable development.

The 7th International Conference **ECOLOGICAL & ENVIRONMENTAL CHEMISTRY 2022** is an important international event, which attracts scientists and engineers from Europe, NIS, U.S.A. and other countries.

Ecological Chemistry started to develop in Moldova in 1985 when the First International Ecological Chemistry School was held. For more than 35 years this field has been intensively expanding, being among the priorities for the sustainable development of national economy.

The 7th International Conference **ECOLOGICAL & ENVIRONMENTAL CHEMISTRY 2022** is part of a series of successful conferences organized in 1995, 2002, 2005, 2008, 2012 and 2017 being supported by UNESCO, MFGS, CRDF/MRDA, ONRG, as well as by Moldovan R&D organizations: Institute of Chemistry, Chemical Society of the Republic of Moldova, Department of Ecological and Industrial Chemistry of Moldova State University, Moldovan Research and Development Association, etc.

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Organizing Committee of the 7th International Conference **ECOLOGICAL & ENVIRONMENTAL CHEMISTRY 2022** highly appreciates the input and expresses the profound gratitude to the remarkable personalities, who are not any more with us, for their essential contribution to the development of ecological and environmental chemistry domain:

COVALIOV Victor, *Prof., Moldova State University, Moldova*

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EEC-2022 Conference Topics

A. Fundamental Aspects of Ecological and Environmental Chemistry

- Oxidizing and reducing agents (antioxidants) in environment, technology and living organisms
- Electron transfer reactions in redox processes
- Thermodynamics and kinetics of redox processes in ecological systems
- Photochemical processes in the environment
- Modeling of the redox processes in environment
- Chemical risk assessment and analysis

B. Water Science and Society

- Ecological chemistry of natural waters, pollution and self-purification
- Industrial and municipal waste water treatment and reuse
- Modern approach and advanced methods to pollution control, monitoring and prevention: physico-chemical, biochemical and remote sensing methods, water quality indicators, etc.
- Transboundary waters and disasters management
- Water, sanitation and health

C. Climate Change and Atmospheric Chemistry

- Redox processes in troposphere and stratosphere (air emissions, acid rains, precipitations, smog, etc.)
- Air quality monitoring, pollution prevention, control and modeling
- Air pollution impact on climate change
- Air quality and health

D. Food, Soil and Waste Chemistry

- Food safety and security
- Chemical aspects of crop nutrition, soil fertility and degradation prevention
- Physico-chemical transformations of soil pollutants
- Wastes management, treatment and reuse in agriculture, food and wine production
- Hazardous wastes (POPs, hospital, pharmaceutical, etc.) detoxication

E. Ecological & Environmental Chemistry within the Knowledge Triangle: Research-Education-Innovation

- Methodological aspects in assurance of high quality knowledge, skills, innovation, technologies and solutions towards the ecologically balanced future
- Innovative policies, strategies and solutions addressing the global challenges for environment and sustainable development
- Environmental transnational rights, legislation and control
- Sustainable use and circular management of natural resources
- Household chemicals in everyday life: safety and efficiency
- Pollution impact on the health

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The 7th International Conference of Ecological and Environmental Chemistry

March 3-4, 2020, Chisinau, Republic of Moldova

Session A

FUNDAMENTAL ASPECTS OF ECOLOGICAL AND ENVIRONMENTAL CHEMISTRY

FUNDAMENTAL ASPECTS OF ECOLOGICAL AND ENVIRONMENTAL CHEMISTRY

Gheorghe DUCA

President of the Chemical Society of the Republic of Moldova,
Research Centre of Physical and Inorganic Chemistry, Institute of Chemistry, ***Moldova***

Science usually involves the fundamental and applied research. Fundamental research means the basic, core studies. The task of fundamental research is to discover and substantiate the laws that underlie the existence and development of nature and society. Generally, the basic knowledge in science is a relatively small part of the scientific theories that researchers use for the applied research, which is much broader and generates added value in education, culture, business, environment, including science. The fundamental science is also called academic, because it is developed mainly in the academic institutions and universities.

The fundamental ideas lead to the revolutionary changes, to the “discoveries” and “breakthroughs” in knowledge. Huge sums of money are being spent in the world for basic research, because only if it is successful, although less often, may lead to the serious changes in science and society. The Republic of Moldova, with regret, is an exception. Financing of fundamental research, as well as of applied research, is miserable, around a total of 15 million dollars, or $ 5,000 per researcher in 2021. At the same time, in Switzerland the annual funding allocations are of $ 406,000 per researcher, in the USA – $ 360,000 per researcher, in Germany - $ 295,000 per researcher. Let us take another example: funding for the Faculty of Natural and Environmental Sciences at the Newcastle University, UK, reaches ₤ 40 million a year.

We should not forget that the immediate goal of the applied research is to implement the results, by using the results of fundamental nature, to solve the problems in social or industrial practice. In spite of under-financing of research activity in Moldova, we have have successfully completed the fundamental studies in ecological and environmental chemistry. Theoretical and experimental results allowed elucidating the key role of chemical, physico-chemical and biochemical processes in the environment, including the redox phenomena, pollutants’ transformation, self-purification of natural waters and formation of chemical composition of the environment appropriate to the biological value of habitation. Etc. This approach is fully in line with the science of ecological chemistry which we have been promoting for over 30 years, and all seven international conferences organized to date have been to the results of this fundamental and applied research. The redox reactions are considered a real driving force of many natural processes, such as photosynthesis, respiration, water quality formation, self-purification, etc.

To accurately estimate the ecological status of the environment, we used a variety of research methods, including the studies of physical, chemical and biological processes that take place in ecosystems, treated as “open”, dynamic systems. Many chemical processes in the environment are catalytic, or occur under the solar irradiation – photocatalytic processes. The most important natural oxidants we have used are O_2, H_2O_2 and their free radicals (superoxide and hydroxyl) which have been investigated over the years, but the detailed mechanisms of their primary generation and subsequent behavior in the presence of labile metal ions, which could underlie the quantitative modeling, are still unclear. For this reason, on behalf of the Institute of Chemistry, State University and Technical University of Moldova, we have proposed a project “Physico-chemical mechanisms of redox processes with electron transfer involved in vital, technological and environmental systems”, No. 20.80009.5007.27, with the main objective to determine the mechanisms of the redox processes in vital systems, food and environment by studying the electronic structure, thermodynamics, kinetics and catalysis of the antioxidants interaction with oxidants to substantiate the electron transfer reactions.

The situation is complicated by the fact that in the environment, unlike the laboratory experiments, there is no purity of reagents, but there is always a whole mixture of participating transition metals. There is a cross-influence of species that react over time and so the question of the mechanisms of reactions is still open.

Our concept is that the redox processes with participation of O_2 and H_2O_2 in the presence of metal ions with variable valence always go first and foremost through the formation of complex intermediate compounds. And only then they can contribute to the emergence of different types of free radicals and / or various intermediate forms of chemicals.

Our goal is to create a new unified theory or revise the current variant of the redox processes in environment, based on the fundamental research of the chemical reactions' mechanisms with the participation of natural oxidizing agents in the presence of transition metals.

To this end, we have performed the comprehensive studies of the mechanisms of chemical reactions involving the natural oxidants, including the kinetic studies of different systems, mathematical modeling and related problems solving, and instrumental determination of intermediate particles present in the detectable amounts. The research was focused on the study of the redox-processes' mechanisms, of non-radical and redox nature, including the activation of oxygen and hydrogen peroxide by the reduced metal ions, as well as the redox processes accompanied by the formation of free radicals and complex compounds with partial charge, studying their reactivity towards the certain types of pollutants.

Acknowledgements: This work has been performed within the State Program of the Republic of Moldova (2020-2023), Project Nr. 20.80009.5007.27 "Physical-Chemical Mechanisms of the Redox Processes with Electron Transfer in Vital, Technological and Environmental Systems". The author is grateful to following researchers involved in the fundamental and experimental studies: Prof. Serghey Travin ("N.N.Semenov" Federal Research Center for Chemical Physics, Russian Academy of Sciences, Moscow, Russia); Prof. Igor Cretescu ("Gh.Asachi" Technical University of Iasi, Romania); Dr.hab. Olga Covaliova, Dr. Lidia Romanciuc, Ph.D. students: Natalia Bolocan, Crina Vicol, Corina Tașcă (Institute of Chemistry, Moldova); Conf. Viorica Gladchi, Prof. Maria Gonța, Conf. Elena Bunduchi, Assistants: Vlad Blonschi, Angela Lis, Larisa Mocanu (Moldova State University); Prof. Rodica Sturza, Assoc.Prof. Iurii Subotin, Assoc.Prof. Ecaterina Covaci (Technical University of Moldova).

DEVELOPMENT OF THE APPLICATION OF THE MONTE CARLO METHOD FOR SOLUTION OF ECOLOGICAL CHEMISTRY TASKS

Serghei TRAVIN

N.N. Semenov Federal Research Center for Chemical Physics Russian Academy of Science, Moscow, ***Russia***

Abstract. The possibilities of application of the Monte Carlo method for the purpose of simulating the consequences of burst emissions of pollutants in the case of their specific adsorptive binding by the underlying surface (water, soil) are considered. A review of the historical development of this class of modeling methods is carried out. The limiting cases of the modes of diffusion, drift, and chemical degradation of the pollutant are considered, as well as all kinds of their combinations. The results of model calculations by Monte Carlo are compared with the results of numerical integration of the differential equation for the pollutant distribution obtained for identical conditions. The complete adequacy of the simulation model is shown and its advantages associated with the stability of the solution and lower costs of computer time are demonstrated. The basic techniques for the implementation of the model in the VBA-Excel environment are shown. The possibilities of the developed software toolkit for the application of the Monte Carlo method to solving problems of the spatio-temporal dynamics of a pollution spot in natural conditions are demonstrated. Effective methods of obtaining kinetic curves for the concentration of a pollutant for a selected square on the field and constructing contamination profiles for a specified time are analyzed and formulated. The estimation of the necessary parameters of the model for obtaining high-quality kinetic curves was performed and recommendations for their optimization are given.

THE H-BOND IN ENVIRONMENTAL REDOX PROCESSES AS A PSEUDO-JAHH-TELLER EFFECT

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The majority of environmental processes are essentially based on chemical transformations that involve either electron, or proton transfer, or both. Therefore, revealing the micro-mechanisms of the latter is crucial for the understanding and possible manipulation of these processes. On the other hand, the vibronic coupling theory, mostly the pseudo-Jahn-Teller effect (PJTE), as the only source of spontaneous symmetry breaking of high-symmetry configurations of polyatomic systems [1], was shown to control the proton transfer between two molecular systems, often termed as the Hydrogen (H) bond [2-4]. This, in turn, allowed us to estimate the main parameter of the H-bond, the energy barrier for the proton transfer between the interacting molecular systems.

In this presentation we show how the PJTE influences the energy barrier for the proton transfer, in general, with several illustrative chemical processes as examples. These include a number of proton-bounded 30entral such as $(\text{pyridine})_2H^+$, $(\text{butanone})_2H^+$, and other systems. Particular attention is paid to intramolecular proton transfer in excited states (ESPT) using the example of a neutral malonic aldehyde molecule, in which the transfer of a proton occurs through the intramolecular H-bond involving a five-membered ring. This process is compared with the proton transfer in similar systems in which the ring size changes to four and six and in which the systems have a common negative charge.

It is shown that in all the considered cases the low-barrier hydrogen bond can be described within the framework of the pseudo-Jahn-Teller effect. The functional dependence of the potential energy on the instability coordinate, following from the PJTE theory, with parameters estimated using quantum chemical calculations, can serve as a parametrized analytical model of the adiabatic potential, which can be used to simulate the proton transfer process in such systems.

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RENEWABLES AND CHEMISTRY

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One of the most important challenges of the 21st century is the issue of sustainable, clean and affordable future energy provision. Contemporary societies are faced with needs for urgent transformations in the sector of energy production and use, by using complex ways to provide ecologically acceptable energy. At present, the renewable energy sources are treated as the ecologically acceptable solution, which provides opportunities as well as challenges for sustainable energy future. Regardless of "greenness" renewables come in many shades.

Majority of the world's energy is still obtained by ecologically unacceptable energy sources. In those processes beyond carbon dioxide (CO_2) which causes the global warming, even more dangerous is carbon monoxide (CO), the gas that is released during the incomplete fuel combustion. Furthermore, surface ozone is just one of the many more problems that are connected with energy generation and use.

As the global demand for energy continues to grow there is need for more efficient methods of production, storage and utilization of energy based on cleaner, more sustainable methods for the synthesis of chemicals and materials, as well as use of new technologies and methodologies. That includes the investigation of the properties and behavior of materials for batteries, supercapacitors and photovoltaics.

Batteries are becoming important part in the alternative energy systems. Such, lithium-ion batteries have higher energy density. The redox-flow batteries have the large energy capacity, and they can discharge rapidly. Metal-air batteries offer even higher energy densities than lithium-ion batteries. To achieve progress, those working in battery research will need to connect more solid-state chemistry and electrochemistry.

"Green chemistry" enables and accelerates the next phase of the energy transition by improving the recycling and recovery of waste, by using biological components as feedstock for biofuels and chemicals, by reducing industrial process emissions through green and circular chemicals and fuels, and by carbon capture technologies. Furthermore, the design of new nanoscale catalysts for fuel cells and sustainable chemical synthesis, which coupled with surface science studies of their functions are opportunities for substantial gains in energy efficiency. The one of the most important challenges that Chemistry has to tackle today is the need for secure energy supplies and limiting society's reliance on non-sustainable fossil-fuel derived feedstocks.

In large, Energy and Sustainable Chemistry are interrelated by many subjects such as Catalysis, Synthesis, Kinetics, Dynamics and Mechanism, Advanced Materials and Interfaces, Innovative Measurement and Photon Science, and Theory and Modelling of Complex Systems.

ABOUT THE CASCADE OF DEVELOPMENT OF EMERGENCY SITUATIONS AND THEIR CAUSE-EFFECT SCENARIOS

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In modern technical literature, there is traditionally a stereotype about the hardware-machine cascade of the development of man-made emergencies (from tank to tank, etc.). At the same time, it is believed that world industrial production has its roots in those distant times when the first man-made chemical reactors (bonfires) and the first industrial product (charcoal) appeared [1].

These conclusions (assumptions) suggest that chemical processes are the forerunner (basis) of industrial production. In this regard, the comparison of a series of technological patterns of the development of the world economy with the history of the formation of chemical science reveals a certain correlation between them and the exponential growth of various types of emergencies (natural, man-made, biosocial) [2], which was marked especially by the end of the XX – beginning of the XI centuries [3].

Large-scale forest fires, floods, earthquakes – natural emergencies (emergencies), as well as man-made emergencies (emergencies) cause a response in the form of various biosocial manifestations (BSPs) – from protest actions of the population [4] to environmental and political terrorism [5, 6] and contrariwise. Having analyzed the consequences of any kind of emergency, it can be argued that they are a kind of impulse for the cascade transition of one into another.

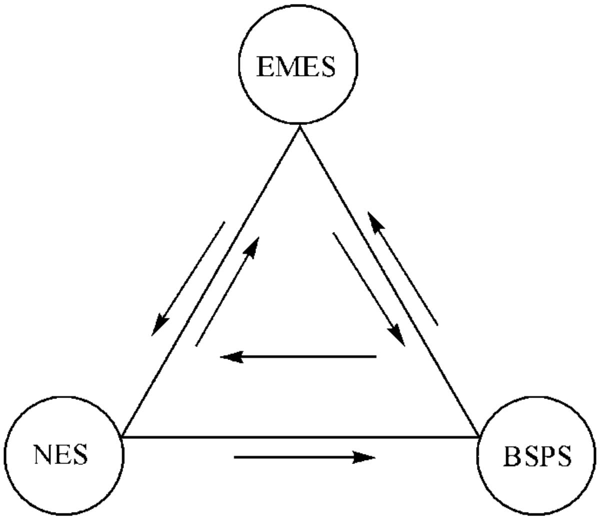

Fig. Triangle of cascading development of emergency situations

For example, man-made accidents at oil and gas complex enterprises lead to large-scale environmental pollution, which has both serious environmental consequences and causes activation of protest moods among the population.

In turn, manifestations of environmental or political terrorism – arson of forests or low technological culture in production leads to fires and explosions, provoking the entry of numerous pollutants into the atmosphere, hydro and lithosphere.

Another example is the shortage of both drinking and irrigation water due to climatic or geographical reasons, leading to incidents and accidents at economic facilities and the emergence of armed interstate confrontation aimed at the redistribution of water resources.

Thus, there are reasons justifying the cascading of the mutual transition of one type of emergency into another, graphically displayed in the form of a corresponding triangle graph (see Fig.), marking the separation of methodological approaches and the transition to a higher level of understanding of their genesis and transformation: from hardware-machine-to cause-and-effect scenarios.

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MODIFIED 3D-ELECTRODES FOR THE EFFICIENT HYDROGEN PRODUCTION

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Although hydrogen is considered to be a secondary energy carrier, i.e. it's cost is generally higher than that of the natural fuels, its application is expedient in many cases, being economically feasable and environmentally friendly. Electrochemical technology is one of the most important among hydrogen production technologies, as it allows to obtain 99-99.5% gaseous H_2. Advantages of this method involve process simplicity, continuity, possibility of automation, absence of moving components in elecrolytic cell, obtaing of precious by-products, such as heavy water and oxygen. However, conventional hydrogen electrolysis is connected with the high overvoltage of hydrogen evolving from water solutions, provoking the elevated energy consumption. In terms of electrochemical hydrogen production costs, according to various sources, they make in average \$4-5/kg H_2.

Therefore, the main task of this research was to elaborate the type new electrode materials to be used as cathodes for the essential reducing of hydrogen evolving overvoltage on their surface, and thus, to make the hydrogen electrolysis more efficient and cheap. To obtain the type new electrode material with the developed surface, making it possible to apply the lower current intensity during the electrolysis and at the same time to reach the optimal current density for hydrogen evolution, the coatings were deposited on the new 3D materials – metal foams (Cu and Ni). Chemical-catalytical deposition process was performed without the application of external current and had the autocatalytic nature. The advantage of this plating process is a possibility to metalize the dielectrics, to obtain the uniform layers on details with complex configuration. $NaBH_4$ and DMAB – dimethylamine borane – $(CH_3)_2$ $HN^{\cdot}BH_3$ were used as reducing agents. To ensure the comparability of results while studying the effect of doping Ni-B alloys with Mo, W or Re, pyrophosphate solutions with rather similar compositions have been selected. The studies of structural-phase transformations of Ni-B coatings were performed using the electronographic, X-ray and thermoderivatographic methods. The effect of potassium molybdate, sodium tungstate and potassium perrhenate concentration on main parameters of metal ion chemical-catalytic reduction and hydrogen emission was studied. The mechanisms of coating processes were considered, including the possibility of auto-catalytic electrochemical reactions. Chemical state of elements and coatings' composition was studied using the X-ray photoelectron spectroscopy. Amount of molecular hydrogen evolved was determined volumetrically and that of hydrogen adsorbed by the deposit was measured using the vacuum extraction method at 400^0 C.

Catalytic activity, chemical composition and structure of Ni-Mo-B, Ni-W-B and Ni-Re-B coatings were studied. The aim of this study was to elucidate the causes for nonlinear, volcano-like dependence of partial rates of DMAB hydrolysis and hydrogen evolution on the doping element concentration in the alloy. It was found that the doping element (Mo, W and Re) introduction into the Ni-B alloy has substantially modified the catalytic activity of the alloy's surface with regard to the concurrent partial reaction, including heterogeneous hydrolysis of DMAB, reduction of Ni ions, and evolving of the molecular H_2. With the increase in the alloying element amount, B contents in coatings was sharply decreased. Effect of alloys composition on H_2 evolving overvoltage was studied in acidic and alkaline mediums by the potentiodynamic polarization curves. It was shown that alloying of Ni-B with Re (11 wt.%) reduces the overvoltage of hydrogen evolution by 200 mV. Due to the low overvoltage of H_2 emission on the alloy Ni-Re-B surface, it was used as a cathode for H_2 from water in the electrolytic cell with novel design and improved technical-economic indicators.

Based on these studies, the new 3D electrode materials, with high active specific surface, were proposed ensuring the low hydrogen evolving overvoltage, for using in the reactors for hydrogen electrochemical generation with the improved power efficiency.

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COMPARATIVE EVALUATION OF ANTIDOTE EFFECTIVENESS ACTIVE CARBONS

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Detoxification of soils from pesticide residues is an important factor in the greening of the agro-industrial complex. Recently, these works have become especially relevant in connection with the adoption of Federal Law No. 280-FZ of 03.08.2018 "On Organic Products and on Amendments to Certain Legislative Acts of the Russian Federation".

Vegetation experiments on soil detoxification were carried out in accordance with the traditional method, according to which the sod-podzolic soil was treated with the herbicide Singer SP at a dose of 0.4 g/ha using a laboratory sprayer. A day later, AU samples were introduced at a dose of 100 kg / ha. After a day, the prepared soil was distributed into waxed disposable paper cups with a capacity of 600 g of soil and the test plants of rapeseed of the Ratnik variety were sown 3 pcs. For each vessel. The repetition of the experiment is 5 times for each dose of the studied AU samples.

The cultivation of test plants was carried out under controlled conditions of the artificial climate laboratory (LIK) in the Fetch chambers (Germany). After 25 days, the aboveground mass of test plants was cut and weighed. The level of antidote effectiveness of the experimental samples of active coals was judged by the mass of the aboveground organs of the test plants in comparison with the control variant without herbicide and active coal. The decrease in the mass of test plants in the experimental variants relative to the control was calculated by the formula:

$$B=100-(A/K * 100), \%,$$

where B is the decrease in the mass of test plants in the experimental variant relative to the untreated control;
A – the average value of the mass of test plants on the experimental version;
K – is the average value of the mass of test plants in the control variant.

The data obtained are shown in table 1

Table 1

Test results for a comparative assessment of the antidote effectiveness of various brands of AU
(LIK FGBNU VNIIF, Department of Herbology, 2021)

n / a	Variant	Dose of AU, kg / ha	Dose of herbicide Singer, SP, g / ha	Aboveground mass of test plants, g						Weight reduction of test plants, % to control
				by repetitions					average	
				1	2	3	4	5		
1	Agrosorb-SO	**100**	**-**	5,7	57	5,7	5,8	5,8	5,7	3,3
2			**0,4**	4,3	5,5	11,1	10,8	4,7	7,3	-23,7
3	Agrosorb-N	**100**	**-**	6,3	6,7	5,9	5,4	6,2	6,1	-3,4
4			**0,4**	7,1	6,8	5,8	10,7	6,3	7,3	-23,7
5	UPK-1B	**100**	**-**	4,3	3,8	4,1	4,6	4,7	4,3	27,1
6	(Δ = 450 g/dm^3)		**0,4**	7,6	4,2	4,3	4,1	5,4	5,1	13,6
7	VSK-830 act.2	**100**	**-**	6,7	6,4	7,5	7,2	8,0	7,2	-22,0
8			**0,4**	9,2	6,1	5,4	6,9	5,4	6,6	-11,9
	Control (Singer)		**0,4**	5,3	4,2	3,1	3,6		4,1	30,5
	Control without AU and herbicide		-	5,5	5,0	5,7	7,2		5,9	0

Note: negative values – stimulation of plant growth.

As follows from the data given in Table 1, the introduction of active coals into the soil contaminated with the herbicide makes it possible to neutralize its depressing effect on the test culture of rapeseed, while the best results were obtained by the active coals of Agrosorb-SO and VSK-830.

THE ‘GASEOUS’ SWORD OF DAMOCLES OVER OUR CIVILISATION

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Our world has experienced five, so-called, great dying cycles in its long history, the most recent dated 65 millions of years ago. The best studied one, 252 millions years ago, marking the Edge of Permian-age, has shown massive extinction of living organisms on Earth: up to 96% of marine and about two thirds of terrestrial life, trees, animals and even microbes. Some say that we just begun our sixth route towards big dying, based on observations of quick extinction of living species, e.g. the overall weight of insects in our climate zone has dropped by two thirds over the past decade (!).. The present ppper provides information about methane and its becoming role in the fast approaching end of our civilisation. Knowledge about it is not secret, however it is rarely included in forecasts, models etc, for rather obscure reasons, perhaps due to incomplete understanding of supramolecular interations between methane and water in the form of clathrate compounds.

From chemical standpoint clathrates display rather bizarr characteristic, they are non-stoichiometric compounds. The products are represented by the formula below being the essence of Van der Waals and Platteeuw theory and it shows the thermodynamic condition of clathrate stability: $\delta(T)$ stands for the chemical potential difference between the host structure in its modifications: clathrate ad non-clathrate, **m** represents a structure factor (the number of hosts molecules forming a cage), and Θ stands for the minimum filling extent above which the clathrate is thermodynamically stable.

$$ln(1-\Theta)=\frac{-m\delta(T)}{kT}$$

Water is capable of forming more than just one clathrate structure but, from the point of view of the present paper we may limit ourselves to one of those, namely the clathrate hydrate type I.) Methane molecules can enter both types of the two types of cavities and the extent of filling is different. The ‘small’ cavities are filled almost completely whilst the ‘big ones’ in about ¾ fraction, please see the formula below

$$-\Delta\mu^{o}_{w} = [3\ln(1-\Theta_L) + \ln(1-\Theta_S)]$$

where $\Delta\mu^{o}_{w}$ stands for the difference between chemical potentials of host modifications, as discussed earlier, and Θ is the minimum filling extent of, respectively, small (s) and large (l) cavities.

We note that the methane contained in the deposits in the amount estimated at 10^{19}grams and in some estimations in the literaturę, it is more than the amount of oxygen in the atmosphere. Sudden evolution, e.g. s the result of cosmic catastrophe, would mean a total dying of biological life. Slow seeping must lead to enhanced greenhouse effect and this, in turn, accelerate destabilization and leading to positive feedback effect. I will be discussed in detail.

$$\ln(1-\Theta)=\frac{-m\delta(T)}{kT}$$

APPLICATION OF METAL OXIDE NANOPARTICLES FOR PHOTO-CATALYTIC TREATMENT OF WATER ENVIRONMENT

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Various types of nanoparticles active in photochemical processes, the most important of them being oxides of Ti, Zn, Ni, Re, Zr, etc. have been successfully tested and applied in the water environments treatment, in view to provide the decomposition or even complete demineralization of toxic persistent pollutants, especially or organic nature, as well as to destroy the pathogenic bacteria and other microorganisms detrimental for human health.

The destruction of the aforementioned toxic components in water, under the photocatalytic treatment, is connected with the formation of a series of active radicals, especially formed under the UV-irradiation with the wavelength of 100-400 nm, penetrating through the quartz walls of the reactor. The suspended nanooxide particles acting as photocatalysis promote the production of active free radicals with high oxidative capacity. Under their impact, the destruction of molecules structures of both the organic pollutants and pathogen microflora in water cells occurs, Thus, in the classical case of TiO_2, under the UV-irradiation on the fine dispersive surface of particles the charge separation proceeds, due to the formation of positive holes (h^+) and free electrons (e^-), according to the scheme: $TiO_2 + h\nu \rightarrow e^- + h^+$, which, in their turn, promote the formation of superoxide-radical: $e^- + O_2 \rightarrow \bullet O_2^-$ with subsequent process: $TiO_2 (h^+) + H_2O_{ads} \rightarrow TiO_2 + \bullet H_{ads} + H^+$. Generally, the photocatalytic activity of metal oxides is ensured by generation of two radical types: $\bullet O_2^-$ radicals formed by the reduction of O_2, and $\bullet OH^-$ radicals resulted from oxidation of OH^- anions. Both radicals react with the pollutants and toxicants to degrade or transform them, with the obtaining of non-toxic or less harmful products. After the chemical transformations of the reactants, the chemical composition of catalyst is regenerated.

In case of sunlight action, another series of photochemical reactions will occur, also providing the detoxification of polluted water systems. Thus, as a result of water radiolysis under the IR-irradiation with the wavelength 700-3000 nm and higher, mainly the short-living hydroxide-radicals ($\bullet OH^-$) are formed having even higher reactivity as compared to the longer-living superoxide-radicals. Therefore, a metal oxide can be activated either with the UV-irradiation, visible light or combination of them both, accompanied with the photoexcitation of electrons transferred from the valence band to the conduction band, creating the electron-hole pair capable to rapidly oxidize or reduce a polluting substance in water absorbed on the photocatalyst's surface.

Although titanium dioxide was among the first particles that have demonstrated the high photocatalytic efficiency in treatment processes, the other metal oxides (including the mixed oxides, or even more complex structures) with light adsorption properties and proper electronic structure with charge transporting ability, thus producing the electron-hole pairs, have also been tested showing good results, among them: ZnO_2, SnO, CeO_2, Cr_2O_3, V_2O_5, etc. The detoxified water can be used for the technological needs, whereas the filtered metal oxide particles, following the washing and drying, can be repeatedly applied in the similar treatment processes.

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THE ROLE OF CHELATES IN ECOLOGICAL STABILITY OF THE ENVIRONMENT

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To date, production of ecologically clean agricultural products with high quantitative and qualitative indices is one of the most topical problems. One of the crucial roles in solution of this problem is played by essential microelements. They may be applied to agricultural crops in the form of fertilizers, while agricultural poultry and animal premixes will get them in non-chelate and chelate form. Microelements in non-chelate form are distinguished by high toxicity, low rate of digestibility and efficiency. On the contrary chelate forms of microelements have low toxicity, high rate of digestibility and, respectively, increased degree of efficiency when used in small doses that in its turn predetermines ecological safety of microelements' use in this form.

It should be noted that in 2003 in European countries there was adopted the legislative act on maximum allowable doses of microelements in poultry and animal manure. As for the problem, as we already mentioned before, it can be solved through use of the mentioned microelements in chelate form only. This fact is evidenced by the results of studies conducted for years by both foreign scientists and by us. In particular, in the agrarian chemistry laboratory of Tbilisi State University there were established synthesis conditions and were synthesized essential microelements containing chelate compounds with general formula: $M(Lig)_n \cdot mH_20$, where M = Mn; Fe; Zn; Co; Cu; Cr. Lig = methionin; glutamine acid; cystine; arginine, $n = 1 \div 3$; $m = 0 \div 6$. Fertilizers and premixes are prepared on the basis of synthesized chelates. Chelate fertilizers are tested in field conditions on different agricultural crops, while premixes are tried on poultry and rabbits. Effect of chelate microelements on earthworm protein mass and multiplication rate are studied in vermiculture, as well [1-3].

On the basis of studied carried out on agricultural crops (wheat, vegetables, kidney bean, corn, citruses) under field conditions it was established that chelate fertilizers' application provided: increase of quantitative and qualitative productivity indices and digestibility of microelements (N, P, K); improvement of physiological state and metabolic processes taking place in plants, prolongation effect of fertilizer, soil enrichment and structure improvement, enhancement of stability against unfavorable environmental factors (drought and cold), pests and different diseases.

Chelate premixes use provided maximal reduction of broilers, egg-laying poultry and rabbits mortality, live weight gain, meat quality improvement, keeping of physiological and biochemical indices within permissible rates, avoidance of different infectious diseases, feed consumption decrease at the expense of increased efficiency of its digestibility, rise of nutritive value and qualitative parameters of the feed; gain in egg shell strength among egg-laying poultry, increase of egg laying and quality.

Thus, it is established on the basis of carried out researches that the application of chelate form of microelements provides avoidance of its excessive accumulation in the environment and respectively the stability of ecological state of the environment.

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ON THE TECHNICAL POSSIBILITY OF PHOTOSYNTHESIS INTENSIFICATION TO FIGHT THE "CARBON PRINT"

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Water is not just a liquid, water is life, one of the main riches of the Earth. Its resources are inexhaustible, it is an inexhaustible source of energy, it contains not only the world's reserves of deuterium – the fuel of future thermonuclear energy, but also colossal amounts of chemically bound hydrogen – an alternative to hydrocarbon and "green" energy. The well-known statement of the Nobel laureate L. Montagnier that water determines not only the health, but also the well-being of the world's population is confirmed.

A method is proposed for controlling not only the physicochemical properties of water (saturated vapor pressure, surface tension, osmotic pressure, etc.), but also successfully changed its chemical characteristics (pH and redox potential (ORP)).

Given the technical simplicity of such a modification – processing with alternating electric potential, its successful application in agriculture is possible — an increase of more than 20 percent in crop yields while reducing irrigation water consumption. To explain such impressive practical results, the experimentally established fact of intensification of the photosynthesis process was confirmed (due to increased assimilation of atmospheric carbon dioxide by plants due to a decrease in the value of ORP in electrophysically modified water and an increase in pH to 7.4).

Thus, the so-called "carbon" agriculture becomes possible and rational, aimed not only at ensuring food satisfaction of the population, but also at minimizing the so-called "carbon print" of man-made activities.

The next step, taking into account the fact of increasing osmotic pressure in electro-physically modified water, becomes likely the success of the fight against viral infections.

The unique physicochemical properties of electrophysical modified water (an increase in the pH of blood plasma and intercellular fluid) lead to an increase in the amount of hemoglobin-bound oxygen, and changes in osmotic pressure and viscosity minimize thrombosis and initiate "osmotic shock" (ruptures of cell membranes).

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SYNTHETIC ZEOLITES MODIFIED WITH SALTS TRANSITION METALS IN THE REACTION OF CHEMISORPTION-CATALYTIC OXIDATION OF SULFUR DIOXIDE BY AIR OXYGEN

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Sulfur dioxide is known as the most widespread environmental pollutant. Various chemisorbents and catalysts are commonly used to reduce its concentration in the air. The most effective chemisorbents are natural and synthetic zeolites, activated carbons, carbon fiber materials, metal oxide. The analysis of low-temperature methods for air purification from SO_2 in the concentration not exceeded 15 MPC (150 mg/m^3) showed that the application of chemisorption-catalytic processes with the participation of transition metal salts deposited on various carriers is promising. In the work, commercial synthetic zeolites of NaA and KA brands were used as carriers of transition metal salts. Chemisorption-catalytic compositions $MX_2/\overline{S}$ ($\overline{S}$ = NaA, KA; M^{2+} = Cu, Mn, Co, Ni; X = Cl^-, NO_3^-) for the oxidation of sulfur dioxide with air oxygen at ambient temperature and high humidity were obtained. The initial carriers and chemisorption-catalytic compositions were studied by XRD, SEM, FT-IR spectroscopy, TG, DTG-DTA. Zeolites NaA and KA have the same parameters of the crystal structure, which do not change when modified with transition metal salts. Under their influence, a slight decrease in the relative crystallinity was observed. The study has shown that NaA and KA samples differ in morphology. Clearly faceted cubic particles with a size of 0.7-1.0 microns were observed for zeolite NaA. Zeolite KA is characterized by aggregated particles of irregular shape of cubes and spherulites. When applying salts of transition metals, the shape of these particles is slightly disturbed. According to the data of thermogravimetric analysis, it has been found that copper (II) ions practically do not affect the temperature of the first (and only) endothermic effect, however, they reduce the content of OH groups due to the reaction of surface complexation. It was found that the adsorption capacity of NaA zeolite relative to SO_2 is 100 times higher than that of KA zeolite (figure); the time of protective action of NaA and KA zeolites increases upon modification with transition metal salts and with an increase of their content in the compositions.

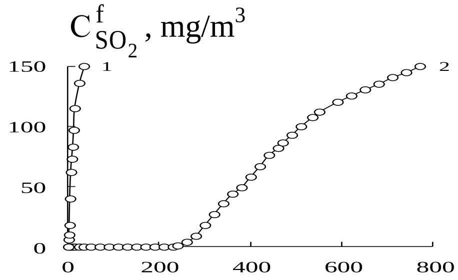

Figure. Time dependence of $C^f_{SO_2}$ for adsorption of SO_2 from gas-air mixture by air-dry zeolites KA (1) and NaA (2)

Taking into account the literature data regarding the mechanisms of SO_2 oxidation with oxygen in the presence of transition metal ions, the possible mechanisms in the presence of MX_2/compositions have been analyzed. It has been proven that the chemisorption-catalytic process ends with the oxidation of SO_2 to sulfuric acid.

INFLUENCE OF ACID MODIFICATION OF NATURAL PHLOGOPITE ON CATALYTIC ACTIVITY OF SUPPORTED Pd(II)-Cu(II) COMPLEXES IN THE REACTION OF OXIDATION OF CARBON MONOXIDE BY AIR OXYGEN

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Carbon monoxide with the maximum permissible concentration in the working area is 20 mg/m^3 (MPC_{CO} = 20 mg/m^3), is a danger to the environment and humans. Although carbon monoxide is a strong reducing agent ($\varphi_{CO_2/CO}$= -0,12 V), direct reaction with oxygen due to steric hindrance is either at high temperature, or in the presence of catalysts. According to the form of the active component, the catalysts can be oxide, metal and metal complex, and according to their temperature characteristics they are divided into low-temperature and high-temperature. The development of catalysts for low-temperature oxidation of CO for personal protective equipment of the respiratory system (RPE) is urgent. Respiratory catalysts must ensure stable air purification to a CO concentration lower than or equal to the MPC_{CO} at ambient temperature and high humidity of the gas-air mixture. Analysis of research in the field of development of catalysts for low-temperature oxidation of CO showed that Wacker-type metal-complex catalysts deposited on various carriers, containing palladium (II), copper (II) salts and other additives, are high potential.

The natural mineral phogopite (N-Phl) was first used as a carrier for palladium – copper complexes that catalyze low-temperature oxidation of carbon monoxide by atmospheric oxygen. It was found that active catalytic compositions K_2PdCl_4-$Cu(NO_3)_2$-KBr/$\overline{X}$H-Phl-1 are formed only on acid-modified phlogopite samples. Phlogopite was modified by the reflux method in a solution of nitric acid of various concentrations $\overline{X}$ = 0.25; 0.5; 1.0; 3.0; 4.0; 6.0 and 8.0 mol/l for 1 hour. Samples (supports and catalysts) were characterized by XRD, SEM, FT-IR spectroscopy and pH metry. It was found that only at $\overline{X} \geq 3.0$ mol/l, the phlogopite samples undergo structural and morphological changes and the pH of the suspension decreases, which in total contributes to the achievement of such catalyst activity, which ensures stable air purification from CO to a concentration below the MPC_{CO} = 20 mg/m^3 for the working area.

TARAXACUM OFFICINALE ACTS AS A POWERFUL ANTIOXIDANT

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Background.

The cell developed a series of antioxidant agents which protect it against harmful effects of free radicals. The superoxide dismutase (SOD) by a redox reaction converts superoxide anion (O_2^-) into oxygen and hydrogen peroxide. The last can also damage important cells' structures, therefore is degraded by enzymes such as catalase (CAT), found in peroxisomes. The roots of *Taraxacum officinale* (TO) are rich in phenolic and terpene compounds, sesquiterpene lactones, fructosans and inulin, which alone or in combinations demonstrated great antioxidant abilities.

The aim of present research was to assess the influence of different TO roots (TOR) ethanolic and dimethyl sulfoxide (DMSO) extracts on red blood cells (RBCs) SOD and CAT activity.

Material and methods.

The TO were harvested from a natural habitat in Republic of Moldova. The extracts for analysis were prepared from grinded dried roots (2 weeks at room temperature). DMSO and ethanol of different concentrations (20, 25, 40, 50 and 80% (v/v)) were used as solvents. The influence of TOR extracts on healthy persons RBCs' SOD and CAT activity was evaluated in accordance with Ryzhikov S.L. et al. (2011) method, modified by Gudumac V. et al. (2010, 2012).

The statistical analysis included calculation of mean and standard deviation (M±SD), Mann-Whitney *U* test (control *vs* experimental groups) and Spearman (r_s) correlation (ethanol concentration *vs* enzymes activity). The *p*-values equal or less than 0.05 were considered statistically significant. The study was approved by the Research Ethics Committee of the "Nicolae Testemitanu" State University of Medicine and Pharmacy.

Results.

SOD activity was dependent on the type of extractant. The ethanol concentration of the extract did not statistically significantly correlate with the influence of TOR on SOD activity (r_s=0.087, p=0.38); nevertheless an increase in the enzyme activity was found in comparison with the control values for all TOR extracts (10% – $33.94\pm1.83^*$ (+10.1%), 20% – $36.08\pm0.86^*$ (+25.5%), 25% – $31.4\pm0.48^*$ (+3.5%) 50% – $42.23\pm1.66^*$(+54.9%), 80% – $38.02\pm0.65^*$ (+23.3%), except 40% ($26.25\pm0.68^*$ or -9%). DMSO extracts determined an increase in RBCs SOD activity ($50.10\pm10.73^*$ or +83.9%).

A strong negative correlation was identified between ethanol concentration and CAT activity in RBCs (r_s=-0.73, p=0.001). DMSO ($26.17\pm9.84^*$ or -42.3%) and all TOR alcoholic extracts (10% – 55.06±4.52 (-21.7%), 20% – $48.04\pm0.73^*$(-13.3%) 40% – 41.72±0.16 (-7.3%), 50% – 41.88±11.67 (-15.6%), 80% – 41.71±2.49 or -11.4%), except 25% ($56.12\pm3.26^*$ or +47.5%), reduced the CAT activity compared to control values.

Conclusion.

Taraxacum officinale roots act as potent modulators of the antioxidants system, affecting SOD and CAT activity. This action depends on the type of solvent. The greatest stimulating effect on SOD activity are exerted by the TOR extracts in DMSO and 50% ethanol. The increase of alcohol concentration in extracts diminishes CAT activity, except extracts in 25% ethanol. Further studies are needed to elucidate the mechanisms of TO influence on the antioxidant system.

Key words: *Taraxacum officinale* roots, red blood cells, SOD, CAT, antioxidants.

THEORETICAL STUDY OF THE THREE-STAGES RADICAL MECHANISM OF THE REACTION OF DIHYDROXYFUMARIC ACID WITH THE STABLE RADICAL DPPH$^{\bullet}$

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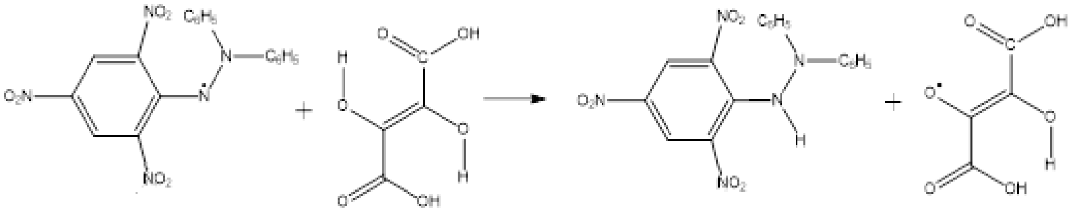
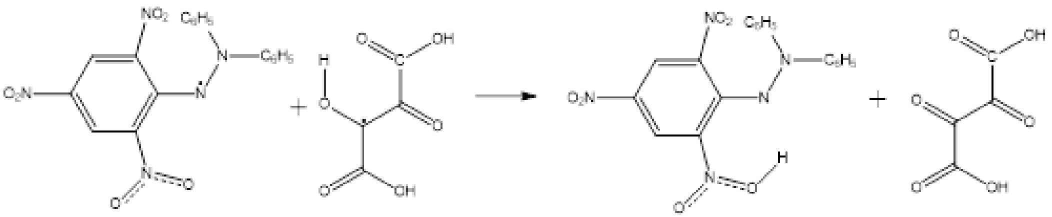
The so-called ‘SPLET’ mechanisms of reaction of dihydroxyfumaric acid (DHFA) with the Stable Radical DPPH$^{\bullet}$ has an ionic character and includes the formation of the charge-transfer complex as the main stage, which is formed from the protonated DPPH$^{\bullet}$ molecule and the anion of DHFA arising due to their electrolytic dissociation in the water-methanol medium [1].

In its turn, it was found by us (by the usage of the program GAUSSIAN09 [2]) that the radical (HAT) mechanism is being realized in the three stages shown below:

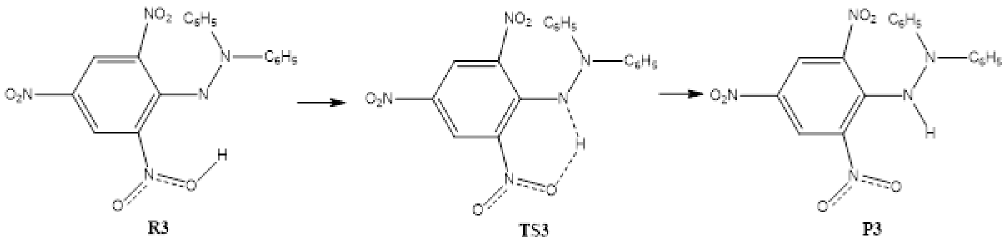
Step I: Direct transfer of the hydrogen atom from the –OH group of DHFA to the functional group –N$^{\bullet}$-N = of the DPPH radical. As the result, the radical of DHFA$^{\bullet}$ is obtained, which is a monodehydrogenated form of DHFA.



Step II: Transfer of the second hydrogen atom from the hydroxyl group of the above formed radical DHFA$^{\bullet}$ to the nitro group of the second DPPH$^{\bullet}$ radical.



Step III: intramolecular hydrogen atom transfer from the nitro-NO_2 group to the –N-N= functional group of DPPH resulting in two neutral molecules DPPH and one molecule of dioxosuccinic acid – DOSA.



Acknowledgement: This work has been performed within the State Program of the Republic of Moldova (2020-2023), Project Nr. 20.80009.5007.27 “Physical-Chemical Mechanisms of the Redox Processes with Electron Transfer in Vital, Technological and Environmental Systems”.

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SYNTHESIS OF SILICA-CELLULOSE HYBRID MATERIALS AND MESOPOROUS SILICA PRODUCTS VIA SOL-GEL MINERALIZATION

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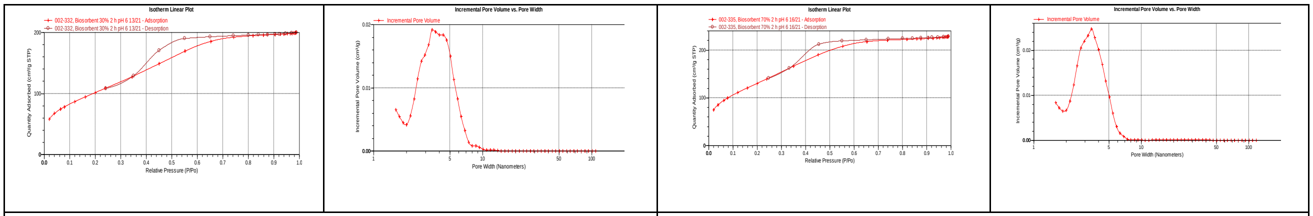
Sol-gel synthesis of hybrid silicas was carried out by the deposition of silicic acid on nematic liquid-crystalline cellulose templates, which are partially ordered suspensions of rod-like cellulose nanocrystals with a size of ≈ 5 to 30 nm in diameter and from 100 to 300 nm in length. Porous silicas of Type SBA-16 were obtained by stepwise heat treatment of hybrid xerogels. The formation of silica-cellulose hybrid materials and mesoporous silica products under concentrations of sulfuric acid of 30, 45, 60, 70 wt%, temperatures of 20 – 45°C, and pH values of 6-10, were investigated using nitrogen sorption analysis, scanning electron microscopy, thermal analysis, FT IR- spectroscopy and X-ray examination.



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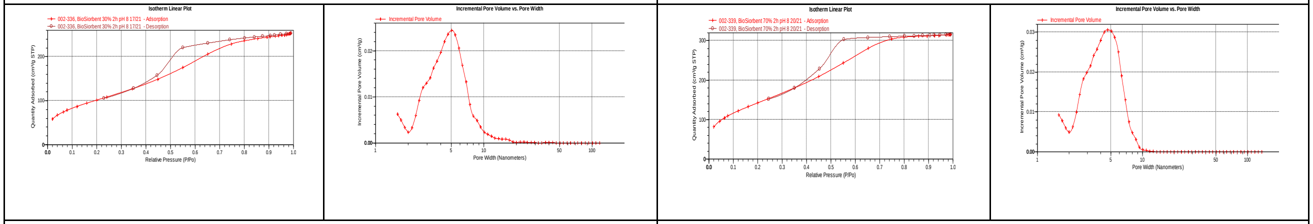

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Figure – Isotherms of low-temperature adsorption-desorption of nitrogen and PSD curves for fully mineralized mesoporous silica samples obtained on a cellulose template hydrolyzed with sulfuric acid for 2 h at different pH values and H_2SO_4 concentration: 002-332 – pH 6, 30%; 002-335 – pH 6, 70%; 002-336 – pH 8, 30%; 002-339 – pH 8, 70%.

Table – Physical adsorption of nitrogen by fully mineralized silica samples

Sample	pH	Time, h	[H_2SO_4]	A_{BET}, m^2/g	A_{ext}, m^2/г	$V_{sp\ des}$, cm^3/g	$V_{BJH\ des}$, cm^3/g	D_{des}, nm	$D_{BJH\ des}$, nm
002-332	6	2	30	377	420	0,31	0,30	3,3	3,4
002-335	6	2	70	484	550	0,35	0,30	2,9	3,2
002-336	8	2	30	377	414	0,39	0,43	4,1	3,9
002-339	8	2	70	529	584	0,49	0,55	3,7	3,7

It was shown that the combination of silica and cellulose imparts new textural, structural and surface properties to the hybrid material. The creation of an ordered mesostructure of cellulose nanorods and SiO_2 framework facilitates template mineralization and increases the thermal stability of the material. Cellulose and silica hybrids with ordered mesopores, narrow pore distribution (5-6 nm) and additional active centers in the form of carbonyl, carboxyl or hydroxyl groups can be used in water purification as adsorbents of metals or larger molecules. The proposed method is variable, cost-effective and environmentally friendly.

THE APPLICATION OF IRON HYDROXO AND OXALATE COMPLEXES IN ECOLOGICAL PHOTOCHEMISTRY

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Fe (III) carboxylate complexes are photoactive natural compounds that are intensively studied and are considered to be one of the promising systems for the degradation of pollutants in the so-called advanced oxidation processes (AOPs) [1]. They demonstrate high quantum yields of photolysis and efficient generation of $^{\bullet}OH$ radicals under the action of UV radiation [2] However, there is very little information on the quantum yields of $^{\bullet}OH$ radicals (ϕ_{OH}) upon excitation of such systems. At the same time, the ϕ_{OH} values and the reactivity of $^{\bullet}OH$ with respect to the target compounds are the most important parameters for the application of any photosystem in AOPs.

This work presents valid approaches to determining the ϕ_{OH} values during UV photolysis of natural Fe(III) carboxylate complexes and determining the rate constants of hydroxyl radical reactions (k_{OH}) with priority environmental pollutants.

The first approach is based on the use of the $FeOH^{2+}$ hydroxocomplex as a reference system with the well-known ϕ_{OH} value and benzene as a selective trap for $^{\bullet}OH$ radicals. For the first time, ϕ_{OH} was determined for the most popular Fe(III)-oxalate photosystem in a wide range of initial parameters (pH, excitation wavelength, concentration of oxalate and Fe(III) ions). Also, the oxidative potential of the oxalate photosystem was tested on a set of resistant organic herbicides, and the quantum yields of photodegradation of these herbicides were compared with the ϕ_{OH} value.

The second approach is based on the application of the method of laser flash photolysis using the $FeOH^{2+}$ complex as a standard source of hydroxyl radicals at pH 3, and methylviologen dication (MV^{2+}) as a selective probe for the $^{\bullet}OH$ radical. The use of MV^{2+} makes it possible to determine the k_{OH} values even for those compounds that do not themselves form optically detectable adducts in the reaction with hydroxyl radicals. The applicability of this approach has been tested on a wide range of resistant organic herbicides, and its main advantages and disadvantages are discussed compared to existing stationary and time-resolved methods [3].

Asknowledgement:

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MOLECULAR ORBITAL NATURE OF THE ATMOSPHERIC REACTIONS BETWEEN THE NO_3 RADICAL AND C3 – C10 N-ALKANES: DFT STUDY

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One of the main night-time oxidants in the atmosphere is the nitrate radical NO_3. In the atmosphere NO_3 is generated by the reaction (I) between NO_2 and ozone O_3:

$$NO_2 + O_3 = NO_3 + O_2.$$

In its turn, NO_3 reacts with different hydrocarbons including the title n-alkanes. The reactions between NO_3 and hydrocarbons essentially influence air quality and climate. However, in many cases there is an incomplete understanding of the mechanisms of the reactions between NO3 and volatile organic chemicals. Here we present our results connected with theoretical calculation of the reaction rate constants k describing the interaction of NO_3 with C3 –C10 n-alkanes at 298K and 0.1Mpa. In order to do it we have used the following Equation (1), which was received in our work [1]:

$$-\lg k = A + B/(E_{oxd} - E_i) \qquad (1)$$

with the newly defined constants A, B, and E_{oxd}, which equal to 17.5404, 50.9904, and 807.38 kJ/mol respectively. Eq. (1) shows that the specific occupied molecular orbitals SMOs of the studied n-alkanes with the energies E_i play the predominant role in their reactions with NO_3. These SMOs include 1s-AO of all the hydrogen atoms of these n-alkanes with one common sign (+ or -) (see [1]). The following Table 1 demonstrates the calculation of the constants k of the given n-alkanes be means of Eq. (1).

Table 1. The usage of Eq.(1) for the calculation of k

n- Alkane:	E_i (kJ/mol)	$-\lg k_{calc.}$	$-\lg k_{ex}^{*}$
Propane	873.56	16.77	16.77*
Butane	863.34	16.54	16.63
Pentane	845.16	16.06	16.19
Hexane	841.27	15.96	16.04
Heptane	837.02	15.82	15.82
Octane	835.47	15.72	15.73
Nonane	833.73	15.64	15.61

[*] The experimental data were taken from [2].

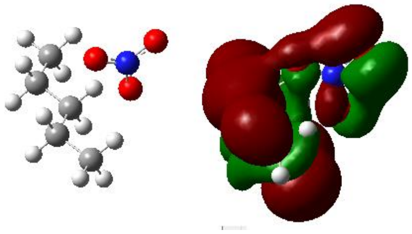

Fig. 1. Formation of three-center C-H-O bonding MO between n-pentane and $NO_3^{\bullet}$ radical.

Acknowledgement: This work has been performed within the State Program of the Republic of Moldova (2020-2023), Project Nr. 20.80009.5007.27 “Physical-Chemical Mechanisms of the Redox Processes with Electron Transfer in Vital, Technological and Environmental Systems”.

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NEW OPPORTUNITIES IN THE DETECTION OF ENVIRONMENTAL POLLUTANTS

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It is known that the search for new detection systems remains relevant. Recently, a new class of artificial ferments, so-called nanozymes has been proposed [1].

The prospects of using natural enzymes as detection systems are limited by their high cost and low operational properties. Overcoming these shortcomings became possible by the creation of artificial mimetics of enzymes – nanozymes. Nanozymes are nanomaterials with their own enzyme-like activity, they are able to combine both the catalytic properties of enzymes and the properties of nanoscale materials. Compared with natural enzymes, nanoferments have better stability, can be mass-produced at lower cost, their properties can be quickly developed and adapted to various requirements. Thanks to these advantages, they have demonstrated wide application in the monitoring and cleaning of the environment [2].

The presented report provides a comprehensive overview of nanozymes used in environmental analysis. Main attention is paid to the generalization of principles and methods for the determination of typical pollutants, including such as: toxic ions, pesticides, phenolic pollutants, antibiotic residues, hydrogen peroxide and pathogens. In particular, acid rains (pH <5.5) is currently a serious environmental problem worldwide. High acidity of rain occurs as a result of the oxidation reaction of H_2O_2 with dioxide and nitrogen oxides in the atmosphere. Thus, the concentration of H_2O_2 is an important indicator providing information about the environment.

We have developed a colorimetric sensor with the property of peroxidase based on heterojunction. Determination of the hydrogen peroxide content in rainwater was carried out using a $ZnFe_2O_4$/ZnO film sensor manufactured by magnetron sputtering, Fig.1. The minimum detectable concentration of hydrogen peroxide in rainwater was 0.02 μM

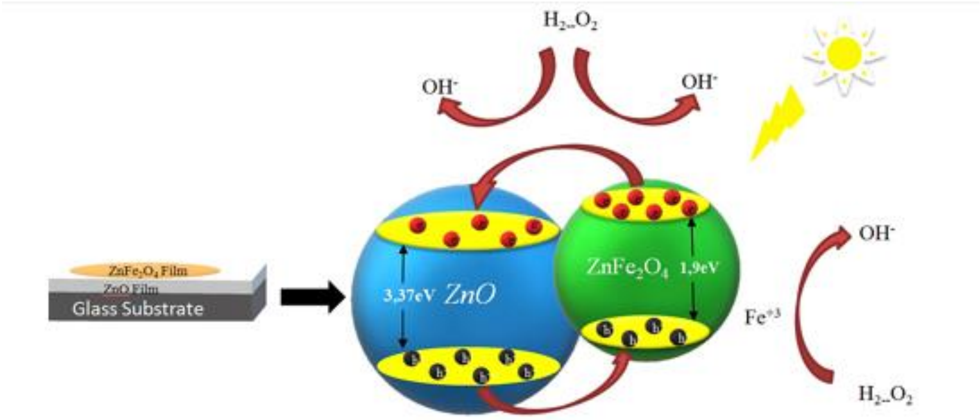

Fig.1. Peroxidase activity of the $ZnFe_2O_4$/ZnO film heterojunction
and the mechanism of the color oxidation reaction of TMB.

Acknowledgement: This work has been performed within the State Program of the Republic of Moldova (2020-2023), Project Nr. 20.80009.5007.11: "Funcțional Nanostructures and Nanomaterials for Industry and Agriculture".

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SORPTION-LUMINESCENCE METHOD FOR DETERMINATION OF YTTERBIUM

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Yb(III) ions, complexed with some organic ligands, exhibit intense luminescence. The light energy is absorbed by the organic part of the molecule of the complex, then there is an intramolecular energy transfer from the organic ligand to the Yb(III) ion. During the sorption of Yb(III) on the solid matrix, the intermolecular energy transfer is suppressed, which provides the increase of the luminescence intensity, and the effect of selective preconcentration is achieved. Promising materials for solid-phase spectrofluorimetry are natural zeolites. Sorbed Yb(III) on these natural nanomaterials retains the ability to interact with organic ligands. In order to develop a sorption-luminescent method for the determination of Yb, the ability to luminescence of Yb(III) ions sorbed on natural Transcarpathian clinoptilolite in combination with 1-(2-pyridylazo)-2-naphthol (PAN) was studied. Luminescence composition «clinoptilolite-Yb(III)-PAN» is observed in the IR region of the spectrum with a maximum λ=978 nm. Luminophore samples were excited by a laser with λ=532 nm. The optimal conditions for obtaining this luminophor have been found. To prepare an effective luminophor «clinoptilolite-Yb(III)-PAN» it is necessary to use precalcined at 300 ^{o}C samples of clinoplololite, heated at 50 ^{o}C samples «clinoptilolite-Yb(III)», and the final luminophor heated at 50 ^{o}C. Sorption of Yb(III) on clinoptilolite is carried out from weakly alkaline solutions at pH 9.0. The developed sorption-luminescent method allows to determine Yb in the presence of 10-fold excess of La(III) and Eu(III), as well as 5-fold excess of Lu(III), Tm(III), Gd(III), Pr(III), Tb(III) with a detection limit of 5.0 $ng \cdot mL^{-1}$. The method is tested on model solutions and intermetallics. The method provides a high enrichment factor, a wide concentration range of Yb determination (12.5-1000 $ng \cdot mL^{-1}$).

THE EFFECT OF HALIDE IONS ON THE ACTIVITY OF D-METAL COMPLEXES SUPPORTED ON NATURAL BENTONITE IN THE REACTION OF LOW TEMPERATURE OZONE DECOMPOSITION

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The use of ozone as an oxidizing agent is associated with certain difficulties: its utilization rate is low at a relatively high cost, so various catalysts are used in ozonation reactions to increase this characteristic. But even in this case, the residual concentration of ozone may exceed the maximum permissible concentration (MPC), so for its decomposition we apply thermal, reagent and catalytic methods. Despite their limited use of supported metal complex catalysts have advantages over other types of catalysts, such as variation of activity due to changes in the nature of the central atom (Me^{n+}), ligands (L) and carriers, relatively simple production technology.

The effect of halide ions (X = Cl^-, Br^-, I^-) on the kinetics of ozone decomposition by compositions supported on the natural bentonite of the Dashukovske deposit in Ukraine (N-Bent(D)) has been studied. It was shown that the activity of the KX/N-Bent (D) composition in the ozone decomposition reaction increases in the series KCl << KBr < KI, which correlates with an increase in the reducing properties of halide ions. The complex composition K_2PdCl_4-$Cu(NO_3)_2$-KX/N-Bent(D) demonstrates the maximum catalytic activity in the decomposition reaction in the presence of bromide ions. Such effect is caused by the expansion of the halide ions functions, which play not only the role of reducing ions, but also form the coordination sphere of palladium(II) and copper(II). It was found that with an increase in the KBr concentration in the composition of the K_2PdCl_4-$Cu(NO_3)_2$-KBr/N-Bent(D), the initial reaction rate and the amount of decomposed ozone increase; however, a stationary decomposition of ozone is observed only at $C_{KBr} \geq 3.0\times10^{-4}$ mol/g. It is shown that the bimetal composition K_2PdCl_4-$Cu(NO_3)_2$-KBr/N-Bent(D) demonstrates the longest protective action time (τ_{MPC}

= 1800 min) at ozone concentration of 1 mg/m^3 (Table), by such conditions the ozone concentration is less than the MPC (0.1 mg/m^3) at the outlet of the reactor.

Kinetic and stoichiometric parameters of ozone decomposition reaction with mono- and bimetallic compositions

($C_{Pd(II)} = 2.72\times10^{-5}$; $C_{Cu(II)} = 2.9\times10^{-5}$; $C_{KBr} = 1.02\times10^{-4}$ mol/g; U = 4.2 cm/s)

Compositions based on N-Bent(D)	τ_0, min	τ_{MPC}, min	$C^f_{O_3}$, mg/m^3	$Q_{exp}\times10^6$, mol O_3**
N-Bent(D)	-	-	1.0	0.9
KBr	18	30	0.1	0.4
Cu(II)-KBr	30	50	0.1	0.6
Pd(II)-KBr	1260	1500	0.1*	33.6
Pd(II)-Cu(II)-KBr	1260	1800	0.1*	37.6

* – the stationary mode is established; ** – Q_{exp} is an experimental amount of O_3 moles

PHOTOCHEMISTRY OF FEEDDS COMPLEX AND ITS EFFICIENCY IN $^{\bullet}$OH GENERATION

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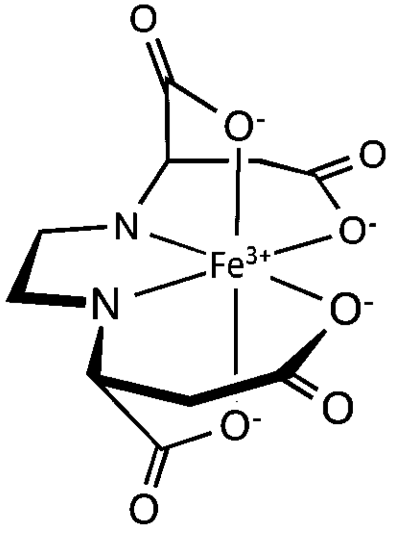
Fe(III) polycarboxylate complexes in photo-Phenton systems are investigated as perspective agents in advanced oxidation processes (AOPs). They demonstrate high photolysis' quantum yields and great efficiency in •OH generation under UV excitation. Hydroxyl radicals are able to non-selective oxidation of large number of organic pollutants.

As ligands in those complexes can be used widely known ethylendiaminetetraacetic acid (EDTA) or its structure isomer – etilendiamindisuccinic acid (EDDS). Advantage of EDDS, in contrast of EDTA, consists in the fact, that EDDS is naturally recycled by some types of bacteria. However, there is very little information about photolysis' mechanism and the quantum yields of $^{\bullet}$OH radicals (ϕ_{OH}) upon excitation of this system. This work presents a detailed study of complex photolysis' efficiency and its efficiency in $^{\bullet}$OH radicals' generation in a wide range of experimental conditions (pH, excitation wavelength, oxygen content, initial ligand and Fe(III) concentrations).



Using steady-state and laser flash photolysis methods in combination with spectrophotometry and high performance liquid chromatography, we got the following results:

1. Primary intermediate is a long-lived (1.8 ms) radical complex [Fe(II)…EDDS•], which is formed in the electron transfer from ligand to Fe(III) ion (λ_{max} = 520 nm).

2. Quantum yields were showed to be dependent from initial concentration of iron, ligand, dissolved oxygen and solution acidity and have achieved value ~0.7 in optimal conditions at neutral pH.

3. $^{\bullet}OH$ quantum yield was showed to be dependent from initial concentration of iron, ligand and solution acidity and has achieved value ~0.1 in optimal conditions at neutral pH.

Received results are important in understanding both fundamental photochemistry of Fe(III) coordination compounds with polydentate carbonic acids and for application of such complexes in advanced oxidation processes of wastewater treatment.

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CONTROLLED SYNTHESIS AND PROPERTIES OF MESOPOROUS Fe-N-C HETEROGENEOUS FENTON-LIKE CATALYSTS

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Highly effective techniques like *Advanced Oxidation Processes* (AOPs) for the removal of hazardous organic pollutants from wastewater have attracted considerable research interests due to its significant impacts on environments and ecological systems. It's known that the generation of reactive oxygen species (ROS), such as $HO^{\bullet}$, $HO_2^{\bullet}$, $O_2^{\bullet -}$, $SO_4^{\bullet -}$, $SO_5^{\bullet -}$, $CO_3^{\bullet -}$ and other radicals, in heterogeneous photocatalysis and Fenton-like processes is an efficient method for the degradation of organic pollutants (pharmaceutically active compounds, pesticides, dyes, etc.) [1]. AOPs means carrying out a catalytic experiment in one of or a multifactorial combination of conditions: when exposed to a light source (ultraviolet, visible), ultrasound, in the presence of transition metal ions (i.e., Fe^{2+}, Fe^{3+}, Mn^{3+}, Mn^{4+}, etc.) and/or nanoscale zero-valent metals (Cu, Fe, Ni, etc.) in the catalyst structure. Thus, the optimization of the conditions of AOPs, in particular, the obtaining of effective catalysts and the development of new methods for its synthesis is an urgent task.

Fe-N-C composites are promising heterogeneous Fenton-like catalysts. These materials demonstrate superior catalytic activity, kinetics of destruction, high chemical stability, etc. in comparison with heterogeneous Fenton-like catalysts based on iron-containing compounds (e.g. $La(Bi)FeO_3$ perovskites, Mfe_2O_4 spinel oxides, iron oxides (γ-Fe_2O_3, Fe_3O_4), oxyhydroxides (γ-FeOOH)), photocatalysts based on graphitic carbon nitride (g-C_3N_4). However, the data on the influence of the conditions of formation of iron-containing compounds in the graphitic carbon nitride system are fragmentary.

In this work, we propose for the development of heterogeneous Fenton-like catalysts based on Fe-N-C composites and a new one-stage method for its synthesis. The combination of highly dispersed iron oxides, zero-valent iron and graphite-like carbon nitride in composites will avoid the drawbacks of catalysts based on the above individual compounds. Systematic study of the effect of synthesis conditions on the physicochemical (crystal structure, morphology, etc.) and catalytic properties of the obtained composites will make it possible to create highly efficient heterogeneous catalyst for practical applications (pharmaceutical and petrochemical industry, agro-industrial complex, municipal water treatment plants, etc.).

Acknowledgements
This work was supported by the Belarusian Republican Foundation for Fundamental Research and the National Natural Science Foundation of China (grant №Х22КИ-018).

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THERMODYNAMIC DETERMINATION OF THE PRECIPITATION CONDITIONS IN MIXTURES OF ANIONIC AND CATIONIC SURFACTANTS

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A thermodynamic model has been developed and used to predict the precipitation conditions using the solubility product relationship between surfactant monomer concentrations, in order to calculate the monomer-precipitate equilibrium, in the mixtures of anionic and cationic surfactants for a wide range of pH variation and various initial chemical compositions of the studied heterogeneous mixtures. The developed model could predict the amount of precipitate that formed in the mixture of cationic and anionic surfactants, the results proving to be in agreement with the experimental measurements. Mixture of sodium dodecyl sulfate (*SDS*) and dodecylpyridinium chloride (*DPCl*) has been shown to react in solution with the formation of a precipitate in a wide range of concentrations. When the micelles are not present in the solution, this reaction can be modeled by a simple solubility product between the total surfactant concentrations. In addition, the developed approach provides an explicit equation which predicts the amount of solid phase which forms in any *NaDS-DPCl* mixture, so that surfactant equilibrium concentrations (after precipitation) can be determined. The chemical composition in each monomer phase, which is determined in the computerized calculation process, helps to understand and predict the solution compositions corresponding to the precipitation limits of anionic/cationic surfactants. The results of the calculation of the global Gibbs energy variations of this system for different chemical compositions show that with the decrease of the total concentrations of the surfactants the areas of existence of the solid phase, $DSDP_{(S)}$, narrows. For the concentrations $C(DS^-) = C(DP^+) = 1 \cdot 10^{-3}$ mol·L^{-1} the precipitate $DSDP_{(S)}$ exists in the whole studied range of pH values. From the obtained data it is possible to determine the pH of the coexistence of two solid phases, lauric acid $HDS_{(S)}$ and dodecylpyridinium dodecyl sulfate $DSDP_{(S)}$. Thus, conditions can be predicted in which there is only one phase or when the precipitation of one or both surfactants can be avoided. The obtained results are in agreement with the existing experimental measurements.

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BIOPOLYMER MATERIALS BASED ON CHITOSAN CONJUGATED WITH SULFODERIVATIVES OF ZINC(II) PHTHALOCYANINES AND GOLD NANOPARTICLES

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Over the last decades enhanced emphasis has been made on the environmental aspects of chemical processes, the preference being given to “green” technologies and materials.

Chitosan is considered one of the most promising biopolymer due to its unique characteristics which include biocompatibility, biodegradability, non-toxicity and solubility in aqueous media, thus making it very promising for medical, biochemical and ecological applications [1]. The presence of reactive amine groups in chitosan structure allows for linkage to acidic fragments of other molecules facilitating its solubility and enhancing the efficiency of the resulting composites.

Metallophthalocyanines (MPc) are gaining continuously increasing attention in biomedicine especially as photosensitizers for photodynamic therapy (PDT) from a tumor-centered approach [2]. MPc conjugated to naturally occurring polymers doped with noble metal nanoparticles are even more effective as anticancer compounds [3].

Considering all these, the purpose of the research was synthesis and investigation of biopolymer materials based on chitosan conjugated with zinc(II) tetrasulfophthalocyanine, thioacetic acid and gold nanoparticles.

UV-Vis spectrophotometric investigation of the solutions of chitosan conjugated with zinc(II) tetrasulfophthalocyanine and thioacetic acid demonstrated the presence of absorption bands in 680-720 nm range. The maximums of the bands shift towards longer wavelengths upon aggregating with gold nanoparticles, which is beneficial for photodynamic therapy. The results of molecular toxicity study test have shown satisfactory results, making the resulting composites convenient candidates for medical use.

Acknowledgement: This work has been performed within the State Program of the Republic of Moldova (2020-2023), Project Nr. 20.80009.5007.16: “Photosensibilizers for applications in photodynamic and photovoltaic therapy”.

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IONIC QUASI-SPLET MECHANISM OF THE INTERACTION OF SOME ORGANIC ANTIOXIDANT ACIDS WITH THE RADICALS ABTS$^{\bullet +}$ AND DPPH$^{\bullet}$

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The classical SPLET mechanism of antioxidants’ action of chemical compounds is based on the supposition that the proton transfer from an antioxidant molecule to an oxidant free radical particle is its first stage. The second stage of the given mechanism includes the following electron transfer which occurs between two the newly formed ions (the former antioxidant and oxidant molecules). Thus, the presence of active hydrogen atoms, which can abandon (at experimental conditions) the studied antioxidant molecules in the form of the corresponding protons, can indicate on possibility of the SPLET mechanism. However, it was shown in our recent [1] and previous [2] works that in the reactions of the certain antioxidant food acids with the radical ABTS$^{\bullet +}$ along with the reaction of dihydroxyfumaric acid with the radical DPPH$^{\bullet}$ (see [2]) there is not any direct transfer of protons from molecules of the given acids to the above radicals. In both these cases the corresponding redox reactions begin from the dissociation of these acids in the ethanol–water medium (see [1,2]) and the formation of their anions in the studied solutions. Their former protons are bonded with solvents’ molecules. Then, for the food acids their anions form charge transfer complexes with the radical cation ABTS$^{\bullet +}$ and transform it in its diamagnetic derivative. In the case of dihydroxyfumaric acid the protonation of the radical DPPH$^{\bullet}$ occurs due to the passing of needed protons from protonated molecules of the solvents (ethanol and water) to the given radical [2].

Thus, in both cases considered, the primary proton transfer proceeds from neutral antioxidant acids molecules to solvent ones. At the same time the second stages of the studied redox reeactions include the formation of the corresponding charge transfer (electron transfer) complexes with the participation of the anions arising during their first stages. In this connection it seems to us reasonable that one can call the such type of antioxidant mechanism as „quasi-SPLET" one. I.e. the quasi-SPLET mechanism can be characterized by the following particularities: firstly, the absence of the direct transfer of protons from antioxidant molecules of the acids to the studied radicals; secondly, the active participation of solvents' molecules in both the processes: the passing of protons to the studied radicals (their protonation) and the formation of acids'anions, which, in their turn, take part (via the formation of the charge teransfer complexes) in the process of donating of their electrons to the protonated (DPPH$^{\bullet}$) or positively charged (ABTS$^{\bullet+}$) radicals and, therefore, transform these radicals in their diamagnetic derivatives.

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WHAT IS THE CHEMICAL SYNERGISM?

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The variety of physical factors and chemical agents used makes it necessary to study the general laws of the manifestation of synergy. It is well known that the maximum effect of the combined action of two agents is achieved with their simultaneous action. The classics of the theory of chemical equilibrium have already in the last century found out for themselves that the formation of mixed complexes is an indispensable condition for the appearance of synergy. However, since then, the attention of researchers has been focused on the external conditions for the manifestation of synergistic effects, neglecting this necessary condition. In this paper the common feature for all synergistic chemical processes has been elucidated. Frequently this common feature does not come to light, being "hidden" and thus the phenomenon of synergism is explained in various ways, depending on investigated chemical processes and their peculiarities, namely the chemical structures of the involved reagents, their mechanism, kinetics, energetics, etc. The authors have proved for all chemical processes used in various physicochemical methods of analysis and research and different fields of applications, that the common feature of the phenomenon of synergism is the formation of a mixed complex. The paper intends to focus attention, describe and characterize this common feature as a suitable tool for search and design of new synergistic effects with required properties for different chemical processes.

The authors have formulated the following rule: the formation of mixed complexes is a necessary, but not sufficient condition to explain the occurrence of the chemical synergism. To prove the synergistic effect, it is necessary to measure a certain physicochemical or physical quantity, which proves the superiority of the non-additivity phenomenon over a simple summation of the properties of individual components. In other words, *the theory of chemical equilibrium* cannot serve as a basis for predicting synergy, but *it can be post-proof of this phenomenon*. The knowledge and the application of the ideas and general patterns of synergy described can be useful for specialists using the simultaneous action of various agents to optimize combined technological schemes. It was also concluded that the overall universal pattern of the manifestation of synergy is its dependence on the intensity of the agents used. The existence of universal patterns of synergy indicates the need to develop a new paradigm and theoretical concept of chemical synergy, which should take into account the identified patterns. *A prior* knowledge of this common feature gives the possibility of a deeper understanding of this phenomenon and of target search or prediction of required or pre-planned synergistic effects. Subsequent research on chemical synergism in order to predict this phenomenon should focus on finding sufficient conditions for synergistic systems, in which the formation of the mixed compound is well known and their comparison with other non-synergistic analogous systems, in which a mixed compound is formed. To explain the lack of synergism in the systems where the formation of the mixed compound takes place, additional knowledge is needed from other sciences, which studies the structure and reactivity of chemicals.

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ECOLOGICALLY FRIENDLY METHODS USED IN HETEROCYCLIC CHEMISTRY

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Five and six member ring azaheterocyclic derivatives are reported as highly valuable scaffolds in modern medicinal chemistry and pharmacy (drugs, as antibacterial, antifungal, anti-inflammatory, antihypertensive, anticoagulants, diuretics, anticancer, antidepressant, etc.), organic materials for opto-electronics (fluorescent and electroluminescent materials, semiconductor devices, sensors and biosensors) and agriculture (mainly herbicides and grow up factors), etc. As a result, obtaining of such derivatives continues to arouse a strong interest from academia and industry.

During the last decades, microwave (MW) and ultrasound (US) assisted reactions has become a successful tool applied in modern organic and medicinal chemistry. In comparison with conventional thermal heating (TH), both microwave and ultrasound irradiation have several important advantages: spectacular accelerations of chemical reactions, increased selectivity, shorter reaction times, higher yields and higher product purities. The MW and US assisted reactions become in many cases ecologically friendly, having milder reaction conditions, suppressing side reactions, energy saving, using small amounts, or no organic solvents, lower costs and simplicity in handling and processing. Also, in some cases described in the literature, reactions that did not occur under classical TH were only successful if carried out under MW and/or US irradiation.

As part of our ongoing research in the field of azaheterocyclic derivatives, we present herein the main results obtained in the last few years by our group in the field of synthesis and developing of new environmentally friendly methods for preparation of these derivatives using MW and US technologies. The main reaction pathway studied was acylation, alkylation, quaternization, esterification, etherification, halogenation, 3+n cycloadditions reactions, etc. Certain advantages of microwave (MW) and ultrasound (US) assisted reactions was observed: better selectivity, higher yields, decreasing of the amount of used solvent comparative with TH, decreasing of the reaction time from hours to minutes, decreasing of the consumed energy, milder reaction conditions; consequently these reactions could be considered environmentally friendly.

The anticancer, antibacterial, antifungal and antituberculosis activity of some azaheterocycles derivatives was determined, some of the compounds having an excellent biological activity. Some of the obtained compounds are promising leading drug candidates.

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THERMODYNAMIC ANALYSIS OF PRECIPITATION CONDITIONS OF ANIONIC SURFACTANTS BY CALCIUM AND MAGNESIUM IONS

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Sodium dodecyl sulfate (SDS) is an anionic surfactant that has found application in personal care products, detergents, in cosmetics and cleaning products. An obvious disadvantage of using anionic surfactants as detergents is the formation of the precipitate with calcium (Ca^{2+}) and magnesium (Mg^{2+}) ions contained in hard water. Below the CMC level, the solubility of SDS as a function of Ca^{2+} or Mg^{2+} concentration is governed by the solubility product (K_S) and decreases with increasing its concentration. Information on the solubility of surfactant salts, determined by the dissolution of pure substances, is of limited utility. Apparent K_S may be exceeded by orders of magnitude without the appearance of the solid phase, due to the surfactant association, the ion pairs formation, the complexation of the solutions, etc. In the paper, the equations for calculating the variation of the global Gibbs energy of the precipitation processes – dissolution of lauric acid and alkaline earth metal dodecyl sulfate have been deduced. The elaborated ΔG(pH) diagrams offer the possibility to determine the areas of thermodynamic stability of the solid phases depending on the chemical composition and acidity of the system. If $\Delta G > 0$, then the compound precipitates and the system is biphasic, while for the values of $\Delta G < 0$, all components are soluble in water, i.e. there is a homogeneous, single-phase system. It has been shown that as the concentrations of the surfactant and the metal ion increase, the range of precipitate formation, either slightly soluble salt or slightly soluble acid, expands, in all cases by some pH units. Thus, the conditions can be established when the formation of precipitates is avoided. Using the developed thermodynamic model, the areas in which the solid phase is formed at the interaction of the anionic surfactant with the calcium and magnesium ions have been determined.

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INFRARED SPECTROSCOPY OF URINARY STONES OF PATIENTS FROM REPUBLIC OF MOLDOVA IN 2016-2021

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IR spectroscopy is used in diagnostic medicine to study the structure of urinary stones and to reveal their chemical composition. The chemical composition of urinary stones obtained from 183 patients with urolithiasis for the period 2016-2021 was studied using IR spectroscopy. A Spectrum 100 Fourier transform spectrometer (Perkin Elmer, USA, 2007) was used to determine the composition of urinary stones. The spectra were recorded using an ATR attachment in the form of a fine powder. There were found in the urinary stones such chemical components, as uric acid, uric acid hydrate, ammonium urate, wedellite $CaC_2O_4{\cdot}2H_2O$, wevellite $CaC_2O_4{\cdot}H_2O$, calcium phosphate $Ca_3(PO_4)_2$, struvite $MgNH_4PO_4{\cdot}6H_2O$, calcium carbonate $CaCO_3$, brushite $CaHPO_4{\cdot}\ 2H_2O$, cystine. These components were found both in an individual state and in the form of mixtures of substances. Very often (up to 40%) there were stones of a mixed type, including, for example, $CaC_2O_4{\cdot}2H_2O$, $CaC_2O_4{\cdot}H_2O$ and $Ca_3(PO_4)_2$ in different ratios. The interpretation of IR spectra was carried out using a database on IR spectra of urinary stones, as well as literature data on IR spectroscopy. The figure 1 shows the IR spectrum of a kidney stone containing vedellite $CaC_2O_4{\cdot}\ 2H_2O$ and $Ca_3(PO_4)_2$. The spectrum shows absorption bands in the regions of 1611 and 1314 cm^{-1} correspond to symmetric and asymmetric stretching vibrations of the C-O and C=O of the oxalate group. The band in the region of 780 cm^{-1} indicates the presence of deformation vibrations δ(O-C=O) in the oxalate group $CaC_2O_4{\cdot}H_2O$.

The presence of strong absorption bands in the region of 1027 and 961 cm^{-1} indicates the content of calcium phosphate in urinary stones.

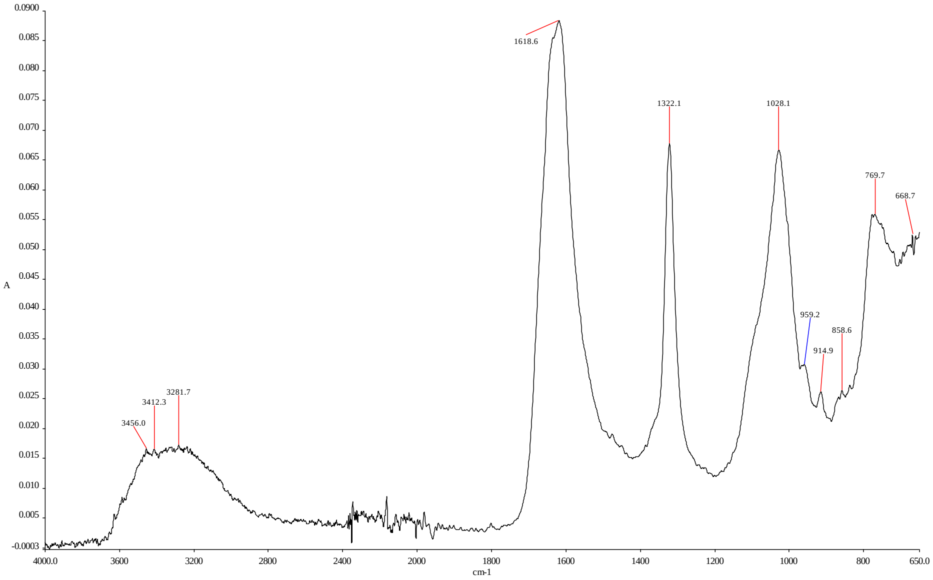

Fig.1. IR spectrum of a kidney stone containing vedellite $CaC_2O_4 \cdot 2H_2O$ and $Ca_3(PO_4)_2$.

Acknowledgement: This work is a part of the Moldovan State Program (2020-2023) “Study and management of pollution sources to develop recommendations for implementing measures to mitigate the negative impact on environment and human health”, Project number: 20.80009.7007.20.

THERMODYNAMIC ANALYSIS OF PRECIPITATION CONDITIONS IN THE MIXTURE OF ANIONIC AND AMPHOTERIC SURFACTANTS

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Surfactants have a wide range of applications: in addition to their industrial use as detergents, being at the same time a serious source of drinking water and waste pollution, they play an important role in analytical and preparatory chemistry and biology as a means to reduce surface tension. An example of the precipitation phenomenon is laundry detergents, in which anionic surfactants provide cleaning, and cationic surfactants offer fabric softening/antistatic properties. A thermodynamic model for establishing the domains of phase stability in mixtures of anionic and amphoteric surfactants for a wide range of pH variation and various initial chemical compositions of the analyzed heterogeneous mixtures has been developed. A mixture of anionic and surfactants, consisting of three components at intermediate pH levels: anionic, cationic (protonated amphoteric) and zwitterionic (non-protonated amphoteric) was studied. Knowledge of the composition of each surfactant in both monomer and micellar forms (monomer-micelle equilibrium) and in the form of a precipitate is important in applications using this mixture.

The systems studied in this paper contain sodium dodecyl sulfate (SDS) and dimethyldodecylamine oxide (DDAO$^+$), which are used in a wide range of consumer products. The pH value has been shown to have a substantial effect on the precipitation of the surfactant mixture when the loading of the surfactant depends on the pH of the medium. The concentration of charged monomers depends on the pH due to the reactions of the surfactant with hydroxyl and hydrogen ions.

Dimethyldodecylamine oxide (DDAO$^+$) is an amphoteric surfactant that may exist as a cationic or zwitterionic surfactant depending on the pH of the solution. The amine group of the surfactant DDAO can protonate in a similar manner to weak acids. By combining the use of the precipitate solubility product constant and the dissociation/protonation constant within the developed approach, taking into account all side reactions, a thermodynamic model was presented and used to predict the solid phase existence conditions. All the global Gibbs energy variation calculations were performed for the concentrations of both surfactants lower than their CMC values. Precipitation of mixtures of dimethyldodecylamine oxide and sodium dodecyl sulfate has been investigated at different pH levels. The protonated form of $DDAO^+$ carries a positive charge and precipitates with the opposite charged DS^-. The precipitation areas of the compound $DDAO^+\text{-}DS^-_{(S)}$ become narrower as the surfactant concentrations decrease. At the same time, when the concentrations of both surfactants decrease, the pH of the coexistence of the two solid phases shifts to its higher values, from a more acidic environment to a neutral one. The ΔG(pH) curve passes through a maximum, then decreases, due to the deprotonation of $DDAO^+$ and the formation of the neutral zwitterionic form of dimethyldodecylamine oxide, $DDAO^0$. The developed thermodynamic model is in agreement with the existing experimental data at different pH levels. The current study provides guidance for handling the precipitation process, as well as a perspective on the entra-chemical phenomena of precipitation and micelle formation in the investigated systems.

Asknowledgement: This work is a part of the Moldovan State Program (2020-2023) “Study and management of pollution sources to develop recommendations for implementing measures to mitigate the negative impact on environment and human health”, Project number: 20.80009.7007.20.

TECHNOLOGICAL PROCESSES FOR REMOVAL OF NITROGEN COMPOUNDS AT NEW WWTP IN THE CAUSENI CITY

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After the commissioning of the WWTP in the Causeni city and the development of the aerobic and anoxic microflora, two variants of the technological processes for removal of nitrogen compounds were tested to ensure the maximum possible treatment efficiency. First of all, in order to estimate the processes that take place in each bioreactor of the WWTP complex in the Causeni city and the effects of nitrogen migration in different forms, research and laboratory investigations of CCO_{Cr}, NO_2^-, NO_3^-, NH_4^+, preliminary analysis of the dynamics of change of forms of mineral nitrogen ($NH_4^+ \leftrightarrow NO_2^- \leftrightarrow NO_3^- \leftrightarrow \ldots \leftrightarrow N_2$) in the solid phase and water after separation (liquid phase) of wastewater throughout the whole treatment course.

The *first variant* tested with the prolonged aeration treatment (sludge age 24-30 days, dose by volume 130-100 mL, dose by weight 2.71-3.21 g/dm^3) demonstrated an insufficient efficacy, which is not complies with the rules for discharge of NH_4^+ and NO_2^- into the aquatic environment. The elimination of organic substances and nitrification take place completely, and during the period when the loading of organic substances take place as a result of the activity of an economic agent (cannery) in the area, the denitrification takes place only in the secondary decanter, being unacceptable and leading to an unstable treatment process due to sludge flotation.

The *second variant* tested, with the inclusion in the treatment of the “aeration – anoxic – aeration” zone (sludge age 30 days, dose by volume 130-190 mL, dose by weight 2.9-3.4 g/dm^3), showed a sufficient efficiency. In this case, however, the quality of the treated water does not fall within the norms of discharge into the aquatic environment only towards NO_2^-. This is explained by the lack of oxygen in the biofilter, due to technical reasons of air aggregates and can be overcome by their adjusting. At oxygen deficiency below 2 mg/dm^3, the rate of multiplication of the bacterial mass at the first stage of nitrification $NH^{4+} \rightarrow NO^{2-}$ is higher than the rate of multiplication of the bacterial mass at the second stage $NO_2^- \rightarrow NO_3^-$, as a result the accumulation of nitrites in treated waters.

In order to increase the sustainability of the technological process and to ensure wastewater at discharge with the quality corresponding to the existing norms even during periods of flow fluctuations or pollutant loading, WWTP Causeni will adjust the technological equipment for testing the *third variant* after implementing advanced UCT technology developed by the University of Cape Town for the elimination of biogenic substances and its intensification through the carousel regime. The consistency of anaerobic and aerobic treatment has been shown not to significantly increase the elimination effect of biogenic substances. The inclusion in the consecutive scheme of the biological treatment of the anoxic area amplifies this effect in the same technological volumes with the reduction of the air consumption for aeration by using oxygen from nitrates.

Asknowledgement: This work is a part of the Moldovan State Program (2020-2023) “Study and management of pollution sources to develop recommendations for implementing measures to mitigate the negative impact on environment and human health”, Project number: 20.80009.7007.20.

STUDY OF SYNERGIC AND ANTI-SYNERGIC INTERACTIONS OF SOME GRAPE ANTIOXIDANTS WITH ORGANIC ACIDS

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Grape is one of the world’s largest fruit crops widely cultivated because of its economic importance in making wine, juice, jam, and raisins [1]. Grapes have been found to possess notable antioxidant capacities mostly due to the abundance in polyphenols [1], as well as due to the presence of several antioxidants that are known to have protective effects against many diseases [2]. Grape phenolic compounds are mainly found in skins, pulps, and seeds that are partially extracted during processing. In grapes, they have a special significance because they contribute to the color, taste and aroma of fresh fruit and also to the color, taste and quality of wines, juices and other products.

Such a complex system like the one found in grapes assumes the occurrence of synergic or anti-synergic interactions between its compounds. According to Tsao [3], synergistic combination of compounds with antioxidant activity can be advantageous, as long as it increases the individual antioxidant effects when two or more compounds are combined. From a technological and ecological point of view, this phenomenon is favorable due to the significant increase in the effectiveness of food preservation, the reduction of the amount of food additives required and, in particular, due to the decrease in the application of synthetic antioxidants that can be toxic [3].

In this study, the influence of tartaric, citric and gallic acids on the antioxidant activity of some grape polyphenols is reported. The experiments were performed using the DPPH method [4] that involves the interaction of the antioxidant compounds with the free radical 2,2-diphenyl-1-picrylhydrazyl. The results are expressed as g-equivalents of ascorbic acid per liter. The half maximal effective concentration, which can be defined as the concentration required to obtain a 50% free radical annihilation effect, was determined in order to ensure an easier comparison between each antioxidant. The synergic and anti-synergic effects were calculated for each sample tested, using the equations described in the literature [5].

Acknowledgement: This work has been performed within the State Program of the Republic of Moldova (2020-2023), Project Nr. 20.80009.5007.27 “Physical-Chemical Mechanisms of the Redox Processes with Electron Transfer in Vital, Technological and Environmental Systems”.

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BACTERICIDAL AND BACTERIOSTATIC ACTIVITY OF IRON(III) COMPLEXES WITH SCHIFF-BASED LIGANDS ON *STAPHYLOCOCCUS AUREUS, ESCHERICHIA COLI* AND *CANDIDA ALBICANS* CULTURES

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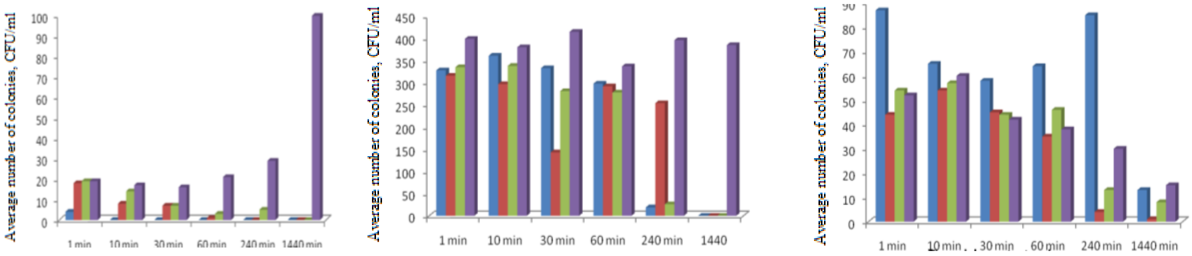
The pathogenic bacteria *S. aureus* and *E. coli* are the main cause of community and hospital-acquired bacteremia. *C. albicans* is the most common fungal pathogen of humans. It is known that, the substances with bacteriostatic and bactericidal effect significantly influence the level of synthesis and elimination of antioxidant enzymes in pathogens.

In order to identify compounds with antimicrobial properties, three coordination compounds of iron(III): $[Fe(H_2L^1)(H_2O)_2](NO_3)_3{\cdot}1.5H_2O$ (**1**), $[Fe(H_2L^2)(H_2O)_2](NO_3)_3{\cdot}5H_2O$ (**2**) and $[Fe(H_2L^3)(H_2O)_2](NO_3)_3{\cdot}2.5H_2O$ (**3**) (where H_2L^1=2,6-diacetylpyridine bis(isonicotinoylhidrazone), H_2L^2=2,6-diacetylpyridine bis(nicotinoylhidrazone) and H_2L^3=2,6-diacetylpyridine bis(picolinoylhidrazone)) were tested for bactericidal and bacteriostatic properties against bacteria *E. coli* and *S. aureus,* as well as yeast-like fungi *C. albicans.* The antimicrobial effect was determined by counting the colony forming units (CFU) resistant to the action of analysed compounds. This method allows the kinetic study of the compound action on microbial cultures and determination of the time in which the complex manifests bactericidal properties. The obtained data are reflected in Figure.



(a) *(b)* *I*

Figure. Colony-forming units of *E. coli (a), S. aureus (b), C. albicans (c)* after exposure to complex **1** (blue), **2** (red), **3** (green) and control, without treatment (violet)

The tested compounds showed a pronounced activity on *E. coli* from the first minutes of contact, showing a decrease to zero of the CFU number. Thus, for complex **1**, the bactericidal effect was observed after 10 minutes of contact, for compound **2** – after 240 minutes, and for compound **3** it was observed only after 24 hours, when a significant decrease of the number of *E. coli* colonies compared to the control sample was observed (Figure, a).

A special behaviour was found in the case of gram-negative bacteria *S. aureus*, which showed resistance to all complexes during the first 60 min, after which there was a sudden decrease in the number of colonies in the presence of complexes **1** and **3**, and after 24 hours the bacterial colonies were absent in all samples (Figure, b).

The results of microbiological tests showed the lack of antifungal activity of analysed complexes against *C. albicans*.

Acknowledgements

This work has been performed within the State Program of the Republic of Moldova (2020-2023), Project Nr.20.80009.5007.28: “Elaboration of new multifunctional materials and efficient technologies for agriculture, medicine, technics and educational system based on the “s” and “d” metals complexes with polydentate ligands”.

ECOLOGICAL CONDITIONALITY OF THE CHEMICAL STRUCTURE OF THE MAIN CLASSES OF NATURAL PIGMENTS

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Expression of the qualitative characteristics of solar radiation is cyclical and can cause a similar response in biological systems, manifested as adaptations both at the zonal (latitudinal) and seasonal levels. Biological adaptation could follow the path of the forming light-sensitive surfaces in living organisms, the absorption maximum of which coincides with the spectral maximum of the incident radiation. For such surfaces, the general laws of absorption of electromagnetic radiation are satisfied. They determine the relationship between the amount of absorption and the amount of absorbing substance (pigment). Pigments are characterized by a specific molecular structure, namely, the presence of a system of conjugated double bonds. Depending on the position and number of double bonds, the pigment absorbs the light of some parts of the visible (white) spectrum, with a certain wavelength. Therefore, each pigment has a corresponding color and a specific light absorption curve. The more double bonds in the pigment molecule are, the longer its absorption wave. According to the Grotthuss-Draper law (Protti & Fagnoni 2009), the chemical transformation of a substance can only be caused by the light absorbed by this substance, or in other words, only such light chemically acts on a colored body, the color of which is complementary to the body color, that is, which complements body color to white

In the presented work, the distribution of representatives of the main pigment classes by months and depending on the qualitative characteristics of solar radiation (position of maximum) is given. The ecological conditionality of the structure of natural pigments is substantiated. Special attention is paid to the seasonal migration of K, Ca, and Mg in biological objects and their influence on the anthocyanin coloration. The synthesis of pigments by biological objects is considered as an adaptive unambiguous response to solar radiation in the range complementary to the color of the pigment.

By the example of the potential flora of the Northern Region of the Republic of Moldova, the seasonal convergence of corolla color of flowering plants and the selective seasonal causation of pigment synthesis are proved.

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APPLICATION OF INFRARED SPECTROSCOPY IN QUALITATIVE ANALYSIS OF ACTIVATED SLUDGE

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With the help of the Infrared (IR) spectroscopy, the presence of organic and inorganic components was established by the absorption bands within the IR region in the activated sludge after wastewater treatment. Its IR spectra contained absorption bands of functional groups of aromatic compounds, polysaccharides, peptides, proteins, lipids, aliphatic chains, ester compounds, nitrates, nitramines, nitroso compounds, nitrosamines, nitro compounds, amine salts, ammonium salts, silicates, phosphates PO_4^{3-}, HPO_4^{2-}, $H_2PO_4^-$. When comparing samples of activated sludge obtained by different methods, a difference was revealed in the intensities of the bands within the range of 1500-1400 cm^{-1}, 1236 cm^{-1}, related to the characteristic absorption bands of components containing nitrogen, as well as within the range of 1100-900 cm^{-1}, characteristic for absorption bands of components containing phosphate ions and polysaccharides. The Spectrum 100 Fourier transform spectrometer (Perkin Elmer, USA, 2007) was used to study the composition of activated sludge. The spectra were recorded using an ATR (Attenuated Total Reflectance) accessory in the form of a fine powder in the range 4000-650 cm^{-1}. The Figure 1 shows the IR spectra of two sludge samples 1 and 2. Their spectra have differences in the intensities of the absorption bands. In spectrum 1 the intensity of the peak at 1236 cm^{-1} (nitrites NO_2^-) is several times more pronounced than that for sample 2. There is an increase in the intensity of peaks 1450 and 1406 in sample 1, which is perhaps associated with an increase in the content of organic components containing nitrogen by a factor of 2 (Fig. 1)

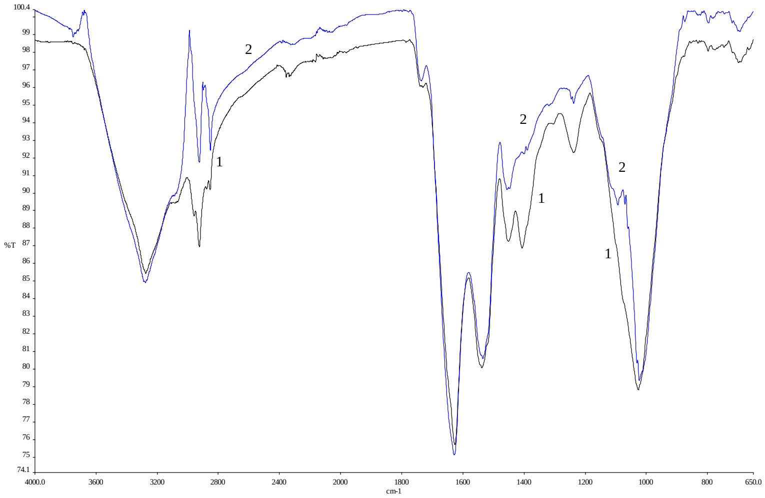

Fig. 1. IR spectra of activated sludge samples 1 and 2 obtained under different conditions.

Asknowledgement. This work is a part of the Moldovan State Program (2020-2023) “Study and management of pollution sources to develop recommendations for implementing measures to mitigate the negative impact on environment and human health”, Project number: 20.80009.7007.20.

AB INITIO STUDY OF HEXAAMMINE COBALT(III) CATIONS INTERACTION WITH MONO- DIANIONS AND NEUTRAL MOLECULES IN MULTI-COMPONENT COMPOUNDS

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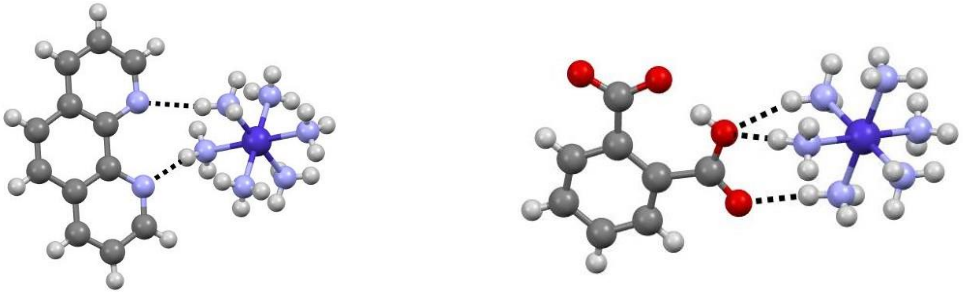
The energy decomposition analysis of the intermolecular interaction energy was performed using the SAPT method to study the non-covalent bonding interactions of $[Co(NH_3)_6]^{3+}$ cations with mono- dianions and neutral molecules (Fig. 1) in a series of multi-component compounds. The series involves $[Co(NH_3)_6]Cl_3 \cdot 2(phen) \cdot 3H_2O$ (**1**), $[Co(NH_3)_6](Hbdc)(bdc) \cdot 3H_2O$ (**2**), $[Co(NH_3)_6]Cl_2(Hpht) \cdot 4H_2O$ (**3**), $[Co(NH_3)_6]Cl(Hpht)_2 \cdot 3H_2O$ (**4**) $[Co(NH_3)_6]Cl(2,3\text{-}pdc) \cdot H_2O$ (**5**), $[Co(NH_3)_6]Cl(sb) \cdot 4H_2O$ (**6**), (where phen = 1,10-phenanthroline, H_2bdc = diphenyl-4,4′-dicarboxylic acid, H_2pht = *o*-phthalic acid, H_2pdc = 2,3-pyridinedicarboxylic acid, H_2sb = 4-sulfobenzoic acid). It was found that the calculated binding energy is minimal for compound **1** (the absolute values of E_{int} are decreases in the following order $E_5 > E_6 > E_2 > E_4 > E_3 > E_1$). In all selected pairs the electrostatic term dominates in calculated binding energy followed by induction interaction. Additionally, the compounds **1-6** have been tested *in vitro* against *Rhizobium* (Agrobacterium) *vitis*, an oncogenic bacteria that causes the formation of tumors in plants. Compound **1**, comprising hexaammine cobalt (III) chloride and 1,10-phenanthroline, shows the highest inhibitory potential and is thus qualified for an application against bacterial cancer in plants. The minimal among the studied compounds binding energy of **1** points out that both cation and neutral ligand might affect on biological activity of **1**.



$[Co(NH_3)_6]^{3+} \cdot (phen)$ $[Co(NH_3)_6]^{3+} \cdot (Hpht)^{-}$

Figure 1. View of selected pairs for estimation of its interaction energies in **1** and **3**.

Acknowledgement: This work has been performed within the State Program of the Republic of Moldova (2020-2023), Project Nr. 20.80009.5007.15: “Implementation of crystal engineering approach and X-ray crystallography for design and creation of hybrid organic/inorganic materials with advanced physical and biologically active functions”.

MULTIPLE COMPONENT IONIC COMPLEXES OF HEXAMMINECOBALT CHLORIDE WITH TWO PHARMACOPHORIC ACIDS

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Multiple component pharmaceutical solids attract special attention as upgraded remedies that provide complemented or synergetic actions often accompanied by the improved pharmaceutical profile (stability, solubility, biocompatibility) in comparison with single pharmacophore [1]. Using drug cocktails combining two or more therapeutic agents with different modes of action and non-overlapping toxicities becomes a common practice in the clinical treatment of cancer and other diseases [2]. We report here two ionic supramolecular complexes obtained by co-crystallization of hexamminecobalt (III) chloride, $[Co(NH_3)_6]Cl_3$ (“Cohex”), that reveals a wide spectrum of antiviral properties [3], with two pharmacophores, NSAID mefenamic acid (2-(2,3-dimethylphenyl)aminobenzoic acid (*Hmef*) [4] and 4-amino-1,2,5-oxadiazole-3-carboxylic acid (*Hoxa*). The crystals with compositions $[Co(NH_3)_6][mef]_2Cl{\bullet}2H_2O$ (**1**) and $[Co(NH_3)_6][oxa]_2Cl{\bullet}H_2O$ (**2**) represent H-bonded systems with inclusion of *mef* or *oxa* as anionic components in the matrix of $[Co(NH_3)_6]2Cl{\bullet}2H_2O$ due to the metal’s second-sphere coordination (Figure).

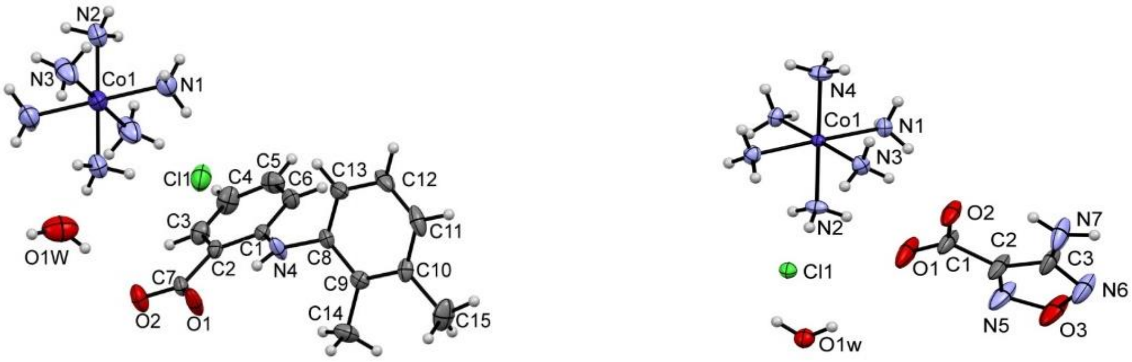

Figure. ORTEP drawings for the components in **1** (left) and **2** (right).

The triclinic (**1**) and monoclinic (**2**) monocrystals are characterized by unit cell parameters a=7.0746(4), b=7.1361(5), c=19.1363(12) Å, α=80.552(5), β=85.770(5), γ=19.1363(12)°; a=7.0175(3), b=18.9329(9), c=7.4775(5) Å, β=105.231(5)°.

The details of supramolecular architecture in the solid state are discussed. In conclusion, two given examples show that Cohex may be potentially useful in a combination drug therapy.

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SYNTHESIS OF QUERCETIN FUNCTIONALIZED CHITOSAN AND DETERMINATION OF ANTIOXIDANT PROPERTIES

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The functionalization of chitosan managed to obtain a method that benefits from a good property in terms of the object of a prepared material with better characteristics. In the study of the data, regarding the low molecular weight chitosan, it is necessary to provide the oxidation of chitosan in the presence of hydrogen peroxide and its functionalization with natural antioxidants – quercetin by the method of grafting, a study of antioxidant properties compared to a compound commonly used to graft industrial chitosan with chitin as well as to graft oxidized chitosan with the same flavonoid. It has been established that the decrease in the molecular weight of chitosan favored grafting may have a concentration, and the result may be composed in order to be able to have a higher antioxidant concentration.

Acknowledgement: This work has been performed within the State Program of the Republic of Moldova (2020-2023), Project Nr. 20.80009.5007.27 “Physical-Chemical Mechanisms of the Redox Processes with Electron Transfer in Vital, Technological and Environmental Systems”.

OCTANUCLEAR COBALT(II) CLUSTER WITH A DIALDEHYDE LIGAND

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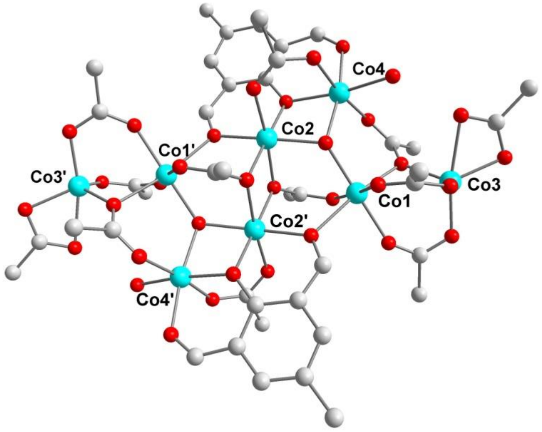
The interesting magnetic properties of cobalt polynuclear clusters arise from the paramagnetism of cobalt(II) ion, with the possibility to exhibit a strong Ising-type anisotropy. An efficient synthetic procedure of high-nuclearity clusters preparation is the use of carboxylate source and auxiliary ligands with bridging ability. Rezulting compounds are convenient objects for studying the type and magnitude of exchange interactions.

Herein we report the structural characterization of a new octanuclear cobalt(II) pivalate cluster $[Co_8(OH)_2(H_2O)_2(L)_2(piv)_{12}]$ (**1**), where L- is deprotonated 2,6-diformyl-p-cresol and piv – pivalate anion. The crystal structure consists of centrosymmetric octanuclear clusters co-crystallized with solvate MeCN molecules in 1:2 ratio. The coordination environment of the Co^{2+} atoms is different. Six of them (Co1, Co2, Co4 and symetrically related) are hexa-coordinated in slightly distorted octahedral geometry. Considering that chelating carboxylate groups occupy only one coordination position, the coordination geometry of Co3 and Co3' atoms can be described as distorted tetrahedral.



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REDOX PROPERTIES AND CATALYTIC ACTIVITY RELATIONSHIPS IN METHANE COMBUSTION FOR Pt-CeO_2/TiO_2 SUPPORTED CATALYSTS

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Aim and methods: The great interest and continuous efforts are dedicated to obtain better catalysts for conversion of the saturated hydrocarbons from air. One of the less explored strategies to enhance the catalytic activity of supported noble/transition metal catalysts is the addition of a second transition metal to the first one. For this purpose, Ce can be a good alternative for the oxidation catalysts reason why this paper evidences the effect of ceria on redox properties and catalytic activity of Pt/TiO_2 high dispersed on mesoporous silica (KIT-6, SBA-15) support. The obtained materials were characterized by various techniques and catalytic activity was tested in total oxidation of methane from air, as a model for understanding the mechanisms of oxidation and catalytic combustion on such catalysts.

Results: Characterization results showed that ceria addition (1%) increased Pt dispersion, reduced the crystallinity of metallic platinum and modified its percentage on the surface. Significant is the different effect of the interaction of Pt species with TiO_2 and CeO_2 which influences the concentration of Pt^0 on the surface. XRD, TPR and XPS results evidenced the effects of ceria immobilization method, Pt (0.25, 0.5, 1%) and titania (5, 10, 30%) loading on Pt^0/Pt^+, Ce^{4+}/Ce^{3+}, TiO_2/TiO_x atomic ratio on the surface with significant influence on redox properties, respectively catalytic reaction. Thus, considering that combustion of methane on these catalysts is a Mars van-Krevelen type reaction, with CH_4 chemisorbed on surface Pt atoms, C-H bond dissociation is the rate determining step due to the relatively large activation energy and greater entropy loss for this molecule. The oxidation on PtO species with lattice oxygen provided by TiO_2-CeO_2 and finally refill of the oxygen vacancies by gas-phase O_2. Ti and Ce oxides high disppersed on the support are the oxygen carriers and the existence of PtO and metallic Pt is essential to provide activity. This explained the reduction in catalytic performance for sample with Pt coated by ceria for which the XPS results indicated the absence of PtO on the surface. In oxidation reactions the oxygen storage capacity provided by the redox couple Ce^{4+}/Ce^{3+}, ratio which varied around 1.1, under a small variation of Ce and Ti species on the surface. High combustion of methane (100% conversion) at low temperature (300-500 °C) was obtained for catalysts with 1% Pt. More significant on the conversion was the increase of the concentration of Pt and TiO_2, in the conditions of a low concentration of CeO_2.

Conclusions: This study showed that both CeO_2 and TiO_2 are beneficial to stabilize the active PtO and Pt^0 playing important role in the complete oxidation of methane. Their loading and dispersion, with significant influence on redox properties, determine the catalytic activity.

APPLICATION OF BIS(TRIETHANOLAMINE)-COBALT(II) DINITRATE IN THE PRODUCTION OF ENZYMES BY MICROORGANISMS

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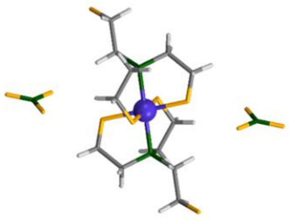
Coordination compounds of 3d metals revealed excellent catalytic activities in the past years and these complexes play an important role in the directed synthesis of biologically active substances, including the production of enzymes by microorganisms. A new coordination compound, $[Co(H_3tea)_2](NO_3)_2$ (**1**), were prepared by the reaction of cobalt(II) isobutyrate with triethanolamine (H_3tea) in the presence of $Dy(NO_3)_3 \cdot 6H_2O$ in MeCN, and characterized by IR spectroscopy and a single-crystal X-ray diffraction studies. The biological properties of this complex have been tested for its ability to increase the biosynthesis of enzymes. The addition of **1** to the nutrient medium of *Rhizopus arrhizus* CNMN FD 03 micromycete in concentration of 5 and 10 mg/L increases biosynthesis of lipases on 54…91.3% depending on the applied concentration and duration of cultivation of the microorganism (Table). Our present results show that the Co(II) triethanolamine containing compounds can been used as biostimulators of the microorganism enzyme synthesis in various biotechnological processes.

Table. The influence of **1** on lipolytic activity (U/mL) of *Rhizopus arrhizus* CNMN FD 03 micromycete.

Compound	Concentration, mg/L	1 day		2 days		3 days	
		U/mL	%, to control	U/mL	%, to control	U/mL	%, to control
 $[Co(H_3tea)_2](NO_3)_2$, **1**	5	30187	100.0	37500	100.0	28125	145.6
	10	57750	191.3/ 154.0	67500	180.0	50625	262.1/ 135.0
	15	24937	82.6	56250	150.0	19687	101.9
Control	-	30188	100.0	39200	100.0	19096	100.0

Acknowledgements: This work has been performed within the State Program of the Republic of Moldova (2020-2023), Project Nr. 20.80009.5007.15: "Implementation of crystal engineering approach and X-ray crystallography for design and creation of hybrid organic/inorganic materials with advanced physical and biologically active functions" and 20.80009.5007.28: "Elaboration of new multifunctional materials and efficient technologies for agriculture, medicine, technics and educational system based on the "s" and "d" metals complexes with polydentate ligands".

PRELIMINARY RESULTS ON ^{13}C NMR STUDIES REGARDING THE RADICAL SCAVENGING ACTIVITIES OF ASCORBIC ACID AND DIHYDROXYFUMARIC ACID USING 1,1-DIPHENYL-2-PICRYLHYDRAZYL

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Dihydroxyfumaric acid (DHF) is a natural compound discovered in 1890s as an oxidation product of tartaric acid [1]. In small quantities it is found in grapes, being involved in the metabolism of the fruits during the ripening period [2]. Due to the ene-diol moiety, DHF exhibit nucleophilic and electrophilic character which support the ”glioxylate scenario” [3], where DHF serves as a source molecule for the formation of a variety of biogenic molecules [4]. On the other hand, it was demonstrated that DHF possesses strong antioxidant activity against the free radical DPPH in alcoholic solvents and in wine matrix [5], having the antiradical power similar to that of ascorbic acid (AA). In virtue of the high reactivity of DHF, in aerobic conditions and in acidic media, it easily decarboxylates to form glycolaldehyde [6].

In extending our recent ^{13}C NMR investigations of radical scavenging activities of two wine antioxidants: AA and resveratrol [7], the current study was aimed at finding of some potentially synergic interactions between DHF and AA, since both compounds can be found in grapes. We have used the analytical approach reported by Sawai et al., which employed ^{13}C NMR spectroscopy in determining the properties of different tea polyphenols to regenerate each other [8].

The interactions of DHF and AA with free radical 1,1-Diphenyl-2-picrylhydrazyl (DPPH) were studied in the mixture of deuterated solvents acetone-d_6 –methanol-d_4 in the NMR tube. Three approaches of performing the reactions were considered, including different sequence of mixing antioxidant(s) and DPPH. The results of the exploratory studies show that neither AA nor DHF can be regenerated from their oxidized forms, in the case of DHF the decarboxylation due to the acidic media being hypothesized.

Acknowledgement:

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A 2D CADMIUM COORDINATION HOST FRAMEWORK WITH INCLUSION OF 4,4′-DIAMINODIPHENYLMETHANE AND 4,4′-BIPYRIDINE GUEST MOLECULES

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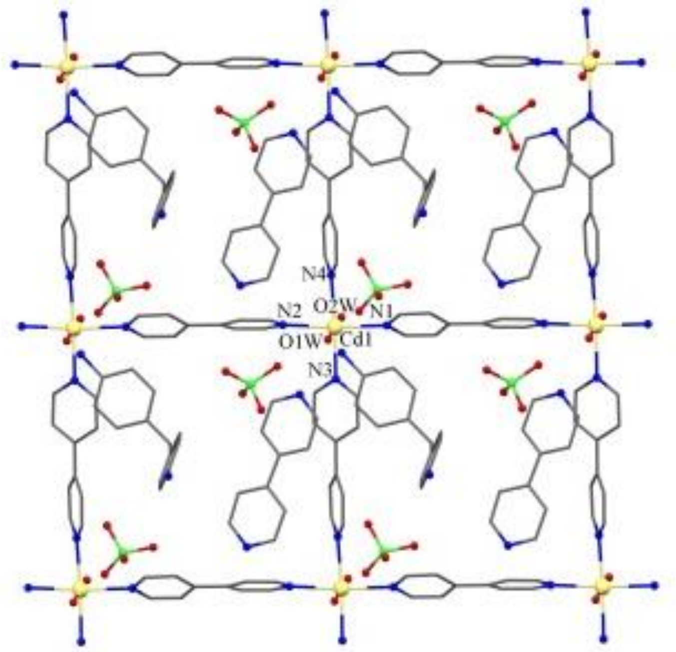
The rapid development in crystal engineering of metal-organic coordination polymers continues to create various solid state structures with new compositions and topologies, which manifest potential applications in host-guest chemistry, catalysis, ion exchange, magnetism, nonlinear optics, molecular recognition and separation. The assembly of these complexes strongly depends on the selection of both the metallic centers and the ligands. Compared to 4,4′-bipyridine (*bipy*), the 4,4′-diaminodiphenylmethane (*dadpm*) molecule forms the hydrogen bonds via terminal amino-groups and it is a good candidate as a ligand in supramolecular architecture [1,2]. Here we report the preparation, IR characterization and X-ray investigation of a new 2D coordination polymer $\{[Cd(bipy)_2(H_2O)_2](ClO_4)_2(bipy)_{0.5}(dadpm)\cdot 2C_2H_5OH\}_n$ using the exo-bidentate N,N-bipyridyl-based ligand such as rigid rod-like *bipy* and angular *dadpm* as a guest molecule (Figure). The reported compound was obtained as a result of the reaction between $Cd(ClO_4)_2\cdot 4H_2O$, bipy and dadpm in C_2H_5OH solvent. The IR specta of the coordination compound and the pure ligands dadpm and bipy were measured and confirm the presence of organic ligands used in the synthesis. The absorption bands observed at 3450-3373 cm^{-1} are assigned to asymmetric and symmetric stretching vibrations $\nu(NH_2)$, while deformation vibrations $\delta(NH)$ were registered at 1600 cm^{-1}. The bands at 2826-2886 cm^{-1} are assigned to the $\nu_s(CH_2)$ and $\nu_{as}(CH_2)$ stretching vibrations. The C-N absorptions are found in the 1065, 1181 cm^{-1} regions. The compound crystallizes in the monoclinic space group $P2_1/c$: a = 11.7324(3), b = 11.7462(3), c = 32.5247(11) Å, β = 95.812(3)°, V = 4459.2(2) $Å^3$. The Cd cation adopts a slightly distorted octahedral surrounding with the N_4O_2-set of donor atoms going from the four *bipy* ligands at equatorial positions and two water molecules at the apical positions. The Cd – N bond distances range from 2.326(5) to 2.357(5) Å and Cd – O distances are 2.323(4) and 2.376(5) Å. In the crystals the 2D coordination polymer layers are united by O−H···O and O−H···N and N−H···O hydrogen bonds through going between uncoordinated chlorine anions, *bipy* and *dadpm* molecules into 3D supramolecular net.



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2D AND 3D Nd(III) COORDINATION POLYMERS ASSEMBLED VIA BRIDGING 1,4-BENZENEDICARBOXYLATE AND OXALATE LINKERS

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Lanthanide-containing solids are amongst the luminescent materials for potential applications in lasers, optical-fiber polymers, and near-IR immunoassays [1]. An attempt to incorporate NHC-luminophores, triimidazo[1,2-a:1′,2′-c:1″,2″-e][1,3,5]-triazine and triimidazo[1,2-*a*:1′,2′-*c*:1″,5″-*e*][1,3,5]triazine in the Nd(III) first coordination sphere to provide an antenna effect resulted in 2D coordination network $[Nd(oxa)Cl\cdot(H_2O)_3]_n$ (oxa=oxalate) and 3D MOF $[Nd_2(bdc)_3(dmf)_2(H_2O)_2]_n$ (bdc=1,4-benzenedicarboxylate). $[Nd(oxa)Cl\cdot(H_2O)_3]_n$ is monoclinic, sp. Gr. $P2_1/n$, a=5.8602(2), b=15.9365(5), c=8.3689(4) Å, β=103.903(4) °, V=758.68(5) Å^3, Z=4. The 2D coordination network is built of centrosymmetric Nd(III) binuclear units with Nd(1)···Nd(1*)=4.4603(5) Å, where each metal atom is nine-coordinated with the ClO_8 set of donor atoms, Nd-O distances ranging 2.441(4)-2.644(5) Å, and the binuclear units are interlinked via tetradentate and hexadentate oxa ligands (Fig.). The MOF $[Nd_2(bdc)_3(dmf)_2(H_2O)_2]_n$ is triclinic, a=8.7229(4), b=10.1533(5), c=11.2003(6), α=65.460(5), β=71.496(5), γ=78.322(4), V=852.85(9) Å^3, Z=1. In crystal each Nd(III) atom is nine-coordinated by oxygen atoms from four bdc residues, and coordinated dmf and water molecules, Nd-O distances ranging 2.420(3)-2.708(3) Å. Two Nd ions are bridged by two carboxylate groups to generate binuclear units with Nd(1)···Nd(1*)= 4.3504(4) Å, which are interlinked by bdc ligands in three directions giving rise to a 3D porous framework (Fig.).

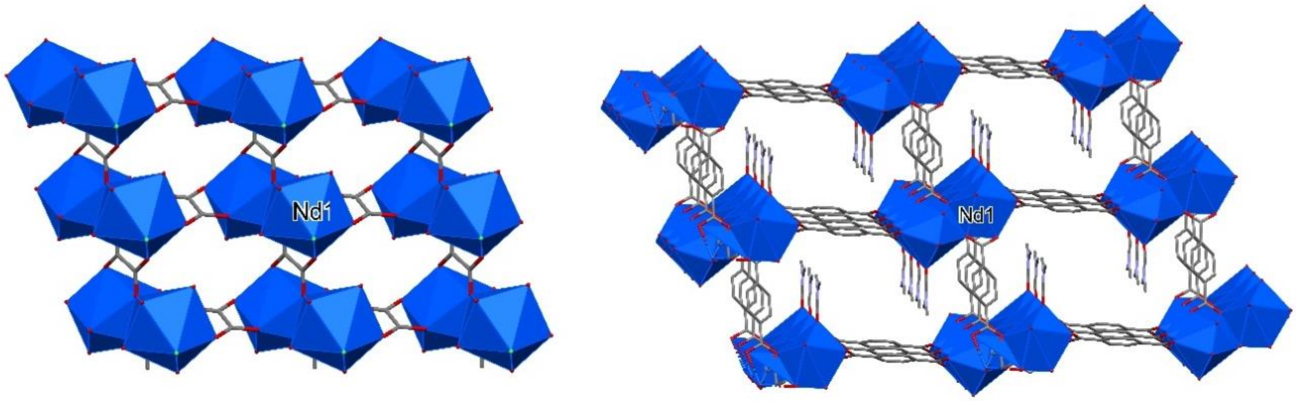

Figure. Coordination grids in $[Nd(oxa)Cl\cdot(H_2O)_3]_n$ (left) and $[Nd_2(bdc)_3(dmf)_2(H_2O)_2]_n$ (right).

Compounds $[Nd(oxa)Cl\cdot(H_2O)_3]_n$ and $[Nd_2(bdc)_3(dmf)_2(H_2O)_2]_n$ are the missing members in the series of isomorphous complexes $[Ln(oxa)Cl\cdot(H_2O)_3]_n$ (Ln=La, Gd, Pr) and $[Ln_2(bdc)_3(dmf)_2(H_2O)_2]_n$ [Ln= Eu, Gd, Tb, Dy, Er, Tm, Yb] [2].

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DFT MODELING OF ADSORPTION OF $[Sr(H_2O)_6]^{2+}$ IONS ON ACTIVATED CARBONS

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One of the most effective methods of removing metal ions from water is the adsorption method using activated carbons [1]. This work aims to computational study the process of adsorption of $[Sr(H_2O)_6]^{2+}$ ions on the surface of activated carbons (AC) containing carboxylic groups. The DFT/B3LYP/3-21G calculations confirm the experimental results and revealed that the adsorption is influenced by the protonation of the carboxylic groups [2]. In case the carboxylic groups are protonated, then the $[Sr(H_2O)_6]^{2+}$ ion is adsorbed on the surface of AC by forming hydrogen bonds of O···H···O type, without modifying the octahedral coordination polyhedron of the strontium. When carboxylic groups are deprotonated or dissociated depending on the pH value, the oxygen atom O36 coordinates at $[Sr(H_2O)_6]^{2+}$. In this case, the Sr–O(COO) bond is formed, and the strontium ion becomes heptacoordinate (Figure 1). At the same time the strontium ion is bound and stabilized by the intermolecular hydrogen bonds of O···H···O type, such as O48-H50-O36, O37-H53-O51 and bifurcated H···O···H bond as is H55-O39-H49.

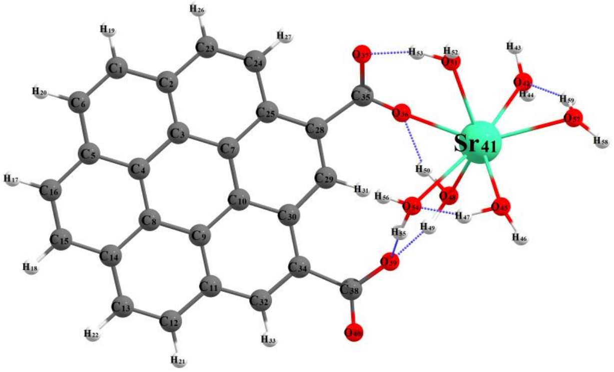

Figure 1. Adsorption of the $[Sr(H_2O)_6]^{2+}$ ion on the activated carbon surface.

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UNPRECEDENTED ATOM TRANSFER RADICAL ADDITION – HIDROGEN ATOM TRANSFER SEQUENCE UNDER VISIBLE LIGHT PHOTOREDOX CATALYSIS

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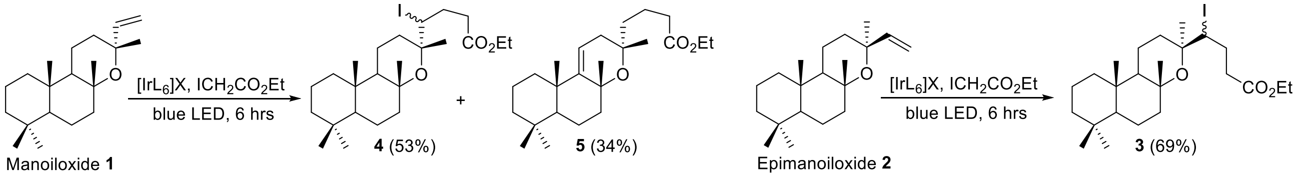
Green chemistry principles announced on the eve of the current century have set a clear strategic line for the global community of chemists. One of the essential elements of the Anastas' and Warner's paradigm represents the need to implement catalytic processes, which are more efficient, provide a better atom economy and diminish the negative impact on the environment that is characteristic for most stoichiometric transformations.

In this line, the visible light photoredox catalysis has emerged in the last decade as an efficient synthetic tool, in particular for free radical mediated processes. Of those, atom transfer radical addition (ATRA) is a simple transformation that allows to achieve a simultaneous alkylation and heteroatom addition to an alkene. The aim of the current work was to investigate ATRA to manoyloxides **1**, **2** under the conditions of visible light photoredox catalysis. The investigated substrates possess the carbon skeleton of forskolin – a well-known natural diterpenoid that increases the level of adenosine monophosphate in living cells. In our view, molecular editing of manoyloxides by functionalization with heteroatoms is the most convenient way to generate new derivatives with biological activity.

This study established that ATRA of ethyliodoacetate to epimanoyloxide **2** under photochemical conditions takes place in a normal pathway, resulting in epimeric iodides **3**, isolated with a very good yield. On the other hand, the manoyloxide **1** provided under similar reaction conditions a mixture of the expected 1,2-addition products **4**, along with an unusual unsaturated compound **5**. Formation of this product was interpreted on the basis of a hypothetical ATRA, followed by a hydrogen atom transfer (HAT) from the tertiary position of the neighbouring cycle which ends with an elimination and formation of olefin **5**. The initiation of the free radical chain takes place on the single electron reduction of the R-I bond which is effected by the iridium catalyst $[IrL_6]X$ excited on blue LED irradiation and following reduction by a sacrificial reductant. Reaction conditions have been optimized for a better yield of olefin **5**. Possible mechanistic pathways of the unprecedented ATRA-HAT sequence will be under discussion. The obtained results represent the first example of triggering two simultaneous free radical processes under conditions of visible light photoredox catalysis. The unsaturated ester **5** represents a convenient substrate for the synthesis of manoyloxide functionalized derivatives, similar to forskolin.



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ADSORPTION OF A CATIONIC DYE ONTO ALGINATE-BASED MAGSORBENT: MACHINE LEARNING AND MOLECULAR MODELING APPROACHES

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Alginate (ALG) is an important biomaterial, with particular properties, which showed its utility for various applications in chemical and environmental engineering, biomedical science, and other industries (*e.g.* food, packing, paper, and textile) [1]. We report herein a machine learning approach based on an artificial neural network (ANN) to estimate the adsorption performance of a composite adsorbent with magnetic properties. This magsorbent was formulated as a cross-linked alginate matrix with glutaraldehyde (ALG-GA) that incorporated 15% wt. inorganic nanoparticles of cobalt ferrite ($CoFe_2O_4$). The produced magsorbent ($CoFe_2O_4$@ALG-GA) was well characterized by instrumental physical-chemical techniques (FTIR, VSM, SEM, and EDX). Afterward, this magnetic material was utilized for the adsorption of a persistent organic pollutant (Rhodamine, Rh6G) from synthetic wastewaters. Adsorption assays were done to evaluate the kinetics, isotherms, and thermodynamics parameters. According to Dubinin-Radushkevich isotherm, the computed free energy of adsorption (E_S) varied from 9.4 to 10.6 (kJ/mol) revealing an ion exchange as the predominant retention mechanism [2]. The adequate prediction capability of the trained ANN-model allowed determining the optimal adsorption conditions by using model-based optimization. Under optimal conditions established, the maximal removal efficiency of 96.54% was confirmed experimentally for an initial concentration of 110 mg/L of the Rh6G pollutant. In addition, the details about the interactions at the molecular level were estimated by the molecular modeling methods. Hence, the molecular docking results suggested that the binding of the Rh6G cationic dye (ligand) to the cross-linked alginate matrix (receptor) was based on the hydrophobic and electrostatic interactions. Moreover, the molecular dynamics simulation highlighted the stability grade of the docked complex *versus* the simulation time (**Fig.1**).

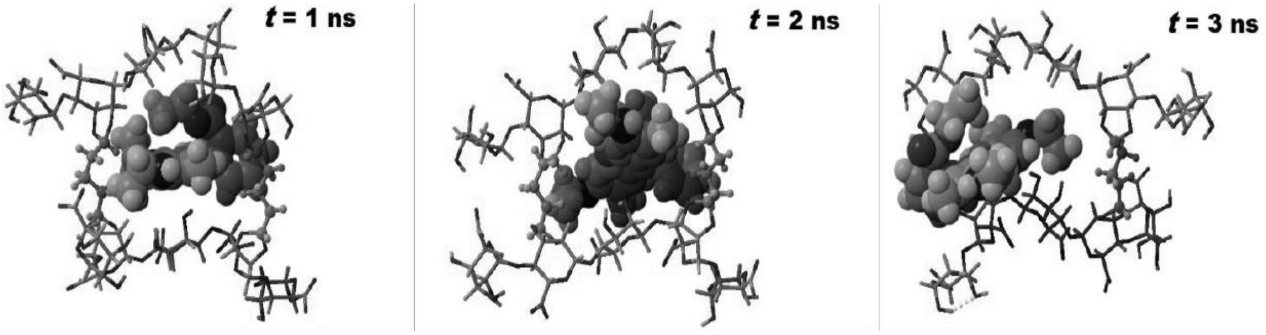

Fig.1. Molecular dynamics results showing the interactions between ALG-GA (receptor) and Rh6G (ligand).

Acknowledgment. This work was supported by a grant of the Romanian Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PN-III-P1-1.1-TE-2019-0594, within PNCDI III.

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PHOTOCATALYTIC ACTIVITY OF TITANIA AND IRON TITANATES FILMS IN THE PROCESS OF LIGNIN TRANSFORMATION

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Iryna LAGUTA[3], Oksana STAVINSKAYA[3], Roman IVANNIKOV[4], Oksana LINNIK[3]

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Photocatalytic conversion of lignin is a perspective route of “green technologies” in the application of “raw” waste biomass in the synthesis of organic compounds. The efficiency of photocatalytic transformation of lignin depends on its concentration, the composition of the photocatalyst, and light source. The electronic structure of the photocatalyst determines the mechanism of photocatalytic transformations and, in turn, the conversion efficiency and reaction products.

The water-soluble fraction of lignin was obtained from plants by extraction in ethanol with the following dissolution of solids in ammonia solution. The photocatalysts were obtained by sol-gel method according to the procedure reported in [1,2]. The photocatalytic experiments were performed using the aqueous solution of lignin liquor at pH 2 in the presence of titania, iron titanate or nitrogen doped iron titanate films under simulated solar light or visible irradiation during 6 h.

HPLC results have shown that the products of the lignin conversion, as namely phenol, vanillic acid, resorcinol, *p*-coumaryl alcohol, have been formed over the photocatalyst as a result of partial depolymerization under light exposure. High yield of phenol formation is observed after photolytic transformation or photosensitization reaction in the presence of TiO_2 film under visible light irradiation. Iron titanates films were inactive towards phenol formation under given experimental conditions. The photocatalytic reaction over titania films led to the formation of the mixture of compounds: phenol, vanillic acid, resorcinol and *p*-coumaryl alcohol whereas the films based on iron titanates exhibited high selectivity towards vanillic acid and *p*-coumaryl alcohol. It is shown that nitrogen doped iron titanate films can be used for the synthesis of vanillic acid, and iron titanate films showed high-selective formation of *p*-coumaryl alcohol under irradiation with simulated solar light.

The efficiency of lignin depolymerization / conversion according to the LDI MS results was increased over titania and nitrogen-doped iron titanate films under simulated solar light. The most effective transformation of complex polymeric structure of lignin molecule under visible light was observed in the presence of nitrogen doped iron titanates.

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EFFECT OF SOME PLANT EXTRACTS ADDITION ON THE OXIDATION STABILITY OF BIODIESEL

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Stabilization of biodiesel against oxidation is known to be an important task for its storage and effective use. One of the convenient approaches to solve this task is the introduction of antioxidant additives. Since no particular inhibitor is found to be useful for every biodiesel type, it is of current importance to search for and to study novel efficient antioxidant additives. The antioxidant-rich extracts from plants of various origin may be a promising source for such kind of additives. The aim of this work was to study the extracts from the leaves of thirteen plants and from the eight samples of vegetable oil production wastes as potential additives for the improvement of biodiesel stability against oxidation.

Composition and antioxidant properties of the extracts were studied by means of HPLC, MALDI MS, Folin-Ciocalteu and DPPH methods. All the extracts were found to contain large amount of phenolic compounds, with the nature and quantity of the antioxidants being dependent on the raw material used for the extract preparation. Hydroxycinnamic acids and quercetin glicosides were the main constituents of the majority of the extracts, while hydroxybenzoic acids and catechin derivatives prevailed in several extracts. In spite of significant distinctions in phenols content, all the extracts were found to possess very high antioxidant activity in both Folin-Ciocalteu and DPPH assays. The overall amount of phenolic compounds in the extracts was up to 350 mg/L.

Five extracts with the highest antioxidant ability was also tested as an additive to stabilize the biodiesel against oxidation. The biodiesel stability was studied according to accelerated procedure at 43°C for 12 weeks (that is equivalent of 12 months of diesel maintenance at room temperature), with the changes in the acid value of the samples being the criteria of fuel oxidation. The results showed that the extracts can provide the deceleration of biodiesel oxidation by 5-25%, as determined by comparison of acid number for the diesel samples with and without antioxidant additives.

The HPLC and LDI MS studies have shown that after maintaining two biodiesel samples for 12 weeks at 43°C a set of the compounds related to the products of original fat acid esters oxidation are formed. The oxidation of original esters in biodiesels was found to be inhibited by up to 15% upon extracts addition. These data are in agreement with the results of biodiesel oxidation test and confirm the stabilizing effect of the plant extract components. Among all the extracts studied, the ones from *Silybum* and *Camellia japonica* L. were found to provide the greatest inhibition of biodiesel oxidation; these extracts can be considered as a promising stabilizing additive to reduce the biodiesel oxidation.

Acknowledgement. This work was financially supported by National Research Foundation of Ukraine (Project No2020.01/0136 «Efficient use of renewable plant resources and photocatalytic conversion of biomass as eco-innovative approaches for environmental protection and human biosafety»).

CRYSTAL STRUCTURE AND HIRSHFELD SURFACE ANALYSIS OF A MULTI-COMPONENT COMPOUND COMPRISING HEXAAMMINE Co(III) CATIONS AND 3-PYRIDINESULFONATE ANIONS

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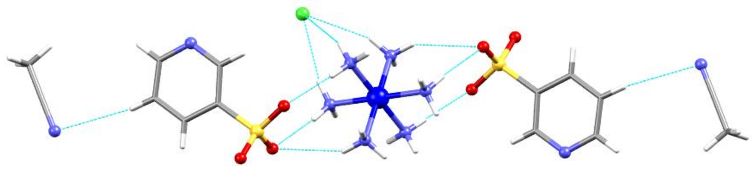
Cobalt(III) complexes have been found to possess both antiviral and antibacterial activities. Recently, we showed that compounds based on hexaammine cobalt(III) trichloride and 1,10-phenanthroline can be applied in various chemical and biotechnological processes as an inhibitor of the development of bacterial cancer in plants [1]. This study investigates the role of 3-pyridine sulfonic acid in the structure formation of a new Co(III) complex focusing on multicomponent mononuclear compound with potential biological activity. A new Co(III)-containing compound, $[Co(NH_3)_6]Cl(pys)_2 \cdot 2MeCN$ (**1**), was obtained from the reaction of $[Co(NH_3)_6]Cl_3$ with 3-pyridine sulfonic acid (Hpys) in the presence of triethanolamine in MeOH/MeCN (1:1) mixture. The single crystal X-ray diffraction analysis indicates that **1** is an ionic compound and its components in the crystal are associated by extended charge-assisted hydrogen bonds between cations and anions and other interactions such as C–H…N bonds and π-π stacking into supramolecular chains (Fig. 1a,b). The use of Hirshfeld surface analysis in combination with fingerprint plots demonstrates that these interactions are important for both local packing and crystal packing: the close contacts are associated with relatively weak H...H (45,9%), H...O/O...H (30,8%), C...H/H...C (8,8%), and Cl...H/H...Cl (12,1%) interactions. The total d_{norm} surface (ranging from −0,4791 (red) to 1,3073 (blue) Å) has been shown in Figure 1c, in which the red points (spherical depression spots) correspond to O–H...O interactions in the crystal. For examination of the influence of π-π stacking on the molecular packing, an analysis of the Hirshfeld surface mapped over the shape-index properties has been made (Fig. 1d).



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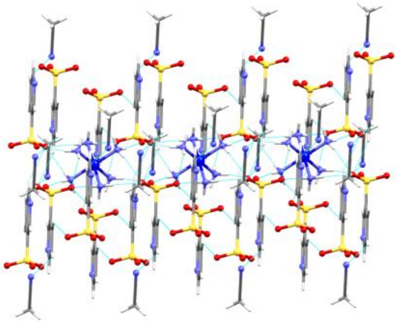

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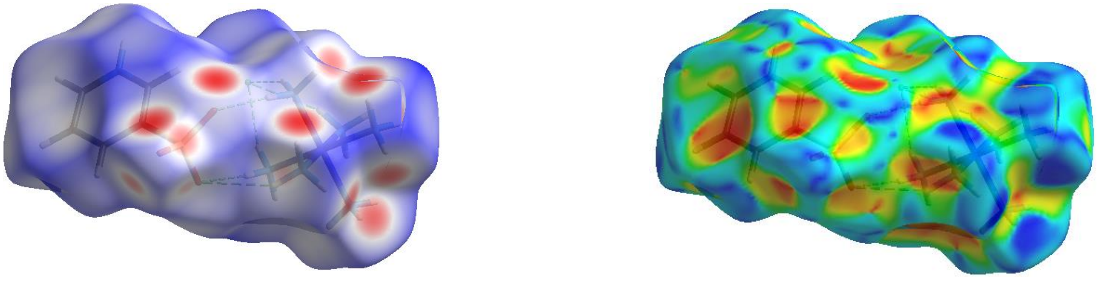

c

d

Fig. 1. Molecular structure of **1** showing intermolecular hydrogen bonds (a). Fragment of a hydrogen-bonded supramolecular chain (b). The Hirshfeld surface of **1** plotted over d_{norm} (c) and shape-index (d).

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SYNTHESIS, STRUCTURAL CHARACTERIZATION AND THERMAL ANALYSIS OF Co(II) MONOMER BASED ON 2,3-PYRIDINEDICARBOXYLIC ACID

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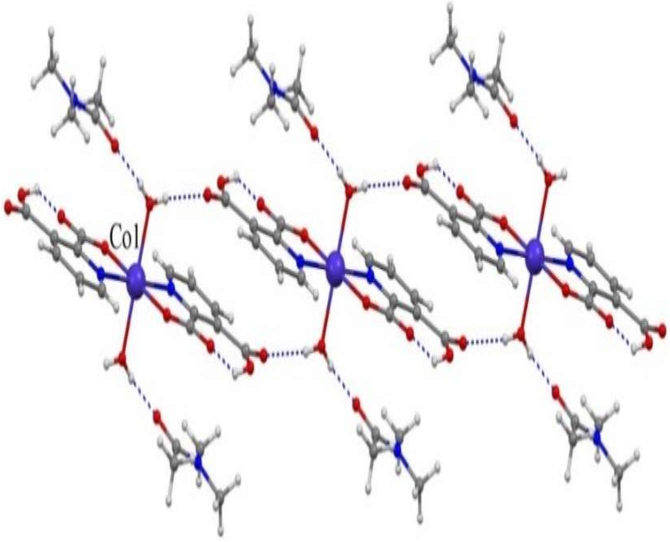
Dicarboxylate ligands are widely used to assemble supramolecular networks organized by coordination bonds, hydrogen bonds and π–π stacking interactions. Due to the sets of N- and O-donors, pyridindicarboxylic ligands can contrast versatile structural motifs, which eventually aggregate to generate various supramolecular architectures with exciting properties. The design and synthesis of metal coordination polymers can be influenced by many factors, especially by the nature of metal ions, anions, and ligands. As one of the dicarboxylate ligands, 2,3-pyridinedicarboxylic acid often acts as a bidentate chelating ligand through the nitrogen atom and one oxygen atom of the carboxylic group to form a discrete complex or 2-D layer. Here we report the preparation of new compound $[Co(2,3\text{-}pyd)_2(H_2O)_2]\cdot Me\text{-}DMF$, which was analyzed by X-ray diffraction, IR spectroscopy and thermogravimetric analysis. This compound was obtained as a result of interaction between $Co(NO_3)_2\cdot 6H_2O$ and 2,3-pyridinedicarboxylic acid (2,3-pyd) in CH_3CN and DMF solvents. The compound crystallizes in triclinic *P*-1 space group: *a* =



7.5963(5), b = 9.3731(7), c = 9.4277(7) Å, α= 88.599(6), β = 74.846(6), γ = 83.113(6)°, V = 643.23(8) Å^3 and represents a mononuclear Co(II) complex where 2,3-pyd works as a bidentate ligand (Figure). The Co atom is coordinated by N and O atoms from two 2,3-pyd ligands and O atoms from two water molecules, forming a distorted N_2O_4 octahedral coordination environment. In the crystal, the monomers are united via O−H···O hydrogen bonds forming supramolecular chains.

Infrared spectroscopy showed the presence of organic ligands used in the synthesis. The band at 3319 cm^{-1} is attributed to the hydrogen-bonded O–H stretching vibration. The absorption bands at 2934 and 2880 cm^{-1} correspond to the asymmetric and symmetric aromatic C–H stretching vibrations respectively. The C=O stretching vibration of 2,3-pyridinedicarboxylic acid is observed at 1659 cm^{-1}. The COO^- asymmetric and symmetric stretching vibrations appear at 1562 and 1388 cm^{-1} respectively. The difference $\Delta\nu = \nu_{as}(COO^-)-\nu_s(COO^-)$ is equal to 174 cm^{-1}, which tells us about the bidentate mode of coordination of the pyridinedicarboxylate anion in the compound. The aromatic C–C stretching vibrations are exhibited at 1477 and 1505 cm^{-1}. The C–H bending vibration is observed at 755 cm^{-1} and the C–N stretching vibration appears at 871 cm^{-1}. The thermal analysis was performed in inert atmosphere. The first stage occurs in the range of 95-158 ^{o}C accompanied by an endothermic process due to the elimination of water molecules. The second step starts up at 239 ^{o}C and ends at 268 ^{o}C with a mass loss of 22.76 % (theor. 22.56%), that is assigned to the loss of the Me-DMF molecules. In the next step that begins at 351 ^{o}C, decomposition of the carboxylate ligand occurs. The final residue is a cobalt oxide.

Acknowledgements. This work has been performed within the State Program of the Republic of Moldova (2020-2023), Project Nr. 20.80009.5007.15: "Implementation of crystal engineering approach and X-ray crystallography for design and creation of hybrid organic/inorganic materials with advanced physical and biologically active functions", and 20.80009.5007.28 **"**Elaboration of new multifunctional materials and efficient technologies for agriculture, medicine, technics and educational system based on the "s" and "d" metals complexes with polydentate ligands".

IMMUNE RESPONSE MODELING UNDER VIRAL LOAD

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The creation of adequate mathematical models in immunology is becoming an even more priority and urgent task. In this work, the model "lymphocytes (killer cells) – antigen" is proposed. This model, in its minimal form, looks like:

$$\frac{\partial x}{\partial t} = c_x x - a_x xy; \tag{1}$$

$$\frac{\partial y}{\partial t} = c_y(x - bx^2)y - ay + p \tag{2}$$

Here x-concentration of antigen, y-killer lymphocytes, the first term of equation (1) describes the increase in antigen concentration, the second term is responsible for the destruction of antigen by killer lymphocytes. The second equation in the system describes the dynamics of killer lymphocytes. In it, the first term describes their multiplication (at small values of x, the proliferation of lymphocytes is stimulated, at large values it decreases (the so-called "crowding effect"). The second term in the second equation corresponds to the death of lymphocytes when they interact with the antigen, the last term corresponds to the influx of lymphocytes from stem cells Depending on the values of the parameters, a pair of differential equations (1), (2) can be solved numerically.There are three types of solutions.

Case I corresponds to an absolute insufficiency of immunological surveillance, the integral curves tend to the point (∞, 0), which means a catastrophic increase in the antigen and a decrease in the concentration of lymphocytes to zero values. Case II corresponds to a situation where the disease is under control and depending on the initial conditions, the recovery scenario may differ slightly. Case III corresponds to a quick recovery and absolute immune competence (possible as a result of prior vaccination or innate immunity).

Acknowledgement: This work has been performed within the State Program of the Republic of Moldova (2020-2023), Project Nr. 20.80009.5007.27 “Physical-Chemical Mechanisms of the Redox Processes with Electron Transfer in Vital, Technological and Environmental Systems”.

A HEXANUCLEAR {Fe_6} PIVALATE CLUSTER BASED ON AMINOALCOHOL LIGANDS

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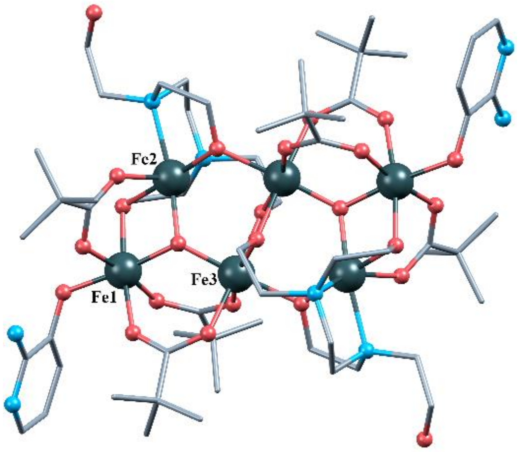
The control of water pollution has become one of the most pressing issues in recent years. The increasing demand of textile and fibers lead to the use of dye in order to dyeing these materials. The chemicals used in the textile industry cause environmental and health problems. There are several methods of dye removal from the waste waters which include coagulation, ozonation, ultrafiltration, photodegradation, ion-exchange, chemical precipitation and absorption. Applying these methods in water treatment reveal that absorption on various materials like clay, biomass, activated carbon, zeolites, cellulose and other polymers is relatively cheap, compatible and eco-friendly. Metal-organic frameworks (MOFs) and polynuclear coordination clusters attracted attention of scientist as alternatives of above-mentioned materials. Coordination compounds based on aminoalcohols contains hydroxylic groups which enhance absorption of perilous dyes. Hexanuclear iron clusters have been investigated as potential candidates in process of dye absorption [1]. Herein we report the synthesis and structural characterization of a new homometallic hexanuclear iron pivalate cluster containing aminoalcohol ligands as promising materials for dye removal in water treatment.

Compound $[Fe_6O_2(piv)_6(Hteed)_2(ahpy)_2]$ (**1**) (where Hpiv = pivalic acid; H_4teed = N,N,N’,N’-tetrakis(2-hydroxyethyl)ethylenediamine; ahpy = 2-amino-3-hydroxypyridine) was obtained by ultrasonic treatment of trinuclear $[Fe_3O(piv)_6(H_2O)_3](piv)$ cluster, H_4teed and ahpy in acetonitrile solution. X-ray structural analysis revealed that compound **1** crystallizes in the triclinic *P*-1 space group with following unit cell parameters: a = 12.600(3), b = 13.760(3), c = 24.530(5) Å, α = 92.83(3), β = 99.11(3), γ = 105.18(3)º. Inorganic core consists of two $\{Fe_3O\}^{7+}$ fragments, connected via μ_2-O^{2-} bridges from hydroxyethyl branches of two triple deprotonated $Hteed^{-}$; six bridging pivalates additionally bind iron atoms in **1** (Fig.). Coordination environments of iron atoms are different, displaying O_6 (Fe1 and Fe3) and N_2O_4 (Fe2) distorted octahedrons. The bond distances Fe–O are in the range 1.820(5) – 2.027(6) Å and Fe–N bond distances fit the interval of 2.202(6) – 2.230(7) Å. The BVS calculation and charge balance prove the Fe(III) oxidation state of all iron atoms in the cluster. Further absorption studies will reveal the efficacy of this compound in dye absorption process.



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Acknowledgement: This work has been performed within the State Program of the Republic of Moldova (2020-2023), Project Nr. 20.80009.5007.15: “Implementation of crystal engineering approach and X-ray crystallography for design and creation of hybrid organic/inorganic materials with advanced physical and biologically active functions”.

THE MODERN PROBLEMS OF ECOLOGY

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In the paper the modern problems and challenges in the field of ecology will be presented. Author will try to explain why today the problems of ecology so important and why now the world pays much attention to this field. Also, will be explained connection between the ecological problems, green economy and informational technologies. Some examples of various countries which effectively used achievement of informational technologies in ecological problems will be given.

SYNERGY EFFECT OF VITAMINS E AND C ON THE EXAMPLE OF LIPID PEROXIDATION REACTION

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The paper presents an theoretical model for the kinetics of lipid peroxidation (LP), which takes into account the synergy effect of vitamins C and E for 5 reagents: InH, In •, R •, ROO • and ROOH:

$$dR/dt = w_i + k_{R1}SR_1 - k_{R}YR - k_iI_1R \,, \qquad (1)$$

$$dR_1/dt = k_{R}YR - k_{R1}SR_1 - k_{i1}I_1R_1 - k_{2r1}R_1^2 \,, \qquad (2)$$

$$dP_1/dt = k_{R1}SR_1 + k_{i1}I_1R_1 - (k_{d1} + k_{d2})P_1 \,, \qquad (3)$$

$$dI_1/dt = k_aI_2A - k_iI_1R - k_{i1}I_1R_1 \,, \qquad (4)$$

$$dI_2/dt = k_iI_1R + k_{i1}I_1R_1 - k_aI_2A \,, \qquad (5)$$

here the following designations are introduced: S = [RH], Y = [O_2], R = [R •], R_1 = [ROO •], P_1 = [ROOH], I_1 = [InH], I_2= [In •], A = [AscH–]. And also k_{d1} and k_{d2} are the rate constants of lipid hydroperoxide decomposition, k_i and k_{i1} are the rate constants of inactivation of R • and ROO • radicals, k_{R1} are the rate constants of radical oxidation of the RH substrate by the ROO • radical, k_{2r1} is the rate constant of quadratic recombination of the ROO • radical. In this model, it is believed that the lipid substrate RH, oxygen O_2, and ascorbic acid AscH– are present in excess; in a first approximation, their concentrations can be considered constant: $S \approx S_0$, $Y \approx Y_0$, $A \approx A0_0$ For different types of cell membranes and different physicochemical conditions for the initiation and course of the peroxidation process, this model, when using an appropriate set of model parameter values (reaction rate constants and initiation rate), makes it possible to determine the concentrations of conjugated antioxidants that are optimal for effective control.

Acknowledgement: This work has been performed within the State Program of the Republic of Moldova (2020-2023), Project Nr. 20.80009.5007.27 “Physical-Chemical Mechanisms of the Redox Processes with Electron Transfer in Vital, Technological and Environmental Systems”.

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Session B

WATER SCIENCE AND SOCIETY

DECENTRALIZED ATMOSPHERIC WATER HARVESTING – A STEP TOWARDS FUTURE OF WATER SUSTAINABILITY

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Ghitu Institute of Electronic Engineering and Nanotechnology, Chisinau, ***Moldova***
Riga Technical University, Biomedical and Nanotechnology Institute, ***Latvia***

Water is fundamental to human survival. Although present abundantly on earth, the supply of clean and safe water in adequate amount and sustainable manner is a global challenge, since the presence of organic and inorganic contaminants, with unknown toxico-kinetics, in waterbodies has developed one of the most alarming issue. The technologies that are employed for water treatment and its desalination remain inefficient in removing many contaminants, especially the ones that are present in trace concentrations, including micro/nano plastics, pharmaceuticals, pesticides, long-chain hydrocarbons, etc. Thus, we must revisit the global reserves of water in an attempt to utilize sources which may be under-utilized and/or cost effective. Out of 2.5% of total freshwater reserve available globally, it seems that over 30.1% is ground water, 68.6% is polar ice and the remaining 1.3% is distributed among various forms such as lakes ~0.26%, ice/snow ~0.97%, rivers ~0.006% and atmospheric water is about 0.037% - which is significant amount considering that nature uses atmospheric condensation for rain and snow. It appears logical to tap into atmospheric water, as an obvious choice for sustainable water production. This presentation investigates various ways to capture atmospheric water as a decentralized way to produce clean water globally and its feasibility. Various technologies are currently used for capturing atmospheric water. We present several chemical formations and nanomaterials-based frameworks for capturing water, their efficiency of production and cost/benefit analysis of atmospheric water harvesting as a means future of water sustainability.

Keywords: water, sustainability, harvesting, nanomaterials, toxicokinetics

ESTIMATION OF WATER QUALITY IN GHIDIGHICI AND DĂNCENI LAKES IN ORDER TO USE THEM FOR IRRIGATION

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The Ghidighici and Dănceni reservoirs are part of the surface water bodies in the Dniester river basin, which is a main water artery for the Republic of Moldova. The Ghidighici accumulation lake is formed on the Bâc river, which flows into the Dniester river, and the Dănceni accumulation lake is formed on the Ișnovăț river, a tributary of the Bâc river. Both lakes are used for recreation purposes, but also for uncontrolled and unauthorized irrigation of soils. That is why it is important to know the chemical composition of the waters in these lakes and to estimate these waters as sources of water for irrigation.

In order to estimate the water quality from Ghidighici and Dănceni lakes in order to use them for irrigation, traditional methods were used. For the calculation of the respective coefficients, the average values of the content of the main ions during the years 2015-2020 were used.

The danger of soil salinization was estimated by the average value of mineralization and the total hardness of the water. Hazards of alkalinization, secondary soil alkalinization, soil alkalinization due to magnesium and sodium ions were estimated by calculating the ratios of the multiannual average values between $(Na^{+}+K^{+})/Ca^{2+}+Mg^{2+}$(mmol/dm^3); $(Na^{+}+K^{+})/\sum$cations (mmol/dm^3); Sodium Absorption Ratio (SAR=$(Na^{+}+K^{+})/\sqrt{(Ca^{2+}+Mg^{2+}/2)}$); $Na^{+}/\sum$cations (mmol/dm^3 %); Mg^{2+} %$\cdot\sum$cations (mmol/dm^3%).

Calculations show that the waters of Lake Ghidighici have increased alkalinity, excessive mineralization, increased content of sodium ions, which can contribute to salinization and alkalization of soils. The use of these waters for irrigation purposes is limited.

Calculations show that the waters of Lake Danceni have increased alkalinity, excessive mineralization, increased content of sodium ions, which can contribute to salinization and alkalization of soils. According to the empirical coefficient of irrigation, this water cannot be used for irrigation purposes.

Acknowledgement: This work has been performed within the State Program of the Republic of Moldova (2020-2023), Project Nr. 20.80009.5007.27 "Physical-Chemical Mechanisms of the Redox Processes with Electron Transfer in Vital, Technological and Environmental Systems".

IMPROVING THE WATER RESOURCES MANAGEMENT ON THE SULINA CANAL (DANUBE DELTA, ROMANIA), BASED ON PREVIOUS DATA AND OWN RECENT INVESTIGATIONS ON THE WATER QUALITY

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*"Gheorghe Asachi" Technical University of Iasi, **Romania***

The Danube Delta is a natural protected area in the South-Eastern part of Romania, declared a Biosphere Reserve through the UNESCO "Man and Biosphere" Programme. Water is a determining factor for all the human settlements in the Biosphere Reserve, the whole Danube Delta being structured by the three branches of the Danube (Chilia, Sulina and Sfantu Gheorghe (Saint George)). Our study case is focused on the Sulina branch, namely also as Sulina Canal. The improvement of water resources management is the main topic of this study, in terms of water quality indicators, which were carried out in a twenty-nine monitoring points, starting since a few years ago and updated to nowadays. During the study period, significant exceedances of the limit value were detected in case of N-nitrate-N (3.9-4.6 mg /L) in the Saint George branch and in the Sulina Channel after the WWTP discharge area, as well as near two settlements, at Gorgova and at Maliuc, that are caused by the leakage of the ageing drain pipes or of the lack of these in the case of the last two settlements. We would like to emphasize that as inhabitants in Maliuc obtain drinking water from shallow, 2-6 m deep drilled wells, due to the risk of exceptionally high nitrate concentrations in surface waters, special attention should be paid to monitoring drinking water quality. Residents living along the Sulina Channel engage in fishing and agricultural activities that also have a significant impact on the nutrient load of the surface water. These findings show that the major point source is the wastewater (not enough treated and untreated) and the main diffuse source is the run-off of agricultural fertilizers. A main conclusion could be drawn related to the nutrients distribution (~85% of nitrogen emissions and ~70% of phosphorus emissions) in the Danube catchment, which is generated by diffuse sources.

In order to avoid the health risks of the population in the Danube Delta, it is necessary to assure a continuous monitoring of the drinking water quality by regional operators who ensure the water supply, as well as the monitoring of water quality from the wells. Potential sources of surface water pollution, like direct or uncontrolled discharge of untreated wastewater, must be eliminated, as well as for soil and groundwater pollution, through the occurrence of leaks in sewage networks. In settlements where there is no water supply system, it is necessary to build and expand such a system to provide the population with the necessary drinking water. From the settlements located along the Sulina channel, only Maliuc, Crișan and Sulina have sewerage systems and domestic wastewater treatment plants, but not completely in function, and therefore there are still many issues related to the wastewater management in terms of domestic wastewater canalization, treatment and discharge.

In order to improve the water management in terms of water quality, we proposed the implementation of an automated water quality monitoring system on a passenger's ship, which could provide an early warning message to the water authorities and stockholder responsible with the water management on the Sulina Canal.

THE STRUCTURING OF THE CATIONIC POLYMER ZETAG 9014 WITH THE CHANGES OF THE pH

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The main applications of organic polyelectrolytes in potable water production are in coagulation and flocculation, and in the dewatering of treatment plant sludges. The water production processes are usually followed by sedimentation and filtration, although with only slightly contaminated waters the sedimentation step may be omitted. The sludges obtained from the various separation processes have very high water contents and must be further concentrated to minimize transportation costs; polymers have a role in this sludge conditioning. Polymers have been utilized in coagulation/flocculation processes for water purification for at least four decades.

For many years cationic polyacrylamide flocculants have been used in the sludge dewatering process. The water treatment chemicals including flocculants and coagulants especially designed for the solid–liquid separation processes in the industrial and municipal wastewater treatment sector.

The structure of the cationic polymer ZETAG 9014 under the influence of changes in pH of the medium was studied in an aqueous solution. Cationic polymer type ZETAG 9014 is structured under the influence of pH changes. When reducing the pH of the medium, there is a clear trend, in which the average particle size reduces and the size distribution narrows. Conversely, at higher pH values (alkaline region), the average particle diameter broadens the PSD. It is important to note that the type of pH modifying agent (in particular, acid) can also affect the polymer structuring process. The chemical agents used to modify the pH of the suspension (medium and polymer) were NaOH, KOH, $Ca(OH)_2$ and HN_4OH.

STUDY ON THE IMPACT OF SOME LOCAL THIOLS ON THE WATER SELF-PURIFICATION CAPACITY OF DANCENI LAKE

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Sulfur derivatives of biogenic origin, such as some of the thiols, have strong reducing properties and actively participate in redox processes in the natural aquatic objects. On the example of cysteine and glutathione, thiol derivatives, which are formed as a result of biochemical processes inside of the water bodies and waters of Danceni Lake, from the Dniester river basin, has been conducted the researches to determine the load of substance that will not hinder the development of self-purification processes that form self-purification capacity of the natural aquatic system.

The research was conducted on microcosm systems, using lake water from the summer season. Thiol concentrations were selected in such a way as to model the pollution situation in natural waters and were of the 10^{-4} M order. The monitoring of self-purification processes was performed according to the parameters: degree of oxygen saturation (GS), permanganatometric oxidability (CODMn) and inhibitory capacity ($\sum ki \cdot [Si]$).

Research has shown that both thiols, in concentrations of the order $(0.8\text{-}2.0)\cdot 10^{-4}$ M, affect the self-purification capacity of the natural aquatic system, by reducing it, because it consumes in its own transformation processes oxygen and its active forms from the water, us hydrogen peroxide and OH radicals. At the same time, it was found that the chemical-biological self-purification system of Lake Danceni neutralizes the negative effect of „redox-toxicity”, caused by the presence of thiols in concentrations of the 10^{-4} M order, for a maximum 48 hours.

Acknowledgement: This work has been performed within the State Program of the Republic of Moldova (2020-2023), Project Nr. 20.80009.5007.27 “Physical-Chemical Mechanisms of the Redox Processes with Electron Transfer in Vital, Technological and Environmental Systems”.

CELLULOSE CONTAINING COMPOSITE SORBENTS TO REMOVE HEAVY METALS FROM WASTEWATER

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The most common and effective method for heavy metals removal is sorption method. The advantage of this method is that it is possible to purify wastewater that contains a large amount of impurities (for example, organic or inorganic). In recent years, for water purification, much attention has been paid to natural sorbents or sorbents based on materials of natural origin.

Natural sorbents are widely used due to their low price. The cost of natural sorbents is ten times less than the cost of artificial sorbents. In the past few years, chemically modified carriers have been proposed to improve the adsorption selectivity towards ions. The most promising carriers were ion exchange resins, cellulose, activated carbons, natural minerals. The application of these materials led to the development of several new sorbents.

Cellulose is the most common biopolymer in the world and the presence of several hydroxyl groups in the structure of its molecules allows modifying its surface properties with the introduction of several chemical groups. Cellulose and its derivatives are used as an adsorbent to remove several contaminants. After chemical modification, cellulosic materials exhibit new properties that are more effective than starting materials. These new modifying groups on the surface of cellulose increase the interaction with pollutants (metals, dyes, drugs, etc.) in the process of absorption from the aqueous medium, which strongly depends on the pH of the solution. Cellulose materials modified by various functional groups are promising for use in the removal of pollutants from the aquatic environment.

By ICP-MS method, the sorption properties of organic-mineral composite sorbents are investigated. The diatomite of the Jradzor deposit and bentonite of the Sarigyuh deposit (Armenia) were used as inorganic constituents. Diatomite serves as a structure-forming component and provides mass transfer due to its high porosity ($V=2.0\ cm^3/g$) and large pore sizes, the size of which is 150-200 nm. Bentonite is responsible for the functionality of the sorbents. The organic component is also responsible for the functionality of the resulting sorbents. As the organic component used paper, pre-treated with acids (nitric and phosphoric). A synthetic solution containing cations of heavy metals was used as an object of study. The experiments were carried out in a static mode on the device Jar-Test.

STUDY OF TN/TP RATIO CHANGES DEPENDING ON WATER LEVEL VARIATION IN THE LAKE SEVAN

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As the largest lake in the southern Caucasus and one of the great freshwater high mountain lakes of Eurasia, Lake Sevan is an Armenian natural and cultural treasure. Among its many features, Lake Sevan is the most important source of fresh water in the South Caucasus region.

The water volume and surface area of Lake Sevan have varied significantly over the past century, due to the numerous natural and anthropogenic impacts. Thus, the variations have led to the changes in hydrochemical regime of the lake and activation of eutrophication processes. In 1933, before the artificial dropping the water level of the Sevan lake, bioproduction processes, unlike many lakes, were limited to nitrogen rather than phosphorus (the amount of phosphorus in the lake was high and the ratio of total nitrogen to total phosphorus (TN/TP) was small). Then, in the 1930s, due to the artificially dropping the water level of the Sevan lake, transfer of large amounts of nitrogen from the sediments to the water was observed, as a result of which the nitrogen content in the lake water increased about 30 times and the phosphorus concentration decreased by about one order. After 1981, then the water level was started to rise, it was found that a slow increase in phosphorus content in the water of Lake was observed in 2010-2020.

In 2010-2020, the total phosphorus content in the water of Lake Sevan ranges from 0.073-0.081 mg/l (eutroph-hyperotrophic state), while in natural lakes, in the transition from mesotrophic to eutrophic state the phosphorus content is estimated at 0.02-0.025 mg/l. Prior to the water level dropping of the lake, the concentration of phosphorus in the water ranged from 0.32 to 0.02 mg/l. It is obvious that the nitrogen-phosphorus ratio (TN/TP) in the lake differs from the behavior typical of natural lakes.

THE INFLUENCE OF THE RĂUT RIVER ON THE MINERALIZATION OF THE NISTRU RIVER WATERS (PERIOD OF YEARS 2015-2020)

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The Dniester river is a cross-border watercourse, which streams from the Ukrainian Carpathians, starting near the border with Poland and reach the Republic of Moldova flowing through the eastern to the south part of the country. It forms a portion of Moldova’s border with Ukraine to the northeast, then crosses the territory of the country, reaches again the border of Ukraine in the southeast and then flows into the Black Sea. The total length of the Dniester river is 1362 km, of which 657 km arewithin the Republic of Moldova’s territory. The perimeter of the Dniester river basin area is about 19 thousand km^3 within the country, and the average of annual flow is 10.7 km^3. The Dniester river is the main water artery of the Republic of Moldova, its river basin occupies about 60% of the country’s territory and represent the main source of drinking water for more than 1 million of the country’s population. The waters of the Dniester are intensely polluted by sewage, municipal and domestic wastewater, negatively influencing to the river water quality. From the Dubasari dam accumulation reservoir to Chisinau, the Raut and Ichel tributaries flow into the Dniester at the right side of the river. Raut River is the largest tributary of the Dniester, with a length of 286 km and the water accumulation basin surface – 7,760 km^2. Within the basin of both above listed tributaries the large administrative points, industrial and agricultural objects are located. On the Raut river the cityBalti is located with a population of about 150 thousand people, where the city’s treatment plant is discharging the suvage waters into the river. Apart from Balti, there are located some large localities such as Marculesti, Floresti, Orhei and others. The biggest part of the Raut basin on its course towards the Dniester captures the waters of the polluted streams from small rivers Copacianca, Cubolta, Cainari, Ciuluc, Cula, Cogalnic. Therefore, Raut flowing through many urban and rural localities, represent the additional sources of pollution due to the untreated wastewater discharge, sanitary protection areas uncontrolled grazing, significant anthropogenic impact on the main river, which poses a danger to the functioning of the aquatic ecosystem. In addition, these tributaries flow into the Dniester in the immediate vicinity of the water collection stations, which are conditioned and subsequently used for centralized water supply of Chisinau – the capital of the Republic of Moldova.

In order to have a complex and objective image of the Dniester river ecochemical state, as well as to assess theRaut impact were organized the seasonal hydrochemical expeditions during the years 2015-2020.The part of the Dniester river selected for observation lasted from the Dubasari dam, upstream from the Raut river to the Criuleni town at the Raut river downstream. During the years 2015-2020, the 27 hydrochemical expeditions in total were made. Downstream of the Dniester River, the essential changes in the formation of the chemical composition of the waters were identified. The hydrochemical water index indicates the dominant anion and cation changes in the water composition. Only 55% of the samples belong to the class of hydrogen carbonate water – typical for the waters with medium mineralization and for the Dniester in general. At the same time, over the 40% of samples indicate the phenomenon of chloride sulfate ions appearance as the main anion, or their competition with the traditional dominant anions – HCO^{3-}. Likewise, in about of 20% of samples as dominant cationsthe Na^+ and K^+ ions were identified, which determine the water group not characteristic for the Dniester waters. For this sampling point, a high correlation was identified between the content of hydrogen carbonate ions and mineralization (r^2 = 0.70) and the content of chlorides and mineralization (r^2= 0.60).

A reasonable correlation was found between the content of the main ions and the total hardness of the waters and between the content of hydrocarbons and hardness (r^2 = 0.50). The data obtained indicate the total hardness values increasing of the Dniester waters after the Raut river flows into it. Higher values of water hardness were recorded in 2015, 2016 and 2019, as well as in the Dniester upstream Raut sampling point. In general, after the Raut river flows into the Dniester, its water hardness increases by about 13%, which confirms the negative influence of the tributary to the main river.

The same trend is observed for the water mineralization annual average values. The results obtained indicate increasing by almost 40% the water mineralization average in the sampling point on the Dniester downstream of the river Răut compared to the samples collection point on the Dniester upstream of the Răut. Moreover, during the monitoring period it was observed the change of ratio between the main ions equivalent content in the Dniester after the discharging of the Răut river. The analysis of the data obtained shows a significant increase in the share of chlorides (2.6 times) and monovalent cations (1.6 times) in the Dniester waters after the discharging of the Raut river, due to the more obvious decrease of Ca^{2+} ions (by 25 %) in the weight and hydrogen carbonates (by 22%). This phenomenon is related to the penetration into the Dniester thepolluted water with household waste and untreated or poorly treated domestic and municipal waters.

Therefore, the waters of the Răut significantly influence the content and distribution of the principal ions, as well as the hydrochemical index of the waters of the Dniester river.

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HYDROCHEMISTRY OF THE GHIDIGHICI ACCUMULATION LAKE (YEARS 2015-2020)

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The Ghidighici accumulation lake is part of the Dniester river basin and is built on the Bâc River, which flows into the Dniester – a main water artery of the Republic of Moldova. During the years 2015-2020, alkaline water masses were formed in the accumulation lake, with an average pH of 9.2 with a permanent content of carbonate ions. The pH values varied within the tight range between 8.7 and 10.2, which corresponds to alkaline or strongly alkaline waters and exceeds the permissible values for surface waters. Increased alkalinity of water can contribute to the formation of toxic conditions and the development of pathogenic microorganisms and bacteria.

The content of the main anions was linearly dependent on the water mineralization values. It showed a strong degree of correlation for HCO_3^- and SO_4^{2-} ions and an average degree of correlation for Cl^- ions. The seasonal dynamics of mineralization demonstrate the minimum average values in winter and its increase in spring. The total hardness of the waters did not undergo seasonal multiannual changes.

The hydrochemical parameters of mineralization and total hardness also varied in the multiannual context. For the values of mineralization the changes were the most pronounced. The maximum annual average mineralization was observed in 2015 (2477 mg/dm^3), after which there is a continuous decrease of these to 982 mg/dm^3 in 2019, which is 2.5 times less compared to the first year of monitoring. For the values of the total annual hardness, a similar trend is observed, but with a decrease not so essential and for the pH values no essential change was observed and these during the permanent observations indicated the alkaline character of the lake waters.

The dissolved oxygen content during the research period varied in the lake between 3.1 mg/dm^3 to 15.7 mg/dm^3, the multiannual average being 9.3 mg/dm^3. The degree of water saturation in oxygen varied between 36% (quality class IV – polluted waters, orange code) and 147% (quality class I – very pure waters, blue code), the average being 88%, which corresponds class II waters – pure waters, code green.

The waters of the accumulation lake during the research period contained substantial amounts of organic substances. The average content of biodegradable organic substances, which is determined by the parameter BOD_5, was 4.7 mg O_2/dm^3, which by over 50% exceeds the allowable values for surface aquatic ecosystems and assigns water to class II. The content of biodegradable organic substances varied between 0.3 mgO_2/dm^3 (class I – very pure waters) and 12.7 mgO_2/dm^3 (class V – highly polluted waters, red code). Of all the processed water samples, over 50% contained biodegradable organic substances in concentrations exceeding their permissible limit concentration. In more than 40% of the samples the content of biodegradable organic substances more than 2 times exceeds the admissible values.

The analysis of the obtained data denotes an advanced pollution of the waters with biodegradable organic substances, which can be formed in the lake as a result of metabolic processes, but can also enter with sewage, drainage, untreated or poorly treated domestic water, from zootechnical units, etc. In other words, Lake Ghidighici has an increased impact of biodegradable organic matter, which contributes to the formation of states with dissolved oxygen deficiency in water and the possibility of rapid eutrophication of the lake.

In addition to the biodegradable organic substances, in the waters of the lake were detected enormous quantities of hardly degradable organic substances, the content of which is reproduced by the COD_{Cr} parameter. The content of these substances practically permanently exceeded the allowable values and presented a real danger for the lake ecosystem. During the research, the average value of bichromatic oxidability (COD_{Cr}), which characterizes the presence of hardly degradable organic substances, was 36.3 mgO/dm^3, which exceeds more than 2 times the permissible limit concentration. This parameter varied over the years in the wide range between 5.7 mgO/dm^3 and 108 mgO/dm^3, all being from the range of heavily polluted waters (class V – red code). The least impactful organic substances had the lowest degradation in 2015 (20.3 mgO/dm^3), and the highest intervention of these substances was recorded in 2016 (47.8 mgO/dm^3).

The ratio between permanganate and bichromatic oxidability during the study years was on average 0.40, which indicates that during the investigated period the tank was subjected to the impact of untransformed fresh organic substances (proteins, fats, etc.). The content of organic substances was subjected to seasonal dynamics. The maximum average value of the COD_{Cr} parameter was observed during the winter, and the decrease of the respective valves was observed during the summer. Therefore, the waters of the accumulation lake have been subjected to increased anthropogenic impact. Various mineral forms of nitrogen and phosphorus were permanently present in the waters of the Ghidighici accumulation lake, the content of which varied depending on the season or the year of studies.

The total content of nitrogen mineral forms was 3.91 mg/dm^3, of which the basic weight is nitrates, with an average content over the years of 3.4 mg/dm^3. Nitrates make up 87% of all mineral forms of nitrogen. The share of nitrites is 1.4%, and of ammonium ions – 11.6%. For nitrite ions a very wide variety of values was detected – from their total absence, to 0.95 mg/dm^3. The average ammonium ion content was 0.34 mg/dm^3, which does not exceed the maximum allowable concentration. On average, the waters of the lake by the content of these ions can be attributed to class III – moderately polluted waters, yellow code. The data obtained indicate the presence of phosphates in very large quantities – up to 29 mg/dm^3. This fact contributes to the rapid course of eutrophication processes of the lake, which can have undesirable consequences in the studied ecosystem, in the ecosystem of the Bâc River and the Dniester.

According to the average content of the mineral forms of nitrogen and phosphorus (N_{tot} = 3.91 mg/dm^3; P_{tot} = 0.63 mg/dm^3) Lake Ghidighici during 2015-2020 can be characterized as a strongly eutrophic aquatic object. In 2015 and in the summer of 2016, the content of mineral phosphorus exceeded the content of mineral nitrogen, which in these cases was the limitation in the development of aquatic plants. On average, the N_{tot}/P_{tot} ratio was 6.2.

The maximum average concentration of phosphates was observed in summer, and the minimum – in autumn. Ammonium ions in larger quantities were detected in winter (class IV – polluted waters, code orange), when metabolic processes are slowed down, but the decomposition of dead organisms with the formation of these ions is performed, and the minimum content was detected during spring winter (class III – moderately polluted waters, yellow code), when all biochemical processes are carried out very quickly. The maximum average values, in terms of nitrite content, were detected in summer, and in autumn their content was minimal. Average nitrate concentrations did not vary significantly in different seasons.

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SYNTHETIC AND NATURAL ADSORBENTS FOR WATER TREATMENT AND DETOXIFICATION OF THE HUMAN BODY

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The environment in the last 70 years has been intensely polluted as a result of a reckless human activity. The accelerated development of industry, the intense chemicalization of the agriculture, the increase in the number of inhabitants on the Earth planet and the living conditions of the population on the one hand and the elaboration, the slow implementation of environmental treatment technologies on the other hand, have contributed to the pollution of water, air and soil.

The ecological chemistry has a special importance in the solving of environmental problems. The results of the studies of the processes and mechanisms of transformation, migration, catalytic decomposition, immobilization, adsorption etc. of organic and inorganic pollutants that enter the objects of the environment are at the basis for the development of high-performance technologies for environmental treatment.

Synthetic and natural adsorbents have a wide application in water treatment, as well as in the detoxification processes of the human body.

The paper presents the results of scientific research obtained in the Laboratory of Ecological Chemistry of the Institute of Chemistry in the field of synthesis, study of structural parameters and adsorption capacity of activated carbons obtained from renewable raw material from the Republic of Moldova by water vapor activation methods, in fluidized bed, microwave heating and chemical activation. The results of the research on the processes and mechanisms of sorption of heavy metal ions, organic pollutants on carbon adsorbents in the aquatic environment are also presented, which were the basis for the development of technologies for natural water purification and wastewater treatment.

The scientific communication also presents the results of the chemical modification of the surface of pectins obtained from apple fruits by oxidation processes and the efficiency of removing lead and mercury ions from biological solutions from individual solutions and from mixtures of ions of these metals. The results of carbon enterosorbent tests in the process of elimination of exogenous metabolites and non-pathogenic bacteria from biological solutions are also presented.

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BIO-BASED PLASTICS FOR ENVIRONMENTAL SUSRAINABILITY AND REDUCTION OF MICRO/NANOPLASTICS IN AQUATIC ECOSYSTEMS

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The diversity of polymers and the versatility of their properties have transformed our everyday life. While their widespread use and disposable aspects was anticipated, some of the recent reports associated with the extent of nano/microplastics environmental pollution was not anticipated. Presence of microplastics in treated tap and bottled water have raised concerns about the impact that microplastics in drinking-water might have on human health and aquatic well-being. We present an overview of monitoring and management of nano/microplastics and plastics in the environment to appropriately assess risks associated with human health, including several key knowledge gaps, to implement appropriate management actions. Addressing issue related to mitigating microplastics using nanotechnologies offers a wide range of solutions. We present methods that include identification of microplastics and mitigation strategies that include hydrogels, catalytic decomposition, nanofibers and preparing biodegradable and bio-based polymers. Hydrogels are materials consisting of a permanent, three-dimensional network of hydrophilic polymers and water filling the space between the polymer chains with applications in diverse fields ranging from bio-medical applications and stimuli sensitive systems for agricultural, personal care, environmental, and industrial applications. Using 3D printing technology, we have developed composite structures to capture polymers, large chain hydrocarbons, including pharmaceuticals. Although, the investigation is in its preliminary stages, we anticipate using meta-materials as catalysts to detect and capture organic materials, volatile organic compounds, as an extension of our work on capturing pharmaceuticals. Since, hydrogel composites contain cellulose fibrils derived from wood, response to environment is likely to produce bio-mimicking to external stimuli. Additional anticipated methods range from separation of micro-plastics and specialized polymers used by the healthcare industries. However, to reap benefits of plastics while keeping pollution to a minimum, it is critical to identify specific uses that offer clear advantages and to refine national and international standards and associated product labelling to indicate appropriate usage and appropriate disposal methods.

Keywords: Microplastics, Nanophotonics, Additive processes, 4D printing, bio-mimicking

IMPACT OF DETERGENTS ON THE NITRIFICATION PROCESS OF AMMONIUM IONS IN NATURAL WATERS

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The evaluation of individual effects of surfactants or other ingredients does not reflect the influence of a detergent on the aquatic environment, being important to estimate the effects of detergent as a whole. In the present study is evaluating the influence of 3 types of detergents on the NH_4^+ nitrification process in water: 2 solid detergents (DS-1 and DS-2) and one liquid detergent (DL). The nitrification process was evaluated in the water from the river Nistru, near Palanca village, in which were added of 2,2-2,5 mg/dm^3 NH_4^+, 1-10-100 mg/dm^3 of DS-1 and DS-2 and 0,1-0,5-1,0 ml/dm^3 of DL.

The $NH_4^+ \rightarrow NO_2^-$ step in water without detergent lasted 8 days. At the addition of 1-10 mg/dm^3 of DS-1 and DS-2 the process took 9-10 days and at 100 mg/dm^3 was in 19-24 days. It was shown that at the addition of 0,1 ml/dm^3 DL the step lasted 19 days, and in the presence of 0,5-1,0 ml/dm^3 after 30 days there were still 56-88% of ammonium ions left.

The $NO_2^- \rightarrow NO_3^-$ step in water without detergent lasted 13 days. When adding 1-10 mg/dm^3 of DS-1 and DS-2 the process lasted 13-17 days and in the presence of 100 mg/dm^3 the stage duration was 26 days for DS-1

and more than 30 days for DS-2, finally nitrates formed after nitrification being 14,6-19,8 mg/dm^3, and in water without the addition of detergents – 22,4 mg/dm^3. DL has a specific influence in the second stage of nitrification. At the addition of 0,1 ml/dm^3 DL the step lasted 20 days, and in the presence of 0,5-1,0 ml/dm^3 after 30 days in solutions were only 0,6-2,5 mg/dm^3 NO_2^-, in final being only 1,01-1,68 mg/dm^3 of nitrates.

Thus, it is necessary to evaluate the influence of detergents (not only surfactants) on water quality, including in the wastewater treatment process.

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BACTERICIDAL MATERIALS BASED ON NATURAL ZEOLITES

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In the context of the coronavirus pandemic, not only the demand for all kinds of disinfectants has increased, but also the interest in obtaining new antibacterial and antiviral materials, among which metal-containing zeolites are recognized as very promising. The purpose of present work was to obtain bactericidal materials using Georgian natural analcime, phillipsite and heulandite-clinoptilolite, to study their properties and use them for water disinfection and as a filler for the production of bactericidal paper.

After pretreatment, the zeolites were enriched with silver, copper and zinc by solid state ion exchange. It is shown that the enrichment procedure practically does not affect the structure and physicochemical characteristics of zeolites containing up to 230 mg/g of silver, 75 mg/g of copper, 86 mg/g of zinc, and the bacteriostatic activity of metal-containing samples is determined not only by the amount of released ions of bioactive metals, but also by the type of zeolite matrix. In a liquid medium, the obtained materials are active against a wide range of microorganisms, and a synergistic effect has been established – against gram-negative bacterium *Escherichia coli* and gram-positive bacterium Bacillus subtilis, as well as against fungal pathogenic yeast Candida albicans and a fungus Aspergilus niger, a mixture of zinc and copper forms of heulandite is most effective, and against Staphylococcus aureus any mixture of silver, copper and zinc forms in a molar ratio of 1:1.

Finely dispersed heulandites containing silver (130 mg/g), copper (63-72 mg/g) and zinc (30-58 mg/g) were used to make paper on the production lines of the GPM Company (Tbilisi, Georgia). The colony forming unit assay indicates the greatest activity against *E. coli* by paper with a high content of zinc, against staphylococcus, by paper with a high content of copper, opening up the possibility of replacing silver.

THE INFLUENCE OF DRINKING WATER QUALITY FROM THE CITY OF FĂLEŞTI ON HUMAN POPULATION HEALTH

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Water is the environmental factor with the greatest impact on the health of the population, given the permanent vital need for its presence for physiological, biochemical processes in the human body, as well as for hygienic and household needs.

The purpose of the paper is to determine the chemical composition and the influence of drinking water on the health of the population in the city of Făleşti.

The physico-chemical analysis of drinking water aims to determine the natural components of water, as well as those caused by pollution. As a result, the control of drinking water quality was performed by performing current, complete and special analyzes, depending on the purpose of the research. The most common are pesticides, detergents, lead, nitrates and fluoride, the presence of which in the water signals a risk of disease for the consuming population.

The study determined an increase of the hardness index over 14 mg/dm^3, in the wells in the city of Falesti. Water hardness, with concentrations higher than 12 mg/dm^3, favors the appearance of osteoarthritis, osteopathies, renolithiasis, cholelithiasis. Also, with the increase of the average allowable concentration of the indices that determine the mineralization (calcium, sodium, magnesium, hydrogen carbonates), is observed the increase of glycemia and uric acid in the body. The hardness of water favors the dissolution in water of some metals such as: cadmium, cobalt, nickel, chromium, manganese, which, in turn, have a negative action on the cardiovascular system. Ca, Mg compounds are the major determinant of hardness, which have a favorable effect. The results of this study determined a high level of nitrates and nitrites in the waters of the wells, which is the etiological factor in the occurrence of acute disorders of the population's health.

Conclusions: Drinking water from the wells of Făleşti does not fully meet the standards. Indices of alkalinity, hardness, fixed residue, ammonium concentration exceed the norm; but pH indices, nitrate concentration, the concentration of chlorine and sulfates corresponds to the norm. This imbalance of water quality indices leads to metabolic disorders, the formation of stones and the gradual onset of other pathologies.

EVALUATING THE SUITABILITY OF GROUNDWATER FOR DRINKING PURPOSES FROM CAUSANI REGION OF THE REPUBLIC OF MOLDOVA

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This work describes the results of the research of underground water from artesian wells and wells in Causani region of the Republic of Moldova. In the studied region in spring, 2021, 13 samples of water from artesian wells and 9 samples from wells were taken. All the sampled wells are important sources of drinking water. All samples were analyzed for various chemical parameters, such as hydrogen sulfide and dissolved sulfides, ammonia and ammonium ions, nitrites, total harness, sodium ions, iron ions, fluorides, sulfates, chlorides, oxidability, total dissolved solids. All the parameters were determined according to standard techniques. It was shown that water from different artesian wells and wells of Causani region of the Republic of Moldova are considerably different.

Water from artesian wells are characterized by elevated content of ammonia and ammonium ions, hydrogen sulfide and dissolved sulfides, sodium ions and fluorides. At the same time, the content of hardness salts is below the minimum allowable value for all the samples. In water samples from wells, the most commonly exceeded parameters are nitrates, hardness salts, sodium ions, sulfates and total dissolved solids. For quality assessment of the analyzed water sample we used water quality index (WQI). WQI allows to transform extensive water quality data to a single value, reflecting water quality level, thus erasing the differences between the parameters used in the assessment independently.

WQI was calculated by 11 chemical indices, maximal allowable concentration of are set in the national legislation (Law № 182/19.12.2019).

WQI was calculated in four steps. The first step was assigning a weight (w_i) to each parameter depending on its effect on human health. The worse the effect on human health, the higher the weight assigned. The allotted weight ranges between 1 to 5. The second step was the calculation the relative weight (W_i) using the formula: $W_i=\frac{w_i}{\sum_{i=1}^{n} w_i}$, where the relative weight is represented by W_i, w_i indicates the individual parameter weight, n represents number of groundwater parameters. The third step was to estimate the quality rating scale (q_i) of each parameter using Equation: $q_i=\frac{C_i}{S_i}*100$, where C_i is the concentration of each parameter in mg/L, S_i is the standard permissible value for the i parameter in mg/L. The fourth step was to calculate the WQI using Equation: WQI=$\sum_{i=1}^{n} W_i$* q_i. Based on the WQI value the water is classified into five categories: excellent (WQI<25), good (25 <WQI<50), poor (50 <WQI<100), very poor (100 <WQI<150) and unsuitable for drinking (WQI> 150).

Quality assessment of water from Causani region of the Republic of Moldova on the basis of WQI showed that 15,4% of water samples from artesian wells belong to the category poor, 53,8% - very poor и 30,8% - unsuitable for drinking. Quality assessment of water from wells on the basis of WQI showed that 66,7 % of samples belong to the category very poor, 11% - poor and 22% belong to the category good. Using WQI method, it was shown that none of the analyzed samples from the artesian wells was in the categories excellent or good. Only 2 water samples from wells were in the category good. The present research revealed an important challenge of providing the population of Causani region with the access to a good quality drinking water and showed the importance of up-to-dated technologies of water purification for facing this challenge.

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QUALITY RATING OF GROUNDWATER FROM ARTESIAN WELLS AND WELLS FROM DIFFERENT REGIONS OF MOLDOVA

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This work summarizes the data on chemical composition of ground water from artesian wells and wells from different regions of Moldova. A comparative analysis of chemical composition of the water samples was carried out, and indices most commonly exceeding the maximal allowable concentrations for both waster types were evidenced.

In this work, 209 water samples were analyzed, 115 of them were water samples from artesian wells and 94 samples from wells. Water quality assessment for use as a drinking water was done according the criteria set by the national regulation – Law 182/ 19/12/2019.

The research show that in most cases, the maximum allowable concentrations in the samples from artesian wells were exceeded for ammonia and ammonium ions (0,58 -7,51mg/l) in 70,7 % samples, for hydrogen sulfide and dissolved sulfides (0,15-33 mg/l) in 43,1 %, sodium ions (218-1095 mg/l) -37,9%. Water hardness was evaluated according to two criteria – minimal value 5˚Ger, and maximal value of hardness 7 mol/m^3 (since the maximal allowable value of the hardness is not set by the national regulatory documents, we took the maximal value of hardness as 7 mol/m^3. This value was in effect in Moldova until 2007). The hardness below 5˚Ger (<0,28-4,2 ˚Ger) was in 22,4% of samples, and above 7 mol/m^3 (7,5-21 mol/m^3) was in 35,3% of wells. Iron ion content (0,33-5,9 mg/l) was exceeded in 32,8% of artesian wells, fluoride content (1,81-10,4 mg/l) – in 20,7% of samples, permanganate index (6,06-26 mgO_2/l) – in 11,2%, nitrates (64-149,9 mg/l) –in 8,6%, sulfates (290,7-954 mg/l) –in 6,9% of cases. As for total dissolved solids (1583-2747 mg/l), chlorides (255-421 mg/l), nitrites (0,73-2,1 mg/l), the exceedance is found in 5,2%, 4,3% and 1,7% of wells, correspondingly. The values of the exceedance vary a lot for each index.

In water samples taken from wells, most common is the exceedance of hardness (10-31 mol/m^3) in 67% cases, nitrates (66-678 mg/l) in 50% cases, dry residue (1583-3012 mg/l) in 20% samples, sodium ions (221-490 mg/l) in 18,1%, and sulfates (291-954 mg/l), ammonia and ammonium ions (2,3-4,89 mg/l), iron ions (0,35-0,96 mg/l) and hydrogen sulfide and dissolved sulfides (0,85-2,33 mg/l) in 14,9%, 7,44%, 5,3%, and 4,3% correspondingly. Permanganate index and nitrites did not exceed the maximum allowable concentrations in any of the analyzed well water samples. Besides, in water samples from both artesian wells and wells, toxic metal ions such as chrome (total), nickel, led, cadmium, copper and zinc were determined. No exceedance was detected in any of the analyzed samples. Out of 115 water samples from artesian wells, 111 samples (96,5%) did not meet the requirements for drinking water by at least one parameter, and out of 94 water samples from wells, 93 samples (98,9%) did not meet the requirements for drinking water. Water from artesian wells and wells was shown to be rather different by chemical composition. The indices most commonly exceeding the maximum allowable concentration for both water types are evidenced.

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ACTIVATED CARBON SUPPORTED METAL CATALYSTS FOR NITRITE AND SULPHIDE IONS OXIDATION IN WATER

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Carbonaceous materials have great potential as catalyst supports since a high metal loading and dispersion can be achieved. Also, it is well known that the role of the support is not simply that of a carrier; the interaction between the active phase and the support can also affect the catalytic activity.

The aim of this work was to develop catalysts on the basis of carbonaceous adsorbents by their impregnation with metals (Cr, Ni, Mn, Fe, Cu) for catalytic oxidation of nitrite and sulphide ions in water.

Impregnation with metal ions and oxides was performed by different methods, and the catalytic properties of carbonaceous adsorbents depend on the nature and state of the metal (ions and oxides) bound on the surface, as well as on the support surface nature. The catalysts general properties were determined by standard methods (BET surface, SEM-EDX, XRD etc.), and the catalytic activity was evaluated by chemiluminescence in luminol/H_2O_2 system and by ABTS cation-radical method.

By applying the chemiluminescence method (luminol/H_2O_2 system) the dualistic behaviour of activated carbons was revealed. According to the activated carbon structure characteristics (well-activated/graphitized structure, functional groups, π electrons, quinone/hydroquinone couple, etc.) under different conditions activated carbon has a dualistic behaviour: on the one hand, it captures free radicals from different systems, and under other special conditions the activated carbon itself can form free radicals. Activated carbon, by means of the redox couple (quinone/hydroquinone) on the surface, in the luminol/hydrogen peroxide system contributes to the formation of free radicals that react with hydrogen peroxide, thus generating hydroxyl radicals OH• analogous to the Fenton reaction. Following the oxidation reaction of luminol with dissolved oxygen, the superoxide radical is produced:

$$CA/CA(Cu) + H_2O_2 \rightarrow CA/CA(Cu) + HO^{\bullet} + HO^{-} \quad (1)$$

$$CA/CA(Cu) + O_2^{\bullet -} \rightarrow CA/CA(Cu) + O_2 \quad (2)$$

The formed OH• radicals are quite reactive and, following the reaction with luminol, form an emission of chemiluminescence.

Comparative analysis of the developed catalysts ability to remove/oxidize sulphur ions highlight samples modified with copper, nickel and manganese ions; the relative capacity (RC, %) decreases in the series CAT36Ni≈CAT36Mn>CAT36Cu>CAT36Cr>CAT36Fe. In the process of sulphide ions removing from water in the presence of samples modified with nickel and manganese ions, colloidal sulphur is formed in considerable quantities. The results reveal that there is a dependence between the amount of metal immobilized on the surface of activated carbon and the amount of colloidal sulphur formed.

The testing of catalysts (on the activated carbon as support) for removal (adsorption/oxidation) of nitrite ions from water highlights the samples modified with copper oxides from the *E* series and the samples modified with manganese from the *C* series. Meanwhile, the removal capacity of nitrite ions from water in presence of catalysts modified with copper oxides (E-Cu-Na_2CO_3, C-1-Cu-Na_2CO_3) reaches ~90% and is in agreement with the redox activity of the catalysts evaluated via the chemiluminescence method.

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COMPARISON OF ADSORPTION PROPERTIES OF HYDROLYZED LIGNIN AND EXPANDED GRAPHITE IN RELATION TO BRILLIANT GREEN

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Hydrolyzed lignin (HL) is a large-tonnage waste of the pulp and paper industry and therefore its utilization is being intensively studied. Expanded graphite (EG) is formed as a result of the rapid heating of intercalated graphite at high temperatures (800-1000°C) [1]. Due to the functional groups (HL) and high porous structure (EG), these materials are widely used in the treatment of wastewater from oil and oil products, heavy metal ions, and synthetic organic dyes.

The purpose of this study is to compare the adsorption of Brilliant Green (BG) dye by two cheap adsorbents, i.e. HL and EG from model wastewater. The purpose of selecting BG dye as a model contaminant is that this dye is a cationic dye and it is known that cationic dyes are more toxic than anionic dyes [3]. BG dye causes burning in the eyes, cough, shortness of breath, skin irritation, nausea, diarrhea, and vomiting. This makes it important to treat wastewater contaminated with BG dye without discharging it directly into water bodies [2].

To compare the sorption properties of HL and EG, BG solution with a concentration of 1-50 mg/l was adsorbed with 0.03 g HL and 0.03 g EG for 24 hours in a static condition. The equilibrium concentration of BG (C_e, g/ml) was determined on a visible spectrophotometer at a wavelength of 625 nm (Thermo Scientific ™ GENESYS 30). Based on the results obtained, the sorption capacity (q_e, mg/g) and removal percentage (%) were calculated using the formulas $q_e=((C_0-C_e)\cdot V))/m$ and $R=((C_0-C_e)/C_0)\cdot 100\%$, respectively (where V is the volume of the dye solution (L) and m is the amount of sorbent (g)). The calculated values are presented in the Table.

Table. Comparison of adsorption capacity and removal percentage of HL and EG

HL	C_0, mg/L	1	5	15	20	25	30	35	40	45	50
	q_e, mg/g	0.8	3.94	11.7	15.2	16.3	17.2	18.1	18.2	18.2	18.25
	R, %	80	78.8	78	76	65.2	57.3	51.7	45.5	40.4	36.5
EG	C_0, mg/L	1	5	15	20	25	30	35	40	45	50
	q_e, mg/g	0.6	2.7	7.9	10.2	12.7	13.5	14.65	14.6	14.6	14.7
	R, %	60	54	52.7	51	50.8	45	41.9	36.5	32.4	29.4

As can be seen from the table, the removal percentage of both HL and EG sorbents is high at relatively low initial concentrations of the dye solution. Also, the sorption capacity and removal percentage of HL are higher than EG at all values of the initial concentrations of the dye solution. This may be because the hydroxyl (-OH) groups of HL and only the pores of EG are involved in sorption.

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SORPTION OF CEFTRIAXONE FROM WASTEWATER BY NATURAL ZEOLITES

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Throughout the world, municipal, agricultural and industrial waste discharges into the environment are ubiquitous, which means that antibiotics can be found in significant concentrations in many rivers, sediments and soils. Because antibiotics and antibiotic-resistant bacteria come from the same source, they are often found together. Due to the incomplete removal of drugs at treatment plants, as a result of their discharge into wastewater, they are released into surface water. Purification of these waters is carried out by different methods, usually in a complex manner, which significantly increases costs. The high price of purified natural water leads to the need to find cheap and effective materials for water purification. Recently natural zeolites have been used for solving practical water purification problems. The adsorption method using natural zeolites is characterized by the absence of secondary contamination, cost-effectiveness associated with the possibility of multiple use of the sorbent.

This study contains data on the adsorption of β-lactam antibiotic ceftriaxone (CEF – $C_{18}H_{18}N_8O_7S_3$) from the group of cephalosporins from aqueous solutions on natural zeolites clinoptilolite and mordenite and their acid-modified forms. Acid modification of natural zeolites leads to an increase in the sorption activity of zeolites, which is associated with an increase in the pore size as a result of unblocking the channels of the aluminosilicate framework of the sorbent, which contributes to a greater accessibility of pollutants to active sites. The study of the adsorption capacity of the studied samples to ceftriaxone was performed under dynamic conditions on a flow-through installations. The change in the concentration of the antibiotic at the outlet of the adsorption column was determined by HPLC. The main information about the work of the sorbent layer at different parameters was obtained by plotting the output curves (isoplan) in the C/C_0- t coordinates. The experiments were performed until the zeolite layer was completely worked out (until the concentration of water behind the sorbent layer appeared to be equal to the concentration in the initial mixture C_0). Analysis of the experimental data obtained showed that the best characteristic adsorption parameters were possessed by samples of mordenite and clinoptilolite modified with 5N HCl solution.

It was established that acid-modified forms of zeolites are effective, competitive adsorbents for removing frequently used antibiotics from wastewater. It is very important from the economic point of view that it is possible to reuse worked out sorbents after their regeneration.

NEW ASPECTS OF ASSESSING THE STATE OF NATURAL WATERS

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Oxidative processes play an important role both in assessing the quality of natural waters and in the metabolism regulation in biological objects of varying complexity. Any biologically active substances, when ingested, affect the intensity of lipid peroxidation processes (LPO) and the structural state of biological membranes (Burlakova, 2005). Previously, the similarity functioning of the physico-chemical system of LPO regulation on the membrane and organ levels was revealed (Shishkina et al., 2013). This made it possible to consider the LPO regulation system as the basis for environmental monitoring and to propose a model system of spontaneous lecithin oxidation to assess the effects of toxicants on biological objects (Shishkina et al., 2020, 2021).

The purpose of this work was to study the effect of natural waters on the physico-chemical properties of the membranes of biological objects, using the ability of natural phospholipids to form nanosize particles in a polar medium. The objects of the study were samples of the rivers Dubna and Sestra (Moscow region), Usman (Voronezh region), Don (Rostov region) and well water (Voronezh Reserve). The analogue of natural phospholipids was soy bean lecithin, which contains from 55% to 80% phospholipids in total lipids. Using the methods of thin-layer chromatography, dynamic light scattering, UV spectrometry, the following indicators were measured: the hydrochemical composition of water, the size of lecithin micelles, their Z-potential, UV spectra of lecithin solutions and their mathematical processing using the Gauss method.

The results obtained are discussed from the point of view of the influence of the hydrochemical composition of natural water on the physico-chemical properties of natural phospholipids and the search of new indicators for assessing the state of natural waters.

ADSORPTION PROPERTIES OF GEORGIAN PERLITE IN THE PROCESS OF WATER PURIFICATION FROM Cu (II) AND Fe (II) IONS

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Environment pollution is a process accompanying scientific and technical progress. Even today this issueis topical, that is why human protection and preservation of safe living environment is a priority task for any country.

Origination of sewage waters polluted by large amounts of heavy metal ions is one of the negative sides of development of industrial technologies. Heavy metal ions have high toxicity even when their concentration doesn’t exceed permissible limits. Copper and iron are considered as less toxic among heavy metals when presented in low concentrations (<5mg/l for copper and<0,3mg/l for iron), but if concentration exceeds the above mentioned figures, their presence gives rise to different diseases: Wilson disease, kidney, liver, myocardium diseases; has an impact on blood composition, provokes allergic reaction, can cause visceral injuries etc.

Investigation and development of simple processing methods of water purification from Cu(II) and Fe(II) ions is very topical in this regard. There are many methods of sewage waters treatment from heavy metal ions, and among them an adsorption method is considered as one of the most important ones. The most attention is paid to those sorption systems, when cheap, effective natural alumosilicates and minerals of different structure, which are distinguished by high adsorption capacity and economical efficiency, are used as adsorbents. Perlite is one of such minerals. Perlite is a natural, vitreous volcanic mineral with high porosity and specific surface. It is chemically inert and safe for the environment. Perlite stands out with water presence in two forms: free and constitution. More than 1% presence of constitution water attaches perlite expansion (foaming) properties at 900-1100°C, at that its volume increases 4-20 times and porosity – by 70-90%. Perlite is used in different branches of national economy.

The present work is devoted to the study of adsorption capacity of Georgian expanded perlite in the process of water purification from copper and iron ions using adsorption method. The dependence of adsorption degree and volumetric capacity of Georgian perlite on adsorbent dosage, contact time, concentration of solution under study and on change of pH of medium in the process of copper and iron adsorption has been studied.

Tests have been conducted mainly under dynamic conditions. Standard solutions of Cu(II) and Fe(II) of given concentration have been used as adsorbates. Optimum conditions for Cu(II) and Fe(II) adsorption on expanded perlite are selected. Maximum efficiency of Cu(II) adsorption is 94%, when perlite amount is 5g, contact time–1h and pH of medium – 8,0; in case of Fe(II) a maximum adsorption degree was 91%, when perlite amount equals to 5g, contact time – 1h and pH of medium – 6,0. Volumetric capacity under such conditions was equal to 1,12 mg/g in case of Cu(II) and 1,82 for Fe(II).

So, one may conclude that Georgian perlite has demonstrated perfect adsorption properties in the adsorption process of copper and iron ions.

DETOXIFICATION AND DISINFECTION TECHNOLOGIES OF DANGEROUS CHEMICAL SUBSTANCES (DCS) USED IN INDUSTRY AND AGRICULTURE

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The synthesis of new compounds used in various fields of human activity requires completely new purification technologies. The paper presents new technologies of detoxification and disinfection of pollutants under the influence of UV irradiation developed by us and tested in industrial and natural objects. The efficiency of purification was controlled by biotesting methods that allow quantifying the total toxic effect of the initial DCS and products of their transformation.

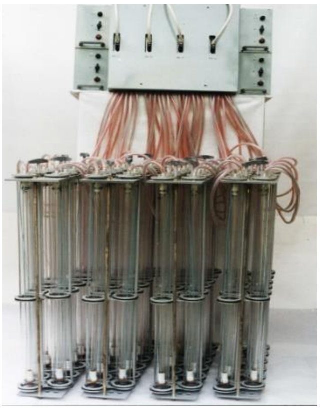
It was shown that the effect of UV light with $\lambda = 254$ nm or in the near UV region ($\lambda > 340$ nm) on benz (a) pyrene (BP) in the sorbed state leads to its direct photolysis. Under the influence of visible light ($\lambda > 430$ nm), BP is effectively oxidized only in the presence of a sensitizer.

The results of the study indicate that the toxic effect of PAHs may be associated with their participation in the initiation of OH radicals directly in the nonpolar phase of biological macromolecules. In the absence of sensitizers, the source of singlet oxygen can be hydrogen peroxide, for example, during its catalase intracellular decomposition.

A method of combined purification of mixed municipal and industrial wastewater with UV treatment and subsequent biological purification in an aerotank has been developed. Production tests of this method were carried out at the wastewater treatment plant of Belgorod. The result is an improvement in the functional state of activated sludge microorganisms, an increase in the throughput of aerotanks by 30-50% while improving the cleaning parameters according to generally accepted indicators.

Conclusion: before supplying wastewater to the aeration tanks of treatment plants, it is necessary to treat them with hydrogen peroxide in combination with UV radiation ($\lambda \geq 220$ nm) with intensive aeration.

The technology of disinfection of natural drinking waters from surface water sources with the use of UV radiation from low-pressure mercury lamps – instead of primary chlorination has been developed. The technology has passed successful production tests at the Pervomaisk drinking water treatment plant in Nizhny Novgorod. The figure shows: a cassette of UV-radiation lamps in a quartz casing and a drinking water flow at the Pervomaiskaya treatment plant in Nizhny Novgorod, passing through a system of cassettes.



This technology is also applicable for disinfection of wastewater after its biological treatment using the original design of water-submersible UV installations of tray-type.

Under the influence of UV radiation, nitrate and nitrite ions serve as initiators of free radical processes in the aquatic environment. A method for the denitrification of wastewater containing nitrate and nitrite ions, simultaneously with destructive purification and detoxification of multicomponent effluents due to the photoinitiation of OH-radicals, leading to a symbatic decrease in the concentration of the toxicant, toxicity and denitrification has been developed.

Photoozoning technology in combination with subsequent microbiological treatment with immobilized adapted bacterial strains for destructive purification and detoxification of wastewater containing difficult-to-decompose surfactants has been developed. With microbiological degradation of photoozonation products, the toxicity of anionic surfactant solutions decreases by 2-3 times, and in the case of nonionic surfactants – until complete detoxification.

REMOVAL CEPHALEXIN FROM AQUEOUS SOLUTION BY PHOTODEGRADATION

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Removal of pharmaceutical compounds from the aqueous environment is one of the most significant priorities in the field of wastewater treatment. Having a complex composition, these pollutants are difficult to remove by conventional or biological methods, and the application of photochemical methods is an effective alternative. It is known that the viability of photochemical methods depends on the source of hydroxyl radical formation (·OH) and the quantum yield of the substrate.

Examples of advanced oxidation process (AOPs) include chemical (O_3/H_2O_2), photochemical (UV/H_2O_2), and photocatalytic (UV/Fenton, UV/TiO_2) methods. In all these cases, the reaction generates hydroxyl radical which is a highly reactive oxidizing species with a high oxidation potential (E^0=2.8 V). Radical hydroxyl acts non-selectively on pollutants in the aqueous environment, and in the presence of catalysts the degradation performance is significantly increased. Consequently, oxidation occurs at a high rate of 10^6-10^{10} $M^{-1}s^{-1}$, and the oxidation process takes place with the complete mineralization of cephalexin to CO_2, water and inorganic ions.

The aim of this study is the degradation of cephalexin (CEX) from aqueous solution by applying direct (CEX/UV) and indirect (CEX/H_2O_2/UV, CEX/H_2O_2/Fe^{2+}/UV, and CEX/H_2O_2/TiO_2/UV) photolysis at λ = 365 nm.

According to research, it has been established that the removal performance of CEX depends on the one hand on the source of radical hydroxyl ·OH, and on the other hand on the irradiation time that influences the rate of degradation. In this study, the kinetics of the CEX antibiotic removal was studied in optimal conditions and using pseudofirst order kinetics models. The rate constant (k) obtained for CEX antibiotic removal was 0.0209 sec^{-1} using direct photolysis and 0.023, 0.0255, and 0.046 sec^{-1} (CEX/H_2O_2/UV, CEX/H_2O_2/Fe^{2+}/UV, and CEX/H_2O_2/TiO_2/UV) respectively using indirect photolysis. Furthermore, the half-life ($t_{1/2}$) of cephalexin removal using the photodegradation process were 33, 30, 27, and 15 sec. Degradation and mineralization was on average, 50% in first minute and continued increase up to 80-90% within 120 min contact time.

The results of this study, as well as data from the literature indicate a high efficiency of photocatalytic methods in the oxidative degradation of cephalexin antibiotic in aquatic environments. As a result of degradation, antibacterial activity is reduced by the action of hydroxyl radicals at the nucleus of penicillin, toxicity decreases and two stereoisomers of penicillinic acid are formed.

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INFLUENCE OF H_2O_2 ON THIOUREA PHOTOCHEMICAL TRANSFORMATIONS IN THE PRESENCE OF Cu(II) AND Fe(III) IONS IN AQUATIC SYSTEMS

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Thiourea (TU) is a substance of anthropogenic origin in aquatic systems, which has reducing properties, respectively directly influences their self-purification processes. At the same time, TU has a toxic influence on hydrobionts, by inhibition their activity. This researches were performed in order to establish the kinetic parameters and phototransformation mechanisms of TU in aquatic systems in the presence of H_2O_2, as an artificial source of OH radicals, in the absence and presence of Cu(II) and Fe(III) ions, as catalysts.

The researches were performed on model systems, and the concentrations of the components added to the system were selected in such a way as to model situations as close as possible to the real situations of the aquatic systems. As a radiation source was used the Solar Simulator, Oriel Model 9119X, equipped with three different filters, which simulate the quantity and quality of solar radiation, which reaches the ground. The research results have shown that TU undergoes photochemical transformations with H_2O_2, on irradiation with the mentioned artificial radiation sources. It was found that the rate of TU transformation depends and increases with increasing of its concentrations, of H_2O_2 concentrations like as of Cu(II) and Fe(III) ions concentrations added to the system. At the same time, it has been found that the rate of TU photochemical transformation also depends on the quality and quantity of used radiation. It has been found that TU leads to complexation of the Cu(II) and Fe(III) ions into stable complex compounds, thus excluding them from the aquatic systems. It was determined that, in aquatic systems, TU will undergo photochemical transformations according to the radical and very complex mechanisms. So we can conclude that TU has a negative influence on the aquatic systems, because on the one hand it consumes oxidative equivalents, and on the other hand it excludes Cu(II) and Fe(III) ions, which act as catalysts in aquatic self-purification processes.

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USE OF BY LOW-TEMPERATURE PLASMA ELECTROLYSIS FOR WATER PURIFICATION FROM BACTERIA AND VIRUSES

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The development in the field of high-energy chemistry, in particular, with the use of low-temperature plasma electrolysis (LTPE), for the study of liquid-phase processes is important in the way of creating completely new technologies that are distinguished by high efficiency and the possibility of their wide application in industry. The uniqueness of the LTPE method lies in the fact that one electrode is located in the liquid phase, and the other is placed at a certain distance from the surface of the liquid, which makes it possible to induce nonequilibrium redox processes in the treated liquid, the implementation of which is impossible when using traditional electrolysis or the effect on plasma liquid of arc, crown, Townsend, or barrier discharges.

Previously, we studied the purification of waters of various origins from organic substances and radioactive elements and showed its high efficiency.

In this study, we have studied the effect of low-temperature plasma electrolysis on solutions containing various types of bacteria and viruses, both when processing certain volumes of liquid media and during electrolysis in a reactor with a dynamic liquid film. The influence of LTPE on solutions containing pathogenic, conditionally pathogenic and indicator bacteria is considered. The high efficiency of the effect of low-temperature plasma electrolysis in the disinfection of bacterially contaminated drinking and waste water has been shown. The influence of LTPE on the death of viruses in water was investigated. Established high virulence against poliomyelitis virus and coliphages.

An experimental study of the effect of various modes of disinfection of drinking water and wastewater on the survival of bacteria: *Salmonella*, *Clostridia*, bacteria of the *E. coli* group, lactose-positive *E.coli* was carried out according to the following bacteriological indicators: total microbial count, lactose-positive *E.coli*, clostridia, enterococci and salmonella.

It is shown that carrying out electrolysis in an electrolysis cell with a dynamic liquid film of solutions containing various microorganisms makes it possible to efficiently process solutions at concentrations of microorganisms significantly exceeding the maximum permissible norms.

ENVIRONMENTAL ASSESSMENT AND POLUTION OF ZABRAT LAKE OF THE ABSHERON PENINSULA

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Zabrat Lake – it is a small lake in Absheron located in a tense ecological condition. Zabrat lake is situated at the Absheron Peninsula in Sabunchu region of Baku city.

Wastewater is disembarked from household, other facilities and private houses which are built around the lake and not equipped with the sewerage systems in the Sabunchu district of the city. At present 8000 m^3 of payable and household water is supplied into the lake from various sources every day. One of the main sources of the lake pollution is the household waste dump in the Zabrat district in the Sabunchu region in the eastern part of the lake.

The main source of the pollution of Zabrat lake was the discharge of household wastewater. In accordance with the mineralization of water, Zabrat lake belongs to the group of salt-water is much higher than that of others. The oxygen regime of the lake is completely disrupted. One of the basic reasons of soluble oxygen's weakness in the water of Zabrat lake is the acceleration of biological processes as a result of ghe oxidation of pollutants. For this reason the biochemical oxygen consumption in Zabrat lake is much higher. Since the 1970s, fecal, domestic wastewater has been discharged through the open channels without a purification process into the lake which seriously worsened the sanitary state of Zabrat, the bottom of the lake and the coastline are polluted with the household waste. Due to the evaporation of waste in hot weather, light fractions of organic waste waste are released into the atmosphere and cause a pungent odor. As a result of the influence of natural factors and wastewater into the lake, the concentration of cations and anions in the water also sharply rises with an increase in the mineralization of Zabrat lake. Cu, Cd, Fe, Zn, Mn and other heavy metals are the main pollutants of Zabrat lake and exceed the MPC by several times. Along with the wastewater, synthetic surfactants enter the lake water. Synthetic surfactants contain sodium polyphosphates in which detergents are dissolved, as well as a number of additional ingredients that are toxic to aquatic organisms: fragrances, bleaching agents (persulfates, perborates), soda ash, carboxymethyl cellulose, sodium silicates. Changes in the level of the Caspian Sea also affect the ecological conditions of the lake and its hydrological regime. As the sea level rises, the water table also increases, and as a result, the amount of water in the lake increases. When the sea level drops, the opposite process occurs.

A state program for the socio-economic development of the city of Baku and its settlements for 2014-2016 has been prepared, approved by the order of the President of Azerbaijan I. G. Aliyev dated January 17, 2014, a project for environmental rehabilitation has been developed to improve, protect and use the lakes of the Absheron Peninsula. The project of ecological rehabilitation of the lake will be implemented in two stages. Work is underway at the present time, and the results are good. At the same time, serious work has been organized to ensure safety, the protection zone of the lake and the prevention of pollution of the lake and coastal areas from household and construction waste.

ADSORPTION OF BACILLUS CEREUS, BACILLUS SUBTILIS AND PSEUDOMONAS FLUORESCENS BACTERIA FROM ACID WATER SOLUTIONS ON ACTIVATED CARBON

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Microorganisms can be dangerous contaminants, and their elimination is very important for human and animal health. Adsorption is often used at the end of a treatment sequence due to a high degree of purification that can be achieved. Activated carbon is the most popular adsorbent used for the application of the adsorption technique. They represent complex and heterogeneous materials and can be obtained from different plant sources with unique adsorption characteristics influenced mainly by the porous structure, surface and chemical structure of the surface. Granular activated carbon has an extremely large adsorption surface, which offers an exceptional ability to absorb many types of materials on its surface.

There is some evidence that the additional use of activated carbon in the treatment of people with gastroenteritis has shortened the duration of diarrhea and reduced the recovery time compared to standard rehydration monotherapy. Activated carbon has a strong ability to attract and eliminate ingested toxins from the gastrointestinal tract, thus preventing their adsorption. The porous texture of the carbon has a negative electrical charge, which makes it attract positively charged molecules, such as bacterial toxins and intestinal gases. So, preventing the adsorption in the body of these adverse entities, makes them suitable for the treatment of diarrhea. Because the normal stomach pH is in the range of 1-2, this study was performed to test the ability of activated carbon obtained from apricot peels to adsorb bacteria from the gram-positive and gram-negative groups at pH 1.97.

To evaluate the bacterial adsorption properties of the activated carbon bacteria from 3 different species (*Bacillus cereus, Bacillus subtilis* and *Pseudomonas fluorescens*) were cultivated on solid pepton agar medium. Subsequently, 3 different bacterial solutions were prepared with an initial optical density of 1.5 after McFarland. The same amount of activated carbon obtained from apricot peels was added to the prepared solutions, around 100 mg. The contact time of the carbon and bacteria varied from 30 to 120 min. The experiments were performed at pH 1.97. After each measurement, the adsorption isotherms were established for each selected bacterium.

Bacterial species	The maximum value of the adsorption of bacteria on carbon adsorbents at pH 1,97 (McF*10^8/g)			
B. cereus	30 min	60 min	90 min	120 min
	0,095	0,112	0,19	0,26
Ps. Fluorescens	0,075	0,14	0,17	0,20
B.subtilis	0,330	0,340	0,450	0,470

The results in the table show that the adsorption process has a specific character, the strongest adsorption being manifested for *B. subtilis* bacteria.

Acknowledgement: This research was carried out with the financial support of the institutional project “The reduction of the environmental and health impact of toxic chemicals through use of adsorbents and catalysts obtained from local raw material” DISTOX, No 20.80009.7007.21

PHOTOCATALYTIC OXIDATION OF THE ANIONIC SURFACTANT SODIUM 2-ETHYLHEXYL SULFATE IN UV/TiO_2/H_2O_2 AND UV/Fe^{2+}/H_2O_2 SYSTEMS

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Surfactants are widely used in the composition of detergents or care products. Their specific characteristics make them be used in various industries such as: agricultural (pesticides), pharmaceutical, textile, food and others. Due to their biotoxicity and non-biodegradability, wastewater containing surfactants must be treated before being discharged into the sewage system. In this work the photo-oxidation process of the anionic surfactant sodium 2-ethylhexyl sulphate (2-EHS) in model systems using UV/TiO_2/H_2O_2 and UV/Fe^{2+}/H_2O_2 processes was studied.

As a result of scientific research it was found that the efficiency of degradation and mineralization of the anionic surfactant 2-EHS depends on physico-chemical parameters such as pH, hydrogen peroxide concentration, catalyst concentration and oxidation time.

From the results it was established that the oxidation process of 2-EHS in the UV/Fe^{2+}/H_2O_2 system was carried out with a higher degradation efficiency compared to the UV/TiO_2/H_2O_2 system. The high mineralization efficiency of the surfactant 2-EHS in the photo-Fenton system can be explained by the formation of OH radicals both by photolysis of H_2O_2, and as a result of catalytic decomposition of H_2O_2, with Fe^{2+}. The given process is a cyclic process because the Fe^{3+} ions formed are reduced to Fe^{2+}, which in turn participates in the decomposition of H_2O_2. As a result of the study, the conditions of photo-catalytic oxidation with the Fenton reagent of the anionic surfactant 2-EHS were optimized and it was established that it undergoes degradation and mineralization with an efficiency of 95% at $[H_2O_2] = 0.3$ mM, $[Fe^{2+}] = 0.8 - 1.0$ mM, pH = 2.0-2.5 and oxidation time (60 minutes).

Oxidation rates of 2-EHS in the UV/TiO_2/H_2O_2 system are lower and the maximum degradation efficiency reaches 90% at optimal conditions: $TiO_2 = 0.1$ mg/mL, $[H_2O_2] = 10$ mM, pH = 5.0 and oxidation time (120 minutes).

Acknowledgement: This work has been performed within the State Program of the Republic of Moldova (2020-2023), Project Nr. 20.80009.5007.27 “Physical-Chemical Mechanisms of the Redox Processes with Electron Transfer in Vital, Technological and Environmental Systems”.

ENVIRONMENTAL ASSESSMENT OF NATURAL WATER SOURCES IN THE VILLAGE OF GUZANLI, AGHDAM REGION

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For research work, samples of natural waters were taken in the territory of the village of Guzanly, Aghdam region. Environmental assessment of 3 samples of natural waters taken from this area was carried out. Samples were taken from the following water bodies:

1. a sample of water taken from the territory of the "Salt Fountain" healing spring;
2. samples of spring and artesian water. The analyzes were carried out in the Central Research Laboratory "Azersu" and in the laboratory of the Department of Ecological Chemistry of the Belarusian State University. In these laboratories, more than 20 parameters of natural waters were determined.

In natural water samples taken from the territory of the Agdam region, nitrate ions were determined by the spectrophotometric method with sodium salicylate, nitrite ions were determined by the spectrophotometric method using the Griss reagent, and phosphate ions were determined by the spectrophotometric method.

According to GOST 2874-82 standards, the content of nitrates in natural waters should not exceed 45 mg/l, nitrite ions – 0 mg/l, and phosphate ions – 3.5 mg/l. Studies have shown that the content of nitrates (1.3 mg/l), nitrites (0.3 mg/l), and phosphates (0.5 mg/l) in natural water samples taken on the territory of the Agdam region is less than the permissible MPC values. The pH in spring water is 7, in artesian water is 8, in the water of the source 9. The amount of dissolved oxygen in the water of the source is 78.5 mg/l, in the spring water is 25.8 mg/l. Dry residue in spring water 519 mg/l, in artesian water 522 mg/l, and in spring water 517 mg/l. The electrical conductivity in artesian water is 19.7, in spring water – 0.779, and in spring water – 24.5. In all water samples, the amount of ammonium ions is within 1.8 mg/l.

ESTIMATION OF THE REDOX STATE OF THE DNIESTER RIVER WATERS BY MONITORING THIOL COMPOUNDS

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The valuable biological status of aquatic ecosystems is ensured by the dominance of oxidative equivalents, especially hydrogen peroxide and which is assessed by the parameter called water redox state. On the other hand, the group of reducing equivalents is represented by a wide range of compounds, including thiols. Due to the fact that the aquatic resources of the Republic of Moldova are limited and about 50% of the country's economy is provided with water needs from the cross-border river Dniester, there is a need to provide and protect it as a living environment for hydrobionts. Thus, the purpose of this research is to indirectly assess the redox state of the Dniester waters by determining the presence of peroxidase equivalents – thiol compounds. During 2021, the content of thiol compounds was monitored in the waters of the Dniester River, in the catchment area of Vadul lui Vodă.

The detected concentrations of thiol compounds fall within the limits of the order of 10^{-6}M, the annual average is $1{,}58\cdot10^{-6}$M. To evaluate the provenance of thiol compounds in the Dniester waters, water samples were taken seasonally. Thus, the following concentrations were detected: in spring – $1{,}52\cdot10^{-6}$M, in summer – $1{,}11\cdot10^{-6}$M and in autumn – $2{,}12\cdot10^{-6}$M. The detection of seasonal variations in thiols indicates their provenance. Thus, if they are products of the metabolic processes of hydrobionts, the concentration of thiols will be maximum during the summer, when the biological activity is high. Minimum concentrations will be in autumn and spring, periods in which biological activity decreases and chemical processes of self-purification of water bodies take place, including redox with the consumption of oxidative equivalents.

Therefore, the seasonal variation was not detected, which indicates that the self-purification processes in the river waters during 2021 are slowed down and / or the source of thiol compounds is mixed, both natural and anthropogenic. Therefore, the redox state of the Dniester waters is unstable, characterized by the dominance of reducing compounds.

Acknowledgement: This work has been performed within the State Program of the Republic of Moldova (2020-2023), Project Nr. 20.80009.5007.27 “Physical-Chemical Mechanisms of the Redox Processes with Electron Transfer in Vital, Technological and Environmental Systems”.

RESEARCH OF POLLUTION LEVEL OF LAKE BINAGADI

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To assess the ecological state of Lake Binagadi, studies were carried out on the physical and chemical properties of water and bottom sediments, as well as the content of heavy metals. For this purpose, in June-August 2021, we took samples of water, bottom sediments and soils for analyzes from different points of the investigated reservoir. Water samples were taken from different depths.

It was found that the oxygen regime of the Lake Binagadi is completely disturbed. One of the main reasons for the small amount of dissolved oxygen in the lake water is the acceleration of biological processes as a result of the oxidation of pollutants. Due to this, the biochemical oxygen consumption in Lake Binagadi is several times higher than the norm. As a result of the influence of natural factors and wastewater discharged into the lake, along with an increase in the mineralization of the waters of Lake Binagadi, the concentration of cations and anions in the water sharply increases. Thus, the amount of Ca, Mg and chlorides is several times higher than the sanitary standard, and the amount of sulfates is several times higher. The concentrations of oil products and phenols, which are the main pollutants of the lake, are many times higher than the MPC. Synthetic detergents in the lake are also in excess of the norm. The main pollutants in the lake are several times higher than heavy metals such as copper, cadmium, iron, zinc, manganese. The radioactive background of the lake is 21 mkR / h. Table 1 shows the results of the analysis of water samples, bottom sediments and soils of the Binagadi Lake.

Chart 1.

Heavy metals	**Water sample from Lake Binagadi, mg/l**	**The soil**	**Bottom sediments**
Si	0,077	31,7	6,23
As	1,76	9,24	5,43
Hg	0,34	0,22	1,59
Cd	0,81	0,44	0,7
Cu	2,63	2,19	2,3
Co	10,15	0,52	1,21
Pb	0,84	0,1	0,78
Ni	2,11	1,03	0,84
Zn	1,16	3,78	17,89
Fe	17,7	116,9	122,5
Al	163,1	109,7	171,68

And in the end, it should be noted that recently our government has been paying sufficient attention to the problem of cleaning the lakes of Absheron. The project to clean up Lake Binagadi is carried out in accordance with the order of the President of the Republic I.A. Aliyev on the approval of the "State program of socio-economic development of Baku and its settlements in 2014 -2016" and the decree "On additional measures in the field of improving the ecological situation, protection and use of Lake Binagadi".

SYNTHESIS, STRUCTURE, AND ADSORPTION PROPERTIES OF ION-EXCHANGE MATERIALS BASED ON Li-Ti SPINEL

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Development of the green technologies and the transition to carbon-free energy are inextricably linked with the creation of new resource and energy storage. Lithium-ion batteries are the most widely used in both – portable electronic devices and electric vehicle batteries. Therefore, considerable attention of researchers is directed to the creation of effective technologies for recycling of spent batteries. This is due to the limited natural lithium resources, toxicity releasing into the environment, and ever-increasing cost.

Recovery of Li^+ ions by the hydrometallurgical methods makes it possible quite efficiently to process high-salt brines. However, the disadvantages of this technology include the large volumes of the resulting liquid effluents, its toxicity, and the difficulty of achieving a deep recovery degree of Li^+ ions. Extraction is superior to hydrometallurgical methods in terms of the Li^+ ions recovery efficiency. The high toxicity and cost of extracting agents make this approach unacceptable for industrial applications with low environmental and economic attractiveness. Currently, electrochemical methods are being actively investigated as a promising alternative, however, the first positive results were obtained only on a laboratory scale.

Inorganic lithium-ion sieves are widely used as adsorbents of Li^+ ions. The most effective selective adsorbents are developed on the basis of Li-Ti and Li-Mn spinels, which is due to the high capacity and affinity toward Li^+ ions, and selectivity with the background of competing metal ions. At the same time, the low kinetics of adsorption-desorption, the complexity of adsorbents regeneration, as well as the low stability of the crystal structure of this ion-exchange materials are the main issues that limit their widespread application.

The present work is devoted to the development of effective Li^+ ions adsorbents based on Li_2TiO_3 spinel, study the relationship between the synthesis conditions, crystal and porous structure, and adsorption properties of obtained adsorbents.

Samples of Li_2TiO_3 spinel were obtained by using hydrothermal, sol-gel, and solid-phase synthesis methods. Hydrothermal synthesis was carried out using precursors TiO_2 and LiOH at 200°C for 10 h. Sol-gel synthesis was carried out by the self-combustion method. For solid-phase synthesis of Li-Ti spinel a stoichiometric mixture of TiO_2 and Li_2CO_3 was preliminarily pressed into tablets under a pressure of 10 Mpa. All samples obtained by the above methods were calcined at 700°C for 5 h.

The report includes the results synthesis and physicochemical properties of Li-Ti spinel adsorbents by using XRD, DTA-TG, FTIR, low-temperature nitrogen adsorption-desorption, SEM-EDX techniques. The main factors determine low kinetics of adsorption-desorption and optimal Li^+ ions adsorption conditions, which make it possible to achieve the maximum theoretical Li_2TiO_3 spinel adsorption capacity, will be discussed.

Acknowledgements

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SYNTHESIS AND PHYSICOCHEMICAL PROPERTIES OF SELECTIVE LITHIUM IONS ADSORBENTS BASED ON Li-Mn SPINELS

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Inorganic adsorbents based on manganese oxides are widely used for the purification of aqueous media from heavy metal ions, radionuclides and organic pollutants. That is due to the features and multiplicity of the crystalline structure, which consist of MnO_6 octahedra, forming layered (birnessite) and channel (cryptomelane, todorokite) structures with a given hollow size in the range of 4-9 Å. Manganese oxides with a spinel structure as adsorbents attract particular attention. Among them Li-Mn spinels with $LiMn_2O_4$, $Li_{1.6}Mn_{1.6}O_4$ and $Li_{1.33}Mn_{1.67}O_4$ composition are one of the most promising materials for the selective Li^+ ions adsorption from natural brines and process waters, which formed during recycling of Li-ion batteries and super capacitors. Ion exchange materials based on Li-Mn spinels are characterized by high adsorption capacity and selectivity to Li^+ ions. However, the low crystal structure stability in adsorption-desorption processes, due to partial dissolution in an acidic medium and the Mn^{2+} ions leaching into solution, are key disadvantages limiting widespread application.

The work aimed to study the regularities of $Li_{1.33}Mn_{1.67}O_4$ spinel synthesis and to determine the main factors affect on the phase composition, structure, and adsorption properties of Li-Mn adsorbents.

$Li_{1.33}Mn_{1.67}O_4$ spinels were obtained by hydrothermal, sol-gel, and solid-phase synthesis methods. To form the spinel structure, all obtained samples were calcined at 500 °C for 5 h. The crystal structure was studied on an Advance D8 X-ray diffractometer (Bruker, USA). The FT-IR spectra of the prepared materials were recorded on an IR spectrometer with a Fourier transducer Tenzor-27 (Bruker, USA). The textural characteristics of the adsorbents were studied by nitrogen adsorption-desorption method on a porosity and surface analyzer ASAP 2020 (Micromeretics, USA). Surface morphology and chemical composition were studied using a JSM-5610 LV scanning electron microscope with a JED-2201 (JEOL, Japan). The adsorption experiment was performed under batch test with lithium nitrate model solutions.

In this work, the physicochemical and adsorption properties of the obtained Li-Mn spinels were studied. The main factors determine $Li_{1.33}Mn_{1.67}O_4$ spinel adsorption-selective properties were established. It was shown that preparation of Li-Mn spinels modified by doping with transition metal ions (Co^{2+}, Ni^{2+}, Cr^{3+}, Mg^{2+}, Al^{3+}, Fe^{3+}) can lead to increase the stability of adsorbents crystal structure during multiple adsorption-desorption cycles.

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ADSORPTION PERFORMANCE OF Zr-Ca-Mg COMPOSITE PHOSPHATES TO Co^{2+} IONS

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Heavy metals are highly toxic and non-biodegradable pollutants that have a negative impact on living organisms due to ingress into water and soil. Therefore, the development of industry and the ever-increasing anthropogenic load determine the urgency of finding novel materials and technologies effective for solving this problem. Synthetic and natural adsorbents are widely used for heavy metal ions removal from aqueous media and for soils remediation. Metal phosphates are characterized by an increased affinity for polyvalent metal ions, while the attention of researchers is directed to the development of methods for the synthesis of these materials using available natural raw materials.

This work is devoted to the study of the adsorption properties of mixed Zr-Ca-Mg phosphates to Co^{2+} ions. The choice of the research object was due to the simplicity of the obtaining method and the use of natural dolomite as a common and widespread raw material. In addition, these materials have shown high efficiency in ^{137}Cs, ^{90}Sr and ^{60}Co radionuclides removal from aqueous solutions of complex radionuclide composition, which makes it possible to significantly expand the adsorbent application.

Zr-Ca-Mg phosphates were obtained by heterogeneous interaction of phosphatized dolomite $Ca_{0.7}Mg_{0.3}HPO_4{\cdot}2H_2O$ with 2.0 wt.% aqueous solution of zirconyl nitrate $ZrO(NO_3)_2$ with a molar ratio (Ca + Mg) / Zr of 1/0.36 (Zr-1) and 1/1.1 (Zr-2). Adsorption of Co^{2+} ions was performed in batch experiment from $Co(NO_3)_2$ aqueous solutions ($C_{initial}$ 50-3500 mg/L, V/m 250 mL/g, contact time 24 h). The initial and equilibrium Co^{2+} ions concentrations were determined by atomic emission spectrometry. To determine the adsorption mechanism, experimental data were calculated using Langmuir, Freundlich, Sips and Redlich-Peterson adsorption models. The correspondence of the experimental data to the specified models was determined by the approximation coefficient and the value of the experimental error.

The adsorption isotherms of Co^{2+} ions by Zr-Ca-Mg complex phosphates had a pronounced vertical section at the initial stage, which indicated a high affinity of the adsorbent to the adsorbate and allows them to be classified as H-type according to the Giles classification. The maximum Zr-1 and Zr-2 adsorption capacity from 0.05 M $Co(NO_3)_2$ solution was 253 and 156 mg/g, respectively. The adsorption isotherms of Co^{2+} ions by Zr-1 and Zr-2 samples were correctly described by the Sips equation, which indicates the adsorption centers heterogeneity of the composite adsorbents. Thus, the obtained results indicated the high efficiency of the studied Zr-Ca-Mg phosphates as Co^{2+} ions adsorbents, which together with the previously obtained data on ^{60}Co radionuclides adsorption, allows them to be used for effective treatment of wastewater and liquid radioactive waste.

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PHYSICOCHEMICAL AND SORPTION CHARACTERISTICS OF LIGNIN-BASED MATERIALS

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The materials with good sorption characteristics: well-developed surface, well-expanded pore system, presence of sorption centers, high selectivity towards solutes, high sorption efficiency, low synthesis costs, high thermal, chemical and mechanical resistance, longevity, low toxic and environmentally friendly are still in demand [1]. On the material market, a wide range of one-component sorbents: silicas, carbons, or zeolites is available, but these materials have certain limitations, therefore new materials with better properties are the subject of search [2].

The entire metallurgical enterprise, as a result of its activities, receives, in addition to the main products, production wastes (secondary products) – blast furnace slags, sludge, dust, scrap metal, etc. In this regard, the solution of the issues of reuse of metallurgical waste is becoming one of the most pressing problems [3].

The presented work is devoted to the synthesis and study of the structural properties of new functional carbon, obtained by pyrolysis of cheap, ecological, renewable and easily accessible raw materials such as induline and furnace dust, which is mainly composed of magnetite and hematite. This approach makes it possible to obtain magnetically sensitive sorbents that can be easily removed from the solution by the action of an external magnetic field.

Carbons were synthesized using two-step method: (i) mechanochemical mixing of kraft lignin (Indulin AT, MeadWestvaco Corp., USA) and furnace dust in a ball mill; (ii) pyrolysis of the mixture in an argon atmosphere at 800 °C. The physicochemical and sorption characteristics of the obtained composites were performed using several analytical techniques: low-temperature nitrogen sorption, thermal analysis, scanning electron microscopy (SEM), and X-ray diffraction analysis (XRD). It was shown that the synthesized composites are microporous with S_{BET} = 107 m^2/g and consist of graphitic domains and metallic phases (Fe^0 – 86%, FeO – 14%). Moreover, the adsorption studies form hazardous substances revealed the potential applicability of biocharin water remediation.

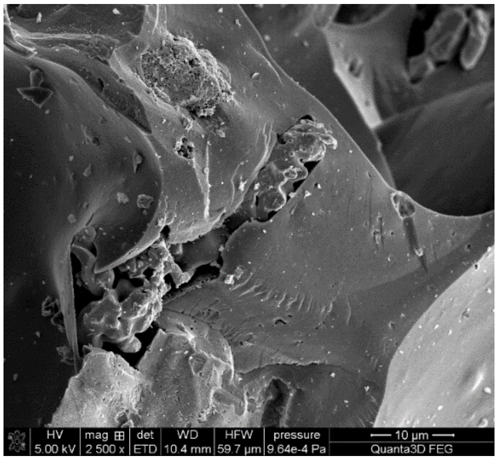

Fig. 1. SEM image of lignin-based nanocomposite.

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PURIFICATION OF INDUSTRIAL WASTEWATER CONTAINING HEAVY METAL SALTS AND RADIOISOTOPES BY LOW-TEMPERATURE PLASMA ELECTROLYSIS

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We have been carried out studies of low-temperature plasma electrolysis (LTPE) action on water and water solutions of different classes of inorganic and organic compounds. The formation of liquid bipolar bifunctional electrode is basis of faraday processes. This fact is difference of LTPE and classic electrolysis. We have carried out studies on the use of LTPE for the purification of industrial wastewater from inorganic heavy metal salts and radioisotopes.

It has been considered the opportunity of LTPE application during the heavy metal salts and trans-uranium and trans-plutonium compounds extraction. The dependence of degree of the purification from initial concentrations of radioactive elements and the number of recycles during processing of liquid in continuous reactor was examined. It has been determined the relative contribution of filtration of the solutions made of nature waters in whole effect of liquid environments purification from trans-uranium elements during the LTPE. Purification degree was shown to depend on particles aggregation time and their subsequent separation by filtration (Fig. 1). For Sr purification degree may be 80% and higher, whereas Cs was shown to be detained slightly on filters during electrolysis (Fig. 2).

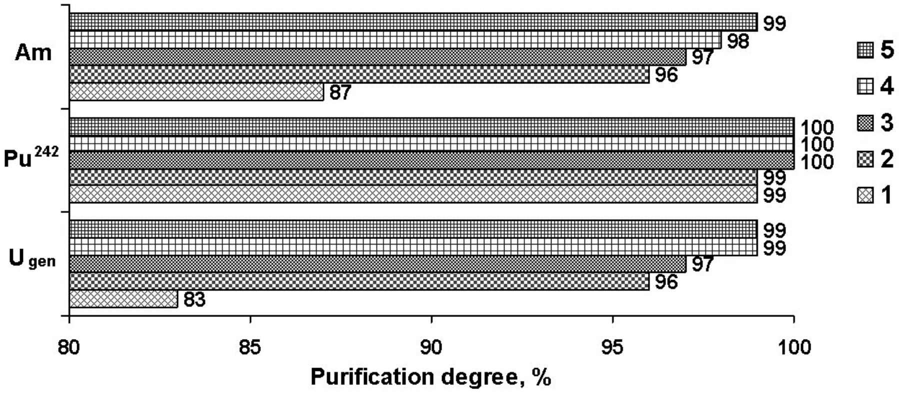

Fig. 1. The purification degree of aqueous solutions of radioactive isotopes: 1 – 5 – recycle coefficient.

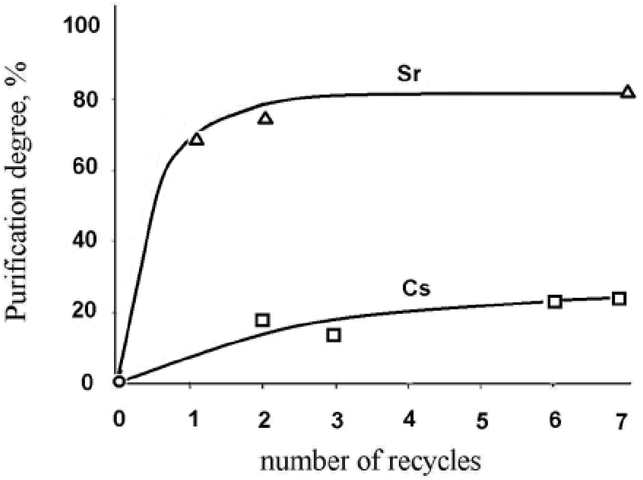

Fig. 2. The effect of LTPE on Sr and Cs extraction.

It has been showed high effectiveness of low-temperature plasma electrolysis method in extraction of heavy metal salts and radioisotopes from aqueous solutions.

MODIFICATION OF LOSS-ON-IGNITION METHOD FOR DETERMINATION OF ORGANIC MATTER IN HIGHLY CALCAREOUS SEDIMENTS

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Biogenic sands are widespread on the planet coasts and in shallow waters (mainly in low latitudes). This type of sediments is composed of pieces the skeletal remains of plants and animals such as clams, sea snails, foraminifera, algae, corals, echinoids, sponges, etc. This biogenic material consists mainly of calcium carbonate.

Determination of organic matter in these sands is associated with a number of methodological difficulties, especially if carbonates constitute the main fraction. There are two main approaches for the determination of organic carbon on marine sediments, namely (1) chemical oxidation of organic matter and (2) high-temperature combustion. Both of these approaches are affected by carbonate harmful influence. Approach (1) is completely unsuitable due to the fact that carbonates react with an oxidizing agent (sulphuric acid and potassium dichromate). Approach (2) is influenced by oxidizing carbonates at high temperature.

The Loss-On-Ignition method relates to approach (2). In the 'normal' case the sample of sediments is treated in a muffle furnace for certain time (usually 1.5-6 hours) at high temperature (most commonly 450-950^o C). The difference between the initial and final sample weights is converted to organic carbon units.

For slightly calcified sediments is recommended to eliminate carbonates by hydrochloric acid with following rinsing, filtering and drying to remove reaction products. But the predominance of carbonates in biogenic sands makes this recommendation difficult to implement. Additionally, flushing and filtration can result in the loss of some of the water-soluble organic matter

The reaction between calcium carbonates and hydrochloric acid leads to the formation of calcium chloride which is highly hygroscopic. We propose the scheme of temperature-controlled weightings after carbonates and hydrochloric acid reaction. The fact is that calcium chloride hydrate contains different amounts of water depending on the temperature. We propose to control this factor by using pure calcium chloride as a 'blank'. This blank should be processed together with the sample after HCl treatment in all stages. There are following stages: drying, combustion, cooling, and weighting. Weighing of the sample and blank should be carried out immediately after each other after stabilization of the selected temperature.

MODELING AND MONITORING OF EURASIAN NATURAL MINERAL WATERS

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Natural mineral waters of Russia, some CIS countries (Belarus, Moldova, Armenia, Azerbaijan, Georgia and Uzbekistan) and Eurasian countries carried to Chloride-Hydrocarbonate type have been investigated. The analytical dependences connecting, entered by authors, characteristic parameters of structure of waters (M, B, Φ) with independent variables of ionic structure and concentration are resulted.

Based on the obtained data a mathematical model of the structure and properties of chloride-hydrocarbonate mineral waters is developed and the principles of formation of waters of a certain type and their distribution into groups and classes are formulated. A general system of classification of Eurasian mineral and low mineralization waters formed during the Late Alpine tectogenesis on the territory of European states has been developed.

Results of research have shown an opportunity to apply characteristic parameters of structure of waters for the organization of national and interstate monitoring natural waters of various genesis and structure. Change of values of characteristic parameters of the mineral water counted on initial data of the chemical analysis of structure, can serve as a quantitative estimation of quality of mineral water and to be used for the organization of system of national and interstate monitoring waters.

In this work it was shown that comparison of values of characteristic parameters of mineral waters and physiological liquids of plants, animals and the person can form a basis for development of recommendations on application of mineral waters for medical, rehabilitation and preventive application in a medical and biologic practice. Characteristic parameters of structure of waters can be used at examination of quality and conformity of mineral water to passport characteristics of declared analogue of reference water, and also for an establishment of the location of a source.

Expansion of geography of a finding of sources of the mineral waters identified on their conformity to reference mineral waters on characteristic parameters M, B, Φ allows to use rationally regional natural water resources and to promote social development of territory of a location earlier sources of mineral waters not taken into consideration.

NUTRIENT LOADS ON THE ENVIRONMENT IN THE BALTI MUNICIPALITY

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Concentration of the mineral forms of nitrogen and phosphor in the limits of urban areas is for 30-40% higher than on adjacent territories used for agricultural activities. Organic forms of both elements predominate in soils and bottom sediments (about 80%). Nitrate form of mineral nitrogen predominates in the surface waters, while in the liquid phase of bottom sediment ammoniac nitrogen consists approximately 70% of mineral nitrogen. The concentration of mineral phosphor in liquid phase of bottom sediments is in 10-20 times higher than in surface waters.

Superficial runoff is an essential source of pollution with nutrients of water ecosystems and in its accumulation in different functional zones of urban areas. The ration between ammonia and nitrate nitrogen in this component is around 1:1, while for mineral forms of nitrogen and phosphorus this is circa 10-12:1. Atmospheric precipitations are responsible for around 1-2% of all nutrient loads on environment in the municipality and ration between mineral nitrogen in superficial runoff and precipitations in average is around 30:1. The content of nutrients in the bottom sediments of lake ecosystems is in 2-5 times higher in comparison with the Raut river sediments.

Such values for nitrogen and phosphorus indicate on permanent and significant pollution of water ecosystems in the Balti town with nutrients and an action plan for its reduction is necessary for general improvement of the state of environment in the municipality.

HYDROCHEMICAL STATE OF SOME FISH PONDS FROM THE REPUBLIC OF MOLDOVA AND ROMANIA

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Water quality is one of the major factors that determine the effectiveness of fish farming in ponds, status of fish health and the quality of fish products. As pond farming is still one of the main branches in fish farming in the Republic of Moldova and Romania, researches have been conducted on the chemical composition of water in various seasons and, respectively, the water quality has been evaluated at different stages of fish rearing. There were investigated six ponds from the Republic of Moldova (Moldovanca, Morozeni, Calugar, Garla, Fagadau from Falesti district and Dusmani from Glodeni district) and two ponds from Romania (Dracsani from Botosani county and Podu Iloaiei from Iasi county). Atmospheric precipitation and small springs are the sources of water supply of theinvestigated ponds from the Republic of Moldova. Dracșani and Podu Iloaiei ponds are fed by the small rivers Sitna and Bahluet, some springs and atmospheric precipitation, including snow melting.

The results of the investigations showed that according to the thermal regime, mineralization and nutrient content the waters in most of ponds are favourable for fish rearing, but in summer the gas regime, including biochemical and chemical oxygen demand, becomes a limiting factor, especially in ponds with high density of fish.

In some ponds, due to the imbalance in the gas regime, of the ratio between nitrogen and phosphorus compounds, the algal blooms are observed. Such periods are characterized by the change of pH values, decrease of the water saturation with oxygen, which can also cause the fish death.

The increase of the content of organic substances and the siltation of ponds, caused by the fact that the pond waters are not replaced by fresh ones for years, especially in ponds where phytophagous cyprinids predominate, can be considered as the most severe problem of pond maintenance. Polyculture is one of the ways for pond remediation, for example, the stocking of ponds with detritophagous species, resistant to increased amounts of organic substances, such as the Far Eastern mullet (pilengas) *Mugil so-iuy Basilewsky*, whose rearing in polyculture has been tested in Moldova (Patent MD 3408).

In summer, due to the shortage of atmospheric precipitation and high temperatures, an increase of water mineralization of up to 4-6 g/l was recorded, for example, in Garla (4.13 g/l) and Fagadau (5.7 g/l) ponds, but no decrease in fish productivity was noticed. Nevertheless, such mineralization is unfavourable for cyprinid larvae and first-year juveniles. Water mineralization and hardness of Dracsani and Podu Iloaiei ponds are suitable for obtaining of fry of freshwater fish and rearing of table fish.

Acknowledgments. The researches were done in the frame of the national project 20.80009.7007.06 – AQUABIO: “Determining the changes of aquatic environment, assessing the migration and impact of pollutants, establishing the patterns of the functioning of hydrobiocenoses and preventing the negative effects on ecosystems” (2020-2023 State Program) and EU project 2 SOFT/1.2/47 – TeamUp HealthyFish.

THE INFLUENCE OF SOME CHEMICAL AND PHYSICO-CHEMICAL PARAMETERS ON THE GLUTATHIONE PHOTOLYSIS

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Natural waters, in terms of thermodynamics, are an open system in which various redox reactions involving oxidants (molecular oxygen, hydrogen peroxide, free radicals, etc.), reducing agents and transition metal ions are constantly taking place. The presence of these components determines the redox state of the aquatic environment. It has been proved that under normal conditions the ecological state of aquatic systems is dominated by oxidants, but natural waters also contain a large number of dissolved organic substances that exhibit a reducing character. One of them are thiols, that are substances containing functional group -SH. Thiols are conventionally divided into autochthonous thiols (glutathione (GSH), cysteine), that are substances entering natural waters as a result of metabolism and biochemical processes involving hydrobionts, and allochthonous thiols (thioglycolic acid, thiourea), that are products of anthropogenic impact on aquatic ecosystems.

In the surface layers of natural waters the concentration of thiols can decrease not only as a result of interaction with oxidants, but also due to photolysis, which positively influences the formation of the redox state of the aquatic environment. Considering that in natural waters the most frequent thiols are autochthonous thiols, glutathione was chosen as the object of study. Based on bibliography data, transition metal ions can influence the photolysis intensity of thiols. The most common transition metals in natural waters are various forms of iron (10^{-5}M) and copper (10^{-7}M).

The kinetics of direct photolysis of glutathione in the presence of Fe(III) and Cu(II) ions was observed by looking at the change of the glutathione concentration, using the Ellman method. A polychromatic lamp model DRT-400 was used as the radiation source. The reaction rates were determined using the Van't Hoff method.

From the rate constants and half-life values obtained for the modelled systems shown below it is seen that in the presence of Fe(III) and Cu(II) ions, the photolysis intensity of glutathione is higher and the half-life of glutathione is almost twice as long. Also, from the data obtained, it is seen that the rate constant of photolysis of glutathione in the presence of Fe(III) ions is lower than in the presence of Cu(II) ions, which may be due to the neutral pH value of the modelled systems, at which the Fe(III) ions pass into the suspended state.

$$\text{GSH} - h\nu\ (k = 2{,}04 \cdot 10^{-4}\ s^{-1};\ \tau_{1/2} = 56\ \text{min}\ 38\ \text{s});$$

$$\text{GSH–Fe(III)–}h\nu\ (k = 3{,}36 \cdot 10^{-4}\ s^{-1};\ \tau_{1/2} = 34\ \text{min}\ 23\ \text{s});$$

$$\text{GSH–Cu(II)–}h\nu\ (k = 3{,}90 \cdot 10^{-4}\ s^{-1};\ \tau_{1/2} = 29\ \text{min}\ 37\ \text{s}).$$

Also, based on bibliography data, it was hypothesised that the intensity of photochemical transformations of thiols could also be influenced by water mineralization. Based on the fact that most of the natural waters in the

Republic of Moldova belong to the hydrocarbonate class of waters, the system GSH – HCO_3^- – hν was modelled. The rate constant ($k = 11,4 \cdot 10^{-4}\ s^{-1}$) and glutathione half-life ($\tau 1/2$ = 10 min 8 s) obtained for this system, showed a significant increase of glutathione photolysis intensity. The explanation is that the pH-value also increases with increasing concentration of hydrocarbonate ions and dissociates the thiol group -SH to form thiolate anion ($C_{10}H_{16}N_3O_6S^-$), which is more reactive than the undissociated group. Another explanation for the increased photolysis intensity of glutathione in the presence of hydrocarbonate ions, according to some bibliography sources, is that hydrocarbonate ions under UV radiation may be electron donors: $HCO_3^- + h\nu \rightarrow (HCO_3^-)^* \rightarrow HCO_3^{\cdot} + \bar{e}$.

Thus, it has been determined that transition metal ions Fe(III), Cu(II) and mainly water mineralization, particularly hydrocarbonate ions, increase the rate of direct photolysis of glutathione, which is a positive factor in the formation of the redox state of water systems and in the processes of chemical self-purification of natural waters.

Acknowledgement:

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WATER AND SOCIETY IN GEORGIA FROM HISTORICAL ANGLE

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The paper describes water resources of Georgia, characterizing them from historical point of view and demonstrating their contemporary role for the country. The discussion further refers to water monitoring system in Georgia, featuring both modern and old irrigation systems used in the country. Various anti-drought rituals practiced in old times are also listed in the paper. Drinking water supply system of ancient times together with old and modern water treatment methods are sufficiently detailed. Parallels are drawn between what alchemists and Georgian King, Vakhtang VI, thought of drinking water purity. Among water treatment plants, Vakhtang VI named swamp plants. In the 21st century, scientists have already proven the importance of artificial wetlands in sewage and wastewater treatment. Vakhtang VI refers to „water“ in various meanings and, like King Philip II of Spain, describes a method, according to which, rose petals, cloves, cinnamon, amber, oak bark and 12 other ingredients should be placed in water. Such water was meant to stand for 15 days. However, it is not clear what was the purpose of using it.

The Georgian king also describes the method of preparation of „body whitening water“. However, whitening the body is likely to mean body healing.

The vegetation were mentioned by King Vakhtang in different context as well, noting that the presence of algae in rivers indicated to various problems. The same were declared by alchemists in medieval era, however, no one would specify what was meant. In fact, it was about eutrophication process.

The paper investigates whether the same issues are faced by the modern science, that were noted in the book by the Georgian king and specifically, what method of water purification was preferred by him. Ancient Georgian baths and material for water utensil production are also reviewed in the article.

Keywords: Water in early Georgia, Water in the Georgian folk, the Georgian Chemist King, Old irrigation systems, Drinking water supply, Utensils, Ancient rituals, Old baths.

SURFACE WATER STUDY IN SEVERAL VILLAGES OF KAKHETI REGION OF GEORGIA

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Water resources are of significant importance in providing favorable living conditions for people, healthy state of the economy and in preservation of the environment. Providing water to the population, industry, energy and agriculture is one of the priority tasks for successful performance of countries.

There are mainly two types of water in Kakheti. The first originates from one of the ravines and runs from taps installed in yards. This type of water undergoes only mechanical treatment. I.e., unlike similar-size villages in neighboring countries, there is no unified wastewater system and therefore, neither natural, nor other type of treatment systems are applied. This type of water is not used for drinking purposes, but for washing, bathing, cooking and for preparation of various hot beverages. Drilled waters originate from mountains, outcropping to the surface of the ground. It is natural, that these waters are not examined, however the people drink them and they taste really good. Drilled water pipes sometimes run directly into the street and occasionally into residents' yards.

The article reviews the chemical composition monitoring results of water, running from taps installed in yards and from the so-called drilled wells in villages of Gurjaani region, Kakheti.

Gurjaani Municipality – Administrative-Territorial Unit in Eastern Georgia, Kakheti Region. Gurjaani municipality is bordered by 5 administrative municipalities. It is bordered by Sagarejo Municipality to the west, Sighnaghi Municipality to the southeast, Telavi Municipality to the northwest, Kvareli Municipality to the north, and by Lagodekhi Municipality to the east. The territory of Gurjaani municipality belongs to the district of moderately humid subtropical climate. To the east, the plain has a moderately humid climate with mild winters and hot summers. There is moderately humid climate on Gombori range, characterized by long summers. The Iori Plateau is known for its dry subtropical steppe climate, with moderately cold winters and hot summers.

The study was focused on the purity of water as it is used by the population in everyday life for drinking, as well as for cooking and other household purposes. In the process of examination, a small amount of iodine was observed in drilled waters, that probably could serve as an explanation to the fact, that there are less cases of goiter problems in this region.

Key words: borehole waters, surface water, metals in the water, iodine in the water.

TECHNOLOGICAL ASPECTS OF WASTEWATER RECEPTION AND TREATMENT

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Summary. The problem of efficient wastewater treatment is increasingly brought into society nowadays. The pollution effect of insufficiently treated wastewater on surface water is manifested by the content of total suspended matter, organic matter, organic nutrients of nitrogen, phosphorus, ammonium and pathogenic microorganisms. The purpose of this research is to deepen practical and theoretical knowledge to improve the wastewater treatment process.

Research period: January-June 2021, the object of study is the Wastewater Treatment Plant in Chisinau. In order, to monitor the technological process of wastewater treatment, five main indicators are checked daily: acidity (pH), temperature (T), biochemical oxygen consumption (BOD), chemical oxygen consumption (COD), total suspended solids (TSM), as well as the content of organic nutrients (N, P). Of these quality indicators, only the pH and temperature fall within the norms of reception-discharge of wastewater, the rest of the indicators do not correspond to the norms recommended for the reception and evacuation of wastewater. However, the Wastewater Treatment Plant in Chisinau is in the process of reconstruction with special

normative evacuation facilities, coordinated with the State Ecological Inspectorate of Republic of Moldova. Considering that an efficiently functional wastewater treatment plant has a certain treatment capacity for the above mentioned indicators that do not fall within the prescribed norms: BOD-70-90%, COD-70%, TSM-90%, NH_4 –N- 70-80%, P-80%, from the obtained results the treatment capacity of the treatment plant is: BOD-78%, COD-64%, TSM-70%. The nutrient content of wastewater before and after treatment indicates that in the Chisinau Wastewater Treatment Plant are discharged wastewater with increased loads of pollutants, which exceed the norms of maximum permissible concentrations, and the treatment capacity is lower: NH_4-N-27-34%, P-78%. Based on these data, we can conclude that the treatment plant has a satisfactory treatment capacity, although the treatment capacity is reduced due to the reconstruction works and the increased concentrations of pollutants received in the wastewater.

Keywords: wastewater, organic nutrients, total suspended solids, biochemical oxygen consumption, chemical oxygen consumption, treatment plant.

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THE QUALITY OF TAP AND SPRING WATER BEFORE AND AFTER TREATMENT WITH THE USE OF HOUSEHOLD EQUIPMENT

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Because tap water often does not meet regulatory requirements in its sanitary and chemical indicators, an increasing part of the population prefers to use spring water as an alternative source of drinking water. However, today springs can also be subject to significant pollution. In this regard, the aim of the work was to assess the possibility of using household equipment for the purification of tap and spring water and to check the filter resource specified by the manufacturer.

The paper presents data on monitoring the quality of tap and spring water before and after treatment using household equipment. Water quality control was carried out according to 25 indicators. Among them are composite, metal compounds and some inorganic substances.

We tested samples of tap and spring water in Ivanovo city, which had undergone additional treatment using filters of the most popular trademarks. We used devices based on different principles of operation: treatment with the use of jug-type filters "Aquaphor" and "Barrier" based on adsorption treatment and the installation "Aquaphor Osmo Pro" based on the reverse osmosis method. With the help of the filter jug and replaceable modules "Aquaphor A5", "Aquaphor A6" 350 liters of spring water were filtered, and with the help of the filters "Aquaphor B100-8" and "Barrier Standard" 350 liters of tap water were filtered.

The results of the chemical analysis of the initial samples of spring water showed an excess of the total hardness (1.37 MPC) and the index of the iron compound (1.08 MPC) in comparison with the MPC. The results of the chemical analysis of the initial samples of tap water also showed an excess of the value of the iron compound (1.04 MPC).

The greatest degree of water purification is achieved when using an installation based on reverse osmosis, namely "Aquaphor Osmo Pro" (90 %). The degree of post-treatment of tap water using the "Aquaphor B100-8" sorption module averaged 38 %, and with the "Barrier Standard" cassette 30 %. The average cleaning degree of the Aquaphor A6 filter was 62 %, and the Aquaphor A5 filter was 32 %.

In the work, the magnitude of the potential danger from the use of this water was assessed. With the constant use of spring and tap water of this quality, there is a possibility of hypertension, as well as diseases such as coronary heart disease and chronic gastritis.

The work estimated the probable damage to the health of an individual from drinking water of this quality. Based on the criteria for the acceptability of damages, the damage caused by this risk can be characterized as minimal and low. Hence:

1) assessment of the magnitude of risks and associated damages showed that these values are small and lie in the area of low damages;

2) resource of filters based on sorption water purification does not meet the manufacturers' indications. On average, the degree of purification is less than 50%, and is produced when filtering 150-200 liters of water;

3) the best water purification device in this study was the "Aquaphor Osmo Pro" filter based on the reverse osmosis method, the purification degree of which was 90%.

NEW NANOSIZE MATERIALS OBTAINED BY THERMAL TREATMENT OF VANADIUM OXIDES WITH APPLICATION IN DYES REMOVAL IN WASTEWATER TREATMENT

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Rapid population growth, urbanization and industrialization pose significant threats to the aquatic ecosystem. A water contamination has a significant impact on environment and has become one of the major problems facing the world today. The discharge of untreated dyes contaminated wastewater causes harmful chemical and biological changes in water bodies as well as human disease. The most common dye used at industrial scale is methylene blue (MB). Recently, numerous metal oxide nano-particles adsorbents such as zinc oxide, magnesium oxide, ceria oxide have been applied for the purpose of treatment of water from dyes and/or other pollutants.

The research work deal with vanadium pentoxide (V_2O_5) nanoparticle adsorbents which were obtained by thermal pretreatment carried out by increasing the temperatures between 90 and 750 °C. In order to obtain more detailed information on the surface chemistry of the newly prepared nanomaterials, the characterization was done by X-ray diffraction, scanning electron microscopic, Fourier transform infrared spectrometry and thermalgravimetric investigation techniques. The prepared nanoparticles were tested for methylene blue removal from water model solution. Initial MB concentration, solution volume and weight of adsorbent were as follows: 20 mg/L, 30 mL and 20 mg, respectively. UV-Vis analysis indicated that high MB removal efficiency (93%) and adsorption capacity (27 mg/g) after 40 minutes of adsorption were obtained over V_2O_5 annealed at 500ºC in comparison with V_2O_5 treated at 90, 250 and 750ºC, respectively. It was also pointed out V_2O_5 annealed at 500 °C has higher sorption properties in comparison with other sorbents reported in literature.

Therefore it might be utilized as potential adsorbent material in dyes depollution control and open new avenues for vanadium pentoxide application. The applicability and suitability of the two kinetic models were tested and the removal mechanism was proposed. The adsorption results demonstrated that the best fit of experimental data was to the pseudo-second order model.

TREATMENT OF AQUEOUS SOLUTIONS CONTAINING HEAVY METAL IONS IN PLASMA SYSTEMS

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Preservation of the hydrosphere with increasing water consumption and water pollution by industrial and domestic sewage is one of the mam environmental problems of modern times. Heavy metals (HM) are criterion pollutants for natural basins.

The new methods that have attracted the close influence of researchers in recent years include high-energy chemistry methods. Their characteristic feature is high efficiency, the absence of the need for chemical reagents, and their use allows avoiding secondary pollution of the environment.

In this work, we investigate the processes of destruction of HM dissolved in water by a glow discharge, the establishment of the influence of various physicochemical parameters, and the study a new method for the synthesis of nickel oxide powders in a plasma-solution system using an aqueous solution of nickel nitrate. Research methods were used: SEM, X-ray structural analysis, EDX microanalysis, TGA-DSC.

The advantage of this method is the absence of contact of the electrode surface with the initial solution. Previously, this method was successfully applied for the synthesis of powders of zinc, copper and cadmium oxides.

It was established experimentally that the effect of a direct current discharge on an aqueous solution of $Ni(NO_3)_2{\cdot}6H_2O$ leads to the formation of powders in the bulk of the liquid anode. The results of studies of the synthesized samples showed that they have a complex composition, and upon high-temperature treatment they form NiO.

It is shown that low-temperature plasma can be used for post-treatment of waste water and a new method for synthesizing nickel oxide powders.

PECULIARITIES OF THE ACCUMULATION OF IRON AND COPPER IN THE DNIESTER RIVER

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The Dniester is the main water artery of the Republic of Moldova. The presence of copper and iron in the waters of the river researchers are noted constantly, therefore it becomes clear practical and scientific interest in the processes of mass transfer of metal species of the studied metals.

The work was carried out in 2017-2021 on the segment of the lower Dniester, in the area of the influx of large tributes of Raut and Ichel. During the work, hydrological, mathematical and statistical aspects were taken into account. From the water samples, using the membrane filtering method were extracted the dissolved-colloid (DCF<0.45 μm) and particulate (PF $\geq$ 0.45 μm) forms of metal species. The copper and iron content was determined by the atomic absorption method on the IL-551 spectrophotometer, also other important hydrochemical (pH, water temperature, oxidability, O_2) and ecochemical (Eh, rH_2) parameters were also defined in water samples.

The nature of dissolved-colloidal forms of metal species changed depending on the object of the study, the Dniester control section. In Raut, you can assume dominance of mineral-organic forms of iron and copper. Ichel can be characterized by the predominance of organic forms of metal species. On the studied segment of the lower Dniester, with the help of indirect methods, has been revealed a change in the nature of the forms of metal species from mineral-organic forms in the upstream cross section of Dniester, to organic coexistent metal forms in the outlet of Dniester. In the outlet cross section of Dniester (Vadul-lui-Voda), according to our data, the chemical channel of self-purification of natural water was established with the participation of free radicals and dissolved-colloidal forms of copper as catalysts. Excesses of sanitary and hygienic standards relating to dissolved forms of metal species have not been detected.

Balance calculations for copper and iron give an opportunity to approximately evaluate accumulation of metals on the studied section of the Dniester. If the metals accumulation processes prevail over the emission processes, then balance calculations give a positive result. Such results for copper us were obtained in 2018, 2019 and 2020, when 29.221 tons, 3.84 tons and 26.184 tons of copper were accumulated on the studied section of the lower Dniester, respectively. In 2017 and 2021, the emission processes prevailed over the processes of copper accumulation for the studied area of the river, as a result of which negative values of -2.028 t and -1.970 tons were obtained, respectively.

In the case of balancing calculations by the iron on the studied area of the river for 2017, 2018 and 2019, negative values are set -5.406 t, -23.834t and – 67.5 tons, respectively. Iron accumulation it was found by us at 2020 and 2021 at the level of 2558.267 t and 157.559 t, respectively. Significant was the flow of iron with the waters of the tributary of Raut, whose amount sometimes exceeded the flow of iron in the upstream cross section of Dniester (Dubasari).

Thus, it can be concluded that in the studied section of the lower Dniester can accumulate to 29.221 t / year of copper and up to 2558.267 t / year of iron, copper emission from the studied area of the river can reach 2.028 tons / year, and iron-67.5 t / year.

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DYNAMICS OF THE CONTENT AND FORMS OF MIGRATION OF Cu AND Zn IN THE PRUT RIVER

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In the Republic of Moldova, the total concentrations of Cu and Zn in surface waters are regulated by the regulation on environmental quality requirements for surface waters, approved by Government Decision no. 890 of 12 November 2013.

The purpose of this study is to analyze the dynamics of Cu and Zn in the waters of the Prut River in the territorial limits of the Republic of Moldova, as well as to establish the ratio between the forms of migration (dissolved and suspended) of these metals in recent years. The study of the concentrations and forms of migration of microelements in the dissolved fraction, suspensions, sediments and aquatic organisms is an imperative for science, especially in the XXI century, when anthropogenic pressure on the environment increasing.

Cu and Zn can penetrate surface waters from both natural and anthropogenic sources. In the Republic of Moldova the main source of water pollution with Cu and Zn is agricultural activity, given the presence of these metals in various chemicals used. The dynamics of Cu and Zn concentrations in recent years, compared to the '80s and' 90s of the last century, show a decreasing trend.

The migration capacity of microelements in surface waters and their forms of migration are conditioned both by the properties of the elements themselves and the physico-chemical peculiarities of the environment, by the redox conditions, the size of pH, temperature, the presence of agents of complexation, of suspended substances, of the vital activity of hydrobionts, etc. The study of the correlation between suspended and dissolved forms of migration of microelements in river waters is important in assessing their influence on living systems and is of great importance in hydrogeochemical research.

Cu and Zn are essential nutrients in the development of living organisms, but can represent toxic effects at higher concentrations. Considerable concentrations of these metals, including other microelements in surface waters can make water unsuitable for use as a drinking source, for food preparation, recreation, household use, irrigation, in industry, etc. And as a result they can have negative effects on the health of both humans and aquatic organisms, but even worse can lead to complete disruption of the normal functioning of the ecosystem. In this context, it is necessary to constantly monitoring the concentrations of metals, including Cu and Zn in aquatic ecosystems, in order to prevent pollution as well as timely intervention.

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APPLICATION OF CNT-COOH/MnO_2/Fe_3O_4 NANOCOMPOSITE FOR THE REMOVAL OF CYMOXANIL FROM AQUEOUS SOLUTION

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In the last years, water pollution and pesticides accumulation in food chain have become a serious environmental and health problems. In agriculture, the pesticides are intensively used due to their capacity to control and eradicated insects, fungi, bacteria, weeds, worms, rodents and other pests. Their constant use results in obtaining healthy and high yield crops but, on the other hand, over time, leads to their accumulation in soil and water with irreversible effects on the environment and health. For this reason, it is imperative to constantly monitor their concentration in the environment and aquatic media.

To improve the extraction of pesticides, new methods and materials are constantly developed. A very promising material are multi walled carbon nanotubes, alone or in combination with other nanomaterials, due to their highly porous and hollow structures, high surface area, thermal stability, high mechanical strength in tension, good thermal conductivity, electrical conductivity, optical activity, mechanical damage resistance and a strong ability to establish $\pi- \pi$ interactions with the pesticides or other organic materials.

Cymoxanil, [1-(2-cyano-2-methoxyiminoacetyl)-3-ethylurea], is an aliphatic nitrogen fungicide, with promising effect like fungicide, alone or in combination with other fungicides, against grape downy mildew, tomato and pepper bacterial spot and lettuce bacterial leaf spot due to his high efficiency, low toxicity and curative activity on plants, but with a lake of literature about the long-time toxicity of cymoxanil accumulation.

The present study evaluates the efficiency of the cymoxanil adsorption on CNT-COOH/MnO_2/Fe_3O_4 nanocomposite. The optimal conditions were established studying the influence of pH (2-10), temperature (20-60°C), initial cymoxanil concentration (7-20 mg L^{-1}), adsorbent dose (0.5-5 g L^{-1}) and contact time (2-30 min) on adsorption process. Isotherms and kinetic models were used to analyze the experimental data. Among the used isotherms, the Langmuir isotherm model provides the best fit for experimental data. The maximum adsorption capacity of cymoxanil on studied nanocomposite was 10.672 mg g^{-1}. Also, cymoxanil adsorption follows the pseudo-second order kinetic model. According to the experimental results, CNT-COOH/MnO_2/Fe_3O_4 nanocomposite can be used for cymoxanil removal from aqueous solution.

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ENVIRONMENTAL ASSESSMENT OF WATER QUALITY IN THE WATER SUPPLY SOURCE IN IVANOVO

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An important factor in health protection is the provision of the population with good-quality drinking water. It is one of the main environmental factors that can have both positive and negative effects on the health of the population.

To assess possible negative consequences for the health of the population, water samples were taken from the Uvod reservoir, which is the main source of water supply for the city of Ivanovo.

The results obtained allow us to conclude that the water body, according to the integrated WPI indicator, for 2021 belongs to the 6th class – very dirty. However, taking into account the dynamics for the period 2019 – 2021, there is a negative trend, which leads to a deterioration in the state of the water body, and as a consequence to a low quality of drinking water. The list of monitored indicators was formed on the basis that they are included in the list regulated by regulations and are typical pollutants for the investigated water body. It was found that the main contribution to WPI and the greatest contribution to the value of general toxic risk (development of chronic intoxication) and the risk of developing adverse organoleptic effects (chronic intoxication) are made by Cu, Mn and Fe. Perhaps this is due to the increasing anthropogenic load, namely, the development of the banks by private households and the use of the facility for recreational purposes.

The results obtained show that it is necessary to implement measures aimed at reducing the level of pollution, both of water in the reservoir and water in the centralized water supply system of Ivanovo.

QUANTIFICATION OF ANTIBIOTICS IN INFLUENT AND EFFLUENT WASTEWATER TREATMENTS PLANT AND ANTIBIOTIC RESISTANCE PROFILE OF ISOLATED BACTERIA

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One of the global health emergency is represented by the antibiotic resistance, which is considered as a consequence of various patterns of antibiotic consumption. The rise of antibiotics usage has led to an exposure of bacterial communities and ecosystems to a significant amount of antibiotic residues. Therefore, the major future needs should estabilish standardizeds methods for the quantification of the antibiotic residues and antibiotic resistance level which are critical in establishing the link between their presence in the environment and their biological effects. Also, it could be an essential tool in the monitoring and surveillance of antibiotic residues in the environmental matrices as a consequence of inadequate antibiotic use. The analysis of influent and effluent wastewater treatment plant (WWTP) could provide useful information about the medication use and misuse.

The aim of the present study is to develop an analytical HPLC/MS-MS method to quantify antibiotics from influents and effluents WWTP. Also, to determine the antibiotic resistance profile of bacteria isolated from wastewaters matrices. This study is focused on the analysis of 7 antibiotics mostly present in the wastewaters of Romania. By incubating the water samples with nutrient agar media, several bacteria were isolated and tested against the detected antibiotics.

Results: Using HPLC/MS-MS technique, several antibiotics were detected in the WWTP influent, such as clarithromycin, doxycycline, ciprofloxacin, azithromycin, piperacillin and amoxicillin. After the treatment process, the following antibiotics were detected in effluent samples of the treatment plant clarithromycin, azithromycin, ciprofloxacin. Several bacteria were isolated from the wastewaters and tested against these main antibiotics, all showing resistance to clarithromycin, but also to amoxicillin and norfloxacin.

Conclusions: After the wastewater treatment process we detected antibiotic residues in the WWTP effluent, which highlights the ineficiency of wastewater treatment process and a potential risk of waters contamination. Also, rise a concern of negative impact on human and ecosystem health. The next step will be to try and determine the exact type of bacteria isolated and establish the resistance mecanism to antibiotics.

RESEARCH ON THE COMPOSITION AND PROPERTIES OF UNDERWATER SEDIMENTS OF THE GHIDIGHICI LAKE

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The purpose of the works. The researches aimed to elucidate the composition and properties of sedimented matter from the water of Lake Ghidighici - a typical example of a eutrophic lake in the geographical area. Samples of mineral and organomineral sediments extracted from the lake bottom were investigated using for this purpose different chemical and physico-chemical research methods - elemental composition analysis, automatic acid-base titration, infrared and UV-VIS spectroscopy, Roentgen analysis, etc. The research was performed using the Metrohnom 848 Titrino plus titrator, Perkin Elmer Lamda 25 and Lomo SFD-46 spectrophotometers, Dron 3 diffractometer.

Research results. Automatic acid-base titration of dispersed systems - solid particles from underwater sediments showed a relatively high buffer capacity for acidic agents and relatively low in the case of basic solutions. The separation of the fractions in the clearing processes were performed by subsequent agitation and sedimentation following the specificity of the sedimentation process over time of the fractions of the dispersed system. A total of seven fractions were separated. Acid-base titrations allow to evaluate the resistance capacity of the underwater sediment to the action of aggressive agents of acidic or basic nature. Knowing the laws of acid-base influence on underwater sediments allows the creation of stability conditions in the aquatic environment. Carrying out the clearing of water basins makes it possible to use underwater sediments as a material to strengthen the durability of soils against erosion and improve the physico-chemical and mechanical properties of soils. The phenomenon of cetyltrimethylammonium adsorption on underwater sediment particles demonstrates that the highest adsorption value has the fine fraction. The decrease of this characteristic is observed in the case of fractions with medium and coarse dispersion. The study of underwater sediments with modern physico-chemical methods allowed the identification in them of a series of minerals (silicates, alumosilicates, carbonates and others) characteristic of the soil in the area, their quantitative assessment and their role in nature, and the prospect of using their specific properties. The determination of the structural-sorbational characteristics and the surface chemistry of solid particles in underwater sediments prove the possibility of obtaining new filter materials and allow the development of original methods for purification of natural and wastewater, and the evaluation of acid-base durability and adsorbent properties of sludge develop soil fortification procedures against erosion processes.

Asknowledgement: This work is a part of the Moldovan State Program (2020-2023) “Study and management of pollution sources to develop recommendations for implementing measures to mitigate the negative impact on environment and human health”, Project number: 20.80009.7007.20.

ASSESSMENT OF THE HISTORY OF POP POLLUTION IN LAKE IACOB, DANUBE DELTA, BASED ON RADIONUCLIDE-DATED SEDIMENTS

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The aim of this work is to assess the history of POP pollution in Lake Iacob from Danube Delta using sediments dated with the ^{210}Pb and ^{137}Cs radionuclides. The amount of 16 Polycyclic aromatic hydrocarbons (PAHs), 20 Organochlorine Pesticide (OCP), and 5 Polychlorinated biphenyl (PCB), were determined in each dated sediment layer by gas chromatography (GC) coupled with mass spectrometry for PAHs and electron capture detector for OCP and PCB. Prior GC analysis the target compounds were isolated from the sediment matrices by ultrasound assisted extraction subsequent by extract purification by open column chromatography.

The ages of the sediment layer were determined using alpha and gamma spectrometry and by measuring the amount of ^{137}Cs and application of the ^{210}Pb dating method for the entire sediment column.

PAH diagnostic ratios, HCH isomer ration, and sum of DDT and Chlordane metabolites were used as a tool for identification and assessment of the pollution emission sources.

The results of the study showed that the POP concentrations detected in sediment samples ranged from 73.81 to 214.54 ng g^{-1} for PAH, 71.78 to 192.69 ng g^{-1} for OCP, and 49.4 to 162.3 ng g^{-1} for PCB, being well correlated with the Danube River flow rate.

As conclusion, the analysis of POP residue in sediments is a suitable method to estimate the pollution history of surface water sources.

Key words: Historical pollution, Iacob Lake, Danube Delta, Polycyclic aromatic hydrocarbon (PAH), Organochlorine Pesticide (OCP), Polychlorinated biphenyl (PCB), radionuclides dated sediment

UTILIZATION OF NANOMATERIALS BASED ON CARBON NANOTUBES FOR TARTRAZINE REMOVAL FROM WATER. ISOTHERMS AND KINETIC STUDIES

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Nowadays, many industries use dyes in various processes and the resulting wastewater is a major source of environmental pollution. A part of these dyes are resistant to degradation and due to their toxicity are harmful to humans and to aquatic organisms. Tartrazine is an anionic dye that is commonly used, as coloring agent, in a variety of foods. This is also used to color capsules used in medicines, cosmetics, vitamins and syrups. In order to reduce its impact on the environment, different treatment methods are used (*e.g.* adsorption, coagulation, flocculation, ozonation, photocatalysis). Among the methods used to retain dyes, it was found that adsorption is the most efficient and with promising results. In addition, adsorption is considered an attractive process because it involves easy operation and simplicity in process. Various materials have been tested for removal of dyes from wastewater, the most widely used being activated carbon. Recently, nanomaterials have emerged as a strong competitor of conventional adsorbent materials due to their unique properties, such as large surface / volume ratio, chemical stability etc. The application of nanomaterials based on carbon, such as carbon nanotubes (CNT), for the adsorption of dyes from wastewater is one of the new trends in this field. CNT are characterized by high adsorption surface and relatively easy attachment of functional groups that give them interesting adsorption properties.

The present investigations concern the application of magnetic nanocomposites CNT-COOH/Fe_3O_4 and CNT-COOH/Fe_3O_4/NiO as adsorbents for the removal of tartrazine, a hazardous dye, from aqueous solutions. In order to establish the conditions for optimal retention of tartrazine, the influence of some physico-chemical

parameters on the adsorption process was evaluated, such as: initial pH of the dye solution, temperature, adsorbent dose, contact time and the initial concentration of dye. The best degree of removal of tartrazine was obtained with CNT-COOH/Fe_3O_4/NiO.

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IDENTIFICATION AND MEASUREMENTS OF ORGANOCHLORINE COMPOUNDS IN DANUBE DELTA

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Persistent organic pollutants (POPs) are complex organic substances that have toxic properties, are resistant to degradation, accumulate in the environment, are transported by air, water and migratory species across international borders and are stored away from their place of origin. Exposure to persistent organic pollutants can cause serious health effects. Organochlorines (Ocs) are chlorinated compounds widely used as pesticides and are included in the category of persistent organic pollutants.

Some of the most toxic organochlorine compounds are polychlorinated biphenyls (PCBs), hexachlorocyclohexanes (HCH), aldrin, dildrine, dichloro-diphenyl-tetrachloroethane (DDT), heptachlor, etc. The main sources of pollution are agricultural practices, storage of polluted waste in landfills, companies that synthesize these compounds, or power energy installations and condensers containing contaminated oils. Many of the pesticides are considered disruptors of endocrine function in both humans and animals / birds. Although they have been phased out due to their harmful effects, many of these pesticides are still detected in the environment.

Concentrations of pesticides and other persistent organic substances are found in most water basins, rivers, seas and oceans. Depending on the 119entra-chemical properties, the contaminants that reach the aquatic environment either remain in the aqueous phase or reach the level of sediments. Thus, for hydrophobic compounds, determining their concentration in sediments describes the distribution of contamination much better than analyzing them in the water column. At sediment level, pesticide-mediated changes can adversely affect the functioning of the ecosystem if tolerant microorganisms cannot compensate for the loss of functionality associated with pesticide-sensitive microorganisms. Moreover, changes in microbial communities can affect the quality and quantity of resources available for aquatic food chains.

In Danube Delta, for the monitored sites, the concentrations of total organochlorine compounds varied between 0.282 $\mu g\ kg^{-1}$ and 46 $\mu g\ kg^{-1}$. Among the monitored chlorinated organic compounds, the highest concentrations were determined for the isomers of hexachlorocyclohexane (HCH) and polychlorinated biphenyls (PCBs). The relatively low values of PCBs in the collected samples from the Danube Delta may be due to the fact that these compounds have been used quite little in Eastern European countries.

In most lakes and sediments, the concentrations of HCH isomers were on average <0.2 $\mu g\ kg^{-1}$. In the Caraorman Basin, the concentration of γ-HCH (Lindane pesticide) was 8.79 $\mu g\ kg^{-1}$, while in Lake Crișan was detected β-HCH in a concentration of 35.58 $\mu g\ kg^{-1}$ and ε-HCH in a concentration of 1.99 $\mu g\ kg^{-1}$. PCB concentrations were on average <0.5 $\mu g\ kg^{-1}$, except for Lake Crișan where higher concentrations of PCB 101 (2.15 $\mu g\ kg^{-1}$), PCB 138 (2.10 $\mu g\ kg^{-1}$) and PCB 153 (2.80 $\mu g\ kg^{-1}$) were determined. Regarding the insecticide DDT (Dichloro-Diphenyl-Trichloroethane) and its degradation products, relatively low concentrations were determined in the sediment samples, between 0.1 $\mu g\ kg^{-1}$ and 0.78 $\mu g\ kg^{-1}$.

ENVIRONMENTAL RISK ASSESSMENT ASSOCIATE TO ORGANIC MICROPOLLUTANTS IN THE FINAL EFFLUENT OF URBAN WASTEWATER TREATMENT PLANTS

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Organic MicroPollutants (OMPs) include a wide number of chemicals belonging to different classes, e.g. pharmaceuticals, drugs of abuse and their metabolites, steroids and hormones, endocrine-disrupting compounds (Barbosa et al. 2016; Chiavola et al. 2019). Increasing attention has been dedicated to OMPs, as a source of a high risk for public health and environment (Rodriguez-Narvaez et al. 2017). OMPs are characterized by low environmental concentrations (about ng/L or μg/L), high toxicity, very low biodegradability, and resistance to degradation in conventional treatments (Patel et al. 2019). The scientific community established that one of the main sources of release to the environment are the wastewater treatment plants (WWTPs), which are not specifically designed and operated to remove OMPs (Di Marcantonio et al., 2020; Luo et al., 2019). As it has been done to address other environmental problems, it is compulsory to determine the maximum permissible concentration on the basis of the acceptable risk for ecosystem and human health, as recommended by the new European Regulation on minimum requirements for water reuse 2020/741/EU. However, one limitation of the present EU approach is the focus on priority substances and on the risk associated with individual substances (Escher et al. 2018). Mixture risk assessment represents a breakthrough compared to European Environmental Quality Standard (EQS) of the European Water Framework Directive for surface water, since it allows to take into account potential synergism or antagonism which may cause adverse effects. The present study aims to compare the different Risk assessment methods. Specifically, the methods proposed by the European medicine agency for individual substances and the method for mixture of substances defined by Backhaus et al (2012) were applied. Moreover, the impact of the dilution factor (D) estimation, related to the flow rate of the receiving water bodies compared to the flow rate effluents from the WWTPs, was also assessed. The methods were applied to the concentrations of 3 illicit drugs, 6 pharmaceuticals and caffeine detected in different full-scale WWTPs in central Italy. The study highlighted that the individual risk for the monitored OMPs was always acceptable and considered medium only for Carbamazepine. In case of mixture of compounds, the risk was medium for the class of pharmaceuticals and low for the illicit drugs.

PHYTOREMEDIATION OF Zn-LADEN WASTEWATER USING A CONSTRUCTED WETLAND TREATMENT SYSTEM

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The aim of the research is to verify constructed wetlands as a sustainable solution for metal-laden wastewater treatment and to discover particular parameters for purification of industrial wastewater with different chemical composition. As an eco-friendly and economical method, bioremediation using plant, phytoremediation, is a promising strategy for removing, accumulating, or decomposing contaminants from water, soil, or sludge. The goal of the paper is to test the ability of metal removal from highly polluted batch systems and wastewater by *Phragmites communis* and *Typha gracilis*.

Two experiments were carried out, firstly industrial wastewater was used. *Typha gracilis* and *Phragmites communis* were planted in two kinds of substrates. Half of the samples were planted in the combination of quartz sand and gravel. The second half of the samples grew in the ceramsite sand. The regular sampling of water (once per week) indicated a very quick removal of zinc ions from zinc-containing wastewater. Therefore, the model experiment followed the research. Samples of *Phragmites communis* were planted into the ceramsite and were watered by water containing zinc in concentrations ranging from 10 to 100 mg/L. Water was collected for analysis once per week. After four weeks, Zn concentration in all samples was below permissible pollution values for wastewater discharged from the selected industrial sector. After zinc removal from the water, all parts of the plant (root, leave, stem) and substrate were taken to analyze in order to gain information about the transfer and accumulation of zinc through the system. Inductively coupled plasma atomic emission spectroscopy as a suitable method for elements analyses of employed plants was used. Results have shown that *Phragmites communis* and *Typha gracilis* are suitable for zinc removal from wastewater.

ANTIBIOTIC POLLUTANTS DEGRADATION WITH PHOTOCATALYSTS BASED ON MODIFIED TiO_2. EFFECTS OF DOPANT, SURFACE AREA AND POROUS STRUCTURE

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Aim and methods: Recent studies evidenced that various ground and surface water sources contain antibiotics residues. These pollutants represent potential threats to the ecosystem due to bacterial resistance development even at low concentrations. Many studies were focused on the utilization of photocatalysis for water treatment due to the obtained successful results. TiO_2 is one of the best material used for these applications. The aim of this study was to obtain new photocatalysts based on modified TiO_2 in order to be used in degradation of different antibiotics from water. The effects of dopant (Au, Ag, Fe, C, P), surface area and porous structure of TiO_2 photocatalysts on antibiotic degradation were evidenced. In order to obtain TiO_2 photocatalysts with high surface area, this was dispersed on support (zeolite Y, hierarchical zolite Y, MCM-48, SBA-15) and to vary the porous structure, titanium dioxide was obtained by the sol-gel method in the presence of a surfactant (Brij 58) and co-surfactant (active carbon obtained from coffee with different phosphorus content). These materials based on TiO_2 were doped with Au, Ag, Fe and were used as photocatalysts in degradation of amoxicillin (AMX), gentamicin (GM), ciprofloxacin (CP) from aqueous solution.

Results: The antibiotics photodegradation was evaluated under UV (254 nm) and visible light (532 nm). The best degradation efficiency, D_{eff} (100%) of AMX was obtained for Au-TiO_2 supported on MCM-48 mesoporous silica. This result was explained by surface plasmonic effect of Au nanoparticles in interaction with TiO_2 (as anatase and rutile, evidenced by XRD and Raman). A similar effect (90% D_{eff}) was achieved, in visible light, for CP photodegradation with Ag-doped mesoporous TiO_2. Under similar conditions, in the presence of mesoporous TiO_2 with P activated carbon and Ag it was evidenced the absence of antibacterian activity after 5 hours of reaction, suggesting antibiotic degradation. For both, Au and Ag samples, XPS spectra revealed the existence of metal nanoparticles on active surface. A significant effect of mesoporous structure and high surface area on antibiotics degradation was evidenced for similar composition and reaction conditions. Thus, a higher D_{eff} value was obtained for hierarchical zeolite Y compared to zeolite Y. In the case of iron doping, a lower degree of amoxicillin (~40%) release was obtained for both types of zeolite, requiring an increase of iron concentration. For all these applications kinetic studies were performed. These were correlated with the optical, structural and textural properties. Photoluminescence results and measurements of antimicrobial activity revealed different mechanisms of reaction under UV and visible light irradiation.

Conclusions: The photocatalytic experiments confirmed the possibility of antibiotics degradation and total reduction of their antimicrobial activity in wastewater.

PHYSICO-CHEMICAL AND MICROBIOLOGICAL ASSESSMENT OF WATERS AND SEDIMENTS FROM DANUBE DELTA

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Aquatic ecosystems are critical components of the global environment. One of the most important issues that has not been elucidated in aquatic ecology concerns the long-term effect of climate change on the ecosystem stability. Due to the role it plays in aquatic ecosystems, understanding how microbial communities respond to climate change is a major challenge. Our investigations focused on the microbial diversity in water and sediments from Danube Delta, in relation with the spatial distribution and geochemistry.

The samples for this study were collected from 11 sites that cover all the important regions of the Danube Delta. The physico-chemical analysis performed for each site indicates the presence of reduced quantities of organochlorinated compounds in most of the analyzed samples. A high content of γ-HCH (Lindan insecticide), respectively the isomer β-HCH and PCB were measured in Caraorman and Crișan sampling points. Illumina MiSeq sequencing of 16S rRNA gene carried out on water and sediment samples highlighted variations of bacterial diversity with the type of habitat, location and geochemical characteristics.

The microbial community consists of several bacterial phylum, of which Firmicutes, Proteobacteria, Actinobacteria and Bacterioidetes are the most abundant. No seasonal variability was detected, the main community members in all samples being affiliated with the Firmicutes and Proteobacteria strains. However, in the cold season (October) it was observed an increase in the relative abundance of Firmicutes, from > 50% to > 60%. Patescibacteria (4.6%) and Tenericutes (25.8%) are present in relatively high abundance in one of the sampling points, being followed by Bacteroidetes and Proteobacteria with a higher relative abundance in other sites.

Associations between microbial diversity and pesticide content indicate the possibility of a link between community structure and the presence of organochlorine pesticides.

ASSESSMENT OF THE DEGREE OF POLLUTION OF SURFACE WATERS IN THE URBAN ECOSYSTEM BALTI WITH ORGANIC POLLUTANTS

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The analysis of the degree of pollution of aquatic objects in the Balti urban ecosystem after COD_{Cr} and COB_5 shows that according to the values of these indices (mg/l), on the first place after the degree of pollution is water r. Răut, str. Locomotivelor, bridge, COD_{Cr} (134.8), and BOD_5 (27.0). According to the values of both indices, the water quality class is (V) (highly polluted). Subsequently, the Orășenesc pond, city Bălți, COD_{Cr} (133.5) and BOD_5 (26.7), the quality class is (V) (highly polluted); on the third place is the Copaceanca river, a tributary of the Răut river, city Bălți, (route) COD_{Cr} (124.5), and BOD_5 (24.9), quality class (V) (highly polluted); follows the Hunters and Fishermen's Pond, city Bălți, COD_{Cr} (121.9) and BOD_5 (24.5), the water quality class is (V) (highly polluted), and the fifth place – Răut river, upstream (confluence with the Copaceanca tributary), city Bălți, COD_{Cr} (116.1) and BOD_5 (23.2), the water quality class is (V) (highly polluted). These data demonstrate the consistency of surface water pollution with light organic (BOD_5) and hard to degrade (COD_{Cr}) pollutants. For the first five aquatic objects, the quality class according to both indices demonstrates a very high degree of pollution of aquatic objects (class V).

Subsequently, the consequence of reducing the degree of pollution is: after COD_{Cr} water r. Răut, downstream biological treatment plant (BTP) Bălți, COD_{Cr} (87.4), (water quality class is (IV), polluted) and after BOD_5 (11.4), is class (V) (highly polluted). According to COD_{Cr} (80,2), the river Răut, upstream of BTP, Bălți, the quality class is (IV), polluted, and after BOD_5 (10,8) the quality class is (V), very polluted. For r. Răut, Dobruja tributary, Sorocii street, bridge, town, Bălți, COD_{Cr} (77.4), the quality class is (IV), and for BOD_5 (17.5), the third quality class. For water r Răuțel (entrance to Bălți), COD_{Cr} (73.5), quality class is (IV), polluted, and BOD_5 (14.7), quality class is (V), very polluted. Downstream BTP, Floresti, COD_{Cr} constitutes (36.0), class (IV) quality (polluted), and BOD_5 for the same water is (7.9), class a (V) quality (highly polluted). Răut, upstream BTP, Floresti, COD_{Cr} is of (32.9) quality class (IV) (polluted), and BOD_5 (7.6), quality class (V), very polluted. Is established, for water r. Flămânda, the tributary r. Răut, town Bălți, COD_{Cr} is less than 30 mgO_2/l, class (III) quality, and for BOD_5 (1,2), mgO_2 / l, class (I) quality (clean water).

The experimental results indicate a high degree of surface water pollution for virtually all aquatic objects located in the Balti urban ecosystem. The high degree of water pollution is caused by the operation of industrial enterprises and anthropogenic household activities. For the waters of the Răut River outside the urban ecosystems of Bălți and Floresti, the main sources of pollution are inadequately treated water at BTP Balti and Floresti.

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CONTRIBUTIONS TO THE ENVIRONMENTAL IMPACT OF THE WASTEWATER TREATED AT BIOLOGICAL PURIFICATION PLANTS

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It is established that the environmental impact caused by purified wastewater at wastewater treatment plants (WWTP) is determined by several factors: the performance of purification plants, the volume and degree of wastewater pollution, the specificity of the pollutants removed and the purification capacity WWTP. The highest degree of wastewater treatment is achieved at the leachate treatment station generated at the landfill in the commune of Bubueci at the Corporation "Regia Autosalubritate", 205/2, Uzinelor Street, Chisinau. This is explained by the fact, that reverse osmosis is used in the installation. This fact ensures a high degree of purification for pollutants (chlorine ions and sulfates), which by the biological method of purification, their removal is only about 10% of their amount.

A high level of environmental pollution is caused by wastewater from M.I. „Vinăria Bardar" Corporation, and treated at the local purification station, which do not meet the requirements of GD 950/2013, Annex 1. Exceedances for COD_{Cr}, are 1.61 times, for the first case and 1.04 times for the second case. For BOD_5 the overruns are 2.54 times, and 1.82 times, respectively for the first and second case. This is explained by the degree of inadequate treatment of wastewater. The characteristic of the water from the "Negară Vasile" pond, according to the requirements of GD no. 890, water refers to the quality of class 2, by the content of nitrate and chloride nitrogen – to quality class 1, by the sulfate content – to class V, total iron – to class IV and by the content of zinc refers to the quality of class III.

An essential impact on the Chisinau treatment plant is caused by JSC "JLC" Lactate, Chisinau. According to HG-950/2013, Annex 1, practically, after all the pollutants from the wastewater discharged into the sewerage, the admissible limit values are exceeded. Exceedances are: COD_{Cr}: 6.9 times; 3.7; 4.1; 33.9 and 5.7 times. For BOD_5: 7.7 times; 4.4; 4.8; 36.4 and 6.1 times, and for chlorides, these are: 1.7 times; 1.3 and 1.1 times. In total phosphorus, the exceedances represent: 2.1 times; 1.2; 1.4; 4.4 and 3.0 times; and for fats, they are: 4.7 times; 11.0; 17.7; 9.5; 12.6; 3.2 and 1.5 times.

Key words: plant performance – leaching – specific pollutants- reverse osmosis – determining factors-pollutant load

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EVALUATION OF THE IMPACT OF THE BIOLOGICAL WASTEWATER TREATMENT PLANT IN FLORESTI ON THE WATER OF THE RĂUT RIVER

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It was established that the exceedances (ratio) of the concentrations of the indices in the downstream Biological treatment plant (BTP) / upstream of BTP occur practically for all the pollutants analyzed, especially for NH_4^+ 7.05 times (28.02.2017), biological oxygen consumption (BOD_5) – 4.22 times (28.02.2017), chemical oxygen consumption COD-Cr – 4.77 (03.09.2019) times. Report of the concentrations of the analyzed indices from the waters, exit from the BTP/ norms established by GD 950 of 25.11.2013, (Annex 2, regarding the requirements for collection, treatment and discharge of wastewater in the sewerage system and / or in water bodies .for urban and rural localities), for the analyzed pollutants took place, for (times): suspended substances in the range 1.16 – 1.77 times; COD-Cr, overruns are 2.36 – 4.77; for BOD_5, they are in the range of 1.46 – 2.40; for NH_4^+, the ratio value is in the range of 2.13 – 10.64 times.

The largest exceedances, as for the ratio of the concentrations of the indices in the downstream BTP / upstream BTP waters, as well as for the ratio of exit from BTP / GD 950 of 25.11.2013, norms, (Annex 2), in the first place are the exceedances for NH_4^+, followed by the exceedances for BOD_5, COD-Cr and suspended substances.

These results confirm that the treated water at BTP Floresti, as in the cases of urban ecosystems Chisinau, Orhei, Telenesti, Balti, is one of the essential sources of surface water pollution.

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PLANKTONIC ALGAE OF THE RIVER RĂUT WITHIN THE LIMITS OF THE BĂLȚI URBAN ECOSYSTEM

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The ecological problems of the urban ecosystem require a complex study to highlight the paths of evolution in the global aspect. The floristic study of urban ecosystems at the current stage of development of human society determined by the urbanization process, which has intensified since the second half of the 20th century.

The terrestrial and aquatic vegetation within the urban ecosystems is subject to a pronounced anthropogenic impact. The taxonomic structure of the flora in these ecosystems differs significantly from the flora outside the urban ecosystem, and the indicator species signal an increased degree of environmental pollution and eutrophication. The data of the study of the chemical composition of the water from the rivers that cross the Bălți urban ecosystem are characterized by increased indices of mineralization and pollution with different compounds that hit the aquatic environment through wastewater from different enterprises.

Algae have the role of capturing compounds and including them in the biogenic circuit. Some species have adapted to a higher degree of pollution, and others are disappearing from planktonic communities. The study indicates the presence of a small number of species in the studied sector of the river and among the detected species we identified 17 species of indicator diatoms algae in relation to different factors: environmental pH, salinity, trophicity, saprobity, etc.

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APPLICATION OF CHITOSANE MODIFIED (O-OXIDATION), IN ADSORPTION OF ORANGE 7 COLORANT

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In this study, the composite of chitosan modified (Oxidation) for the elimination of orange from aqueous solutions.

In order to clarify the adsorption process, batch experiments were carried out to study the effect of the operating parameters on the adsorption process such as: the dose of adsorbent (0.5-2 g/L), the initial concentration in orange (5-100 mg/L), and the temperature (25-45°C) were studied. To describe the adsorption equilibrium, the experimental data were analyzed by the Langmuir isotherm and the Freundlich isotherm. The equilibrium is perfectly described by the Freundlich model, the correlation coefficient of which is greater than 0.99. Thermodynamic parameters such as Gibbs free energy (ΔG^0), enthalpy (ΔH^0) and entropy (ΔS^0) were also evaluated and they showed that the adsorption process was spontaneously feasible and endothermic in nature. The results of the present study show that this composite can be advantageously used as a low-cost biosorbent for the removal of orange 2 from water and wastewater.

Keywords: Adsorption, Orange 2, Biosorbent Chitosan Oxidation

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DYES DEPOLLUTION OF WATER USING PdO-ZnO PHOTOCATALYSTS

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The objective of the study was to investigate the effect of ZnO powder partially coated with a nanometric layer of PdO on the treatment of water contaminated with dyes. In this approach, we successfully synthesized PdO coated ZnO, and tested it on the degradation of basic yellow 28 and malachite, under UV-visible irradiation. The prepared samples were characterized by TG-DTA analysis, X-ray diffraction with Rietveld refinement, and scanning electron microscope coupled with EDX analysis. The XRD measurement revealed that all prepared photocatalysts have a hexagonal ZnO structure, the average particle size is about 32 nm. The EDX analysis confirmed palladium presence in the prepared materials with very good dispersion and homogeneity. The results prove that the partial coating with PdO enhances the photocatalytic activity of ZnO, with almost complete degradation of dyes after 2 h of irradiation. The simple and easy product synthesis, and the remarkable properties allow the partial coating with PdO to be considered as a very promising and innovative material to increase the photocatalytic activity.

THE EVALUATION OF REDOX SELF-PURIFICATION PROCESSES OF SOME NATURAL WATERS

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This paper presents the results of the self-purification processes supervision of some natural waters supported by H_2O_2 and OH radicals, from the period of the year 2021. The monitored objects were Dniester river and its tributaries Raut and Ichel, at the confluence with the river, as well as two accumulation lakes located in the Dniester river basin, Ghidighici and Danceni.

Field measurements revealed good saturation of water with dissolved oxygen, but have highlighted the absence of hydrogen peroxide in suitable concentrations for hydrobionts from the supervised waters.

For the Dniester river it has been established that the dynamic equilibrium between the oxidative equivalent (H_2O_2) and the reducing substances susceptible to the action of this oxidant has been moved to the reducing equivalents. The evolution of the H_2O_2 flow and peroxidase reducers (Red) shows that the period of unstable redox waters state (when in the waters was not found the dominance of either H_2O_2 or peroxidase reducers) registered in the spring and summer seasons, is followed by the establishment of the reducing kinetic redox state in the autumn season, when the peroxidase equivalents prevailed in the waters. At the same time, it should be noted that the reducers content in the monitored waters was not high (0.60-3.10 μg/L). The absence of oxidant amounts within the limits determined as physiologically normal have led to the formation and maintenance of a biologically unfavorable state for the hydrobionts of this natural ecosystem. A similar situation for the flows of H_2O_2 and peroxidase reducers has been identified for the Ghidighici lake waters. The measurement datas confirmed that in the ecosystems of the Dniester tributaries (Răut and Ichel) and of the Dănceni lake there was a permanent consumption of H_2O_2 above the limits of the content resulting from the oxidant formation processes. As a result, also in these waters were lacking the optimal redox conditions for the hydrobionts development.

The amounts of the effective constant of the process of radical chain breaking in the processes involving OH radicals ($\Sigma k_{i,OH}[S_{i,OH}]$) demonstrate that radical self-purification processes have taken place at approximately the same level in the all monitored waters ($\sim 10^5$ s^{-1}). Also, the same amounts highlight the fact that the waters of the Ichel river and Danceni lake are the most polluted with substances which interrupt the self-purification process with OH radicals.

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ALLUVIUM RUNOFF IN TRANSBOUNDARY RIVERS IN THE REPUBLIC OF MOLDOVA

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The actions of erosion caused by precipitation, the alternation between frost and thaw as well as liquid runoff in the receiving basin on the slopes and riverbeds lead to the existence of a significant amount of solid material that is transported by water from the source to the discharge.

The Dniester and Prut rivers are cross-border rivers and are also the largest in the territory of the Republic of Moldova. The volume of alluvium runoff and its variability are determined by several factors, which are discussed below.

The maximum amount of alluvium in the Dniester transports it during the high spring waters (48–50%) and rainstorms (35–45%). In rainy springs, during the high spring waters, 70–90% of the annual volume of alluvium passes through rivers. In dry years the flow of the summer period is about 40% of the annual one.

The alluvium runoff in the Dniester River is regulated by 2 hydroelectric power plants, CHE Novodnestrovsk and CHE Dubasari. They play a major role in the distribution of alluvium in the Dniester River. Thus, for the hydrological post (ph) Hrușca we can speak of 2 periods of observations 1969–1980 and 1981–2019.

Until the construction of CHE Novodnestrovsk, at the entrance to the country, at pH Hrușca the average multiannual alluvial flow was equal to 236 kg/s and had a leakage of 7342 thousand tons. In the second observation period, 1981–2019, the transport of alluvium decreased considerably and amounted to 19 kg/s, and the average leakage was reduced by about 90% and is equal to 806 thousand tons. Currently, the amount of alluvium transported downstream of the dam on the Dniester River is much lower, so the risk of clogging the lakes in the basin has been significantly reduced. The alluvium that is collected from the territory of the Republic of Moldova and transported to the mouth of the Dniester, is retained by the dam of the Dubasari reservoir. Downstream of the lake, the alluvium accumulated over a distance of 275 km, is measured at pH Olănești. Thus, the average multiannual alluvium flow increases and is 19 kg/s. The construction of all dams on the Dniester had a significant effect on the transport of alluvium downstream to the mouth.

The maximum amount of alluvium the Prut transports during the high spring waters (48–50%) and the storm floods (35–45%). In rainy springs, during the high spring waters, 70-90% of the annual volume of alluvium passes through the river. In dry years the flow of the summer period is about 40% of the annual one. Alluvium runoff in the Prut River was assessed based on data from the monitoring network of the State Hydrometeorological Service of the Republic of Moldova at 2 hydrological stations: Şirăuți (located on the border with Ukraine) and the city of Ungheni. Very high turbidity is observed during the passage of intensive rainstorms. An example is the flood of June 1965, when the degree of saturation with alluvium in suspension in the town. Ungheni was 12000g/m^3. The concentration of suspended alluvium increases from the source to the mouth of the river.

ADSORPTION OF PYRIDOXINE FROM AQUEOUS SOLUTIONS USING CARBON ADORBENTS

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Water pollution is one of the most pressing environmental problems in the world and requires drastic and urgent solutions. Pharmaceuticals are a special category of contaminants that are widely consumed in many aspects of life and are increasingly discovered in the environment, greatly affecting the quality of life. Currently, traditional water treatment systems do not offer adequate solutions for pharmaceutical drug elimination and there still isn`t a regulated criterion for their limitation in water. Obviously, it is imperative to develop and implement effective methods to eliminate this category of pollutants. Adsorption is one of the most effective and practical techniques for removing pollutants from water. The use of carbon adsorbents in treatment technologies is justified by the fact that activated carbon is able to remove a very wide spectrum of pollutants, almost entirely.

In this paper we studied the adsorption parameters of vitamin B$_6$ (Pyridoxine, $C_8H_{11}NO_3$, MM 169.18) on three samples of activated carbon (AC-C, obtained from apricot kernels; CAN-8, obtained from walnut shells; Granucol FA, commercial carbon adsorbent). The effects of initial Pyridoxine concentrations, contact time, structural parameters of coals on the adsorption process were experimentally investigated. The adsorption kinetic curves were determined for three values of concentration (0.25 mmol/l, 0.5 mmol/l and 1.0 mmol/l) in a time interval between 10-300 minutes at 25^{0}C. The obtained data indicate that the degree of vitamin B$_6$ immobilization on investigated activated carbon samples grows with increasing contact time between the two phases and depends on the initial concentration of Pyridoxine. The percentage of vitamin B$_6$ removal decreases with increasing initial concentration, although the actual amount of Pyridoxine adsorbed per unit mass of adsorbent increased. It was observed a rapid adsorption of vitamin B$_6$ during the initial stage of the adsorption process, followed by a gradual process. The equilibrium of the adsorption process between vitamin B6 solution and carbon adsorbent surface was achieved in 300 minutes.

The effect of initial vitamin B_6 concentration on the adsorption capacity of the researched coals was studied in the range of 0.25-2.5 mmol/l. The adsorption isotherms of vitamin B_6 on AC-C, CAN-8 and Granucol FA coals were determined after establishing the equilibrium of the adsorption process (contact-stirring time – 300 minutes) at a temperature of 25^0C. The highest value of maximum adsorption (***a_m***) of vitamin B_6 has been registered for autochthonous activated carbon AC-C (1.59 mmol/g), followed by an intermediate value for the CAN-8 sample (0.96 mmol/g). The lowest immobilization capacity of vitamin B_6 was determined in the case of commercially activated carbon Granucol FA (0.74 mmol/g). The obtained results are in accordance with the structural parameters of the researched coals, with an obvious advantage of the autochthonous activated carbon AC-C, which has double value of ***a_m*** compared to the commercial coal sample Granucol FA. The realized research shows that pharmaceuticals such as vitamin B_6 can be effectively removed from aqueous solutions using autochthonous activated carbon AC-C and CAN-8 as economic adsorbents.

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WASTEWATER TREATMENT OF EFFLUENTS CONTAINING ERIOCHROME BLACK T USING AN UV REACTOR. EXPERIMENTAL, MODELLING AND OPTIMIZATION

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In this work, the discoloration of azo pigment Eriochrome Black T (EBT) was analysed using a complete methodology consisting of: i) a hydrodynamic study of the photochemical reactor employed for discoloration; ii) experimental analysis of the efficiency based on Design of Experiments (DOE) approach; iii) efficiency modelling using Response Surface Method (RSM); iv) process optimization based on RSM and Harris Hawk Optimization (HHO) algorithm.

The reactor has a UV-C lamp protected by a quartz tube and was analysed using the tracer method. The Residence Time Distribution (RTD) technique employed used as tracer a sodium chloride solution of 10% mass concentration. The response was registered with a WTW conductivity meter Cond 315i. The classic RTD functions, namely: residence time distribution I, cumulative residence time distribution (F), internal age distribution (I) and intensity function (λ) were plotted as function of dimensionless time (θ), in normalized form. Also, the first, the second, the third and the fourth moments of residence time distribution, usually known as the mean residence time ($\tau = 14.15$), the variance of distributions ($\sigma = 5.81$), the skewness ($s = 6.53$) respectively kurtosis ($k = 4.08$) were determined for debit of 28.99 mL/s. The obtained results indicated the presence of flow short-circuits and dead-zones.

The next step of the applied methodology considered in an experimental study regarding the EBT discoloration based on hv/TiO_2. To this mean, the DOE strategy was applied taking into account the following parameters: the amount of photocatalyst (Z1, g/mL), the contact time (Z2, min) and the initial concentration of the dye (Z3, mg/L).

Based on the experimental data previously obtained and the RSM based approach, the regression equation of the process was determined in Minitab software (Eq. 1). The variance of the model was 97.76%, indicating a good agreement between experimental and predicted.

$$Y = 6.41 + 17.92*Z1 + 0.0314*Z2 – 0.763*Z3 – 7.41*Z1*Z1 + 0.000003*Z2*Z2 + 0.00661*Z3*Z3 + 0.00325*Z1*Z2 + 0.0029*Z1*Z3 – 0.000338*Z2*Z3 \quad \text{(Eq.1)}$$

The last step consisted in the application of a process optimization procedure. In this case, two distinct strategies were applied: i) the RSM approach from the Minitab software and ii) the HHO algorithm (a bio-inspired metaheuristic that simulates the cooperative behaviour and chasing style of Harris' hawks). The results showed that through optimization, the process efficiency was raised from 75.35% to 98.37%, indicating the capacity of the applied methodology to improve the process without the need for additional resources.

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POLLUTION OF LAKE LADOGA ECOSYSTEMS BY ORGANOMETALLIC COMPONENTS OF OILS AND PETROLEUM PRODUCTS

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The ingress of oil, petroleum products and wastewater, as well as toxicants by aerogenic means, discharges of industrial enterprises – this is an incomplete list of ways for pollutants to enter the hydrosphere. As a result, chains of complex transformational, in some cases reversible, processes are launched, which have a significant impact on the content of organometallic compounds and heavy metals both directly in water and in biota [1].

Studies have shown that the Volkhov River is polluted with petroleum products from various sources in the cities of Kirishi, V. Novgorod, Volkhov with their removal to the waters of Lake Ladoga [2]. Oil and petroleum products tend to accumulate in bottom sediments and have a highly toxic effect on the ichthyofauna in early ontogenesis. Oil and petroleum products as sources of organometallic compounds have a particularly strong effect on benthic organisms, and in case of salvo intake – on fish grown by industrial methods.

The migration of various forms of chemical ingredients in the biosphere organisms is a very complex system of many interconnected and to varying degrees closed cycles of elements in individual aquatic ecosystems. Ultimately, intra-aquatic relationships are reduced to the exchange of elements between organisms and the environment. In general, the differences in the biogeochemical cycle of trace elements are due to their concentration in the components of hydroecosystems, which occur in a certain ecotoxicological setting.

Heavy metals as priority toxic substances have a high ability to actively penetrate into the most diverse substances of hydroecosystems: they are found in large quantities in water, soils, internal organs and bones of fish, and their parasites, other aquatic invertebrates, as well as plants [3]. Quantitative indicators of the occurrence and accumulation of metals in the waters and hydrobionts of Lake Ladoga are subject to large fluctuations. The degree of their concentration in the organs and tissues of fish and in the external environment is usually higher near the entry of industrial wastewater into the reservoir. Almost everywhere, a number of heavy metals are found in water, sediments and various organs and tissues of fish in quantities exceeding permissible standards.

Due to exposure to dangerous toxic substances, the fish of Lake Ladoga are severely intoxicated at different stages of ontogenesis, which affects the vital activity of the body. In fish, toxicoses of varying severity, the appearance of neoplasms are recorded. With deep lesions of the vital systems of the body of fish, in some cases their death occurs.

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TECHNO-ECONOMIC ASSESSMENT OF ELECTROCHEMICAL PROCESS FOR SUSTAINABLE REMOVAL OF METHYLENE BLUE

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Methylene blue (MB) is one of the most common organic dyes that contaminates textile wastewater. Since it has many adverse effects on human health when exposed at higher doses than recommended limits, MB in effluents must be treated prior to discharge. In this study, the removal of MB from water using electrochemical reactor with flexible graphite electrodes which are low cost, high conductive and stable material as electrode was studied extensively. The effects of operating conditions such as initial concentration of MB, initial solution pH, electrolyte dose, electrical potential, and operating time were investigated to determine optimum conditions. Box-Behnken experimental design (BBD) was performed to optimize the performance of the system with the minimum number of experiments, and to assess influence of the variables on removal efficiency, energy consumption, operating cost and effluent MB concentration. There was a significantly positive effect of electrical potential and electrolyte concentration on MB removal efficiency. In addition, MB removal efficiency increased with the increasing operating time while the MB removal efficiency decreased with increasing initial MB concentration and initial pH. The combined effects of operating time-electrical potential and electrical potential-electrolyte concentration have a positive effect on MB removal efficiency, while the other combined interaction of operating variables didn't have a considerable effect on removal efficiency. The highest removal efficiency and lowest operating cost were found to be 99.9% and 0.012 $\$$ m^{-3} when operating time of 30 min, initial pH of 4, initial MB concentration of 26.5 mg L^{-1}, electrolyte concentration of 0.6 g L^{-1}, and electrical potential of 3V. As a result, process outputs can be predicted thanks to the mathematical model by BBD without experiments, which provides a promising convenience for applicability in real textile wastewater containing methylene blue.

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Session C

CLIMATE CHANGE
AND
ATMOSPHERIC CHEMISTRY

ON THE TRANSITION TO GREEN AVIATION

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With the growth of cities and the increase in the number of air transportation, the problem of reducing harmful emissions into the atmosphere, reducing noise and vibrations is becoming more and more urgent. Greenhouse gas emissions are a huge problem for all transportation systems, including aviation. Most aviation emissions occur at high altitudes, generating greenhouse gases and, as a result, contributing to climate change. According to estimates, greenhouse gas emissions increase by 1.4% annually and CO_2 by 1.8%. Moreover, more than half of these emissions are accounted for by the combustion of fossil fuels.

In addition to the detrimental effect on the climate, traditional aviation has a strong effect on the quality of the ambient air, which is fraught with various lung diseases among the population of the Planet. The main air pollutant from aircraft flights is NO_x. To solve the problem of emissions, the principles of «green aviation» have been developed, which are based on optimization of flight schedules, changes in the design of aircraft, the use of lightweight composite materials, changes in the principle of operation and in the design of the engine and the fuel used.

IEE RAS adheres to the principles of «green aviation» and is working in this direction. Over the past few years, we have developed a number of powerful switching voltage converters as a part of power plants for electric and hybrid aircrafts, in particular, for charging batteries aboard the airplane. Thanks to the use of modern solid-state electronic components and an ergonomic design, we have managed to achieve a power-to-weight ratio from units to ten kW/kg [1, 2]. In the field of low-temperature plasma physics, our Institute is working at gas electrodynamic flow control systems for aircraft [3, 4], which is of the primary importance for increasing aerodynamic and energy efficiency, thus solving the environmental problem of reducing emissions of carbon and nitrogen oxides and significant fuel economy.

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NEUTRON ACTIVATION ANALYSIS IN THE ECOLOGICAL STUDIES: MOLDOVA CASE STUDY

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Neutron activation analysis is a high sensitive analytical technique used in the environmental studies for the determination elements in a wide range of concentrations. The principle of instrumental neutron activation analysis is discussed and the advantages of this technique in analysis of environmental objects are shown. Examples of research performed on the radioanalytical complex REGATA at the IBR-2 reactor (Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Dubna) in collaboration with scientific institutions from the Republic of Moldova will be summarized. The presentation will be focused on moss biomonitoring studies performed in 2015/2015 and 2020/2020, wastewater treatment procedure, nanotoxicology and assessment of the quality of agricultural products.

ANALYSIS OF NO_2 AIR POLLUTION: CASE OF UKRAINE

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Atmospheric air is the most important life-sustaining natural environment representing the mix of gases and aerosols of the surface layer formed during the Earth and human activity evolution. The international and Ukrainian research results showed that atmosphere pollution is the most powerful factor that constantly affects the environment. The World Health Organization considers the air pollution as one of the main risk factors for human health. By reducing the air pollution level, such diseases as stroke, acute respiratory and heart attack can be avoided. The main pollutants include solid dust particles (PM_{10} and $PM_{2.5}$), nitrogen dioxide (NO_2) and sulfur dioxide (SO_2), hydrocarbons (CnHm), aldehydes (RCHO), carbon monoxide (CO), heavy metals (As, Cd, Ni, Hg), formaldehyde (CH_2O), dust undifferentiated in composition, benz (a) pyrene ($C_{20}H_{12}$) (WHO. Ambient air pollution).

Auto transport is one of the strongest air pollutant in many countries around the world, including Ukraine. Emissions of vehicles are dangerous because they are carried out in the immediate vicinity of sidewalks in the area of active pedestrian traffic (for cities and villages) and along highways (green areas of roads). The largest amount of toxic substances is released during variable modes of engine operation – in particular during start, stop and idling. Therefore, the maximum concentration of toxic substances in cities is observed at intersections and at traffic lights. About 50% of intra-city vehicle emissions are from low-speed roads and less than 25% from high-speed roads (Raza et al., 2018; Anenberg et al., 2019).

The state of air in Ukraine is constantly deteriorating, and has a negative impact on the citizen's health. The cars are the main source air pollutant emissions in Kyiev recent years. According to the latest research of the International Association of Automobile Manufacturers (April 2019), 947 million cars and 335 million commercial vehicles were operated worldwide in 2015 (European Vehicle Market Statistics, 2016). In 2018 in Ukraine were registered: 6 566 thousand cars, 250 thousand buses, about 840 thousand motor vehicles. The World Bank estimated that the number of cars will double by 2050 (Bank, 1017). Exhaust gas toxicity of gasoline engines is mainly due to the content CO and NO_2, but diesel engines – by NO_2 and soot. Impurities of NO_2 entering the atmosphere pose a serious danger to the environmental situation. They are caused acid rains and can be toxic substances that irritate the mucous membranes, affect the respiratory tract and lungs, change composition and reduce hemoglobin in the blood. To reduce the risks, it is necessary to limit the use of petrol and diesel cars within cities and to promote transition to the renewable energy sources.

The NO_2 concentration was studied based on AURA satellite data, obtained in *.txt format. First it was necessary to translate this data into *.img format in EEDAS Imagine space image processing software. The remote sensing data estimation consisted of several steps: 1) Creating a *.grd format file. It needs to be added 5 rows to the original file, which contained the values of columns and rows numbers. Also minimum and maximum coordinates in latitude and longitude. 2) Convert a file from *.grd to *.img format. The conversion was performed using the *Import* function of ERDAS Imagine. 3) Geometric correction of the obtained image, which is performed using the *Geometric Correction* function of the ERDAS Imagine, and is converted into a Geographic coordinate system in degrees. 4) Defining the contour of the Ukraine territory. Using the *Subset* function of the ERDAS Imagine Ukraine was selected in the space image using "Ukraine 500" vector data. After all AURA satellite data determination of NO_2 concentration was converted according to this approach. The average values for each year were estimated, as well as two periods – from January to March and from April to June.

The analysis of air quality monitoring was carried out based on the data collected from 21 pollution monitoring posts within Kyiv at the Boris Sreznevsky Central Geophysical Observatory (CGO). Ten air pollutants were analyzed: suspended solids, sulfur dioxide, carbon monoxide, nitrogen dioxide, nitrogen oxide, phenol, hydrogen fluoride, hydrogen chloride, ammonia, and formaldehyde. The assessment of air pollution was carried out by comparing with the corresponding maximum permissible concentrations (MPC) of substances in the air of cities. Analysis of air quality data for 2018 – 2020 showed the highest average of pollutants concentration in the multiplicity of MPC that is calculated for NO_2. According to the Resolution "On approval of maximum allowable emissions of pollutants standards (June 27, 2006 N 309), the NO_2 belongs to the IV class of danger substances. Further study demonstrated that NO_2 concentration exceed the MPC by 1.1 to 16 times in comparison to other impurities. Operational information of air pollutants concentration changes, such as NO_2, can be provided by satellite regional monitoring.

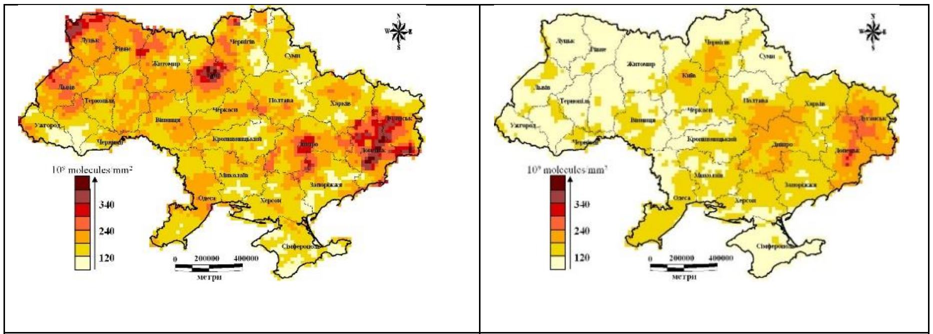
The remote sensing data analysis of NO_2 concentration distribution detected the annual average of CO_2 concentration for 2018 in 134.58 (10^9 molecules/mm^2), for 2019 – 157.51 (10^9 molecules/mm^2), for the six months of 2020 – 153, 27 (10^9 molecules/mm^2). The average values of NO_2 concentration for the first six months each of 2018, 2019 and 2020 were determined (table 1).

Table 1. The average of NO_2 concentration for January – May of 2018 – 2020

Year	Values, (10^9 molecules / mm^2)
2018	123.12
2019	144.15
2020	153.27

The difference in NO_2 concentration values was 21.03 (10^9 molecules/mm^2) in 2019 – 2018 and 9.12 (10^9 molecules/mm^2) in 2019 – 2020 (Lyalko et al., 2020). Thus, there is an increase of NO_2 concentration over the Ukraine, which is usually highest in cities due to the car gas burning.

The analysis of possible reducing of the air quality quantitative characteristics changes on a regional scale, was made on the example of pandemic quarantine restrictions established in 2020. According to the AURA satellite, the value of NO_2 concentration in the atmosphere was calculated for two periods: I period – from January to March, reflects the air quality before the quarantine restrictions; II period – from April to June, showing the air quality within the quarantine restrictions period (Fig. 1).



(a) – I period January – March, 2020

(b) – II period April – June, 2020

Figure 1 – Distribution of NO_2 concentration in Ukraine by AURA satellite data for I period (a) and II period (b) for 2020.

According to the NO_2 concentration spatial distribution in 2020, the following industrial regions with maximal air pollution were distinguished: Donetsk (Donetsk, Luhansk regions); Prydniprovsky (Dnipropetrovsk, Zaporizhzhya); Capital (Kyiv, Chernihiv region, Kyiv city). In spring 2020, the negative effects of forest fires and large dust storm were added (mixed) to usual smoke that was reflected in the first period of 2020, exceeding the MPC of NO_2 concentration by 1.2 – 1.5 times than in previous years. Figure 1 (b), which corresponds to the second period of 2020, showed a significant decrease of the nitrogen dioxide content over the entire Ukraine territory due to quarantine measures which led to a slowdown the economic activity.

Therefore, atmospheric monitoring can be assessed using remote sensing data. The estimation of NO_2 concentration by the spatial quantitative analysis during the pandemic period confirmed that gas pollution is mostly produced by human activities.

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POTENTIAL OF NEURAL NETWORKS FOR AIR QUALITY SENSOR DATA PROCESSING AND ANALYSIS

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Air quality sensors are an emerging new technology of the air quality monitoring. Their main advantage is that they are significantly cheaper monitoring device compared to standard monitoring equipment. Cheap, mass produced sensors have a potential to form much more dense monitoring networks and provide more detailed information about air the pollution distribution. The drawback of the sensor air pollution monitoring is the lower quality of measurements than standard monitoring equipment. Air pollution sensors measurements quality is known to be negatively influenced by meteorological factors, such as temperature or humidity. Neural networks are potentially valuable technique of the monitoring data processing, to transform sensor measurements complemented with meteorological data to more accurate estimations of pollutant concentrations.

Co-located measurements at the three monitoring sites in the Ostrava region in Czechia proved that although the PM_{10} and $PM_{2.5}$ measurements are relatively highly correlated (0.8-0.9) the measurements need to be adjusted because sensor measurements, based on location, under- or overestimate the particulate pollution. Neural network proved to be the method which can significantly raise the quality of measurements. The neural network postprocessing significantly raised precision of measurements as well as the correlation between professional monitoring station and sensor measurements (approx. to 0.95) which make cheap sensor data reaching sufficient quality for air quality monitoring.

AIR POLLUTION MODELING USING REGRESSION MODELS

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Air pollution dispersion modelling using standard Gaussian methodologies is a data-intensive process that requires extensive computing power, high-quality data, and human effort. Land Use Regression (LUR) is an appropriate alternative to standard modelling. LUR work with the presumes that air pollution concentration concludes from environmental factors. These factors are evaluated using spatial analysis and selected based on the ability to express air pollution variability. The main benefits of the LUR modelling are lower compute and data-intensive and substantial elimination of human factor. The significant drawback of LUR modeling is lower accuracy in comparison with Gaussian methodologies. The standard LUR models use linear regression equations for the estimation of air pollution concentrations. We presume that linear regression is not appropriate for describing nonlinear phenomena such as air pollution. Therefore, alternative LUR model was constructed, and linear regression equations were substituted by Artificial Neural Network (ANN)-based regression, which is appropriate to capture non-linear behavior of the phenomena. The presented study assesses two approaches:

1. Construction of the LUR model based on the linear regression using the Gaussian model results dataset or emission data dataset.

2. Construction of the LUR model based on the non-linear regression using the Gaussian model results dataset or emission data dataset.

The accuracy of the estimation was evaluated using the coefficient of determination (R2). LUR models constructed based on the linear regression reached 0.639 for emission data and 0.652 for Gaussian model results data. LUR models constructed based on the non-linear reached 0.937 for the LUR model based on emission data and 0.938 for the model based on Gaussian model results. The LUR model based on non-linear regression provides more accurate results.

ABSENCE OF SOLID PARTICLES GENERATED FROM THERMAL PROCESSES IN THE AEROSOL FROM AN ELECTRICALLY HEATED TOBACCO PRODUCT

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Heated Tobacco Products (HTP) were developed as better alternatives to cigarettes to avoid the release of thousands of chemicals formed when the tobacco is being burnt. One such HTP is the Electrically Heated Tobacco System (EHTS) (from Philip Morris International), in which the tobacco material in the Electrically Heated Tobacco Product (EHTP) is heated instead of being burnt. The significant reduction in emissions from EHTPs compared to combusted cigarettes have been extensively substantiated by independent research groups. The absence of solid particle emissions from the EHTP has also been confirmed in published research. As EHTPs have filter elements between the tobacco portion and the mouth-end, their role associated to the conclusion that no solid particles are formed during use has never been investigated to our knowledge. In this work, aerosol collected from the EHTP with and without filter elements during heating as well as without heating was studied to investigate whether solid particles were formed in any part of the product during use. Two different analytical methods were used and the results from both methods showed that no solid particles originating from thermal processes was present in the EHTP aerosol.

ASSESSING CLIMATE CHANGE IMPACT ON WATER QUALITY OF THE RIVER VOGHJI

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The natural factors influencing the water quality of water resources are theoretically considered to be stable. However, it is evident that the climate patterns of Earth are changing. Climate, as a potential indirect natural factor in the formation of the chemical composition of natural waters, not only leads to obvious hydrological changes but also inevitably leads to hydrochemical changes. The quality of drinking water sources may be compromised by increased sediment or nutrient inputs, as well as changing in mineral composition water.

Long-term observations were shown that precipitation and natural flow of Voghji river in the reference point were decreased by 18% in 2007-2020 compared with the 1961-1990 baseline period. At the same time, significant changes in the ratio of elements of the mineralization regime were observed in the river.

As a result, the nature of the water of the Voghji River gradually becomes strongly hydrocarbonate-sulfate-calcium: the difference in the concentrations of the main ions compared to the baseline period is 4.7-13.6%. If in the baseline period the ratio of calcium and total sodium and potassium concentrations was almost equal, then according to long-term observation data the increase in calcium and sodium, as well as a sharp decrease in potassium are recorded.

SPATIAL MAPPING OF NATIONAL EMISSIONS OF SHORT-LIVED CLIMATE POLLUTANTS IN REPUBLIC OF MOLDOVA

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The spatial distribution of the emission of short-lived climate pollutants (SLCP) is an important issue for the modelling of the air pollution and the assessment of the human exposure. The spatial emission mapping provides an information for policy makers in the decision process for the implementation of environmental policies and measures. The aim of this study is a development of the spatial emission mapping of SLCP using GIS approach based on the last national Informative Inventory Report of the Republic of Moldova for the period 1990 – 2019 years (2021 data (ceip.at) and created national database by the development of Nomenclature For Reporting (NFR) according to EMEP/EEA air pollutant emission inventory guidebook 2019 (https://www.eea.europa.eu/publications/emep-eea-guidebook-2019). The emission mapping supports a link between emission data and air quality models that need emissions information at a proper spatial, temporal, and sectoral resolution. It is also important to improve the linking of the air pollutant emission inventories in line with the UNECE Convention on Long-range Transboundary Air Pollution (CLRTAP) and the EU National Emission Ceilings Directive (NECD). Reported spatial emissions data are an input for models used to assess atmospheric concentrations and deposition, as the spatial location of emissions determines to a great extent their atmospheric dispersion patterns and impact area. The results of model assessments inform national and international policies used to improve the environment and human health (https://www.eea.europa.eu/publications/emep-eea-guidebook-2019/part-a-general-guidance-chapters/7-spatial-mapping-of-emissions/view). EMEP grid with the resolution $0{,}1^0 – 0{,}1^0$ of longitude-latitude in the WGS84 geographic coordinate system was used for the mapping SLCP. The respective maps were created for all principal emission sectors: energetic, transport, industry, agriculture, waste. All territory was divided into cells according to EMEP grid and proxy spatial datasets were created for diffuse pollution sources. QGIS free software was used for the data processing and creation of spatial models of emission for every pollutant. Different maps were created for the visualization of the obtained results. The principal point sources are also characterized on the respective maps. This study is a first result of the spatial modelling of SLCP pollution sources which can be used for the air modelling and the evaluation of hot spot in the Republic of Moldova for the decision-making process in the environmental sector. Further spatial analysis is required for the improvement of model precision and the reporting of the national air pollutant emission inventory.

Acknowledgement: The presented study was carried out within the National Project no. 20.80009.7007.20 “Study and management of pollution sources for the elaboration of recommendations for the implementation of measures to reduce the negative impact on the environment and the health of the population”.

THE SAMGAU PROJECT – THE GREEN TECHNOLOGY TO DELIVER THE CLEAN ATMOSPHERE (AIR) BY THE MEANS OF UNIQUE FEATURES OF EVERGREEN TIAN-SHAN SPRUCE

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The Samgau Project is fully consistent with the One Trillion Trees Global Initiative, announced at the World Economic Forum in Davos at the end of January 2020 and supported by leaders from all over the world. The Initiative is about planting of about 1 trillion trees worldwide until 2030, which by the expert’s analyses will have a significant impact on reducing CO_2 in the planet’s atmosphere. However, our analysis allows us to argue that the correct selection of plant species and their planting sites, in addition to the general task of neutralizing carbon dioxide emissions, will solve the more serious problem faced by many large cities, namely the catastrophic level of accumulation of smog and pollutants.

Unfortunately, historically due to the necessity of those times, the most cities are located in the foothills, in natural narrows, which impedes the process of convection of surface polluted air, which is a natural mechanism of air purification. Physically, the surface heating efficiency, and therefore the convection intensity, depends on two main parameters: the angle of incidence of solar radiation and the absorption efficiency of the surface (Albedo coefficient). The main territory of the formation of vertical convection process in cities is the territory that absorbs more light – dark roofs, roads, agricultural lands of the suburbs, a water mirror of the river, lakes, etc., which intensively absorb the sun during the summer period, warm themselves and the lower layers of the atmosphere that creates a powerful heat flow that can “break through” the blocking layer of smog and ventilate the city. In winter, the intensity of the low-level sun is much lower, the roofs and roads of the city are covered with snow, the sun’s rays are almost specularly reflected from the surrounding forests, slopes, etc., and the convection mechanism stops working.

An elegant, environmentally friendly and at the same time simple and obvious solution that does not require complicated technical decisions and financial investments is to increase the absorption capacity of urban slopes in the vicinity by planting a forest of evergreen trees. Based on the studies, it was concluded that the most suitable type of trees for these purposes, depending on the climatic and geographical features of the region, are conifers, namely various species of pines, spruce, etc., especially the unique Tian-Shan spruce which can easily raise in extreme environments and remain completely black in cross the cross section for the winter sun, which is low above the horizon, even in the snowiest winter, this is due to the fact that the spruce, with its millions of needles, absorbs almost all radiation, that is, it is absolutely the best absorber of light or a direct source of heating of ambient air.

A large spruce has a cross-sectional area of about 100 m^2, given that the density of the sun’s flux is about one kW / m^2, one spruce can generate a flow of 10-100 kW. Having an effective park / forest area of 10-100 km^2, we get the power of the “heat source” up to 100 GW. And if, based on the geographical location of the city, the wind rose, to plant a large forest in the right place (ideally on the southern and / or eastern, western slope of the narrows), it is possible to create a heat source with a capacity of about 100 GW, which will form a powerful upward air flow, destroying and preventing the ill-fated cloud of smog from forming!

THE RISK ASSESSMENT TO HUMANS AND THE BIOSPHERE FROM AIR POLLUTION NEAR SPRINGS

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Linden litter and snow cover accumulate large amounts of substances (including harmful ones), mainly coming from the atmospheric air. Therefore, both snow and litter can be indicators for an indirect assessment of the state of the air pollution level. Observations have shown that the concentration of pollutants in melt water and plant litter is several times higher than in the atmospheric air. Harmful components in the future can enter the upper soil layer, as well as groundwater and exert a negative effect.

The aim of our study was to monitor litter and snow cover near three springs (two in the city of Ivanovo and one in its satellite town – Kokhma).

In the motoring performed, the content of harmful impurities in the studied samples of melt water of the snow cover was controlled by standard methods of chemical and physicochemical analysis (potentiometric, titrimetric, photometric and atomic absorption) in accordance with the standards for the content of substances in water bodies for fishery purposes (TLVrh). Snow samples were taken at five points around each of these springs, as well as near the nearest highways. The pH value and the content of compounds Cu, Cr, Mn, Pb, Zn, Al, Co, Cd, Ni were also under control. In addition to melt water, the level of air pollution, samples of linden blossom and lime litter was also analyzed according to the list of 139entrali pollutants characteristic of the territories under consideration. Data on priority pollutants were obtained from the research paper by S.A. Buimova, A.G. Bubnov "Comprehensive assessment of the quality of spring water on the example of the Ivanovo region" (2012).

The data obtained from the studies of the snow cover showed that all the studied samples were characterized by an increased content of Cu_{gen}, Zn^{2+}, Pb^{2+} compounds. At the same time, in most cases, the presence of pollutants was higher in samples taken during the warm period of 2019. Based on the monitoring results, the risk from air pollution by Zn^{2+}, Mn^{2+} and Co^{2+} compounds for humans, plants and the biosphere as a whole under chronic exposure was assessed. The estimated values can be attributed to an unacceptable (high) degree of risk of atmospheric pollution.

THE TREND OF THE DYNAMICS OF THE MAIN CAUSES OF DEATH OF THE POPULATION IN THE NORTH DEVELOPMENT REGION

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The dependence of the general incidence of the population (especially after the diseases of the respiratory system) on the degree of environmental pollution (air emissions) in the given locality is demonstrated. Diseases of the cardiovascular system remain in second place, with an average value of 194.0 / 10,000 cases and constitute 7.3 percent of the total number. This group of diseases has an increasing character, from 173.0 / 10000 in the year 2010, to (239.0 / 10000 cases towards the year 2017.

The comparison of the average general prevalence on the regions of the republic indicates that the highest value, of the respective index, was registered in the North Development Region (NDR) with 7121.9 cases per 10 thousand inhabitants, followed by RD Gagauzia ATU (6969.4), on the 3rd place and 4 are placed Center DR (6954.8) and South DR with 6020.2 cases. In the structure of the general prevalence of the population in the RDN, it was established that according to the number of diseases, cardiovascular diseases are in the first place, followed by diseases: respiratory, digestive, endocrine and genitourinary diseases.

The dynamics of the general mortality of the population in the Northern Development Region is established. The reduction of deaths by districts takes place in the following order: Donduseni > Briceni > Rascani > Edinet > Drochia > Ocnita > Floresti > Soroca > Sangerei> mun. Balti > RDD Chisinau. Mortality by type of disease indicates that in the first place is the mortality of diseases of the circulatory system, two – mortality caused by malignant tumors, followed by deaths caused by diseases of the digestive system, trauma and poisoning and diseases of the respiratory system. But the analysis of the trends of the main causes of death of the population in the DRN in the period 2010-2020, indicates that from 4 causes of death: diseases of the cardiovascular system, digestive system, and causes of trauma and poisoning, and tumors, indicates that for the first 3 causes of death, they have a downward trend: for cardiovascular system diseases, the downward trend is 4.6%, digestive system diseases - 24.2%, trauma and poisoning – 45.7%, and only for tumors, it is a growth trend over the entire period of 2.2%.

Asknowledgement

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PRESENT AND FUTURE TRENDS IN PHYTOREMEDIATION OF URBAN PARTICULATE MATTER POLLUTION BY ROADSIDE VEGETATION

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One of the most dangerous pollutant created by traffic is particular matter – PM. They can be suspended in the air even for weeks as aerosols, and when inhaled can have carcinogenic, allergic and mutagenic effects. If pollutants have been emitted to the atmosphere only possible method to clean the air is via environmental technology – phytoremediation. It involves growing plants on the surface of which PM are deposited. Nevertheless air pollution has also negative effects on efficiency of photosynthetic apparatus but still there is little data towards such effects of PM.

In this work we focused on the potential of PM accumulation on leaves of trees growing in Polish cities with different level of particulate matter in air. We also studied the reduction of urban particulate matter concentration by trees and shrubs and meadows growing in roadside vegetation barriers and the impact of PM on plants health.

Amount of PM was measured in two categories (surface-PM – deposited on the leaf surface and in wax-PM – phytostabilized in waxes) and three size fraction (10-100μm, 2.5-10μm and 0.2-2.5μm). For the same plants we also measured the concentration of heavy metals and PAHs. To define the impact of PM on plants vitality we used efficiency of photosynthetic apparatus and *a* chlorophyll fluorescence.

We found significant differences in PM amount between plants growing in different cities corresponding with amount of PM in atmosphere. The highest amount of PM was measured on trees growing in Cracow – which have one of the highest level of PM in air in Europe. We also found that green barriers can significantly reduce the spread of traffic PM, heavy metals and PAHs pollution. Moreover flowering meadows can also be more efficient in pollution reduction than regular lawns. However for almost all tested species parameters describing photosynthesis and chlorophyll *a* fluorescence were reduced in comparison with the control plants.

At the present time, phytoremediation technology is becoming more and more popular around the world. In this work we want also present new trends and research plans on the ability of plants to phytoremediate various types of pollutants from the air.

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ASSESSMENT OF ATMOSPHERIC DEPOSITION IN CENTRAL RUSSIA

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Moss biomonitoring technique was applied to study peculiarities of the spatial distribution of atmospheric deposition of heavy metals on the territory of the Moscow, Vladimir and Yaroslavl regions. During the summer 2018 and 2019, samples of the terrestrial mosses *Pleurosium shreberi* were collected at the 282 sites evenly distributed over the territory of investigated regions. The combination of neutron activation analysis and atomic absorption spectrometry allowed to determine more than 30 elements in moss samples. To identify the main sources of air pollution multivariate data analysis technique – factor analysis was applied, while the deposition patterns of pollutants was illustrated using GIS technology. Median values of the elements were compared with the results obtained for other regions in Russia, which participated in moss survey studies. The contamination factors, Geo-accumulation Index and pollution load index were calculated for the following elements As, Sb, Pb, V, Cd, W, Fe, Cr, Ni and Co. Ni. The dominant anthropogenic sources of air pollutants in studied regions can be considered industrial activity and transport.

THE PROBLEM OF ACID RAIN AND TRANSBOUNDARY AIR POLLUTION

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The evolution of the development of the economy and industry of the states of the world has brought on the one hand progress and benefits to the people, but on the other hand it has created and is creating great problems for the environment and our health.

Acid rain is a phenomenon largely generated by anthropogenic activity, both from sources of pollution in the chemical, steel, energy, transport, etc., and from natural sources such as forest and peat fires, volcanic eruptions.

Ordinary rain is known to be a natural meteorological phenomenon, in which water vapor in the atmosphere condenses and turns from gaseous to liquid. But if pollutants from various sources persist in the troposphere in the condensation zone of water vapor, then the process of raindrop formation undergoes a chemical reaction in which molecules of carbon dioxide, sulfur oxides and nitrogen oxides coagulate with water molecules, producing dangerous acids.

The phenomenon of acid rain is studied extensively in terms of the genesis of the formation conditions, but too little is studied as a phenomenon with a risk impact on human health and the environment.

Global and national monitoring networks are increasingly reporting acid rain, and media sources are reporting the consequences. The territory of the Republic of Moldova, along with other territories in Western and Central Europe, is affected by acid rain. The world community is concerned about the impact of this growing phenomenon, which is affecting more and more areas. It is found that the intensity and frequency of these acid rains is directly proportional to the emissions of chemical pollutants dispersed in the atmosphere.

Long-distance transboundary transport of air pollutants and acid rain in places where there are no sources of air pollution has demonstrated the vulnerability and inability of communities to adapt to such a high-impact process.

The hope is to implement and comply with the provisions set out in both the Convention on Long-range Transboundary Air Pollution and Decision 81/462/ EEC on the conclusion of the Convention on long-range transboundary air pollution and the 8 annexed protocols to the Convention to which the Republic of Moldova is part.

The Convention requires the Parties to develop and implement appropriate policies and strategies in special air quality management systems, and the Parties have agreed to make synergistic efforts in the fields of research and development, in particular for the reduction of major air pollutant emissions, monitoring and measurement, emission levels and concentrations, as well as for a better understanding of their effects on health and the environment.

MOSS BIOMONITORING OF AIR POLLUTION IN GEORGIA

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Air pollution is a serious global problem, closely related to the ecological situation, economy and human health. The moss biomonitoring technique was used to provide an assessment of the air quality throughout Georgia. Starting from 2014, Georgia participates in the Moss Surveys carried out in the framework of the UNECE ICP Vegetation (https://icpvegetation.ceh.ac.uk/) on air pollution in Europe. The first moss surveys in Georgia were undertaken in 2014-2017 [1-3] and the results are included in the Report on the European Moss survey 2015–2016 [4]. In the summers of 2019-2021 new moss surveys were undertaken in Georgia. Four moss species (*Hylocomium splendens* (Hedw.) Schimp. (n=6), *Hypnum cupressiforme* Hedw. (n=25), *Pleurozium schreberi* (Brid.) Mitt (n=7), and *Abietinella abietina* (Hedw.) M. Fleisch) (n=14)) were collected from 52 locations.

Concentrations of 41elements (Na, Mg, Al, Cl, K, Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Zn, As, Se, Br, Rb, Sr, Zr, Mo, Sb, I, Cs, Ba, La, Ce, Nd, Sm, Eu, Tb, Yb, Hf, Ta, W, Th, U, Cu, Cd, and Pb) were determined by two complementary analytical techniques, epithermal neutron activation analysis (ENAA) and inductively coupled plasma atomic emission spectroscopy (ICP-AES). Principal Component Analyses was applied to show the association between the elements in the study area. Geographic information system (GIS) technologies were used to construct distributions maps of factor scores over the investigated territory. The concentrations were compared with the previous surveys in Georgia and corresponding values in the literature. The obtained data may serve a baseline data for the deposition of air pollutants and follow up possible dynamics of the air quality in Georgia.

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INVESTIGATION OF TOXIC COMPOUNDS IN THE AEROSOL OF TOBACCO HEATING SYSTEM

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Chemical composition of aerosols of novel tobacco- and nicotine-containing products such as tobacco heating systems requires a systematic study, being a starting point in assessing their level of risk to consumers. Carbon monoxide, benzene, benzo[a]pyrene, 1,3-butadiene, tobacco-specific nitrosamines NNN and NNK, acrolein, acetaldehyde, formaldehyde are included in the lists of priority tobacco smoke toxicants by WHO and various public health organizations, so their quantification in aerosols of novel products is an important step in determining both the absolute and relative (compared to cigarette smoke) product risk, taking into account mode of consumption and design features of these products. Levels of above mentioned toxic compounds were measured in aerosol of tobacco heating systems and in cigarette smoke by the high-performance liquid chromatography with mass spectrometry (HPLC/MS-MS) and gas chromatography with mass spectrometry (GS/MS) in the laboratory of chemistry of the All-Russian Scientific Research Institute of Tobacco, Makhorka and Tobacco Products.

The results demonstrate that the levels of toxic compounds in the aerosol of the tested samples of tobacco heating systems are significantly (by 87–99%) lower than in the 3R4F reference cigarette smoke and the smoke of commercially available cigarettes. This can be explained by specific mechanism of aerosol formation in novel products without pyrolytic and pyrosynthetic reactions. Unlike cigarettes, where combustion is the principle of operation leading to smoke generation, tobacco heating systems form an aerosol without combustion by heating a substrate (tobacco mixture), to evaporate aerosol forming compounds such as glycerine and propylene glycol, along with nicotine and flavour compounds. Nicotine content in the aerosol of tobacco heating systems decreased only by 42.7% compared to 3R4F reference cigarette smoke by and by 33.7 – 40.3% compared to commercial cigarettes smoke, so these products can be a replacement for traditional cigarettes.

INVESTIGATION OF INFLUENCE OF ENVIRONMENTAL POLLUTION ON TREES LEAF PROPRIETIES OF BALTI URBAN ECOSYSTEM (REPUBLIC OF MOLDOVA)

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The aim of this study was to investigate the physiological response of species of tree *Tilia cordata* Mill. From zones with different pollution in Balti ecosystem. The influence of car emissions on vegetation has been determined in function of the intensity of the auto traffic. As it has been demonstrated physiological and biochemical manifestations (the concentration of assimilating pigments and of the total water content) serve as an indicator of the state of plants exposed to stress factors and can be used as a methodology for estimation of the ecological impact of car emissions on vegetation. The impact of certain stress factors (auto emissions) on the bio productivity of vegetation was also estimated. In the municipality of Balti are registered 49453 transport units. The highest number was registered on Stefan cel Mare Street in the perimeter of Nicolae Iorga Street with the bypass of the town. Balti – 1806 units / hour. The ratio of assimilative pigments "a" / "b", as in the case of the total water content in the tree leafs (*Tilia cordata* Mill.) from Balti urban ecosystem proved to be closely related to the number of transport units. Thus, the lowest concentration was established on Stefan cel Mare street, the sector near the bus station and Nicolae Iorga street, where is the largest number of transport units.

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Session D

FOOD, SOIL
AND
WASTE CHEMISTRY

NEW ECO-FRIENDLY MATERIALS FOR VARIOUS FUNCTIONAL PURPOSES

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The development of environmentally friendly materials is an urgent area in agriculture and industry. New eco-friendly sorbent for cleaning the water surface from oil and oil products (KNOP) was developed. It is produced from a mixture of polyacrylonitrile, polyester and wool fibers, which are a waste of textile production. This sorbent doesn't have flowability, which almost excludes its elimination. KNOP structures the liquid hydrocarbon into a three-dimensional compact mass, which can be easily separated and practically does not retain water.

Novel protective masks with high bacterial filtration efficiency have been developed. For their design, non-woven polymeric materials from polypropylene produced by OJSC "SvetlogorskKhimvolokno" (SpanBel, Aquaspan, Meltblown) was used. The developed masks are 3-layered nonwoven fabric (SpanBel – Aquaspan – SpanBel) with upper modified surface layer, which allows to achieve a bacterial filtration efficiency up to 98.6%.

Biodegradable composites based on polylactide (PLA) are promising materials for various applications. The developed PLA-based 3D printing rod are of great interest for educational and medical purpose. PLA-based sheets and films with micro- and nano-fillers (thickness – 0.05 -0.6 mm, width – up to 60 cm) can be used for making biodegradable packaging and consumer goods (folders, boxes, etc.). Adding carbon fiber to PLA-based tape can strengthen the parts of complex shape, and adding lignin is important for the coatings exposed to direct sunlight.

INFLUENCE OF PULSATING ELECTRIC FIELD (PEF) PRE-TREATMENT ON THE EXTRACTION EFFICIENCY OF PHENOLIC COMPOUNDS FROM GRAPE MARC

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The extraction efficiency of bioactive compounds (CBA) can be increased by using the pulsating electric field (PEF) due to the electroporation phenomenon, which influences the permeability and rupture of cell membranes. This phenomenon facilitates the extraction of soluble intracellular compounds without significant increase in temperature, without chemical or physical changes in the plant matrix. The aim of the research was to establish the influence of PEF and extraction temperature (t) on tannins content extraction (CT), antioxidant activity (AA) and the composition of red grape seed extracts (EtOH, 60% (v / v).

It has been shown that PEF parameters, especially the voltage (U) have influenced the rate of tannins extraction, due to the increased permeability of cell membranes. The number of pulses (n) had a lower influence than U. The t had a synergistic effect with the PEF parameters on the tannins yield, as it significantly influenced the fluidity and stability of the cell membrane in the grape seed matrix. At 30°C the phospholipids are packaged in a gel-like structure and their order of extraction decreases with increasing t of the extractant. At 65 ° C the structure of phospholipids changes from the gel phase to a liquid crystalline structure, affecting the stability of the cell membrane. Extraction at 65ºC assisted by PEF (U = 165 V, n = 900) contributed to the increase of tannins yield 2.45 times compared to the conventional extraction method.

The AA of grape seed extracts corresponds to the extraction yield of tannins and constitutes 80.13 – 92.70% of inhibited DPPH. The correlation between CT-AA is $R^2 = 0.928$, demonstrating that the evolution of AA depending on the PEF and t extraction parameters is synergistic with the tannins extraction rate. Phenolic compounds extracted from grape seeds were identified and quantified (HPLC). Experimental data show the presence of 10 identified phenolic compounds: vanillin, resveratrol, qercetin and cinnamic acids, p-hydroxybenzoic, floretic, vanillic, gallic, p-coumaric and caffeic. Another 7 present phenolic compounds could not be identified. The presence of catechin and epicatechin, as well as conjugated polyphenols and their ester derivatives were not attested in this study. Resveratrol (0.047mg/g) was also extracted from grape seeds. The predominant compounds, in descending order, are: vanillic acid – 0.413 mg/g; caffeic – 0.183 mg/g and gallic acid- 0.107 mg/g. This composition reflects a high biological activity of phenolic compounds in grape seeds.

In order to establish the combined influence of t, n and U on CT and AA, the sensitivity analysis was used by applying the first-order Sobol index. Temperature has the greatest influence on CT and AA, n and U is lower than t. The three factors (t, n and U) have more influence on CT and AA at low temperatures (here at 30°C). According to the results of the study, PEF technology presents a promising alternative for CBA extraction from grape seeds, compared to the conventional extraction method.

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SYNTHESIS OF BIOLOGICALLY ACTIVE TERPENOIDS BY VALORISATION OF SOME VEGETABLE WASTES

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Keywords: *apple pomace, clary sage, lavender, sunflower, diterpenes, nitrogen-containing diterpenoids, triterpenes, synthesis.*

The valorisation of vegetable waste from various economic activities, becoming one of the major concerns in many countries around the world. They are trying to develop green and sustainable methodologies for utilization of these important sources of bioactive components that belong to various groups of natural compounds.

A special place in the range of biologically active natural compounds is occupied by diterpenoids and triterpenoids. The products or active principles obtained from them are widely used in perfumery, cosmetics, agriculture, tobacco industry, pharmaceuticals and other fields of human activity.

Researchers from the *Institute of Chemistry of Moldova* have accumulated a rich experience regarding the isolation and chemical transformation of terpene compounds from vegetable waste, including local ones. Using known or new processes, here were isolated diterpenoids – (-)-sclareol from concrete of Clary sage (*Salvia sclarea* L.), *ent*-trachilobanoic and *ent*-kaurenoic acids from sunflower wastes and triterpenoids – ursolic and oleanolic acids from lavender wastes and apple pomace.

The research was focused on the development of original methods for the preparation of new functionalized bicyclic nitrogen-containing diterpenoids based on the available natural diterpenoid – sclareol and designing of natural chiral molecules of interest to the pharmaceutical industry. Bicyclic di- and sesquiterpenoid functionalization was performed both in the lateral chain and in the C-7 position of the B cycle, producing lactams and derivatives containing an amino group, or azine, hydrazide, dihydrazide and guanidine fragments, as well as heterocyclic units.

Experimental work included extraction methods such as Soxhlet or ultrasound-assisted, column chromatographic separations, thin layer chromatography (TLC), gas chromatography-mass spectrometry (GC-MS) and high-performance liquid chromatography (HPLC) analyses. Chemical transformations of starting di- and triterpenoids were performed by conventional and non-conventional (microwave, photochemical, electrochemical) methods of synthesis. The structures of synthetized compounds were proved by spectral methods (IR and NMR), mass-spectrometry and X-rays analysis on single crystal.

As a result of the research, based on the mentioned compounds, dozens of natural analogs, odorous or biologically active compounds were synthesized.

A series of over 50 newly obtained substances was subjected to biological testing, of which 10 showed pronounced antifungal and antibacterial activity, 2 amides showed pronounced antioxidant activity, and two derivatives with guanidine fragment showed high antitumor activity.

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ANALYSIS OF THE MECHANISM OF FORCED OXIDATION OF GRAPE SEED OIL

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Lipid oxidation is one of the major causes of decreased nutritional value of foods, limiting their shelf life. This phenomenon leads to changes in the nutritional and organoleptic quality of the oils. Consumption of metabolites of oxidative degradation of lipids is the cause of oxidative stress of the human body and, respectively, causes multiple morbid conditions for human health. In food, the oxidation of lipids is a process consisting of a series of stages, being influenced by the chemical structure of unsaturated fatty acids, their physical state (liquid or solid), the presence of inorganic oxidants (ions of some metals: Fe^{2+}, Cu^{2+}, Co^{2+}, Mn^{2+}) or organic (haemoglobin, myoglobin), the pre-existence of free radicals, the existence of lipases, the quantity and quality of substances with antioxidant role in food, the way of food processing, the way of packaging and the conditions of food storage. Stopping or inhibiting the lipid self-oxidation process is of practical importance for various industrial applications, especially for the food industry. One of the most rational methods of inhibiting lipid self-oxidation is the use of affordable, relatively inexpensive natural antioxidants that do not affect the health of potential consumers. In order to select antioxidants potentially useful for inhibiting the oxidative process, it was necessary to study and understand the mechanism and kinetics of the lipid self-oxidation process, the influence of various factors on the process kinetics, both in the absence and presence of antioxidants.

Grape seed oil, a local product ("Golden Tear") was used as a substrate. A study was performed on the process of forced oxidation of oil in the presence of hydrogen peroxide and Cu (II) ions. The action of some antioxidants on the oxidation process was researched: α-tocopherol, n-octyl gallate, L-ascorbic acid 6-palmitate and matcha extract (green tea). The oil samples with the addition of different concentrations of H_2O_2 and Cu^{2+} were placed in airtight containers. Periodically, for 800 hours, samples were extracted to determine the peroxide index and the content of conjugated dienes and trienes.

Following the forced oxidation of the researched oils, products of the oxidation reaction (HPLC method) were identified: hexanal, octanal and hydroxinonadienal. It was found that the most intense dynamics is attested in the first 12 hours of exposure to prooxidant conditions. Optimal concentrations of oxidizing agents to accelerate the oxidation process – hydrogen peroxide (10^{-3} M) and Cu^{2+} ions (10^{-3} M) were established. The inhibitory action was demonstrated by the application of the antioxidants α-tocopherol, L-ascorbic acid 6-palmitate, n-octyl gallate, macha extract. The effective action of L-ascorbic acid 6-palmitate and n-octyl gallate has been established. Less effective have been established to be α-tocopherol and matcha extract.

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A SMALL ANGLE SCATTERING STUDY OF POLYSACCHARIDES WITH ANTIOXIDANT ACTIVITY

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Amongst the most common functional ingredients of different food colloids and emulsion formulations are polysaccharides. These natural polymers possess the ability to impact the product shelf life, food texture and colloidal stability, and therefore are regarded constantly for new food formulation developments. The wide range of applications of polysaccharides will primarily depend on their properties in solutions, the conformation stability, aggregation and gelation behaviour. And, although there is a vast advancement made in the recent years in understanding the physicochemical properties of polysaccharides and how to explore these into food hydrocolloid formulations, the topics continue to be challenging.

Small-angle scattering techniques are powerful, non-invasive experimental tools that provide information about the structure and conformation of macromolecules in solution. Previously, small-angle scattering was used successfully for characterizing the structural features of milk proteins in solutions under *in situ* conditions [1-3]. This study reports the results of investigation of the aggregation and gelation behaviour of several polysaccharides possessing antioxidant activity by using small-angle scattering methods.

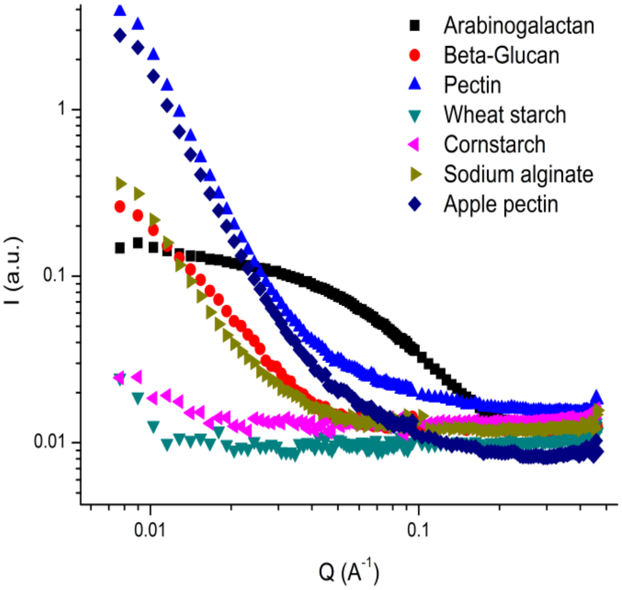

Figure 1. *Small-angle neutron scattering profile demonstrating the structural difference of the studied polysaccharides in solutions prepared under the same conditions. The experimental data were obtained on the KWS-2 small-angle neutron scattering diffractometer.*

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INFLUENCE OF NATURAL ZEOLITES OF GEORGIA ON THE MIGRATION OF TOXIC ELEMENTS IN SOIL-PLANT SYSTEM

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Natural zeolites are widely used in the field of environmental protection. Nowadays, the environment is saturated with various pollutants, including such life-threatening elements as cesium, strontium, etc. These elements in significant quantities accumulate into the soil, pass to the plant, fall into a living organism and poison it.

The purpose of this study is to identify the possibility of application of Georgian zeolites to reduce the migration of Sr+ and Cs^{++} cations in the soil-plant system and protect the environment.

The objects of the study were selected Georgian natural zeolites, lomontite and scoleciite containing rocks.

The sorption and ion exchange properties of these zeolites were studied. Ion exchange properties were studied under dynamic conditions; dynamic exchange capacities (DEC) were established in relation to Cs+ and Sr+ cations. They are important indicators and determine the prospect of natural zeolites application in agriculture. Dynamic capacities were established based on the number of absorbed and washed out cations.DEC of lomontite in relation to Cs^+ and Sr^{++} cations are the same (2.8mg.eq/g); a higher selectivity with respect to Sr^{++} is noticed for scoleciite (3.2 mg/eq/g).

The study of the ion exchange properties of lomontite made it possible to carry out laboratory vegetative experiments to determine the possibility of its application for removing cesium and strontium from soil that decrease in their migration in the soil-plant system. Soils, contaminated by 0.1 N aqueous solutions of cesium and strontium chlorides, were placed on special plates. Granulated, lomontite-containing rock was introduced into the soil in an amount of 10.20 and 30%.

The tests on wheat were carried out in three replications. In the first period of a plant development (in the stem) amount of Cs^+ and Sr^{++} cations were determined. As a result of the introduction of lomontite in amount of 10, 20 and 30% into the soil, 0.7, 0.5 and 0.2% of cesium and 0.6, 0.4 and 0.1 strontium were found in the stem respectively.

According to the results, it can be assumed that the introduction of 10 to 30% lomontite into the soil as an additive reduces amount of both cesium and strontium in the soil and their migration in the soil-plant system and this affect becomes more noticeable with an increase of the amount of zeolite.

MICROBIOSTATIC EFFECT OF BIOACTIVE COMPOUNDS FROM AGRO-FOOD INDUSTRIAL WASTES ON MICROORGANISMS CAUSING FOOD SPOILAGE

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In this research the effect of direct contact of raw materials and agro-food industrial wastes rich in bioactive compounds (polyphenols, carotenoids) on microorganisms that cause food spoilage was evaluated. The aim of the research is to elucidate their microbiostatic action on different types of food matrix.

The research methodology included the modelling of food matrices (emulsions, gels, pastes) and the study of the microbiostatic effect of plant extracts in situ and in vitro. The following methods were applied to determine the chemical composition and biochemical transformations of bioactive components from natural sources: physical, chemical and microbiological analysis, UV / dream spectroscopy, HPLC.

In vitro, the antimicrobial effect was determined by direct contact of various berries (sea buckthorn, rosehip, shrubs, hawthorn) and dried grape marc with microorganisms that cause food spoilage - *S. aureus*, *E. coli*, *K. pneumoniae*. *Staphylococcus* and *Escherichia* are the most common causes of outbreaks of contaminated food in the population. *K. pneumoniae* is responsible for nosocomial, urinary tract (UTI), respiratory tract and bloodstream infections, where contamination is possible after handling food.

The test results show that sea buckthorn powders and sea buckthorn flour have a more pronounced antimicrobial activity than the investigated pathogenic microorganisms.

For *Staphylococcus aureus*, the diameter of the inhibition zone is 22 mm (powder) and 18 mm (dry residue); for Escherichia coli, the diameter of the inhibition zone is 18 mm (powder) and 15 mm (dry residue). For *Klebsiella pneumoniae,* the diameter of the inhibition zones is smaller compared to Staphylococcus aureus and Escherichia coli. The other plant powders (rosehip, grape pomace, chokeberry, hawthorn) have a weaker antimicrobial activity against the pathogens tested. Sea buckthorn powder showed the lowest minimum inhibitory (MIC) and bactericidal (MBC) concentrations for Staphylococcus aureus, followed by sea buckthorn resulting from sea buckthorn, rosehip and grape pressing. Only sea buckthorn powder showed antibacterial activity on *E. coli and K. pneumoniae*.

The greatest inhibitory and bactericidal effect on the examined bacteria, capable of rapidly colonizing food, especially meat products with a high degree of hydrophobicity, was observed for sea buckthorn and rosehip powders, in which the content of biologically active lipophilic compounds (lycopene, b-carotene), zeaxanthin, chlorophyll) is considerably higher than aronia and grape pomace powders, in which flavonoids predominate. At the same time in hawthorn the content of biologically active lipophilic compounds is significant, however, the inhibitory and microbicidal effect was lower than for sea buckthorn and rosehip powders. It demonstrates that the presence of organic acids and active acidity plays an extremely important role, directly influencing bacterial adhesion and, ultimately, the process of inhibiting the proliferation of pathogenic microorganisms.

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NEW ADDITIVES OF BIOACTIVE SUBSTANCES IN THE BIOCHEMICAL DIGESTION PROCESSES

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The liquid wastes from the agro-industrial sector can serve as renewable source of value-added products, following the specific treatment. Such treatment is also important from the ecological point of view, as it may prevent the discharge in natural environment of wastes with varying composition, often containing toxic or environmentally-unfriendly components. Usually, the liquid wastes from agricultural and food sector are being processes through the following methods: sedimentation, decanting in stabilizing ponds, anaerobic digestion, etc. Our research was focused to intensification of anaerobic fermentation processes using the additives of bioactive substances introduced into the digested biomass. As an initial biomass, the vinasse from grain distillation taken from ”Garma Grup” Company, Hâncești region, R.Moldova was taken, as well as the other liquid wastes, including from corn fermentation and beer production.

The technological experiments have been performed using the experimental laboratory set-up, using several addivite types. The biomass mixed with the nutritive solution and additives (2 ml/400 ml biomass) was subjected to anaerobic digestion under the mesophilic conditions (20-32^{o}C). Alcoholic fermentation was traced by the volume of emitted carbon dioxide (CO_2), titrated, following the standard procedure, NaOH. Thus, it was found that in case of tomatin application, higher amounts of emitted gas were observed, whereas in case of menthol, dihydrofumaric acid, sclareol, vanillin the rate of the gas emission was lower. At the same time it became obvious that introduction of higher amounts of additives (in 2-4 times) in many cases makes no sense as it does not provoke further acceleration of digestion process.

The results obtained testify that the substances of natural origin used as additives, render the pronounced effects on alcoholic anaerobic fermentation of vinasse under the mesophilic conditions. The comparative assessment of different additives action in the studied processes have demonstrated that the dihydrofumaric acid caused the emission of 266 cm^3 CO_2 during 76 hours, aescinum – 251 cm^3 during 55 hours, tomatin – 233 cm^3 during 78 hours, sclareol – 232 cm^3 during 55 hours, vanillin – 229 cm^3 during 69 hours, whereas catechin – 180 cm^3 during 61 hours of fermentation, until the process was completed.

The study of the effects of additives of bioactive substances with possible antioxidant properties on biomass from agro-food sector fermentation with identification of these processes mechanisms can be a perspective direction, suggesting the new ways of wastes valorization. The anaerobic digestion products obtained in the proposed technological conditions can have the added value and find further applications. Thus, carbon dioxide can be introduced into the microalgae cultivation basins, promoting their biomass growth and development. In their turn, microalgae can be used for feeding the animals in zootechnical sector (mainly, the poultry), to be used as fertilizers or as a source of second-generation biofuel (or a source of biomethane, biohydrogen, bioethanol). Water seperated from the digested biomass, can be used in technical scopes at the industriel entities, to help constructung the semi-closed or even closed water using cycles. The solid digested fraction, separated from water, can be applied on agricultural fields an efficient fertilizer, specifically, for decorative plants or technical cultures, based on of its composition determination and approval for such uses.

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INFLUENCE OF VEGETABLE POWDERS ON THE RHEOLOGICAL PROPERTIES OF PASTA DOUGH

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Technologies for the manufacture of functional flour products must ensure their quality and consumption properties (sensory characteristics, structure, consistency, etc.), reduce the negative impact of food ingredients, which are not compatible with the functional properties of the protein-carbohydrate complex of flour and increase food security. Currently, an important role in expanding the range of pasta is the use of non-traditional raw materials. To meet the needs of consumers, pasta is fortified with protein, dietary fiber, trace elements, etc. The rheological properties of the dough can be chemically improved, using oxidizing agents (ascorbic acid, azodicarbonamide, calcium peroxide, etc.), acidic substances (lactic, acetic acids) or enzymes. The aim of the presented research is to investigate the influence of rosehip and chokeberry powders on the rheological properties of pasta dough.

The research focused on the following directions: determination of physico-chemical and organoleptic indices of wheat flour and rosehip and chokeberry powders; the chemical composition of vegetable powders, in particular the content of sugar, fat, starch and dietary fiber. Total content of polyphenols, anthocyanin’s and carotenoids was achieved by the spectrophotometric method. Identification of the individual profile of polyphenols, anthocyanin’s, carotenoids by HPLC method. In the case of organic acids, the capillary electrophoresis method was used. The rheological behaviour of the empirical properties of the doughs was performed using the Alveograph apparatus. The first-order Sobol index sensitivity analysis was used to study the influence of powder concentration on dough rheology. Vegetable powders of chokeberry and rosehip were used in quantities of 1.5%, 3% and 5% of the mass of wheat flour. It was shown that in relation to the control sample, the introduction of vegetable powders significantly influenced the increase of the maximum pressure, P, or toughness of the dough and led to the formation of the dough with maximum resistance to deformation.

This phenomenon is due to ascorbic acid in berries, which in the presence of oxygen included in the dough to knead oxidizes the sulfhydryl groups –SH, which belonging to two protein molecules form disulfide bridges –S-S- strengthening the gluten in wheat flour. The increase in dough toughness can also be influenced by the presence of berries. The increase in the L value of the dough is explained by the fact that pectins from powders in water form a strong carcass due to the convergence of hydrophobic methoxyl groups, and free carboxylic groups dissociate into ions, which interact with $–NH_3^+$ groups on the protein surface, thus improving structural and mechanical properties. Of the dough. The content of pectin and organic acids had a significant influence on G. The addition of vegetable powder to wheat flour leads to an increase in the deformation energy. The sensitivity analysis showed that in rosehip powder the greatest influence of the concentration is on W (0.561), and the least on the P / L ratio (0.15). For chokeberry powder the greatest influence is on L and P / L (0.561), and the least – on W (0.270). It is also found that for chokeberry powder the influence of concentration is generally higher than for rosehip powder. Thus, in the rosehip samples the presence of the increased amount of ascorbic acid and organic acids had a predominant effect on gluten proteins, leading to an increase in the dough P. In the case of samples with aronia, pectic substances had an essential effect, which improved the dough.

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EVALUATION OF THE POLYPHENOLS POTENTIAL FROM GRAPE VINIFICATION RESIDUES OF RARA NEAGRĂ AND MALBEC GRAPES VARIETIES HARVESTED FROM PURCARI AREA

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Red grape grapes are an important source of phenolic compounds, which possess important physiological properties. As a result of processing, a certain share of polyphenols passes into wine and contributes essentially to the formation of its structure, physico-chemical, microbiological and organoleptic properties. However, a considerable part of them remain in the pomace, and the transfer rate depends on the ripening state of the grapes and the technological processes applied. In this study, different important groups of polyphenols were determined in the wines and pomace resulting from the *Rara Neagră* and *Malbec* grapes.

The extraction of the active components was performed using two solvents: hydro-acetonic, with the addition of HCl for acidification (S1, acetone-water-HCl conc. 80:20:1, v/v/v), and hydro-ethanolic (S2, 12% ethanol (v/v)), acidified with tartaric acid (5 g/l). The first solvent with lower polarity is preferred for the extraction of less polar organic compounds and is used to determine the quantitative potential of grapes skin and seeds, the second being a benchmark of the qualitative and quantitative composition of the polyphenolic complex, which actually passes into wines under conditions of alcoholic fermentation.

For both Rara Neagră and Malbec, the extractable contents of phenolic substances and anthocyanins are influenced by the harvest season, by the drying temperature of the pomace and by the extractant used. Total phenolic substances reach the maximum level for extracts in solvent S2 from Malbec skin dried at 40^oC, while pigments predominate in Malbec extracts dried at 105^oC. The higher temperature causes an essential degradation of the polyphenolic complex: 2.3 times in Malbec and about 3.3 times in Rara Neagră. The decrease for natural pigments is inhomogeneous: for Malbec the maximum value is reached in the case of grape skins dried at 105^oC, and is 1.4 times higher than for 40 ^oC, while in Rara Neagră the situation is reversed – if drying is done at 40^oC their content is 1.6 times higher than at 105^oC. In solvent S1, the extraction of polyphenols from the grape skins treated at 105^oC is favored for Rara Neagră. The content of similar products extracted from Malbec is slightly higher in samples dried at 40^oC. The trend is also observed for Malbec pigments – at 105°C their content is 2.2 times higher than at 40 °C. Although to a lesser extent (just 1.2 times), this order is similar for Rara Neagră.

Both the drying temperature and the solvent influence the extraction of polyphenols from seeds. The total content of phenolic compounds extracted in both S1 and S2 is maximal in the case of Rara Neagră seeds, harvested late and dried at 40

°C. On the contrary, for Malbec the high drying temperature of the seeds contributes to the higher extraction of polyphenols in both S1 and S2, the effect being considerable (1.6-2.3 times).

It has been shown that actual industrial technologies of wines production from Rara Neagră and Malbec grapes have contributed to the extraction of only about 10-18% of the polyphenols. The predominant amount of phenolic compounds with important biological and nutritional value is still concentrated in pomace, which should be treated accordingly for the extraction of the desired bioactive substances.

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THE COMPOSITION OF THE AROMATIC COMPLEX OF WINES FROM LOCAL GRAPE VARIETIES LEGENDA

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The global wine market is characterized by great competition and the solution to stay in competition, to have a name of its own consists of unique products with authentic qualities specific to the area. Thus, the originality and typicality of the product is an important decision factor in the consumer's choice. The exploitation of local selection varieties offers this possibility. The improvement of the assortment of local cultures in order to connect them to the consumer's requirements results from the strategic development priorities of the wine branch. In the Republic of Moldova there are several varieties approved and recommended for the production of quality white and red wines. The new selection varieties are interspecific varieties obtained as a result of crossbreeding between Vitis Vinifera and other species. Although there are optimal conditions for growing grapes, the interest of wineries in the varieties of local selection leaves much to be desired. This fact can be explained by the small number of researches on the respective grape varieties, including the technological properties and the 153entra-chemical, sensory characteristics of the new selection wines.

The Legenda presents a medium maturing variety, created within the National Institute of Viticulture and Vinification in 1975 by crossing the Royal Vinyard (England) table variety with the pink Traminer variety (Austria). The berries are round, pink, medium in size, with a juicy pulp, with a specific taste and original aromas when ripe. The juice is colourless. The Legenda variety is intended for the production of quality dry white wines, being also used as a raw material for the production of sparkling and blended wines. The wines have a rich aroma of flowers, incense, full and fresh taste. The variety is recommended for cultivation in the southern and central wine regions of the Republic of Moldova.

The purpose of this research is to evaluate the technological properties of Legenda grapes, optimizing the technological process of winemaking in microvinification conditions, with elucidation of the composition of the aromatic complex of wine.

The raw material wines obtained were analysed organoleptically and in terms of physico-chemical parameters. Free and glycosidic monoterpenes were determined by the spectrophotometric method to obtain information on the content of compounds. Volatile compounds, including terpenes, alcohols, esters, aldehydes and ketones, have been identified by the GC / MS method with solid phase micro extraction. The identification of the peaks took place through the mass spectra and the retention time in the mass spectral library. The organoleptic profile of the Legenda wine was determined.

ENVIRONMENTALLY FRIENDLY PYRETHROID DRUG AGAINST PLANT PESTS

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In today's reality, no country in the world can abandon chemical plant protection products, as they are significantly more effective than biopesticides, the efforts of researchers are aimed at using pesticides that are as safe as possible for humans and the environment. One way to reduce the environmental burden is to extend the effective period of the pesticide, since in this case the frequency of its use is reduced.

Taking into account the stricter environmental requirements, an insectoacaricide composition with a low environmental load was developed at the Petre Melikishvili Institute of Physical and Organic Chemistry. In the composition of the developed composition, the auxiliary component of the main active substance (synthetic pyrethroid – cypermethrin) is turpentine oil, which is obtained from plant remains (pine resin).

It was found that the presence of turpentine oil in the composition of the developed composition determines an increase in the period of insect-acaricidal activity from 15-17 days to 25-28 days. The increase in the period of insect-acaricidal activity developed by the composition is probably caused by the formation of a micro emulsion system water – turpentine oil, which creates certain steric difficulties in the release of cypermethrin molecules.

The effectiveness of the composite preparation containing turpentine oil was studied by comparing its effect on the mortality of aphids with the imported insect-acaricidal preparation "Arrivo" (FMC Corporation – Agricultural Products Group, USA). According to the results obtained, the effectiveness of the developed composition is at the level of imported insectoacaricide, despite the low content of synthetic pyrethroid in the developed composition by 60%.

The result of the analysis a residual amount of pyrethroid in nectarine, peach and apple(cypermine) are 0.006÷0.013 mg/kg, while according to The European Food Safety Authority (EFSA) the maximum residue level (MRL) of cypermethrinin these products is 2.0 mg/kg.

Based on the research conducted, we can conclude: Effectiveness of developed composition and the high-quality European and American acaricidal preparations are almost identical.

The content of turpentine oil in the formulation of developed composition determines the sufficiency of low pyrethroid content for the effective action of the drug against plant pests. Therefore, the use of the developed composition against pests is absolutely safe for humans and the environment.

REVIEW OF THE MANAGEMENT OF POPs CONTAMINATED SITES IN REPUBLIC OF MOLDOVA

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The soil is an important and non-renewable natural resource which is a base for life and for supporting livelihoods. Healthy soil is an essential component of the agriculture production with the capability of supporting the ecosystems on which economic activities and livings rely (https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX:52006PC0232, http://www.ipes-food.org/pages/CommonFoodPolicy).

However, soils are under increasing environmental pressure across the globe, and the associated soil degradation is raising extreme values in Europe due to a high population density and its related activities, such as industrial activity, inappropriate agricultural and forestry practices, tourism or urban development (https://esdac.jrc.ec.europa.eu/themes/soil-contamination). The aim of this study is an evaluation of the status of contaminated sites in Republic of Moldova and problems of their management for the sustainable agriculture production. The 16 POPs contaminated sites were studied in 2020 year for the actualization of the current situation after the inventory project in 2009 – 2010 years. More detail risk assessment procedure was realized for the studied sites for the evaluation of possible impact to nearest ecosystems, agriculture production and human health. The obtained results showed that the situation from the past inventory (2009) is not changed essential for POPs contaminated sites. The high level of contamination was identified for the majority of sites, the level and spectrum of pollutants have not changed significantly. All studied sites have high environmental and public health risks. The remediation actions are required for all of them. These actions can include the utilization of in-site remediation technology and dumping of contaminated materials at the site. The special requirement should be elaborate and later adopt regulation for each site based on guides of the European Union, and other actors in the field. The other important factor is to elaborate and approve environmental quality standards that indicate the admissible concentrations of hazardous substances in the soil based on the type of land use: agriculture, residential, commercial, and industrial. One of the most important strategies for the achievement of sustainable development is the promotion of a legislative system coherent with current requirements at the international level.

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THE QUALITY OF SOIL AND VEGETATION COVER NEAR THE OUTLET OF SPRING WATERS BASED ON BIOINDICATION DATA

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Chemical and sometimes microbiological contamination of the soil cover, incl. and due to cross-border transfer processes. Spring water discharge points (moles) are often found near urban infrastructure, which adversely affects the condition of ground surface waters. The quality of soil and vegetation cover near the points of groundwater discharge may indirectly indicate the state of groundwater, therefore, monitoring of these covers is relevant [1]. In this regard, the aim of the work was to assess the quality of soil and vegetation cover near the outlet of spring waters. For this, initially it was necessary to analyze the soil and vegetation cover at the studied objects.

In the course of visual observations of the soil and vegetation cover, the presence of soil animal species was found only in those habitats that provide a full range of conditions necessary for the manifestation of vital activity. And the results of vegetation identification showed that species diversity is interrelated with the level of anthropogenic impact.

It is known that soil invertebrates, due to their natural qualities to quickly respond to changes in environmental parameters, are an informative indicator of the state of soil biota [2]. Plants, on the other hand, can serve as an indicator of the content of xenobiotics, which, upon entering the soil and through plant organs, can enter the groundwater from the soil cover.

In the studied samples of the soil cover, exceeding the regulatory requirements for the following quality indicators was found: Ni^{2+}, Zn^{2+}, Cu^{2+}, Cd^{2+}. As a result of the analysis and systematization of data on the quality of soil cover, vegetation and the presence of soil fauna near the spring waters of Ivanovo during the study periods, priority pollutants were identified – compounds Cu^{2+}, Zn^{2+}, Mn^{2+}, Ni^{2+}, Cu^{2+} и Co^{2+}. Consequently, this is precisely why soil and plant flora and mesofauna are sensitive to the reaction of soil solutions. With the help of plants and invertebrates, it is possible to simply monitor the state of urban ecosystems. In this regard, the use of soil and plant flora and mesofauna in the future will be one of the best methods for bioindication of the state of springs.

Thus, using soil and plant indicators, it is possible to monitor and even predict changes in the OS (in behavior, changes in appearance, quantity and chemical composition).

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DETERMINATION OF HEAVY METALS IN SOIL

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Abstract. *The term "heavy metals" refers to environmental pollution and the toxic effects of elements when they enter the biota. These elements have a great affinity for physiologically important organic compounds. Heavy metals differ not only in the degree of impact on the soil, but also in the condition in which they are located. By its nature, soil is a combination of various clay minerals of organic and inorganic origin.*

Currently, two different terms are widely used to describe almost the same group of chemical elements: trace elements and heavy metals. In total, there are more than 40 heavy metals. Priority pollutants are Pb, Cd, Zn, Hg, As and Cu, as man-made accumulation in the environment is very high. Excessive amounts in the body of living things disrupt all metabolic processes and cause serious diseases in humans and animals. At the same time, many of their elements (Co, Cu, Zn, Se, Mn), as mentioned above, are widely used in the national economy (especially in agriculture, medicine, etc.) under the name of trace elements. The biggest threat to the soil comes from man-made factors. Various industries, where the wastes are heavy metal particles, unfortunately the best filters are equipped in such a way as to allow the passage of heavy metal elements that first enter the atmosphere and then penetrate the soil along with industrial wastes. This type of pollution is called man-made. In this case, the mechanical composition of the soil, carbonate content and absorption capacity are of great importance. Elements N, P_2O_5, K_2O, Na, Fe, Cu, Zn in the 30-60 cm layer of the soil on the basis of the sample taken from the fruit field within the territory of Gakh region are indicated in the measure of more or less than the norm standards.

Code: 23; Area: əibəyli Nr.1; Depth: 0-30 sm; Plant: Meyva bagi
Coordinates: Nr. 41,33327644 E: 46,84144269

Nr.	Parameter	Unit	Norm	Method	Result	Assessment
1	pH (1 : 2,5)	µs/sm	6,5-7,5	ГОСТ 26423-85	7,51	Zəif Gələvi
2	EC	%	0-4000	ГОСТ 26423-85	1728	Duzsuz
3	$CaCO_3$	%	5-15	Seybler	2,54	Az kirəkli
4	Humus	%	3-4	Wolkey Black	2,9	Orta
5	Azot	kg/ha	0,09-0,17	ГОСТ 26107-84	0,17	Yuksək
6	P_2O_5	kg/ha	60-90	Olsen	8,01	Cox Az
7	K_2O	mg/kg	250-500	ГОСТ 26210-91	214,2	Az
8	Na	mg/kg	80-120	ГОСТ 26210-91	480	Cox Yuksək
9	Fe	mg/kg	2,51-4,5	ГОСТ 26210-91	8,88	Yuksək
10	Cu	mg/kg	>0,2	ГОСТ 26210-92	3,2	Yetərli
11	Zn	mg/kg	0,71-2,4	ГОСТ 26210-93	1,04	Orta

It is now known that almost all particles of heavy metals can be present in the soil in the following conditions: in the form of a mixture of oxidized isomorphic particles in the form of salt deposits, in the crystal lattice, in soluble form, directly in soil solution and even part of organic matter. It should be noted that the behavior of metal particles can vary depending on redox conditions, soil composition and carbon dioxide levels.

Depending on the composition of the soil, geographical data and distance from industrial areas, there may be different types of heavy metals in the soil, each of which poses a certain degree of environmental hazard. Because the structure of the soil can be different in different places, redox conditions, reactivity, as well as the binding mechanisms of heavy metals in the soil are different.

EXTRACTIVE PHOTOMETRIC DETERMINATION OF COBALT

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Cobalt (II) plays an important role in biological processes in the body and is an indicator of some diseases. This requires constant monitoring of anthropogenic pollutants and the migration of toxic substances in the environment.

We studied the possibility of using 2-piperidinomethyl-4- (3-methylcyclohexyl) phenol (L) for photometric determination of cobalt (II).

Cobalt (II) forms a colored complex with L, which dissolves in chloroform. In a single extraction with chloroform, 97.6% of cobalt is recovered as a complex. The complex is extracted at pH 4.2-5.5. Optimal conditions for the formation and extraction of the complex are 0.8×10^{-3} mol/l, concentration L. The extract of the complex obeys Beer's law at a concentration of 0.03-3.6 μg / ml of cobalt. The maximum optical density is reached within 5 minutes. The optimal V_{aq}/V_{org} value is 5/5-80/5. The molar absorption coefficient is $\varepsilon_{548} = 3.25 \times 10^4$.

The stoichiometry of the complexes under study was established by the methods of equilibrium shift and relative yield. The ratio of the components in the Co: L complex = 1: 2.

It was found that colored complexes with L also form ions Fe (III), V (IV), Cu (II), Ni (II), Mo (VI), Pt (II), Mn (II), Cd (II), Zn (II) and Pd (II). The selectivity of the determination increases significantly in the presence of masking reagents or when the pH of the medium changes.

Based on the results of spectrophotometric studies of cobalt (II) with L, methods have been developed for the determination of cobalt in plants (beans: 0.20 ± 0.0053 μg/kg Co; peas: 0.11 ± 0.0040 μg/kg Co) in wastewater (0.45 ± 0.05) μg/l Co) and bottom sediments (1.92 ± 0.04 μg/l Co).

INVESTIGATION OF THE CONTENT OF MINERALS IN SAMPLES OF VOLCANIC MUD BY X-RAY DIFFRACTOMETRY

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The content of minerals in samples of volcanic mud taken from the Salyan (Khidirli village), Shamakhi (Gushchu village) and Aghstafa districts was investigated by X-ray diffractometry. Based on the analysis of the samples, the amount of natural minerals such as illite, calcite, quartz, gypsum, tridemite, microcline, volcanic glass, cristobalite, etc. was calculated. For the analysis, a D8 ENDEAVOR diffractometer from Bruker was used.

X-ray diffractometry is the most direct and effective method for determining the quantitative ratios of crystalline and amorphous materials, determining their microstructural properties, such as crystallite sizes and microstrains, as well as macrostructural properties, such as the magnitude of residual stresses and strains in products. The phase composition of materials is traditionally determined by means of X-ray diffraction. To prepare samples for XRF of mud volcanoes taken from the Aghstafa, Shamakhi, and Salyan regions, grinding followed by pressing the samples into tablets was used. All samples of mud volcanoes taken from the

Aghstafa, Shamakhi and Salyan regions include the mineral illite. The high content of micro-components: iodine, boron, bromine, organic substances, as well as mineralization – the advantage of volcanic mud taken from the Aghstafa, Shamakhi and Salyan regions, distinguishing them from silt and peat mud. Other minerals are also part of the volcanic mud taken from the Aghstafa, Shamakhi and Salyan regions.

Table 1 shows the results of the analysis of volcanic mud taken from the Aghstafa, Shamakhi and Salyan regions. For analysis, 15 grams of volcanic mud were taken, pressed and given in the form of tablets to a D8 ENDEAVOR diffractometer. LOI-loss on puncture is 6.45%, 4.01% and 5.72%.

Mineral types%	**Shamakha (Kushchu)**	**Salyan (Khidirli)**	**Aghstafa**
Illite	4,26	6,2	3,42
Quartz	13,29	12,39	9,8
Gypsum	0,4	0,36	0,09
Tridemite	0,25	0,13	0,39
Volcanic glass	59,47	55,5	67,12
cristobalite	1,64	1,66	1,75
microcline	4,77	4,69	4,51
plasiclase	13,16	17,4	12,61
calcite	2,76	1,61	0,33

The amount of minerals found in samples of mud volcanoes taken from these places indicates that these minerals are useful for various purposes, especially as valuable medicinal products in cosmetology and pharmaceuticals.

STUDY OF OXIDES CONTENT IN VOLCANIC MUD SAMPLES USING A HIGH-EFFICIENCY S8 TIGER X-RAY FLUORESCENT SPECTROMETER

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Azerbaijan is a country where mud volcanoes are widespread. Mud volcanoes are included in the ranks of the country's natural resources. Of the 800 mud volcanoes in the world, more than 300 fall on the territory of Eastern Azerbaijan and the border waters of the Caspian Sea. Here you can find all types of volcanoes: active, extinct, land-continental, oil, island and underwater volcanoes. Thus, in terms of the number, variety and active activity of volcanoes, the territory of our republic has no analogues in the world.

Mud volcanoes are widespread, mainly in the territory of Eastern Azerbaijan – on the Absheron Peninsula, in the Shemakha-Gobustan region, in the southeastern Shirvan lowland and in the Baku archipelago.

XRF analysis is one of the best analytical methods for performing elemental analysis of all types of samples. Bruker XRF spectrometers combine the highest accuracy with simple and fast sample preparation for the analysis of elements in a concentration range from 100% to below ppm. Each geological sample is a product of the original source material and environmental conditions that existed during its formation. The geochemical composition of mud volcanoes and minerals is responsible for their distinctive characteristics, which make them a valuable resource for scientific research.

To study the content of oxides in samples of volcanic mud, samples were taken from the Salyan (Khidirly village), Shamakhi (Gushchu village) and Aghstafa regions. Based on the analysis of the samples, the amount of oxides in the volcanic mud was calculated. To prepare samples for XRD analysis of mud volcanoes taken from the Aghstafa, Shamakhi, and Salyan regions, we used grinding followed by pressing the samples into tablets. The high content of micro-components: iodine, boron, bromine, organic substances, as well as mineralization – the advantage of volcanic mud taken from the Aghstafa, Shamakhi and Salyan regions, distinguishing them from silt and peat mud. Table 1 shows the results of the analysis of volcanic mud taken from the Aghstafa, Shamakhi and Salyan regions. For analysis, 15 grams of volcanic mud were taken, pressed and given in the form of tablets to an X-ray fluorescence spectrometer S8 TIGER.

Oxides,%	**Shamakhi (Gushchu)**	**Salyan (Khidirli)**	**Aghstafa**
SiO_2	64,52	65,30	65,47
Al_2O_3	12,40	13,20	12,53
CaO	4,25	3,25	3,95
MgO	0,63	0,84	0,6
SO_3	0,69	0,38	0,19
K_2O	3,45	3,32	3,57
Na_2O	3,15	3,24	3,21
TiO_2	0,3	0,34	0,29
Mn_2O_3	0,09	0,1	0,1
$P_2 O_5$	0,07	0,082	0,068
$Fe_2 O_3$	2,5	2,95	2,47

IDENTIFICATION OF PRIORITY POLYCYCLIC AROMATIC HYDROCARBONS IN ROADSIDE DUST (IVANOVO CITY)

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Priority environmental pollutants include polycyclic aromatic hydrocarbons (PAHs). A complete list of toxic PAHs is established by the US EPA, which includes 16 compounds, while some of this group have carcinogenic, mutagenic and teratogenic properties. Therefore, the purpose of this work was to evaluate the content of 16 priority PAHs in roadside dust in the city of Ivanov. The PAH content in dust samples was estimated by HPLC using a FLUORAT-02M fluid analyzer as a detector.

It was found that the benz(a)pyrene content in the dust fraction varies from 0.6 (northern part of the city (residential private sector) to 102.3 μg/kg (industrial part of the city) with a median and average value of 10.9 and 19.3 μg/kg, respectively. A similar situation is observed with the total content of PAHs. Note that the contribution of BP to the amount of carcinogenic PAHs is insignificant and amounts to less than 1%. It was found that in more than half of the sampling points, the proportion of carcinogenic PAHs was ≥ 90% of the total content, with most of the points located along the roads. These data are in good agreement with the results of measurements of BaP content in the snow cover on the territory of Ivanovo [1].

The totality of the data obtained made it possible to identify criterial pollutants that must be recommended for monitoring and to determine possible sources of income.

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ENVIRONMENTALLY FRIENDLY THERAPEUTIC AND PROPHYLACTIC MEANS AGAINST PLANT PATHOGENS

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Complex compounds (chelates) of polyvalent metals (Fe, Mn, Co, Zn, Cu) with organic ligands were synthesized, in the laboratory of agrarian chemistry of the Institute of Physical and Organic Chemistry, Tbilisi State University. These ligands are obtained in the process of oxidative and thermal destruction of agricultural products (molasses, sugar beet) agricultural waste (rods of corn cob) and natural resources (peat, coal). The resulting chelating compounds are non-toxic and stable in an alkaline environment.

According to the results of the tests carried out, the obtained chelates are effective both for root feeding of the plant and for preliminary soaking of seeds, annual vegetable crops (tomatoes, cucumbers, peppers, eggplants) with a 1% chelate solution. The Chelates enhance the defense reaction of plants against viral, fungal, trachyomycotic and functional diseases. The development of these diseases stops, the plants are refreshing and their development continues within normal limits. Chelate solutions act on the plant and as a growth stimulant.

The tests carried out have shown the effective action of solutions of the developed chelating compounds against fungal, bacterial and vurus diseases of vegetable crops (verticillary wilting of eggplant, rhizoctonic wilting of pepper, mosaic of tomatoes).

Probably, the developed metal chelates of natural compounds cause structural and biochemical changes in plant tissues, the formation of new tissues at the sites of infection, which determines their normal development and an increase of fertility 2-3 times. Along with this, chelated compounds prepared according to an innovative method are absolutely harmless for people and the environment. Along with the above, chelated compounds prepared according to an innovative method are absolutely harmless for people and the environment.

The chelated complexes of natural compounds with practically favorite polyvalent metals are readily available and easily assimilated by the plant. They are effective in combating a number of intractable diseases of annual vegetable crops.

ANTIMICROBIAL EFFECT OF MONOVALENT COPPER IONS, POSSIBLE APPLICATIONS

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It has recently been reported[1,2] that monovalent copper ions have the ability to destroy microorganisms, bacteria and fungi. Although the mechanism of Cu^+ ions' antimicrobial effect is not, yet fully understood recently published results show that conditions of acidic pH, an unfavorable carbon source, and elevated temperatures boost the antibacterial action of Cu^+ ions. In less than 1 min, 0.4mM of Cu^+ ions eliminated a $10^6/cm^3$ *E.coli* bacterial population; microscopic images of *E.coli* morphology showed mortality of bacteria with almost no lysis.

The monovalent copper ion is unstable in water and without a suitable environment will undergo self-redox oxidation, in addition the monovalent copper ion reacts rapidly with molecular oxygen, so the use of monovalent copper ion for disinfection poses a technological challenge.

In this study, we will present systems that maintain an effective dynamic concentration of monovalent copper ions sufficient for complete elimination of bacteria and fungi populations. Including surface disinfections formulas, medical ointments for the treatment of skin infections[3], food disinfectant solutions and water disinfectant systems.

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DYNAMICS OF WHITE WINE OXIDABILITY DEPENDING ON TECHNOLOGICAL FACTORS: SULFUR DIOXIDE, IRON AND COPPER IONS

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Oxidation and the capacity for sufficient ageing potential of white wines are constant problems for winemakers worldwide. In general, it is accepted that certain grape varieties are especially sensitive to oxidation, suggesting that some of the chemical components key to their sensory attributes are strongly modulated by oxygen exposure. Of all the gases that can be dissolved in wine, oxygen and carbon dioxide can be considered the most important. Oxygen must be considered as a highly reactive chemical agent that has the potential to modify wine by oxidation.

The aim of this project is to carry out a detailed study of sulfur dioxide (SO_2), copper (Cu^{2+}) and iron (Fe^{3+}) ions distribution and concentrations in wine and their effect on the wine's quality and characteristics throughout different stages of the winemaking process.

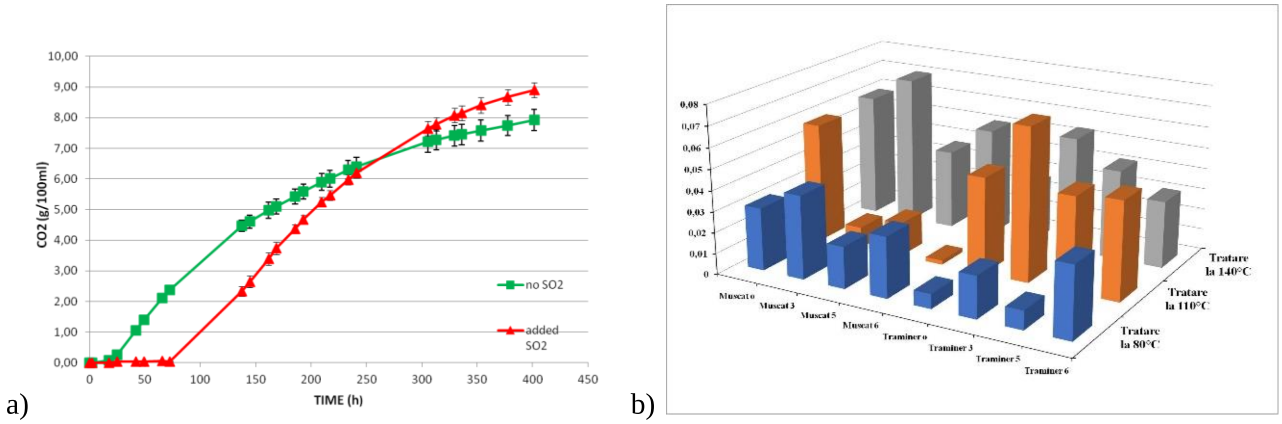

Fig. 1. Description of effects: a) the fermentation kinetics of the grape jus sample in the presence and absence of SO_2 in the fermentative medium and b) the color intensity for the wine samples experimentally oxidized with Iron and Copper ions at different thermal regimes

In laboratory conditions, by monitoring the oxidation processes throughout the technological process 2 dry white aromatic wines were developed. In the dynamics, a series of analyzes on the grapes, must and wine obtained, such as: physico-chemical indices, specific indices (pH, $OD_{420\ nm}$, antioxidant capacity, POM-test, other) were performed.

Generalizing the results of the experimental and applied presented study, it is revealed that the decomposition rates of oxygen in wines described a good correlation with the total concentration of exogenous copper and iron in the wine samples, both for total and residual concentrations compared to decomposition oxygen rates.

The results obtained in this research reveal remarkable new aspects about Cu and Fe speciation in white wine. They open new opportunities for further research on the influence of copper and iron speciation on winemaking.

Acknowledgment: This research has been performed within the State Program of the Republic of Moldova (2020-2023) Project Nr. 20.80009.5007.27 “Physical-chemical redox processes with electron transfer in the vital, technological and environmental processes”.running at Technical University of Moldova, Department of Oenology and Chemistry, Microwinery Center.

STUDY OF THE EVOLUTION OF POLYPHENOLIC CONTENT AND ANTIOXIDANT ACTIVITY OF LOCAL GRAPE VARIETIES AT DIFFERENT MATURATION PERIODS

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According to NBS [1], 462 thousand tons of grapes were cultivated in Republic of Moldova in 2020. Internal grape products are estimated annually at 450 - 500 million US dollars, which is an important contribution to the country’s budget [2]. On the other hand, in 2019, in Republic of Moldova were produced 178 thousand tons of wine, this ranking the country the 10th in Europe for winemaking [3]. Almost 80% of wines were exported, this representing the highest percent registered in the region [3]. This is a good indicator that confirms the high quality of Moldovan grape production and the important development that was achieved in grape and winemaking industry.

Grapes are excellent sources of various classes of polyphenols like phenolic acids, anthocianins, proanthocyanidins and stilbenes, each distributed differently within the grape tissues. At different maturation periods the content of different classes of compound varies significantly. For examples the anthocianins, which are the principal phenolic compounds responsible for the color in red grapes, accumulate in ripe berries. On the other hand, the proanthocyanidins accumulate in the pulp of unripe berries and then garner in the seeds during the veraison and ripening. The accumulation of these groups of compound in grapes is highly desirable due to their antioxidant activity [4] and to the beneficial effects of grapes on human health.

The present research reports the observations related to the evolution of the phenolic content and of the antioxidant activity of four grape varieties: Riton and Viorica – white grapes, and Feteasca Neagră and Copceac – red grapes. These are local grape varieties of new selection, characteristic for Republic of Moldova, this fact implying a big scientific and industrial interest. In order to study the dynamics of particular groups of compounds the sampling and the analysis were performed in unripen grapes, at the veraison and in ripe grapes. Three suitable extraction technics were used in order to ensure the maximum extraction of a specific group of compounds. The total phenolic content, the proanthocyanidins content, the anthocyanins content and the antioxidant activity was determined, and the correlation between this data was defined.

Acknowledgement: This work has been performed within the State Program of the Republic of Moldova (2020-2023) Project Nr. 20.80009.5007.27 “Physical-Chemical Mechanisms of the Redox Processes with Electron Transfer in Vital, Technological and Environmental Systems”.

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SYNTHESIS AND APPLICATIONS OF A NEW CATALYST BASED ON SILVER NANOPARTICLES INCORPORATED ON CATIONIC CLAY

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A facile, eco-friendly and cost effective method involving clay coating with silver was developed to prepare a microporous material BN-Ag^0 core shell with high catalytic and bactericidal /bacteriostatic activities against newly isolated bacterium from sewage sludge, named *ISO SS.* The catalytic activity of this nanomaterial in the mineralization process of Malachite Green and Tartrazine dyes was also tested.

Malachite Green (nature = basic green), classified in the dyestuff industry as a triarylmethane dye, usually used as a dyestuf for materials such as paper, leather, silk and controversially as a strong anti-bacterial, antifungal and antiparasitic agent in fish farming. Effects due to its presence in the environment by the accumulation of sediments in the aquatic environment can cause the disappearance of fish species or even aquatic life in time due to its toxicity. It is highly cytotoxic to mammalian cells and acts as a tumor enhancing agent. On humans, it possibly causes carcinogenic, mutagenic and teratogenic effects, if it may enters in the food chain.

Tartrazine is a stable water-soluble azo dye widely used as a food additive, which could pose potential threats to humans and the environment. It acts as a histological dye and food dye, being one of the most stable, edible and synthetic pigments. It is widely used as a food additive, such as coloring in beverages (juice drinks, carbonated beverages), mixed beverages and confectionery. In addition, it has a wide range of uses in the pharmaceutical, cosmetics, clothing and other industries.

For this purpose, a silica material (BN) coated with silver oxide was prepared, followed by the chemical reduction of silver with sodium tetrahydroborate (BN-Ag^0). The catalytic and antibacterial activities of the clay (BN) and its chemically modified counterpart (BN-Ag^0), along with its recyclability will be examined using diverse characterization techniques. The results obtained are expected to provide valuable findings for the preparation of a good silica core shell material with multiple functionalities.

Keywords: Silver, adsorption, catalyst, catalytic ozonation, dyes, bacteria.

DISINFECTION OF SEWAGE WITH THE HELP OF A SYSTEM THAT GENERATES COPPER IONS

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It has recently been reported[1,2] that monovalent copper ions have the ability to destroy microorganisms, bacteria and fungi. The monovalent copper ion is unstable in water and without a suitable environment will undergo self-redox oxidation, in addition the monovalent copper ion reacts rapidly with molecular oxygen, so the use of monovalent copper ion for disinfection poses a technological challenge.

In this study, we will present water disinfection systems that maintain an effective dynamic concentration of monovalent copper ions sufficient for water disinfection. We will present three different water disinfection systems suitable for batch and continuous disinfection. The first system is based on an ointment that releases monovalent copper ions to the solution (inspired by a patent[3]), the second in the form of a colona that in the first part filled with an ion exchanger loaded with divalent copper ions and in the second part metallic copper and the third based on copper electrodes.

The results of the study show that it is possible to treat wastewater containing microorganisms with the copper-based system. In addition, the quality of the water that had been obtained after the treatment is suitable for use in agriculture in accordance to the Israeli regulations.

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STUDY FOR DEVELOPING DEVICE TO PROCESS HUMAN FOOD WASTE TO ANIMAL NUTRITION

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Food waste is a dual problem, a waste of nutrition source and sanitation problems that accompany waste treatment. A new UN report states that food waste in the world is increasing: in 2019, 931 million tons of food were thrown away, a huge number, which not only embodies a huge financial and social loss, but also accelerates global climate change. So what can be done to reduce this unnecessary and harmful waste?

The discarded food waste has a very high nutritional value; It contains proteins, fats, sugars, vitamins and dietary fiber. The natural organic waste (without the artificial polymers) has great potential to be used to feed animals. The costs of feeding the animals are a significant part of the costs of producing meat, eggs and milk and they range in the range of about 55-72%.

Feeding them food waste can lower the cost range significantly. In addition, food waste may contain good nutritional values; Bioactive compounds such as unsaturated fatty acids, vitamins, carotenoids, peptides and polyphenols, which are present in food in small amounts and provide health benefits. Food waste contains a high liquid percentage of about 50-85%, which can significantly affect shelf life, waste collection and incorporation into animal diets.

Since the 1980s there has been a sharp decline in animal feed in food waste due to the fear of outbreaks of diseases as a result of the spread of contaminants found in food. That is why many countries in the world ban the feeding of animals from food waste.

The challenge: Development of a compact, multi-stage facility, designed to treat food waste in varying qualities and quantities as needed to obtain a dry and sterile product suitable for feeding omnivorous animals or as a food additive for other animals.

In this study, we will present food processing includes grinding, complete disinfection by disinfectant solution which does not harm the quality of the food, squeezing, drying and granulation to obtain a product suitable for feeding omnivorous animals.

RESIN ACIDS AS RAW MATERIAL FOR FABRICATION OF ANTIFUNGAL MICRO- AND NANOPARTICLES OF DEHYDROABIETIC ACID LOADED WITH CYCLODEXTRIN AND CHROMENOL HYBRID

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Vladimir VALICA[2], Livia UNCU[2], Victor KRAVTSOV[3], Dumitru TERTEAC[1,4],
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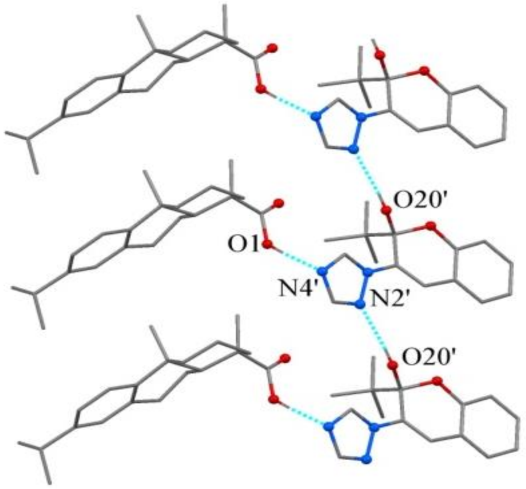
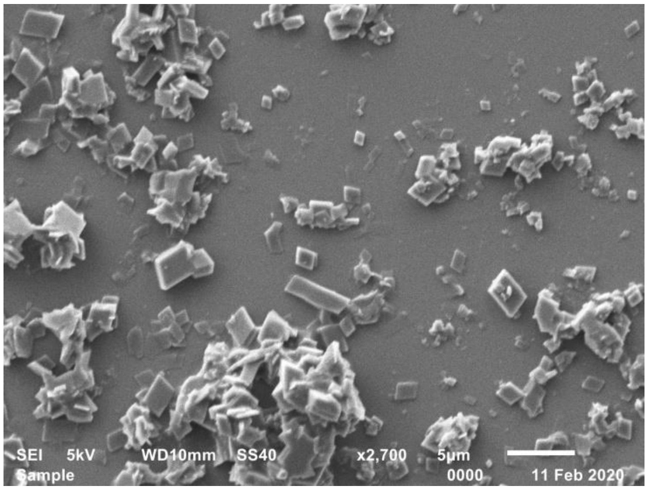
In these presentation methods to fabricate micro- and nanoparticulate systems from dehydroabietic acid and β-cyclodextrin with chromenol-triazol hybrid will be reported. Kneading, co-evaporation and co-precipitation as example of the resolution technology of racemic chromen-2-ol for obtaining micro- and nanoparticles has optimized. The inter- and intra-molecular interactions among ingredients were characterized by X-Ray, IR- and NMR spectroscopies.





The antifungal activity data of the obtained systems will be discussed. It was been shown that β-cyclodextrin microparticulate systems loaded with dehydroabietic acid and chromenol-triazol hybrid are as effective as pure components applied in higher dosages.

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PROPOLIS EXTRACTS FROM CENTRAL ZONE OF MOLDOVA AS AN ACCESSIBLE AND ALTERNATIVE THERAPEUTIC RAW MATERIAL

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Natalia BOLOCAN[1], Gheorghe DUCA[1], Svetlana ARMASU[1,3], Dumitru TERTEAC[1,3],
Vitalie CEBANU[3], Serghei TINCU[4], Alexandru ZNAGOVAN[4], Iulia NEICOVCENA[5],
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In the context of the Covid-19 coronavirus pandemic (SARS-CoV-2) situation, propolis was investigated, as an accessible and alternative therapeutic raw material, which rarely causes side effects. The results of the study of propolis extracts, collected in the central part of Moldova, showed that the nature of the solvent significantly affects the composition of the extracts, which differ in properties and can be recommended for the prevention of several diseases, including Covid-19. There were found 20 amino acids, of which the most abundant are glutamic acid, alanine, leucine and isoleucine. The main constituents of the alcoholic extract are pinocembrin, *n*-heptacosan and naringenin. The aqueous-alcoholic extract is characterized by the content of sakuranin, 4-methoxy sakuranetin, caryophylline oxide, isocaryophylline oxide, trans-longipinocarveol. Some components of the extracts, such as pinocembrine, have previously been proposed for the treatment of cerebral ischemia, intracerebral hemorrhage, neurodegenerative diseases, cardiovascular disease and atherosclerosis, also showing cardioprotective properties and a strong inhibitory effect on SARS-CoV-2 virus.

Acknowledgments: This research has been performed within the State Program of the Republic of Moldova (2020-2023) Project Nr. 20.80009.5007.17 "Hybrid materials functionalized with carboxyl groups based on plant metabolites with activity against human and agricultural pathogens". The authors are appreciates the contribution of the National Collection of Non-Pathogenic Microorganisms for the offering of the microbial cultures for testing.

ECOLOGY OF OIL INDUSTRY

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The oil and gas industry is one of the largest and fastest growing industries in the world today. There are various factors that can lead to oil spills which range from accidents, carelessness to deliberate dumping. Solutions are needed on ways in which we can deal with the devastating effects of oil spills.

Oil and natural gas products touch our lives in countless ways every day. Together, they account for more than 60 percent of our nation's energy.

Oil pollution has become a big problem today affecting the natural habitat of humans and many animals. The thing of human industrial operations, it threatens to mess with the oceanic environment that makes up more than 75 percent of our planet's surface. Tanker accidents are one of the popular causes of oil spills. Tankers can sometimes crash or run into un- expected land causing a crack or hole that allows oil to escape. They are highly publicized by the media and they release large volumes of oil into the oceans. Globally only a small percentage of oil spills occur as a result of tanker accidents such as explosions, hull failure, running aground or even collisions. Tanker accidents result in oil spills that are very harmful because of the large volumes of oil released at once.

As we have seen oil spills do much damage to the environment, Human health and also the economy. Some of the ways to deal with an oil spill include skimming which happens to be a popular method. It involves cleaning oil spills by skimming the oil from the water using skimming equipment with fine filtering instruments. These are chemicals (dispersants) that break down the tension that keeps water and oil separated. The oil will collect in smaller droplets and sink allowing greater natural breakdown. Another method that can be of help is to release biological agents into the water to help bring about breakdown. These agents include nitrogen and phosphorous which promote bacteria in the water helping the oil to disperse and breakdown naturally. N conclusion we know that oil plays a vital role in our lives which means that life as we know it would be hard without oil. Despite this oil spills have devastating effects on our environment, health and also economy leading to many of us calling for an alternative source of energy that can replace oil. Before a replacement for oil is discovered, human beings will have to continue to enjoy the benefits offered by oil and also suffer from the effects of oil such oil spills.

THE VARIATION OF THE BIOACTIVE COMPOUNDS CONTENT IN LETTUCE GROWN IN THE PRESENCE OF HEAVY METALS SALTS

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Heavy metals (e.g., Hg, As, Pb, Cd, and Cr) can accumulate and migrate in soil environments and due to their cumulative effects or long-term interactions can effects in the negatively way the crop yield and its consumers by entering in human bodies by the food contamination. The results can be observed in an increased incidence of chronic diseases (deformity of body or various types of cancer) and can disturb human metabolomics, contributing to morbidity and even mortality. Food security became thus a high-priority concern for sustainable global development. [1]

Scientific papers revealed that fruits and vegetables consumption is the primary pathway of human exposure to heavy metals and recommended to never using sewage wastewater to irrigate vegetables unless it is obligated. [2] They reveals that the untreated wastewater is the primary source of soil pollution, due to contaminated water containing high amounts of heavy metals and microorganisms and lead to increase the concentration of metals and pathogens on the lettuce. Using wastewater for a long time, this may lead to severe risk to consumer's health.

The aim of the present work consists of the evaluation of the heavy metals impact on bioactive compounds (e.g. assimilating pigments, polyphenols) from lettuce. The heavy metals taken into account were: Pb, Mn, Cu, Zn, Ni, Cd, having 3 different concentrations: one under accepted limit, one maximum accepted limit and one above maximum accepted limit. The growth of plants in the presence of different concentrations of the heavy metals salts was compared with those grown in the absence of salts. The influence of heavy metals salts on bioactive compounds and elemental content of lettuce were investigated by UV-Vis spectrophotometry. The correlation between the content of metals and biologically active compounds has also been traced.

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ASSESSMENT THE POTENTIAL OF BIOLOGICALLY ACTIVE SUBSTANCES OF YOUNG RED WINE PRODUCED FROM *RARĂ NEAGRĂ* (LOCAL GRAPE VARIETY)

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Recent trends promoting a healthy and active lifestyle have a negative impact on the consumption of sparkling and aged red wines. Therefore, consumers preferences focus on balanced and lighter wines, which also have a higher biological/physiological value, such as: local variety, country wines, young wines, white and rose table wines.

These varieties are the ones that have appeared on Moldovan land since ancient times, have adapted to the pedo-climatic conditions and have been preserved until the present, mentioning: *Feteasca Albă*, *Feteasca Regală*, *Zghihara*, *Plăvaie*, *Galbena*, *Crâmpoșie*, *Feteasca Neagră*, *Rara Neagră*, *Negru de Ialoveni*, *Francuș* and other.

The purpose of the present work is to establish the potential of *Rară Neagră* local variety producing red wine with characteristics of pedo-climatic *Purcari* areas conditions. Physico-chemical analyses of the wine have been evaluated by the international standards of International Organization of Vine and Wine (IOVV). The data concerning the main wine characteristics are presented in Table 1 and the diagram of grapes components antioxidant capacity evaluated by DPPH radical is included in figure 1. According to achieved results the skin grain present 85,3 % inhibition rate and 50% in pulp respectively.

Table 1. The 168entra-chemical indices of red wine obtained Rara Neagră locale grape varieties

Indices	**Determined parameters**						
	Mass ethanol concentration, % v/v	pH value	Mass concentra-tion of titrable acids, g tartaric acid /L	Mass concen-tration of sugar, g/L	Mass concen-tration of volatile acids, g acetic acid /L	Total poly-PH index mg/L	Conducti-vity at 20°C, µS/cm
Rara Neagră	13,27 ± 0,08	3,42 ± 0,01	5,88 ± 0,04	2,23 ± 0,06	0,39± 0,08	682,45 ± 0,1	1910 ± 6
Organoleptic analysis	Clear red wine, without particles in suspension. Red-ruby colour with bright. Aroma of plums, with no foreign flavors. The taste is complex, balanced with nuance of dry fruits.						

According to these data, the physico-chemical characteristics of red wine Rară Neagră variety are characteristic for a highest quality wine. Also, the major antioxidant capacity of *Rară Neagră* skin grain allows elaborating and implementing a modern technology to produce the high biological vineyards local varieties.

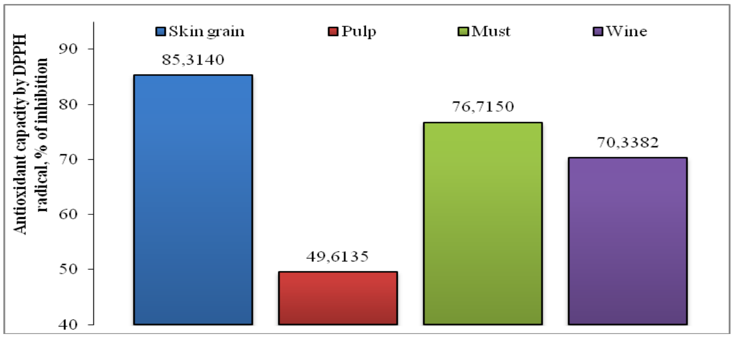

Fig.1. Antioxidant capacity of grapes components by DPPH radical, % of inhibition.

Acknowledgements: The research was funded by State Project 20.80009.5107.09 „Improving of food quality and safety through biotechnology and food engineering”, conducted at Technical University of Moldova, Department of Oenology and Chemistry, Microwinery Center.

STUDY OF ADSORPTION PARAMETERS OF AUTOCHTHONOUS CARBON ENTEROSORBENTS

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Anthropogenic factors of environmental pollution are increasingly affecting the health of the human body, being the cause of many diseases with a negative impact on quality of life. Focused on the elimination of endo- and exogenous toxic substances from the human body, research in the field of enterosorption is in a continuous process of identification of new enterosorbent products. At the top of the demands are enterosorbents prepared from activated carbons of vegetal origin (fruit kernels, walnut shells, grape seeds etc.), because their morphological structure favors the obtaining of adsorbents with a high mechanical strength and increased adsorption capacity.

In the Ecological Chemistry laboratory of the Institute of Chemistry, using different methods and conditions of activation, a set of activated carbons was obtained in order to identify samples with potential of use as enterosorbents.

The testing of the adsorption power of the autochthonous carbon adsorbents was performed with the use of Antipyrine, according to the requirements of the European Pharmacopoeia Monograph (EPM) for enterosorbents. The obtained results allowed us to select two samples of activated carbon (AC-MR and AC-C, obtained from apple wood and apricot kernels) which showed an adsorption power greater than 400 mg/g, which corresponds to the requirements of the EPM. The research of the influence of the granulometric composition of the investigated carbon adsorbents on the adsorption capacity compared to Antipyrine shows a considerable increase (about 30 %) of the adsorption power value with the decrease of the carbon particle sizes (from 800-2000 μm to 90-125 μm).

The Quinacrine dihydrochloride ($C_{23}H_{30}ClN_3O \cdot 2HCl$) was used as adsorbate for the study of adsorption parameters of autochthonous activated carbon AC-MR. The adsorption kinetic curves were determined for two concentration values (200 mg/l and 500 mg/l) in a time interval between 15-300 minutes. Adsorption isotherms were measured, modeling the parameters of temperature and pH according to the values of the human body. It has been established that the adsorption of Quinacrine dihydrochloride on AC-MR is an endothermic process but the influence of the temperature factor (studied values: 25ºC, 35ºC and 45ºC) on the degree of immobilization is insignificant. The increase of the pH from 2.0 to 7.0 is accompanied by a practically double increase in the rate of Quinacrine dihydrochloride immobilization.

The realized study regarding the adsorption parameters of autochthonous activated carbon AC-MR attested the compliance of the adsorption power against Antipyrine with the requirements of the European Pharmacopoeia Monograph and suggests that this sample of carbon adsorbent is of interest for use as an enterosorbent.

Acknowledgments: The research leading to these results has received funding from the institutional project DISTOX, number 20.80009.7007.21: "Reducing the effects of toxic chemicals on the environment and health through the use of adsorbents and catalysts obtained from local raw materials".

THE IMPACT OF SOIL POLLUTION WITH ANTIBIOTICS ON SOIL MICROORGANISMS AND FOOD SAFETY

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Exposure to antibiotic-resistant bacteria from natural and agricultural ecosystems such as soil can significantly affect the health of the human microbiome. Much of the antibiotics excreted by animals and humans reach the soil by applying manure and sewage sludge as organic fertilizers. Inevitably, antibiotics affect native microbes, increasing the development of microbial resistance to antibiotics. Even in small doses, they can cause a toxic effect and form antibiotic resistance of microorganisms. Numerous researchers have studied the accumulation and spread of antibiotic resistance genes in manure-treated soil microorganisms, as well as in vegetables grown on this soil. These studies demonstrated the presence of antibiotic residues and antibiotic resistance genes in manure-treated soil. These residues could persist in the soil for a long time. Meanwhile, antibiotic resistance genes have also been detected in cultivated vegetables.

Varieties of tetracycline and related resistance genes have been detected, especially in soils treated with wastewater from pig farms. Soil quality has been affected by relationships with bacterial abundances and microbial geochemical functions. *Proteobacteria* and *Bacteroidetes* have been spread and positively correlated with antibiotic resistance genes in soils, indicating that there are potentially antibiotic-resistant bacteria in the soil. Antibiotics and antibiotic resistance genes have also been detected in vegetables. Some vegetables from these soils were infested with *Rickettsiales* intracellular parasites (positively correlated with antibiotic resistance genes), indicating potential risks to consumer health. *Rickettsiales* is an order of the class *Alphaproteobacteria,* obligate intracellular parasites of eukaryotes that are responsible for a wide range of important human diseases, including anaplasmosis, rickettsiosis, and typhoid fever. A study of soil samples from agroecosystems grown with peppers (*Capsicum annuum*), vines (*Vitis vinifera*), raspberries (*Rubus idaeus* L.), parsley (*Petroselinum crispum*) showed that the microbial community is characterized by a high content of antibiotic-resistant microorganisms. Anaerobic and aerobic microorganisms with antibiotic resistance were isolated from the soil: *Clostridium perfringens*, *Clostridium oedematiens*, *Clostridium difficile*, *Enterobacter cloacae*, *Enterococcus faecalis*, *Hafnia alvei*, *Bacillus megaterium*, *Bacillus mycoides* and *Pseudomonas aeruginosa*.

The risk of introducing more antibiotic-resistant genes and antibiotic-resistant bacteria into vegetables through organic production procedures requires further investigation. Antibiotic residues can select endophytic bacteria resistant to antimicrobial substances, which are not removed by washing or peeling food raw materials of plant origin. Agricultural management systems must not allow an increase in the burden of antibiotic resistance of harvested crops**.**

Asknowledgement: The work was carried out within the State Program of the Republic of Moldova (2020-2023) Project Nr. 20.80009.5107.08 «Efficient use of soil resources and microbial diversity by applying the elements of organic (organic) agriculture».

SUNFLOWER CROP AND AGRO-ECOLOGICAL APPROACH TO SOIL CONSERVATION AND REDUCING CHEMICAL INPUTS

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Population growth and climate change are the main challenges of the 21st century, and the agricultural sector is directly or indirectly involved in solving both. The vulnerability of the agricultural sector increases as a result of fluctuations in temperature and precipitation regimes, the more frequent manifestation of atmospheric and soil moisture droughts with the subsequent reduction of the yield level. As a result, the rate of chemical inputs in the form of pesticides and fertilizers increases, which in turn has an impact on soil quality and biodiversity.

Among the activities of adaptation to climate change we can mention: the implementation of agro-ecological approach and use drought and heat stress-tolerant crops. Sunflower is a crop that has agro-ecological perspectives and also has increased resistance to drought. Agro-ecological approach aim to: reduce the impact on the environment, by reducing or eliminating chemical inputs; strengthening the sustainability of agro-ecosystems by promoting techniques that increase natural pest control; optimizing the metabolism of agroecosystems by organizing the recycling of nutrients; improving the conservation and regeneration of soil, water resources and biodiversity.

Sunflower can be considered an “organic” crop for several objective reasons:

1. The crop requires a limited amount of N (50-60 kg / ha) fertilizer, which is done directly or indirectly by a low greenhouse gas emitter.

2. In the conditions of our country it is primarily cultivated as a non-irrigable crop, even in the situation where it would be irrigated, it needs limited amounts of water (around 50 mm).

3. With the exception of herbicides, very few other pesticides (fungicides, insecticides) are used in sunflower crops. But it is also possible to control weeds by mechanical work, because the width of the rows is usually 70 cm, thus reducing the amount of herbicides.

4. It has advantages in stimulating the nutrient circuit, because the root system can absorb water and nutrients from the deeper layers of the soil and the rapid degradation of crop residues leads to the return of nutrients to the system and increase their availability for subsequent crops.

5. Sunflower has the potential to provide multiple ecosystem services in various cultivation systems this crop is an important source of pollen and nectar. Its contribution to the aesthetic value of the landscape should be highlighted, although this service seems difficult to assess correctly.

Although sunflower crop is considered by farmers to be traditional, efficient, tolerant of water stress, and easy to manage, it suffers from low productivity due to a number of limiting factors:

1. Plowing is still widely used for primary soil tillage, as sunflower needs uncompacted soils for the formation and branching of the root system.

2. Sensitivity to diseases and pests, which involves a rotation of at least 5-6 years. But the use of pesticides can be reduced by cultural and genetic control. Considering the results of surveys with farmers, this trend is emerging in our country.

In conclusion, we can mention that in the current and future context of climate change, agro-ecological approach can be a solution and sunflower is a perspective crop from this point of view.

THE ACIDIFIER FROM UNRIPE APPLES – SOURCE OF NATURAL ACIDITY

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The unripe apples, obtained from agrotechnical operations or physiological falls, are not used for food. These are a source of natural organic acids, the dominant being malic acid (about 70-90%) [1, 2], and other valuable substances. In the food industry there is a need for sources of natural acidity. For this purpose, experimental samples of acidifiers from unripe apples were obtained [3]. At the same time, the rational use of these fruits will contribute to solving ecological problems [4]. In this paper, the content of dominant organic acids in apple acidifiers was studied.

The acidifiers were obtained from unripe apple fruits of 4 varieties: Coredana, Golden Rezistent, Rewena și Reglindis. These were picked between June 1 and July 24, 2020 from the experimental lots of the Scientific-Practical Institute of Horticulture and Food Technologies, Chisinau, Republic of Moldova. The fruts were harvested during development at 45th, 58th, 71st, 84th and 97th days after the full bloom. The titratable acidity, expressed in malic acid, was determined by titration with alkaline NaOH solution (0.1 N) in the presence of the phenolphthalein indicator [5]. The concentrations of malic and citric acids were determined by the capillary electrophoresis method [6].

In this paper, the titratable acidity and the content of predominant acids in apple acidifiers were studied. According to the literature, the dominant acids in apples are malic and citric [7]. The titratable acidity decreases on average from 29,5 $^{g}/_{dm^3}$ to 12,0 $^{g}/_{dm^3}$. The content of organic acids during fruit development decreases, as a large part of the acids are used in the process of respiration and are converted into carbohydrates. [8].

In acidifiers the content of malic and citric acid varies between the limits 16,35 $^{g}/_{dm}{}^{3}$ and 9,24 $^{g}/_{dm}{}^{3}$ and, respectively, 2,86 $^{g}/_{dm}{}^{3}$ and 1,68 $^{g}/_{dm}{}^{3}$, depending on the variety of apples from which they were obtained and the period of their harvest (figures 1 and 2).

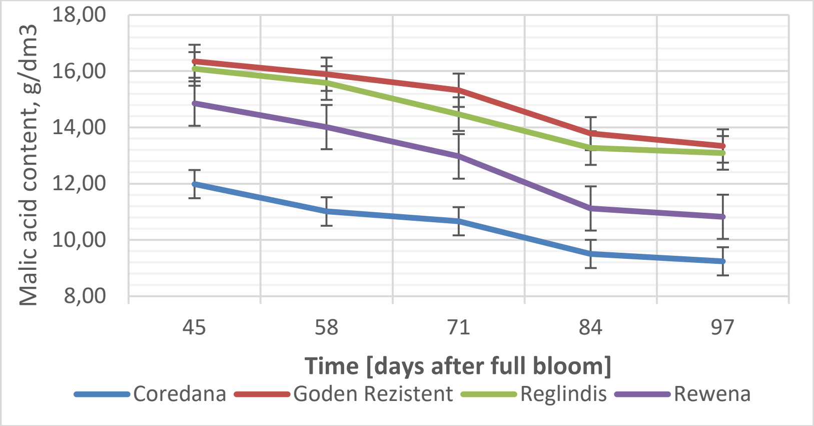

Fig. 1. Malic acid content in acidifiers from unripe apples of varieties Coredana, Golden Delicios, Reglindis, Rewena during the development of fruits. Source: authored

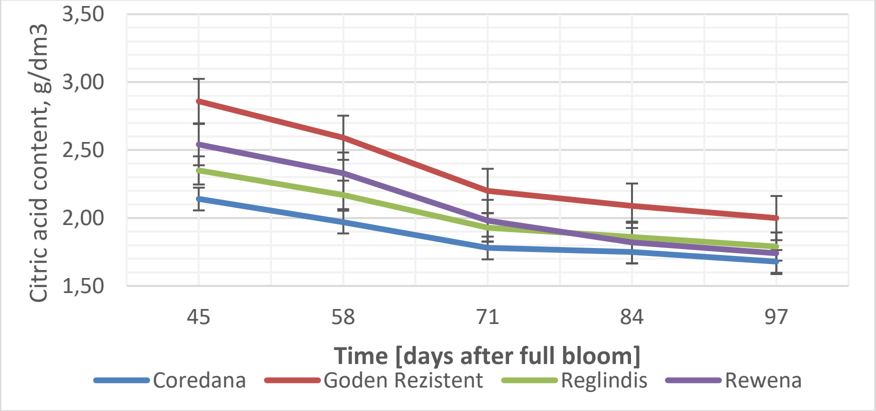

Fig. 2. Citric acid content in acidifiers from unripe apples of varieties Coredana, Golden Delicios, Reglindis, Rewena during the development of fruits. Source: authored

All types of acidifiers contained a relatively high concentration of malic acid and citric acid, representing 71.09% - 81.24% and 8.66% - 14.46% of the total acidity content.

The apple acidifiers contain significant amounts of native organic acids, the dominant acids being malic and citric. They can supply the necessary sources of natural acidity in the food industry, especially in the preservation of fruits and vegetables, substituting acidifiers of chemical / biochemical origin. This can improve the nutritional value of food.

Also, obtaining fo acidifiers from unripe apples as a source of acidity for the food industry is an important direction in the context of sustainable development.

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PROFILE OF LIPOPHILIC AND HYDROPHILIC EXTRACTS FROM *FETEASCA NEAGRĂ* BY-PRODUCTS

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Abstract: Grapes grown in Republic of Moldova are widely used in the wine and juice industry, whereas, the functional compounds, recovered from wine by-products, are not fully exploited. After analyzing the seeds separated from fermented pomace of the local *Feteasca Neagră* (*Black Maiden)* grapes, grown on the vineyards of Nisporeni (F_N), Hâncești (F_H) and Speia village, Anenii-Noi (F_S), in the season of 2020, the physico-chemical indicators as well as the content of the bioactive substances in lipophilic and hydrophilic extracts, were determined. The content of carotenoids and polyphenols, in lipophilic extracts, was determined by spectrophotometric methods. F_N and F_S oils have an increased carotenoid content, of 49.703 ±0.424 and 48.533 ±0.466 mg/100g of oil. The highest concentration of phenolic compounds was recorded for the F_N oil, of 4.89± 0.05 mg GAE/100g of sample (which is approximately 0.005%). The oil quality indices were also determined.

Hydrophilic extracts were obtained by the ultrasound-assisted extraction method. The total content of polyphenols (TPC) and flavonoids (TFC) in the hydrophilic extracts from non-degreased (I) and degreased (II) grape seeds, was determined by colorimetric methods, with Folin Ciocalteu reagent. Results were expressed in mg GAE/g, mg QE/g and mg RhE/g of seeds. It has been proved that seed degreasing leads to a better solubilization of polar substances, therefore, extracts II contain up to 28.30% more polyphenolic compounds, compared to extracts I. However, the spectrophotometric analysis with $AlCl_3$, showed that washing and degreasing the seeds with hexane-n, removes the protective layer of tannins – the soluble proanthocyanidins on the surface of the seeds, and reduces the content of flavonoids in extracts II. Research shows a TPC twice higher in F_N extracts II, if compared to F_H and F_S. Meanwhile, the highest TFC was detected in F_H extract I. The difference between the content of biologically active substances in F_N, F_H, and F_S seeds is permissible within the same grape type, and is largely due to cultivation conditions. After determining the antioxidant activity (the Trolox equivalent antioxidant capacity assay), it was noted that the lipophilic and hydrophilic extracts from *Feteasca Neagră* seeds inhibit the DPPH free radical, the highest value being recorded for the hydrophilic extracts.

Grape seeds are a valuable source of bioactive substances and phytonutrients, which can be recovered and then incorporated into various foods, thus increasing their nutritional value and turning them into functional foods with health benefits.

Keywords: antioxidant capacity, flavonoids, grape, phenols, seeds, oil, waste

Acknowledgment: The research was carried out with the support of the Moldova State Project 20.80009.5107.09 “Improvement of food quality and safety by biotechnology and food engineering”.

STRUCTURAL, SPECTROSCOPIC AND DFT STUDIES OF A COMMON FOOD PRESERVATIVE «E202» AND INVESTIGATION OF ITS IN-VITRO ANTIMICROBIAL ACTIVITY

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Sorbic acid «E200» and its salts like potassium sorbate «E202» are commonly used as preservatives in food. Potassium sorbate may find more frequent applications because of its greater solubility in water. Moreover, Researches during the 1950s demonstrated the impressive effectiveness of sorbate against many microorganisms such as bacterial species, yeasts and molds…. However, microbial inhibition by sorbate is variable, which could lead to defective food products. This study is focused on the investigation of antimicrobial activity of potassium sorbate in presence of numerous microbial species, in different concentrations of sorbate, pH and temperature, in order to define the suitable conditions.

Potassium sorbate has been provided by QUIMIDROGA, LC-MS analyze confirmed its purity. The product has been then characterized by X-ray, ATR, UV and 1H-RMN.

For the first time, the optimized geometry of potassium sorbate was approved with the Gaussian 09 software using DFT functional. The theoretical vibrational frequencies and optimized geometric parameters have been calculated using (DFT/B3LYP-D3), (DFT/M05-2X) and (DFT/M06-2X) with 6-311+G(d) basis set. Considerable level of correlation with the corresponding experimental results has been noticed when using DFT/M06-2X with 6-311+G(d) basis set ($R^2 = 0.99913$).

Furthermore, TD-DFT approach and NBO analyzes were used to explore the excited states of sorbate anion in liquid phase, using SMD model. NMR chemical shifts of the molecule are determined by the gauge independent atomic orbital method.

Nucleophilic sites are found by molecular electrostatic potential. HOMO, LUMO and HOMO-LUMO gap, recorded from -6.30 to -1.55 eV, are used to calculate global reactivity descriptors according to FMO theory. The results show that charging easily transfers in sorbate, and this affects its biological activity, which can explains experimental results on antibacterial and antifungal activities.

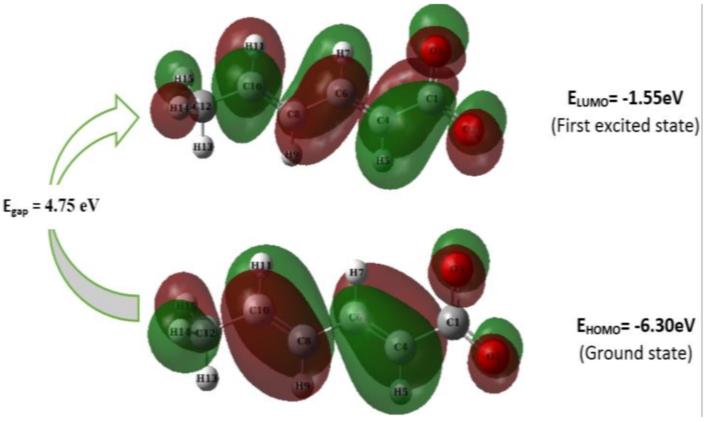

Fig.1.Graphical representation of Calculated HOMO–LUMO.

THE INTERACTION OF RHODOCOCCUS RHODOCHROUS CNMN-AC-05 WITH $CoFe_2O_4$/PEG NANOPARTICLES ANALYSED BY METHOD OF CONFOCAL LASER SCANNING MICROSCOPY

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Bacteria of the genus *Rhodococcus* play an important role both in the processes of soil formation and in their use for bioremediation of soils, as well as for wastewater treatment [1]. Along with this, immobilized *Rhodococcus* cells on various substrates have shown that they can act as effective biocatalysts for the decomposition of carbon-containing pollutants. The interaction of *Rhodococcus rhodochrous* CNMN-Ac-05 with Fe_3O_4/PVP nanoparticles was studied earlier and the effect on cells viability and morphological variability was determined [2]. Thus, the combination of magnetic ferrites and bacterial cells is interesting. Fig.1 illustrates the results of incubation of *Rhodococcus rhodochrous* bacterial cells with magnetic nanoparticles stabilized with polyethylene glycol $CoFe_2O_4$/PEG of dimension 80 – 150 nm, collected in glucose medium after 1, 5 and 24 hours. The study was carried out using a confocal laser microscope ZEISS LSM 900 (Carl Ziess, Germany).

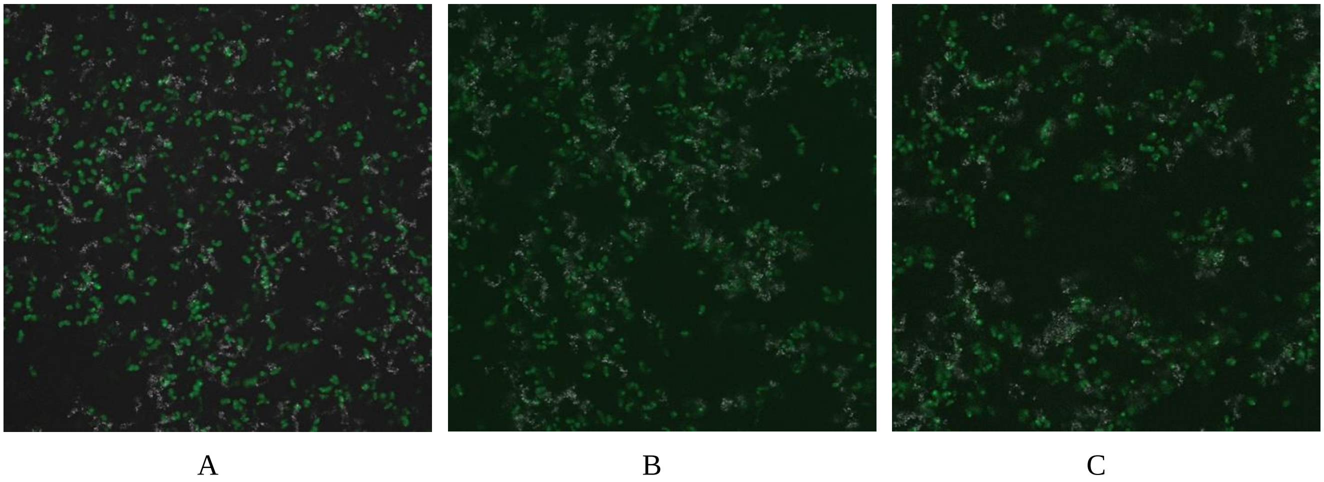

Fig.1. Microfotographs of the bacteria Rhodococcus rhodochrous CNMN-Ac-05 attached to the surface of Nps $CoFe_2O_4$/PEG, at magnification 630 × after 1 (A), 5 (B), 24 (C) hours.

The method of Confocal laser microscopy allows to visualize directly the localization of bacterial cells on nanoparticles. Over time, we observe sequential adherence of bacterial cells to agglomerated nanoparticles and this process is irreversible, which indicates the predominance of chemical interaction over electrostatic, and this is obviously the result of influence of polyethylene glycol film formed on nanoparticles during synthesis. The observed effect can be used for creation of a nanobiocomposite eliminating of pollutants.

Asknowledgement. The work was done within the State Program of the Republic of Moldova (2020-2023), Project Nr. 20.80009.5007.11: "Funcțional Nanostructures and Nanomaterials for Industry and Agriculture".

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ADSORPTION OF *p*-COUMARIC ACID ONTO OENOLOGICAL ACTIVATED CARBONS

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Phenolic substances have been reported as being responsible for wine colour, mouthfeel perception and flavour. From the phenolic compounds, the *p*-coumaric acid is of great interest because in wines its bioconversion by *Brettanomyces* sp. Into ethylphenols damages the quality product.

Nowadays, activated carbons have great applicability in the conditioning of wines: discoloration, removal of foreign taste and smell, correction of organoleptic parameters, etc.

The purpose of this work was to perform adsorption experiments of *p*-coumaric acid from water solutions on two activated carbons: (i) commercial activated carbon FA (Granucol, Germany) and (ii) of local origin ones AC-C, obtained from apricot stones (Republic of Moldova).

The adsorption kinetics of *p*-coumaric acid from solution on activated carbons was studied at different initial concentrations (1, 3, 4.5 mM), at a solid/liquid ratio of 1/1000, for 4-6 hours of contacting. For both activated carbons studied (FA, AC-C), the adsorption equilibrium of *p*-coumaric acid is established in 1-2 hours. At the same time, in the first 10-15 minutes of contact, about 70% of the total amount of *p*-coumaric acid is absorbed.

The adsorption capacity of the studied activated carbons (FA, AC-C) for *p*-coumaric acid was determined from the adsorption isotherms, constituting 1.8 and 2.5 mmol/g for FA and AC-C, respectively.

The obtained experimental results were analyzed by applying the kinetic models: pseudo-first order model, pseudo-second order model and intraparticle diffusion model, as well as theoretic isotherms models of Langmuir, Freundlich, Temkin-Pyzhev and Dubinin-Radushkevich. The experimental data are best described by the pseudo-second kinetic model and Langmuir model suggesting that the adsorption of *p*-coumaric acid onto activated carbons is based on chemisorption.

Acknowledgements: This work was carried out within the Moldovan State Program (2020-2023) Project "Reducing the impact of toxic chemicals on the environment and health through the use of adsorbents and catalysts obtained from local raw materials", Project no. 20.80009.7007.21.

SYNTHESIS AND STRUCTURE OF TANNIN/BENTONITE-DERIVED BIOCHAR

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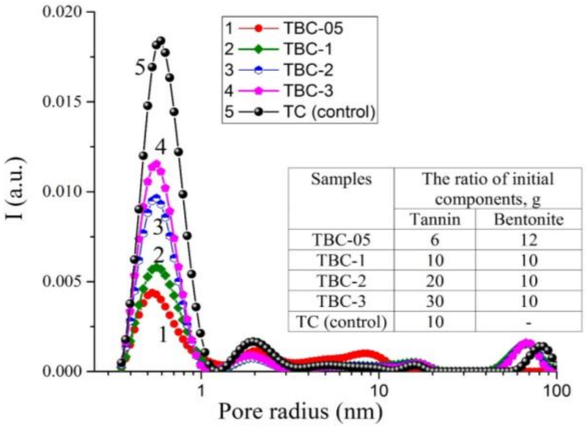
Novel hybrid carbon-mineral composites were synthesized by mechanochemical activation of a mixture of tannin and bentonite in a ball mill with further pyrolysis in an argon atmosphere at 800 °C. Biomass-derived, cheap, nontoxic and abundant tannin was used as carbon precursors. The influence of the tannin content (Table 1) on the morphological, textural and structural characteristics of biochar has been described. It is worth noting that no solvents were used during synthesis process, providing a "Green chemistry" technology. Furthermore, proposed pyrolysis allows synthesizing nanostructured hybrid materials retaining the structural advantages of bentonite (mesoporosity) and adding new structural characteristics due to a carbon component.

The composites were characterized via N_2-adsorption/desorption, TGA analysis, Raman and FTIR spectroscopy. The calculated BET surface area was 84, 127, 194, and 230 m^2/g for TBC-05, TBC-1, TBC-2, TBC-3, and control carbonized Tannin composite (TC), respectively. It was investigated that the increase in tannin content led to an increase in the volume of nanopores (from 0.6 to 0.8 cm^3/g) with a simultaneous decrease in the mesoporosity of biochar (from 0.4 to 0.1 cm^3/g) due to the formation of the carbon phase in the interplanar spaces of bentonite.



Samples	The ratio of initial components, g	
	Tannin	Bentonite
TBC-05	6	12
TBC-1	10	10
TBC-2	20	10
TBC-3	30	10
TC (control)	10	-

Figure 1. Pore-size distributions of composites

Thus, different particle sizes, shapes, specific surface area and degree of graphitization characterize the as-synthesized biochar. These characteristics show the effectiveness of the proposed approach to develop microporous and/or mesoporous structures in hybrid carbon-mineral composites.

SYNTHESIS OF POLYMER SYSTEMS FROM N-VINYLPYRROLIDONE WITH HYDROXYMETHYL DERIVATIVES OF TRANSITION METAL PHTHALOCYANINES FOR PHOTODYNAMIC THERAPY

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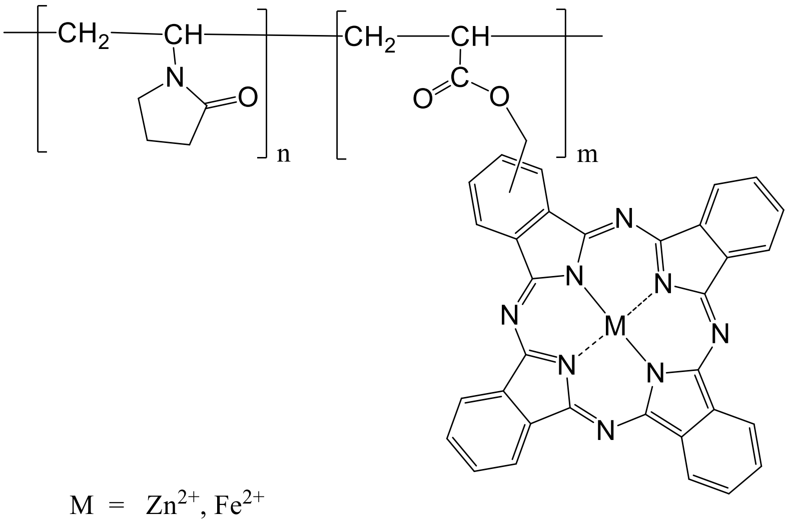
This work describes and presents methods for the synthesis of hydroxymethylphthalocyanines of transition metals (zinc, iron) and the possibility of grafting them to copolymers of N-vinylpyrrolidone (N-VP) with acryloyl chloride (Acl) to obtain environmentally friendly polymers for photodynamic therapy:



M = Zn^{2+}, Fe^{2+}

Hydroxymethyl phthalocyanines were obtained by hydroxymethylation of corresponding phthalocyanines in the presence of urotropine.

Copolymer (N-VP):(ACl) were obtained by polymerization of N-vinylpyrrolidone and acryloyl chloride in the presence of 2.0% azo-bis-isobutyronitrile, at a temperature of 80° C for 4 hours, the ACl content was 10, 20 and 30 mol %. The obtained copolymers were purified by sedimentation from hexane. The intrinsic viscosity of such copolymers range from 0.06 to 0.10.

The grafting of hydroxymethyl phthalocyanines to copolymer (N-VP):(ACl) was carried out in carbon tetrachloride in the presence of triethylamine. The chemical structure of the copolymers (N-VP): (ACl), as well as the polymer analogs with hydroxymethyl phthalocyanines (N-VP): ($AOCH_2Phc$) was confirmed from the IR spectrum data. UV-VIS spectrum data and find toxicity at the molecular level for polymers (N-VP):($AOCH_2Phc$) suggests that these materials are prerequisites for further tests of photodynamic activity.

Acknowledgements

This work was supported by the research project "Photosensitizers for photodynamic and photovoltaic therapy".

MICROBIOLOGICAL CHARACTERISTIC OF SOIL FOR THE BIOREMEDIATION OF POPs CONTAMINATED SITES

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Elena NICOLAU[2], Elena CULIGHIN[2]

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Problems with contaminated sites exist in most European countries and important for Republic of Moldova. The inventory of old pesticide storages in Moldova, executed in 2009 – 2010 years, showed a large quantity of POPs contaminated sites. The risk assessment of contaminated sites provided their ranking and high risks. Despite the realized projects the area of POPs management, still a lot needs to be done for the remediation. In situ soil treatment is a good approach because leaves the soil structure intact, reduces the potential migration of contaminants through soil and water systems, for example in situ bioremediation, phytoremediation, or natural attenuation. In this case, the soil structure is not dramatically transformed and there are no limitations for its future use, as these techniques aim to reduce the total quantity of contaminants in the site. The case study for one POPs contaminated site is presented in this presentation. The toxic substances were studied for the different zones of the selected site for the delineation of different contaminated zones and risk assessment procedure. The interval of the total concentration of POPs substances in soil is changed from 0.31 to 214.9 mg/kg dry soil. The composition of the indigenous population of microorganisms involved in nitrogen transformation and survived in the hard conditions of a long-term toxic stress of contaminated soil was determined for the elaboration of the remediation approach. An analysis of microbial population revealed that the total number of these microorganisms in the polluted soil ($5.31x10^6$CFU/1g dry soil) was by 5.3 times lower than in the reference soil. It has been observed that, under the long-term influence of the toxicants, the restructuring of the soil microbial cenosis took place in the direction of the decrease of the microbial diversity, but with the appearance of more resistant species. The number of bacteria involved in nitrogen transformation processes (bacteria that assimilate mineral nitrogen, oligonitrophilic and ammonifying bacteria) was reduced in polluted soil in 3-8 times in compare with the reference soil. The number of micromycetes and *Azotobacter* spp. was small, the representatives of the group of actinomycetes were not observed.

The preliminary laboratory experiment by the bioremediation showed that the contamination spectrum and concentration as far as the soil microbiological diversity should to be determined for the appropriate remediation project design.

THE PROTECTIVE EFFECT OF VINYL TRIAZOLE DERIVATIVES IN SOME FUNGAL DISEASES IN WHEAT

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Root rot is considered one of the most common diseases in crop plants, including the common winter wheat *Triticum aestivum* L. The disease is caused by various soil pathogens, among which Fusarium fungi are noted with advanced incidence and severity. These pathogens reduce plant biomass due to obstruction of water and nutrients entry into the plant.

As research material served: 1) common autumn wheat grains of 2 genotypes – L SBS and L M / M3); 2) culture filtrate (CF) of the fungus *Fusarium oxysporum*; 3) vinyl-triazolic derivative ((z) -1- (2,4-dichlorophenyl) -5-methyl-2- (1h-1,2,4-triazol-1-yl) hex-1-en-3- one) – EPS 165 in concentrations of 0,005 and 0,01%. CF *F. oxysporum* was prepared by inoculating the fungal mycelium into the liquid nutrient medium Cszapek. The wheat grains well selected on the basis of uniformity and size were treated for 3 hours with the emulsion of the mentioned compound in concentrations of 0,005 and 0,01%, after which they were dried in the open air at room temperature for 48 hours.

The emulsion of the preparation was obtained by adding dimethylsulfoxide of 9%, TWIN-80 emulsifier of 20% and ethanol of 70% to the investigated compound, taken in a concentration of 1%. Wet grains soaked in distilled water for 18 hours served as control I, and grains soaked in CF *F. oxysporum* for 18 hours served as control II.

The outdoor dry mass per plant (mg), determined by weighing, was used as a criterion for resistance/sensitivity to the pathogen. The results obtained are presented in the table bellow.

Table. Influence of study variants on the dry biomass of wheat seedlings at their interaction with *F. oxysporum* (SBS Line)

Nr.	Variant	Dry biomass per plant, mg	σ	In comparison to Control II, %
1	H_2O – Control I	10,77±0,39	0,68	137,9
2	CF *F. Oxysporum* – Control II	7,81±0,23^{v}	0,39	-
3	Compound EPS165- 0,01% + CF *F. Oxysporum*	10,65±0,06*	0,10	136,36
4	Compound EPS165- 0,005% + CF *F. Oxysporum*	10,31±0,04*	0,07	132,01

**- statistically significant difference in relation to "CF F. oxysporum", p≤0.05. –*

v- statistically significant difference in relation to "Control I", p≤0.05.

According to the data from the table, the treatment of common winter wheat grains with compound EPS 165 in concentrations of 0,01- 0,005% leads to an increase in the amount of dry biomass in comparison to the control- *F. oxysporum* by 32,01-36,36%.

Acknowledgement

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BEECHWOOD BIOCHAR FOR THE IMMOBILIZATION OF HEAVY METALS IN CONTAMINATED SOILS: COLUMN TESTS AND SIMULATION MODEL

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This paper presents a one-dimensional simulation model which aims to trace the concentration profile observed by two laboratory columns, filled with soil and biochar, crossed by a solution contaminated with Lead. The laboratory columns are characterized by an alternation of layers, the first of sand and soil and the second of sand, biochar, and soil. Soil is considered the target of contamination. The experimental investigations made it possible to verify that the soil layer induces a delay in the transport process which is further amplified by the presence of the biochar which therefore acts by immobilizing the contaminated solution at least partially.

The simulation model was built starting from the transport equation in which the delay factor was simulated with first-order kinetics for the action of the soil and with pseudo-second-order kinetics for the biochar. In the latter case, the kinetics were experimentally determined with appropriate batch tests; the constant characteristics determined experimentally were used within the simulation model. The results of the model satisfactorily simulate the experimental results; the model could therefore usefully simulate different operating conditions and be a useful tool for remediation activities.

CRITICAL REVIEW OF THE ANALYTICAL METHODS BASED ON THE HPLC-ELECTROCHEMICAL SENSOR COUPLING

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This paper would like to review the literature concerning the coupling of High Performance Liquid Chromatography (HPLC) with the Electrochemical Detection (ED). HPLC is an analytical separation technique to which a detector is coupled at the outlet of the chromatographic column. There is currently no universal detector for HPLC. Electrochemical sensors are competitive with respect to the detectors currently used.

In terms of sensitivity and selectivity no optical detector (e.g., UV-Vis, Fluorescence, Refractive Index RI) nor aerosol-based detector (i.e., Evaporative Light Scattering Detector ELSD, Nano Quantity Analyte Detector NQAD, Charged Aerosol Detector CAD) can compete with the electrochemical detector. Whenever an analyte is electroactive, i.e., can undergo oxidation or reduction, electrochemical detection (ED) can be applied.

HPLC-ED approach is an extremely selective and sensitive detection technique that is applied in many analyses in agricultural, environmental and food field. It should be considered that ED has an enormous linear dynamic range of more than 6 orders of magnitude. This means that concentrations as low as 10 pmol L^{-1} and as high as 500 μmol L^{-1} or more can be detected.

The papers present in literature on the HPLC-ED technique applied to resveratrol, rosmarinic acid, aromatic heterocyclic amines and glyphosate in matrices such as meat, aromatic plants, fruit and tomato juices, will be analyzed and discussed.

The aforementioned papers have shown that electrochemical sensors used as detectors for HPLC can offer better sensitivity values than other detectors. Furthermore, the use of specific working potentials allows to avoid matrix interference by almost exclusively determining the analytes of interest. It follows that the HPLC-ED has a selectivity that allows to limit the sample preparation and clean-up procedures to a minimum, making it quick and easy to apply. In addition, this method offers advantages such as: the possibility of direct analysis, as derivatization is often not necessary, the cost-effectiveness of the instrumentation and the possibility of regenerating the electrodes which allows numerous analyzes in succession.

COMMERCIAL BIOCHAR AS ADSORBENT FOR REMOVAL OF HEAVY METALS AND ORGANIC COMPOUNDS

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Heavy metals and organic compounds are usually presented in the water causing great interest due to environmental concerns. While the first ones are well regulated and their toxic effects on health and the environment are well known, the second ones are not completed regulated and their toxic effects are still not well understood. Due to primary and secondary treatments are not able to completely remove them advanced tertiary treatments are required to improve the quality of the municipal effluents into sensitive receiving water bodies. Among advanced tertiary treatments, adsorption onto granular activated carbon (GAC) has been proven to be a viable technique to remove because of its simplicity, efficiency, and no chemical transformation of compounds, but its main drawback of GAC applications is the need to properly treat and dispose of the spent carbon due to its loss of adsorbent capacity. For some years biochar has been studied as an alternative adsorbent because of its chemical-physical properties such as high specific surface and porosity and it is cheaper than GAC. Biochar is a solid carbonaceous material obtained from the pyrolysis of biomass such as plant and animal waste, and activated sludge, therefore, biochar plays an important role in the sustainable treatment of waste. Even if its main use is as a soil improver, many researchers demonstrated its high removal capacity of heavy metals and organics from water. Most of those studies used biochar produced at scale lab, however few studies used commercial biochar as adsorbent. Hence, this review aims to analyses those studied in which commercial biochar was used as an adsorbent to remove heavy metals and organic compounds considering and the relationship with its properties.

STATE-OF-ART OF FORMALDEHYDE DETERMINATION BY SENSORS IN ENVIRONMENTAL AND FOOD MATRICES

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Formaldehyde, the simplest molecule of the aldehyde group, is in a gaseous state at room temperature and pressure, is colorless and has a strong, pungent odor. It is soluble in water, ethanol and diethyl ether and is used in solution or in the polymerized form. In the atmosphere it is quickly photo-oxidized, it reacts relatively quickly with traces of substances and pollutants. The maximum daily formaldehyde dosage established by the EPA is 0.2 $\mu g\ g^{-1}$ of body weight while that established by the WHO is between 1.5-14 $mg\ g^{-1}$. Human is harmed the most by formaldehyde indoors, where it is released from exogenous sources such as resins, glues, insulating materials, chipboard, plywood and fabrics; other sources can be cigarette smoke, heating, cooking, smoking, cosmetics or endogenous sources. Formaldehyde, despite belonging to category 1A of carcinogens (IARC), is found in aquatic foods due to illicit additions or improper storage, moreover it is widely used in chemical industries, and this causes serious accidents of environmental water pollution.

From an analytical point of view, formaldehyde is analyzed by HPLC with UV-Vis detection. Currently, the need to analyze this compound quickly and in situ is increasing. This work proposes a critical review of methods for analyzing formaldehyde in food and in the environment using sensors.

A search was carried out on the Scopus scientific database, using as keywords “sensors”, “formaldehyde” and “food”, 71 documents published between 2002 and 2021 were found. The increase in interest in the recognition of the presence of formaldehyde in food has occurred in recent years, above all due to an awareness of the damage it can cause to human health.

This paper focuses on some new sensors by analyzing their performance and comparing them with various other methods but focusing on the determination of formaldehyde in food products.

The sensors for the recognition of formaldehyde taken in exams are of various types, but they all share a good LOD, good accuracy, and a reduced analysis time. Some of them are also biodegradable and others have a very low cost, many are portable and easy to use, therefore usable for the recognition of food adulterations on site.

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FINGERPRINTING AND ANTIOXIDANT ACTIVITY EVALUATION OF SOME RED AND WHITE ROMANIAN WINES

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Wine is one of the most consumed beverages over the world. Wine is an alcoholic beverage that contains various polyphenols extracted from grapes during the processes of vinification. The polyphenolic compounds, such as flavonoids, anthocyanins and tannins are considered to have antioxidant activity, protecting the body cells against oxidation. These compounds are present in large quantities in wine, especially in red wines, which may explain so-called French paradox. Moreover, polyphenolic compounds are responsible for the quality of wines, influencing their astringency, bitterness and colour. The viticulture practices, different enological techniques, the varieties and the harvesting year of grapes and the wineries influence the polyphenolic composition of wines. Different studies have been carried out in order to analyze the different compounds from wines, especially polyphenolic compounds.

Romania is the fifth large wine-producing country in Europe, after Spain, France, Italy and Portugal, with an area of about 200,000 ha cultivated with grapevines. The annual production of wine is about 5 million hectolitres and the consumption per person is approximately 27 L. Wine quality assurance and monitoring are of major interest because the accession of Romania to the EU was accompanied with compliance with rules related to authentication of grape and wine varieties. This is due to numerous counterfeit wines that still exist on markets in Eastern Europe.

Thus, two of the principal analytical goals are the development of methods for evaluation of authenticity of the end product and detection of possible adulterations.

CHANGES OVER TIME IN PERSISTENT ORGANIC POLLUTANTS (POP) CONCENTRATIONS IN SOILS IN LOWER DNIESTER REGION, REPUBLIC OF MOLDOVA

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Dniester hydrographic district covers approximately 60% of the Republic of Moldova territory ensuring 63% of the annual water quantity and it encompass ~80% of country’s underground waters. Soils, more precisely, agricultural lands and the practices applied on them serve as a source of point pollution of groundwater and surface waters, in addition to other sources such as the household sector, the food industry, the agricultural sector, the energy sector and other sources of continuous pollution.

Moldova is considered an agrarian country whose main resource and wealth are fertile soils. Substances from the group of persistent organic pollutants (POPs) pose a particular danger to the health of the population and to environmental factors. During the seventies of the last century, organochlorine compounds from this group were widely used in agriculture as insecticides and fungicides. Considering that the impact of the environment on the human body is inevitable, it is necessary to monitor the content of organic pollutants in soils in the Republic of Moldova, aimed at reducing the risk of toxic substances by reducing their impact on living organisms.

The study aims to identify the changes over time of POPs concentrations in the soils from 16 sites along the Dniester River. Results of the research done in 2010 were compared with the investigations in 2020 of the same sites. Random sampling was used, and complex samples were collected from the dept of 0-10 cm. Gas Chromatography coupled with mass spectrometry was used for POPs identification and quantification according to EPA and ISO methods.

The degradation status of DDTs was assessed using the ratio (DDE + DDD)/DDT, which ranged from 0.052 to 0.472 in 2010 and from 0.045 to 8.78 in 2019. These reports show old sources of DDT pollution, indicating that DDT residues were significantly transformed into their degradation products in these areas.

The distribution of HCH isomers varied between soil samples. This may be associated with the isomerization of HCH during the soil transformation process, as well as with differences in physicochemical properties and degradation rates.The value of the ratio of isomers $\beta/(\alpha + \gamma)$ was used for the identification of aged sources of pollution. In the present study, in 53% of the results from 2010 the ratio of isomers $\beta / (\alpha + \gamma)$ was > 1 and for 69% of the analysed soils in 2019. Thus, we can conclude that in these regions the source of pollution is the past use of technical HCH (the share of samples in which the ratio of $\beta / (\alpha + \gamma)> 1$ isomers is greater than 50%).

The value of the α-HCH/γ-HCH ratio varied from 0.12 to 7.8 (2010) and from 0.0 to 8.3 (2019), indicating that there is a slight increase in the HCH transformation under natural conditions and that both lindane and technical HCH were sources of HCH contamination.

In conclusion, the study has shown that the contamination level has not changed significantly over time, subsequently there is a need for the remediation of the studied sites.

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PHYSICO-CHEMICAL PROPERTIES OF VEGETABLE OILS FROM LOCAL TRADE

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Health and nutrition are interdependent categories of vital importance. The availability of harmless and healthy food is one of the inseparable conditions of health care and promotion.

Natural oils have a complex of oily substances extracted by various methods from plants, fruits or seeds without being mixed with products from chemical synthesis. The physico-chemical properties of lipids, which have a special importance in food technology, are determined by their chemical composition and structure, which can be determined by establishing indices of normal chemical composition (iodine index, saponification index) or freshness indicators (acidity index, peroxide index, p-anisidine index).

In the paper are applied a series of chemical and physico-chemical methods for the analysis of commercially oils, with different origins and manufacturing methods. The analyzed oils were mixtures, derived from different oil plants: sunflower, grape seeds, olives, corn germ, pumpkin seeds, flax.

The quality indices of the oil samples were determined by various processes: the acidity (% oleic acid), the saponification index (mg sodium oleate / kg), the iodine index, the peroxide index (meq O_2/kg), the p-anisidine index and the diene content, and conjugated triene.

The experimental study aimed to research oxidative degradation of oils over time, determining by the spectrophotometric method the content of primary and secondary oxidation products. The peroxide (meq O_2/kg) and p-anisidine indices were determined by the spectrophotometric method of iron (III) thiocyanate. For some oils (unrefined sunflower oil, flax, pumpkin seeds) peroxide indices have very low values (0.247 ± 0.02) and their evolution over time is not essential. This indicates that, during the storage of oils, there is a slight accumulation of lipid peroxidation products. A small amount of oxidation by-products (p-anisidine index, 0.037 ± 0.05) is recorded in the mentioned oil samples, which may explain the low values of the peroxide indices.

In contrast, for olive, corn germ and grape seed oils, there are high values of the content of primary and secondary oxidation products compared to the standard of samples, which also have increased during storage. There was a small decrease in the peroxide index during storage due to the increase in the p-anisidine index (1,673 ± 0.06), ie by the accumulation of oxidation by-products obtained by the decomposition of hydroperoxides.

The oils analyzed by the unrefined sunflower, flax, from pumpkin seeds are fresh, but they cannot be kept for a long time. For olive oil the peroxide index exceeds 16 meq O_2 /kg, for corn germ and grape seed exceeds 12 meq O_2/kg. Therefore, these marketed oils already contain primary and secondary oxidation products, ie they show a slight oxidative deterioration.

The difference between the quality indices of the analyzed vegetable oils can be explained by the difference between the production processes (temperature, subsequent purification) and the storage conditions.

THE USE OF SLUDGE RESULTING FROM URBAN WASTEWATER TREATMENT IN AGRICULTURE

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Research has been carried out on the use of dehydrated and stabilized sludge as an organic fertilizer. The physical, chemical and microbiological composition of the sludge from Biological Treatment Plant (BTP) was evaluated, the optimal sludge doses as soil amendatory under different agricultural crops were determined, the soil suitability for the application of the sludge, generated in the domestic wastewater treatment, was evaluated. Methodologically, the works were carried out in accordance with the requirements of Directive 86/278 / EEC on the protection of the environment, and in particular of the soil, when sewage sludge is used in agriculture. It has been established that the sludge accumulated in (BTP) contains sufficient amounts of organic matter and macronutrients (NPK) necessary for the development of plants, while the heavy metal content does not exceed the maximum admissible concentrations for sludge stipulated in the national and European regulations. The experiments demonstrated the effectiveness of the use of dehydrated and stabilized sludge from BTP as a fertilizer under different agricultural crops. Investigations have been carried out on the possibility of composting fresh sludge from wastewater treatment plants with various agricultural waste. The controlled composting technology of sludge with poultry manure contains original elements for the intensification of the composting process by activating the thermophile micro-flora, so that a fertilizer with high physic-chemical qualities and free from helminths and pathogenic microorganisms is obtained. Conducting composting in a controlled way allows the capture of ammonia, carbon dioxide, thermal energy and their use in greenhouses, which also diminishes the polluting impact on the environment.

Keywords*:* fertilizer, heavy metals, sludge, waste

Asknowledgement

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THE NEED FOR SUSTAINABLE USE OF AGRICULTURAL LAND

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The Republic of Moldova, being an agrarian country, needs a radical development in the sustainable management of land resources, which are one of the most precious gifts of nature, which nourishes and helps us to prosper both: society and the country's economy. However, these resources are being degraded at a rapid pace at a worrying rate. Over time, various contents have been suggested regarding the sustainable development of land resources. The conceptual diversity of sustainability reflects the variety of relationships involved in the process of using land resources, such as – sustainability, which is the path to the future desired by all.

The purpose: analysis and elaboration of methodologies regarding the improvement of the system for regulating the sustainable use of land resources.

The sustainability of land resources in the Republic of Moldova were largely influenced by reforms in the field of economy and implementation of market relations, which significantly changed the production process. The cause being the transformation of the state monopoly on land resources into private property. Despite the current stalemate, the future of agriculture and its progress will depend on the harmonious and sustainable development of land resources.

Assessing sustainable land management is an integral part of the process of harmonizing agricultural and food production with often conflicting economic and environmental interests. It is expected that agriculture will continue to be the engine of economic development in these countries but in developing, in order to be realistic, agriculture in the future will have to be more and more productive, more economically efficient and more efficient in the future greener – in a nutshell, more sustainable. Although sustainability will continue to be elusive, learning to assess sustainability must begin now. The task is much too important to wait until we have all the answers.

In addition, it would be beneficial to increase agricultural productivity in order to meet the nutritional needs of the growing population without major environmental degradation. One factor influencing agricultural production is continuous climate change and its impact on the environment, and soil degradation, by non-compliance with anti-erosion measures and which need to be taken into account in identifying and developing sustainable land use practices. Therefore, I set out to conduct more comprehensive studies and propose solutions, based on principles and methodologies for sustainable use of land resources in the Republic of Moldova, to get out of this colossal impact.

CHEMICAL COMPOSITION OF ORGANIC FERTILIZERS OBTAINED FROM POULTRY WASTE BY DIFFERENT METHODS.

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This paper will describe the methods that are used at the enterprise to obtain organic feed from poultry waste. These include conventional composting, vermicomposting, vermicelli production and closed chamber composting. The results of analyzes for the content of the following chemical components in the samples under study will be presented: phosphorus, potassium, organic matter (humus), nitrogen in nitrate and ammonia forms, bound nitrogen, as well as heavy metals and residues of pesticides and antibiotics. Based on the data obtained, a conclusion will be drawn about the advantages and disadvantages of each of the methods for obtaining organic fertilizers.

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THE IMPACT OF TOMATIN BAC ON THE PROCESS OF ALCOHOLIC FERMENTATION OF CEREAL BIOMAS

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The quantity of agricultural waste has been rising rapidly all over the world, many studies has revealed that fruits and vegetables are the main source of bioactive compounds; in most cases, wastes and byproducts generated by the food processing industry present similar or a higher content of antioxidant compounds. Therefore, there is an increasing interest in finding new ways for their processing toward safely upgrading these wastes for recovering high-value-added products with a sustainable approach. Among food waste, the abundance of bioactive compounds in byproducts derived from tomato suggests possibility of utilizing them as a low-cost source of antioxidants as functional ingredients.

The solid residue remaining after the industrial processing of tomatoes (*Solanum lycopersicum* L.), tomato pomace, consists of large amounts of tomato peels and seeds that currently find use as animal feed and fertilizers or are sent to landfill. However, it is still rich in important antioxidant present in the ripened tomato. In this line, numerous approaches have been proposed for the valorization of the unused parts of tomato in various sectors (figure 1).

In the past, people added these byproducts as compost to the soil for agricultural purposes, thus allowing the recycling of nutrients. Today, instead, because of the huge increase in the accumulation of large amounts of waste matter, reducing waste is among the efforts to relieve the pressure on natural resources and move toward more sustainable food systems.

So, a critical and up-to-date review has been conducted on the latest individual valorization technologies aimed at the generation of value-added by-products from industrial food wastes. Waste treatment in wine and alcohol industry is a current problem in Republic of Moldova. The annual volumes of the production and accumulation of liquid wastes are considerable.

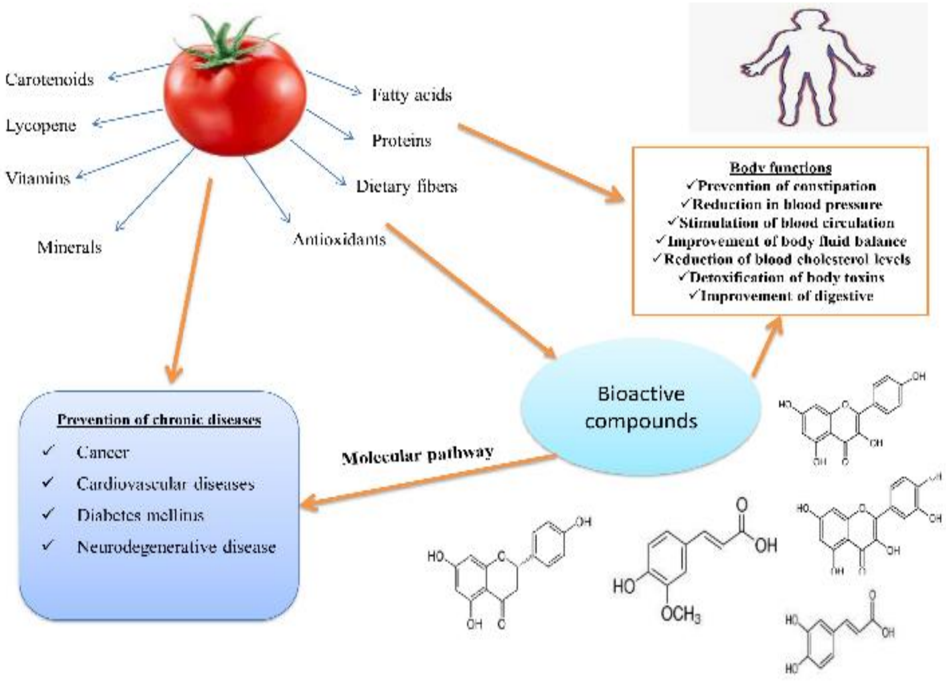

Figure 1. Description of health benefits of tomato.

The aim of the scientifical research is to examine the associated advantages and drawbacks of each technique separately along with the assessment of process parameters affecting the efficiency of the generation of the bio-based products. Research of the influence of tomatine BAC on the process of alcoholic fermentation in the laboratory conditions. The biomass used was the waste from the ethyl alcohol production "GARMA GRUP" L.L.C. Company. The testing of tomatine BAC was performed in order to explore possible activating or inhibiting effect on the alcoholic fermentation process.

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PAULOWNIA FOR BIOREMEDIATION OF URBANIZED SOILS

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At the moment the problems of environmental protection are especially relevant for Russia. Intensive development, industrial activity and high traffic density on the roads contribute to the accumulation of various pollutants in the biosphere. Soil is the most important component of the ecosystem, which accumulates chemical pollutants. Among the numerous pollutants, heavy metals occupy a special place; they bind with mineral and organic compounds, which increases the overall level of soil toxicity.

Paulownia is a fast-growing tree native to China, which grows up to 30 meters in height during a 5-7 year period and a trunk diameter of up to one meter. A distinctive feature of the tree is a rapidly developing root system, which makes the plant suitable for afforestation of areas that are under the threat of erosion. According to numerous foreign studies, Paulownia accumulates nitrates, heavy metals and other elements from the shallow and deep layers of the earth. In Russia now there are no widely known works on the study of Paulownia.

The analysis of soil contamination with heavy metals in the city of Krasnoyarsk was carried out. It was revealed that the main pollutants are manganese, copper, cobalt, zinc, mercury, cadmium. Model soil solutions were prepared, in which Paulownia samples were planted. For three months, Paulownia grew up in a closed system. The soil contained metals with an excess of the permissible concentration by 10 times. After the experiment, a spectrophotographic analysis of Paulownia samples (leaves and stems) was carried out.

The results obtained indicate that, along with the resistance of Paulownia to the high content of heavy metals in the soil, it is necessary to further study the influence of other anthropogenic impurities on the nature of adaptation and plant growth. The results obtained showed that Paulownia actually accumulates heavy metals from the soil into its living tissues.

ECOLOGICAL APRECIATION OF TYPICAL CHERNOZEM

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Recently it has become clear that when describing the soil, it is also necessary to take into account its biological component [2, 4–5], including such a biological and environmental parameter as soil health. The term "quality" of the soil is associated with its suitability for specific purposes, and the "health" of the soil is associated with the performance of its ecosystem functions, which has a broader meaning than "quality" [6, 7].

The aim of our research was a comparative study of the health of a typical black soil of the Republic of Moldova, which has been in agricultural use for a long time. The studies were carried out on the long-term (since 1995) experimental base of the Academy of Sciences of Moldova and on the nearby (~ 100 m) forest strip of broad-leaved trees (Chisinau) during 2008 – 2018. Soil In the experimental plots, typical loamy chernozem. The humus content in the horizon of 0-60 cm is from 2.2 to 3.4%. The sites selected for the study were occupied by plants of two crop rotations of fodder crops in 3 variants: 1 – without fertilizers (control); 2 – mineral background (mineral fertilizers); 3 – organic background: manure.

According to monitoring data, 2/3 of Moldovan soils have a negative humus balance and are characterized by insufficient nitrogen supply [8–10]. Regarding phosphorus and potassium C.L. Zagorcea [11] note that with a relatively high gross content of phosphorus and potassium, the number of their mobile forms is unsatisfactory for plants. According to D.S. Orlov [3], the average composition of humus in soils is $C_{55\text{-}65}N_{3.5\text{-}5.0}O_{25\text{-}35}N_{1\text{-}2}$,%. For the first time in the anthropogenic soils of Moldova, the quality and health of the soil were determined. It was established that the presence of nutrients in the studied chernozem does not satisfy the proportional ratios characterizing their combination in terms of humus content.

Active (microbial) carbon, compared by analogs of indicator of Cornell University, USA [1], showed that they are characterized by values below the average. If, according to the named system, soils with satisfactory (poor) condition contain 284 ppm of active (microbial) carbon, with an average state of health – 601 ppm and with a very high state of health – 1197 ppm. It is obvious that most of the soils studied by this indicator, can be characterized as soils with poor health and only soil fertilized with manure and natural soil are characterized by a tendency to approach soils with average health.

A comparative study of the diversity of micromycetes of a typical chernozem showed that the parallel coexistence of both phytopathogenic and suppressor forms is presented in different ratios. For example, in soil without fertilizers of the control variant, when detecting 17.73% of ***Fusarium*** fungi, ***Trichoderma*** 9.17% of suppressor fungi were found, and in the soil of the mineral background, suppressor fungi were not identified at all, despite the rather high occurrence of phytopathogenic fungus ***Fusarium*** (15.89%). Against the organic background, the presence of both representatives was more balanced, although in this case there were also less suppressor fungi ***Trichoderma***: 3.95 and 4.08%, respectively, in the presence of 6.70-6.91% ***Fusarium*** fungi. Thus, the studied chernozem contains more phytopathogenic fungi of the genus ***Fusarium*** than representatives of the suppressor fungi of the genus ***Trichoderma***. Their unequal ratios indicate an unhealthy development of soil microflora and poor health by this indicator of the soil as a whole. "Father of medicine" Hippocrates said 2500 years ago that human health depends on soil health, so it is very important to take care of the health of agricultural soils. In other words, today it is incorrect to evaluate the properties of the soil only by the criteria of its fertility, the soil. Is deeply erroneous to ignore the biotic block of the soil, which determines the environment-forming functions of the soil ecosystem – its health [4, 5].

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MACRONUTRIENT IN CHERNOZEM FROM LONG-TERM AGROEXPERIMENTS: VARIATION AND PATTERN

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The purpose of these studies was to analyze the content of the main macronutrients of the soil C, N, P, K. The research was carried out in a long-term (from 1953) stationary experiment with different fertilizer and crop types on Calcareous Chernozem (Calcic chernozem in the World reference base for soil resources). Macronutrient dynamics associated with fertilizer rate and residue application were determined. There is a significant decrease in nutrient content compared to the original content when the experiment was set up in 1953.

Acknowledgement: The research was carried out in the research projects: Efficient use of soil resources and microbial diversity through the use of elements of biological (organic) farming (2020-2023).

MEDICAL WASTE PROCESSING IN THE REPUBLIC OF MOLDOVA

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Covid -19 has manifested and is still manifesting a negative impact on public health, global economy and on the environment. The preventive, protection and control measures of coronavirus are continuouslu generating more medical waste: contaminated masks, gloves, used or expired medicine and other infected protection equipment. The improper management of the medical waste could cause unpredicted consequences on the public health and the environment. So, Covid -19 brings challenges in the field of medical waste management as well [1].

The economical agents from the Republic of Moldova have taken this challenge, so SRL Uispac, that has financial support from the National Agency for Research and development, has implemented a project with a technological transfer of neutralization through thermal sterilization of infectious medical waste, using the local machinery Thermoshreder 420 elaborated, created and authorized in the Republic of Moldova.

Neutralization through thermal sterilization of the infectious medical waste using the Thermoshreder 420 is a local solution method, without incineration, of the infectious medical waste processing problem. The process happens and temperatures of 160 – 190^{o}C, with the concomitant chopping, sterilization and destruction of the confidential information keeping units in a single compact space. The machinery transforms the waste from “red bags” (biologically dangerous/biomedical), including the stinging and sharp objects, to municipal sterilized waste [2].

The medical waste treatment process in the local machinery Thermoshreder 420 is closed where the chopping of all the treated medical waste types takes place, and then a further heat treatment of that medical waste takes place. The analysis of this process does not show the drain of any pollutants into the environment, like some pollutants in gaseous, liquid, dust state or any other emissions in any other states. The main disinfection process is represented by the thermal factor, that ensures the total neutralization of the treated medical waste.

In the technological process of the specified plant there is not even residual water formed. In result, it can be confirmed that in the functioning process, the installation does not cause any damage to the environment: there are no emissions into the atmosphere, no residual water and no solid waste.

The processing capacity of the machinery is 420 l, which is equivalent to approximately 42 kg of infectious, liquid and solid waste (if the density verifies the relation 100 l = 10 kg). A cicle takes 45 min.

Neutralization by thermal sterilization of infectious medical waste using Thermoshreder 420 is a method of local solution, without incineration, of the problem of treatment of infectious medical waste. The process takes place at temperatures of 160-1900C, with the concomitant crushing, sterilization and destruction of the confidential information storage units in a single compact space. The device converts waste from "red bags" (biologically hazardous / biomedical), including stinging and cutting objects, into sterilized municipal waste [2].

An operational cycle of the Thermoshreder 420 includes:

- *waste collection:* in a trolley or a crate a special plastic or big autoclavable bags are put to prevent the gluing of the waste on the container. Then, the red bags are put in these containers together with the single-use containers for sharp objects.
- *Preliminary heating:* (at the beginning of the work shift) the machinery is heated for around 90 minutes, depending on the room temperature.
- *Waste loading*: The containers with waste are loaded into the bunker. The waste is chopped using the shredder. Chopped materials fall in the intermediate bunker, then, with the help of the screw, are transported all over the treatment room, where due to the temperature and the shape of the screw, turn into a homogeneous mass, melted and disinfected, that is evacuated through the discharging channel. The machinery reduces the volume of the treated waste by 70-80%. The machinery also transforms the waste in a way that it becomes unrecognizable.

In the adjustment process of the physico-chemical parameters, The National Agency for Public Health has done the microbiological control of the neutralized medical waste with thermoshreder TS 420 and the gas emissions in the working area and has released the positive approval. Also, the ecological examination of the medical waste sterilization machinery was made using the thermoshreder TS 420 by the Institute of Ecology and Geography, that has also released the positive approval. According to the conducted analysis and the project documentation were obtained: The sanitary approval regarding the application in production of the machinery, technological lines, new chemical substances; the sanitary approval regarding the location of the treatment sector through thermal sterilization of the infectious medical waste using the Thermoshreder 420; Approval regarding the establishment of the sanitary area and acceptance of the compartment Environment Protection. Environment Agency has examined the preliminary evaluation file of the environmental impact caused by planned activity regarding the treatment through thermal sterilization of the infectious medical waste using Thermoshreder 420; Project documentation and the compartment Environment Protection has released the approval of state ecological examination for the project documentation, and using this was released the environment Approval for waste management.

Conclusions. At the moment, SRL Uispac has more than 400 contracts signed with medical bugetary institutions and private clinics regarding transportation and neutralization through autoclaving and thermal sterilization of medical waste, resulted from the medical activity. 85% of these contracts are clients from mun. Chisinau and suburbs and the rest form the republic. The neutralized waste quantity at SRL Uispac varies from 20 to 25 t per month.

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Session E

ECOLOGICAL AND ENVIRONMENTAL CHEMISTRY WITHIN THE KNOWLEDGE TRIANGLE: RESEARCH-EDUCATION-INNOVATION

SINERGIES AND COLLABORATION OPPORTUNITIES IN RESEARCH-EDUCATION-INNOVATION FOR RIVER-SEA SYSTEMS

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The paper present collaboration opportunities in *Research-Education-Innovation* fields in the frame of DANUBIUS-RI project. DANUBIUS-RI is a Romanian initiative to develop a Pan-European, distributed Research Infrastructure dedicated to the integrative study of river – sea systems and the opportunities and risks they represent to society. DANUBIUS-RI will provide a unique opportunity to bring together the best existing expertise and facilities in Europe and provide an internationally leading focus to understand, characterize and manage RS systems globally.

ECOPHYSIOLOGICAL AND LIFE-HISTORY ADAPTATIONS OF *GAMMARUS BALCANICUS* (SCHÄFERNA, 1922) IN A SINKING-CAVE STREAM FROM WESTERN CARPATHIANS (ROMANIA)

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Freshwater gammarids are known to colonise occasionally sinking-cave streams, providing contrasting morphological, life-history and ecophysiological adaptations compared to their surface conspecifics. In this study, a subterranean and a surface population of the species *Gammarus balcanicus* was surveyed for one year in a sinking-cave stream from the Western Carpathians (Romania). The results showed that the cave-dwelling population comprised individuals that were significantly larger compared to their surface conspecifics, had larger body-size at sexual maturity and that the females produced fewer, but larger eggs, compared to the population situated outside the cave. The trophic position and the omnivory were significantly higher for the cave-dwelling compared to surface population and the elemental imbalance for C:P molar ratios lower, but similar for C:N. However, the subterranean population did not present troglomorphic characters or longer lifespan as known for other cave-surface paired crustaceans. This, together with the rather extensive hydrological connection of the habitats, suggests active gene-flow between populations and similar response to seasonality for body-size distributions, indicating that the observed ecophysiological and life-history differences are rather the consequence of phenotypic plasticity than the result of genetic adaptation.

INTERACTION OF PROPERTY RIGHT WITH ENVIRONMENTAL LAW FROM HUMAN RIGHTS PERSPECTIVE

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The research is based on the concept of the right of property and the fundamental right of a person for a healthy environment that are present in various national and international acts including the European Convention on Human rights. When talking about the ECHR and its regulation, we should state the fact that a certain provision on the environmental protection we do not have established expressly, but we can deduce it from article 8 mainly, that has in the second paragraph that assures a person’s right for a healthy environment.

When speaking about the property right, it has its regulation in the first additional protocol added to the Convention. The way the Convention treats property right, and the way it is established in the protocol is not very orthodox for the continental European law. It tries to broaden the concept of property in most ways possible and I think, makes it really successful.

Further the research will try to analyse the concept of both fundamental rights establishment in the Convention and try and give some answers to the situations when those types fundamental rights are colluding with each other, for example when one's right of property is colluding with one's right of a healthy environment. This issue keeps getting more attention recently as the aspect of environmental protection becomes more important for a healthy development of humans and its descendants, so there appear more restrictions imposed on several of categories of activities and form of services. That's why there appears a logical question whether those restrictions can be applied or not, are they interfering with another fundamental right, specifically talking about the right of property or not. The other aspect is when the right of property is used to protect the environment and the preserving a healthy environment.

The research will analyse the practices of various EU countries and of course the European Court of Human Rights decisions on this matter (ex. Case of López Ostra v. Spain 09 December 1994 and Case of Guerra and Others v. Italy (116/1996/735/932)

PERSISTENT ORGANOCHLORINE PESTICIDES AND THEIR IMPACT ON HUMAN HEALTH

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The presence of persistent pesticides in environmental components is a major problem both nationally and internationally. This fact is conditioned by the detection of increased amounts of these compounds in various environmental samples, taken in different locations around the world, including from permanently uninhabited territories. Organochlorine pesticides (OCPs) are biocides of anthropogenic origin, used mainly for insect control. They have a high toxicity (groups III – IV), are fat-soluble and can enter the human body by ingestion, inhalation, or contact. Most organochlorine pesticides are banned for production, marketing, and use, which include high toxicity and bioaccumulation in the food chain. OCPs are characterized by persistence in environmental components due to the high level of chemical stability, the half-life varying from a few days to decades.

In the Republic of Moldova, the largest quantities of organochlorine pesticides are identified in soil samples taken from the territory of warehouses for storage and processing of these pesticides (intensively exploited during the Soviet period), as well as in the territories adjacent to these deposits. In some cases, the determined concentrations exceed the maximum permissible value thousands of times. In addition, high values are also detected in the areas of unauthorized dumping. The problem is aggravated by the fact that most of the landfills are in the process of destruction, people and animals having free access to both territories and waste storage lots. In addition, geological and meteorological phenomena contribute to their spread and modification in environmental components.

Studies on soil samples, sediments, food and biological tissues taken on the territory of the Republic of Moldova have highlighted the presence of DDT and its metabolites, hexachlorocyclohexane, hexachlorobenzene, heptachlor, etc., their content ranging from micrograms to grams per kilogram of sample. The content of these compounds in natural waters is relatively low, due to their low solubility in water.

The toxic effects of organochlorine pesticides on organisms are manifested by immune system damage, digestive tract pathologies, respiratory dysfunction, neurotoxic disorders, severe cardiovascular disorders, food allergies, cognitive dysfunction, development of various cancers, increased number of miscarriages and infertility, the birth of children with birth defects, and other serious consequences. The presence of these substances in the atmospheric air is manifested by irritations of the respiratory organs, severe headaches, intoxications, vomiting, etc. The penetration and bioaccumulation of organochlorine pesticides in the human body is a factor in the destruction of both the body itself and the bodies of breastfed children because the presence of these compounds is attested in breast milk.

Therefore, some of the efforts made by state institutions, control bodies, the academic community must be reoriented towards the harmonization of legislation in the field and its connection to international law, identification of existing sources of pollution of environmental components with organochlorine pesticides, organization of restrictive measures of access to contaminated territories, as well as the implementation of technologies for their conservation or remediation.

ISOPROPYL AMINOMETHYL PHENOL – AS AN EFFECTIVE DISINFECTANT AND BACTERICIDAL AGANIST INFECTIOUS DISEASES

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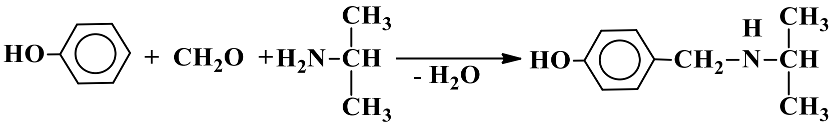
All over the world, 35-40% of agricultural products are spoiled and discarded due to diseases and pests. As a result, the yields of the production is fallen down and the biosphere is harmed. Recently, alkylphenols have been used as pesticides, herbicides, insecticides, bactericides, etc. against diseases and pests in agriculture [1,2].

The proposed 4-isopropylaminomethyl phenol is obtained by the interaction of formaldehyde with isopropylamine:



The article presents the results of obtaining of Mannich base such as isopropylaminomethyl phenol by the interaction of phenols with isopropyl amine and formaldehyde and study its antibactericidial and disinfectant effect aganist the gut microbes. The aminomethylation reactoin of phenol with isopropylamine was carried out at 80^{o}C and for 2 hrs in the presence of solvent (benzene). As a results, p-isopropylamine methyl phenol was obtained with a yield of 72.3%. The chemical structure of the obtained products were confirmed by IR, NMR spectroscopies.

The ^{1}H NMR spectr of 4-isopropylaminomethyl phenol (300 MHz, $CDCl_3$), δ ppm: 1.17(d., 6H, J=6.3Hz), 2.60(s.,1H, NH), 2.92(m., 1H, CH), 3.80(s., 1H, OH), 4.01(s., 2H, CH_2), 6.70-7.25(m., 4H, Ar).

The ^{13}C NMR spectr of 4-isopropylaminomethyl phenol 13C NMR, δ ppm.: 22.42(CH_3), 48.17(CH), 52.95(CH_2), 115.47, 116.50, 119.14, 122.96, 128.68, 157.32(C–Ar).

The obtained p-isopropylamine methyl phenol was tested as a bactericide and disinfectant aganist coli microbes at the Veterinary Research Institute of Animal of the Ministry of Agriculture of the Republic of Azerbaijan. In the institute, it was proved that aminomethyl phenol among 40 samples presented to the institute showed a positive result. Together with the institute, in the field of application of the isopropylaminemethyl phenol, the Eurasian and Azerbaijan patents were obtained.

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OBTAINING OF ANIONIC FORM NANOMATERIAL AND POSSIBILITY OF ITS USE IN AGRICULTURE

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The problem of mineral nutrition in plants is still far from being solved for two main reasons. The first reason is that plant nutrition requires a complex supply of both macro- (N, P, K, Ca, Mg, S) and microelements (Fe, Cu, Zn, Co, Mo, B, etc.). The second reason is the great inhomogeneity of environmental factors (composition and soil properties, moisture, temperature, etc.). Both factors largely determine the quantity of elements required for plant nutrition.

The effect of traditional mineral fertilizers is low, as most nitrogen fertilizers are either washed away or evaporate after application, while most phosphate fertilizers are easily absorbed into the soil and converted to the hardly soluble forms. Therefore, the utilization rate of such fertilizers is very low, no more than 15-25%.

We have proposed a nanotechnological method for obtaining anionic substituents. Method is based on the introduction of the respective desired salt into the zeolite structure in the form of ions so that the resulting material does not lose its zeolite structure and acquires anion-exchanger properties upon the formation of a new phase. Certain amounts of ammonium dihydrophosphate ($NH_4H_2PO_4$), potassium nitrate (KNO_3) and cations (Fe, Ca, Mn, Mg, Zn, Cu, Mo, Co, Sn) mixed with them were introduced into the zeolite-clinoptilolite structure at the nano-level by the melting method.

In order to study the effect of the obtained zeolite fertilizer we chose winter wheat variety. The experiment was carried out in field (open ground) conditions as well as in laboratory conditions.

After harvesting wheat, it was found that under field conditions, the yield increase was 36.6% compared to the variant without fertilizer, and under vegetative conditions – 26%. Particularly noteworthy is the increase in the qualitative indicators of wheat – an increase in protein content, as well as fat and crude gluten.

CLIMATE BOX AS A TOOL FOR ENVIRONMENTAL EDUCATION

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The impacts of climate change are already being observed and are expected to become more pronounced. Extreme climatic events, including heat waves, droughts, and floods, are expected to become more frequent and intense. In Europe, the largest temperature rises occur in southern Europe and the Arctic. To understand the consequences and impacts of climate change, the National Environmental Centre, with the support of GEF SGP Moldova and UNDP Moldova, has introduced teacher trainings on the use of the tool Climate Box, developed by UNDP and adapted to national context in 2019.

Climate Box is a comprehensive learning toolkit that educates school children about climate change and inspires them to act. Designed to make learning fun and interesting, the Climate Box provides up-to-date information on climate change with a range of creative tasks, games, quizzes, and experiments, as well as resources for teachers/educators.

Thus, starting with July 30, 2020, the National Environment Centre organized 13 trainings for 610 teachers across the country about climate change, the Climate Box tool being presented to teaching staff. The training aimed at understanding what is the approach to the subject of climate change in the study hours, how it can be enclosed considering the school curriculum and changes in the educational process caused by the COVID pandemic 19.

The Climate Box tool is comprised of an illustrated educational support for students and teachers, with educational materials and a variety of questions and tasks, designed to be done both individually and in groups, with questions on “Climate change”, as well as methodological guidelines for teachers, regarding the use of the set in classes, for different school objects and a set of questionnaires in the form of a game that could be used to test students’ knowledge.

The teachers who attended this training were enthusiastic about the new educational and methodological support, with recent data and adapted specifically for our country. Also, the question cards aroused their special interest and created ideas for developing interactive activities with students.

HUMAN RIGHTS FOR BETTER LIVE: ENVIRONMENTAL TRANSNATIONAL RIGHTS, LEGISLATION AND CONTROL. ABOUT THE EXPERIENCE OF SOCIOLOGICAL RESEARCH OF PUPILS AND STUDENTS

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In the universities and highschools of the Republic of Moldova, a theoretical and practical concept of teaching environmenal transnational rights is missing. Such a concept would explain in a more accesible and clear way how does the environmental transnational legislation function, taking into consideration especially the specific problems Moldova faces in this certain area. An exception to this situation, are the University courses of the Law Department, where the students are being exposed to a theoretical introduction into the topic, but a practical approach of how do these rights function both in Moldova and abroad is also lacking.

Thus, it becomes obvious, that the lack of knowledge and practice in theoretical and practical aspects of the green ones, for teenagers between 17-22 is an actual problem that arose in the educational system. This problem serves as a basis for development of a bigger problem, which consists in the following: these teenagers that are lacking this knowledge of the green rights, have the tendency to pass their knowledge to a younger generation, in this way creating a bigger knowledge gap of environmental rights in the Republic of Moldova. The educational system of the Republic of Moldova is a 12-year program, full of mostly formal subjects, where the learners get mostly theoretical knowledge, and less practical one. The school day is full, it last 6-7 hours a day. Therefore, a practical way to solve this existing problem, would be creating an inclusive extracurricular program, dedicated to both theoretical and practical aspects of realization of environmental transnational human rights both in the Republic of Moldova and abroad.

Target group of this educational program would be learners of graduating classes of high school and universities aged 16-25 (the age, including higher school pupils and students of Universities).

The goal of this educational program is offering constant and full knowledge and skills in the area of environmental transnational rights. Acquiring these knowledge and skills would help reduce the gap in the area of low environmental law literacy and help improve civic engagement of the country’s youth.

Based on the results of the initial preparation of the educational program, quantitative and qualitative studies were also carried out among the target group, in the form of:

1. An open questionnaire survey aimed at identifying common, problems and difficulties related to human rights, which representatives of the target group are aware of even at the most superficial level of perception.
2. Formation of a target focus group aimed at the most detailed, consistent formulation of specific problems related to the perception of human rights by representatives of the target group.

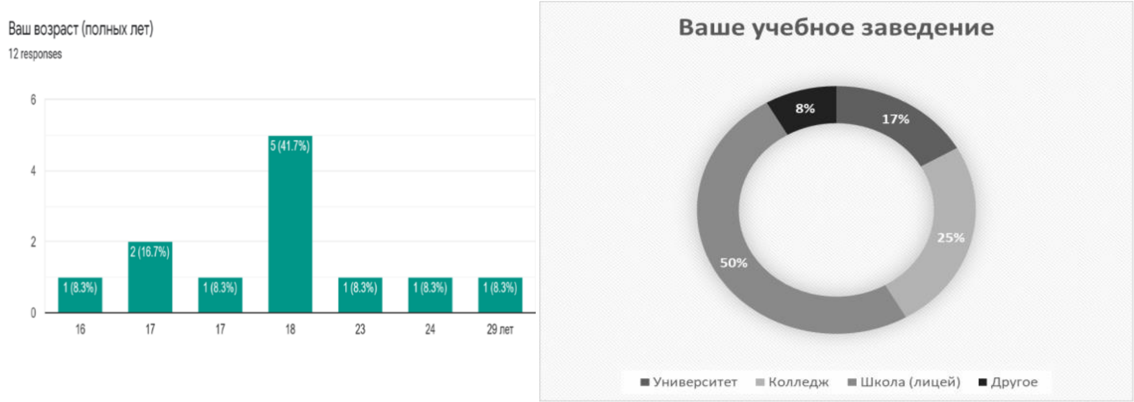

Diagram # 1. Socio-demographic characteristics of the proportion of the target group that took part in the preliminary research

The main conclusions based on the results of the research carried out among the target audience. Schoolchildren note that they are familiar with the concept of “human rights” in general thanks to the discipline “foundations of civic education”, but this knowledge is purely theoretical and extremely superficial.

Quote 1: “*I know that a person has the right to life, work, rest, education, medical care, and freedom of thought. But I think there are still many things that I need to know*.” At the same time, real practical experience in the field of knowledge of their own rights, as well as their defense, is present, as a rule, among students, but in this case, such experience was obtained outside educational institutions, as a rule, at specialized trainings, seminars or volunteer activities.

Quote 2: *“I was a volunteer in a People Traffic organization. Within the framework of this project, we were told about the rights and obligations in employment for work abroad.”*

Quote 3: *“He took part in dozens of actions and protests in the protection of the environment* and *environmental human rights (against the construction of dams on the Dniester, against the use of plastic, etc.). I think the society should be civilly active and savvy in matters of its rights.”* Most of the respondents, even without experience in the field of protection and assertion of civil rights, note that his rights are violated very often – in particular, the right to express his own opinion.

Quote 4: *“They always say, when you grow up, then you will understand”*, as well as the rights to your own, personal space and respect for the individual.

Quote 5: *“In my life I have often come across this. They did not give the right to vote, and very often there was a violation of personal boundaries.”* It is especially important to note that almost all respondents faced the violation of the right to personal freedom, the right to expression, and respect for the individual.

Thus, representatives of the group’s goals under study note **that the knowledge gained in educational institutions in the field of rights and freedoms is categorically insufficient for them.** Life experience at this age stage is also scanty. And the existing examples of violation of rights and complete impunity do not inspire at all, but, on the contrary, incline to a passive, nihilistic position and subsequent socio-political escapism, which does not benefit the development of the Republic of Moldova as a state. Consequently, the creation of a separate educational program aimed at enlightening practical aspects and implementation of human rights is undoubtedly necessary for representatives of the designated target audience.

Thus, representatives of the group’s goals under study note that the knowledge gained in educational institutions in the field of rights and freedoms is categorically insufficient for them. Life experience at this age stage is also scanty.And the existing examples of violation of rights and complete impunity do not inspire at all, but, on the contrary, incline to a passive, nihilistic position and subsequent socio-political escapism, which does not benefit the development of the Republic of Moldova as a state.

Within the framework of the project of such an educational program, on the basis of research of the target audience, the following thematic blocks are planned:

- Experience of national and international youth public organizations in the implementation of legal projects and initiatives (motivation);
- The right to a healthy environment and UN climate negotiations as a tool for public participation in significant decision-making.

In the process of implementing the program, it is planned to use such *methods of interaction and training of the target audience* as presentation, discussion, individual work, work in small groups, brainstorming, reflection, role play, energizer.

The organizational form of the educational program is out-of-school (non-university) training, which includes a variety of modern teaching methods.

The specific, practical results for the target audience of such an educational program, to the maximum extent of its implementation, will be (depending on the intensity and volume of real practice, the number of realized results may vary to a lesser or greater extent):

- obtaining a general volume of theoretical knowledge and the whole range of political and civil rights that exist in Moldova today;
- obtaining and mastering practical tools to protect their civil rights;
- study of international binding documents regulating environmental rights, such as the Aarhus Convention and examples of its successful application;
- gaining skills to actually conduct annual climate negotiations;
- gaining skills to adapt to climate change in everyday life;
- development of a general level of emotional empathy, the ability to empathize with residents of countries that are especially vulnerable to the effects of climate change.

Final conclusions. The educational program, through the gradual and sequential provision of knowledge and skills development, will narrow the gap in the area of low legal literacy among young people. The foundations will be laid for the formation of the basic civic competence – the ability of a person to be an active member of civil society, to participate in its creation and functioning. Knowledge of fundamental rights and freedoms will allow training participants in real life to competently use knowledge of the laws, to defend their point of view reasonably, to analyze the current circumstances in accordance with the existing legislation of the Republic of Moldova and international standards of environmental rights and their regulation in general.

IDENTIFY EMERGING CONTAMINANTS IN AIR, WATER, AND SOIL

Nicolai IASIBAS, Rustam SERHANOV

Lokmera LTD Company, Chisinau, ***Moldova***

Each day scientists identify new and emerging chemical contaminants in environmental matrices requiring further investigation into the affect these toxicants have on humans and biota. Understanding the biochemical and physiological impact of chemical exposure allows government regulators, researchers and producers to determine potential risk and toxicity of newly developed chemicals, and recently identified emerging chemical contaminants through in vitro research exposing live animals, developing larvae, or cells to water or extracts containing chemical contaminants. Changes to cell metabolism, morphology, or mortality suggest a chemotoxic affect that requires deeper investigation.

Identification of the processes up or down regulated in response to chemical exposure necessitates research into physiological processes including metabolic pathways, gene expression and transcription, and protein synthesis, etc. In vitro exposure research using arrays that whole cell and tissue, or subcellular mechanisms allows scientists to quickly identify affected processes and classify the exposure risks. Understanding this risk allows regulatory agencies to protect the public by developing new or updating existing monitoring requirements to reflect changes to maximum levels of chemical release permitted and subsequent presence in the environment.

Agilent's solutions for in vitro life science applications and non-targeted screening provide researchers with the tools required to characterize toxicant impact of biochemical and physiological processes. Our cell metabolism and in vitro assays provide researchers the tools required to quickly and efficiently identify chemicals that pose potential risk. Our portfolio of high resolution mass spectrometry solution deliver the selectivity and sensitivity required to identify new chemical toxicants, in situ degradation or transformation products, and biochemical metabolites. Powerful software facilitates chemical identification and can provide a map to potential metabolic transformation in vivo.

Today's environmental analysis must be done more reliably, more efficiently, and with higher quality results than ever before. Unfortunately, pharmaceuticals, PFAS, pesticides, and other potentially toxic compounds can be difficult to detect in environmental and biological matrices. To complicate matters, several thousand chemicals present in the environment are currently unknown and unidentified. Many of these chemicals could be toxic, but are not regulated in the environment, due to the absence of toxicological data. Lokmera LTD Company offers a comprehensive portfolio of innovative applications from improving lab productivity for chemical analysis, to vacuum systems, to workflow solutions developed to facilitate unlocking the complexities of living systems. We help you stay current with emerging applications and approved methods, while our integrated workflow solutions deliver accurate, comprehensive data helping you make informed decisions accelerating your time to results.

STRUCTURAL-SORPTION DUALISM OF THE BIOCHAR PRODUCED OF SILVERGRASS (*MISCANTHUS* SP) IN ADSORPTION OF FULVIC ACIDS FROM WATER

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The present study reports mathematical analysis of the experimental data based on the paper by M. Konczak *et al.* (https://doi.org/10.1016/j.chemosphere.2021.130447) where two groups of the five biochars (two – residues of sewage sludge or *SS*, three – residues of biogas production or *RBP*) were compared by structure and sorption ability to decontaminate water from fulvic acids. As a reference, a non-waste silvergrass (*Miscanthus* sp or *MI*) biochar was involved. From the experimental results, it was concluded that *MI* structurally is close to RBP and by sorption properties it is as effective, as *SS*. The present research has been developed after the publication and can serve as a theoretical continuation, where mathematical approaches from Data Science, such as 2-Means Clustering, Principal Components and Logistic Regression serve to prove the assumption about the mentioned above duality of *MI*. The experimental data were separated by structural and adsorption criteria, whereupon 2 clusters were established by structure (1: *RBP* + *MI* and 2: *SS*) or by adsorption (1: *SS* + *MI* and 2: *RBP*). Each clustering has been supported by respective Principal Components after removing the variables with the lowest *R2* and highly-collinear interaction. The resulting Principal Components have served, in turn, as variables to build Logistic Regression models to predict and distinguish both clusters: after the iterations, a single Principal Component is enough to describe the clusters as by structural, as by adsorption criterion (Fig.1). The computation results can be helpful to develop machine learning algorithms to classify the biochars by their structural-sorption properties.

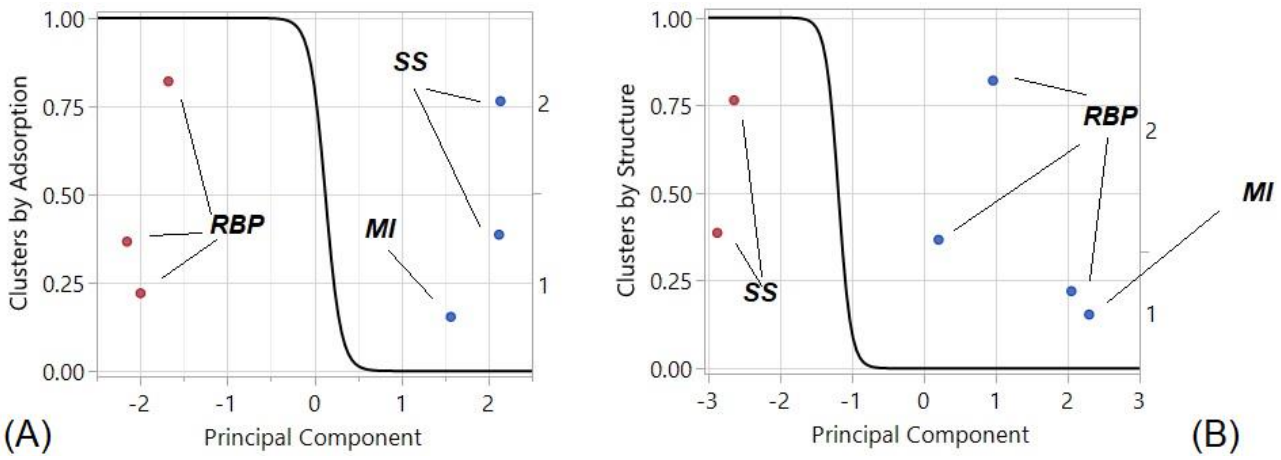

Fig.1. The Logistic Regression plots to classify the clusters by adsorption (A) or by structural (B) criteria of the biochars.

ECOFRIENDLY IONIC LIQUIDS IN PETROCHEMICAL PROCESSES

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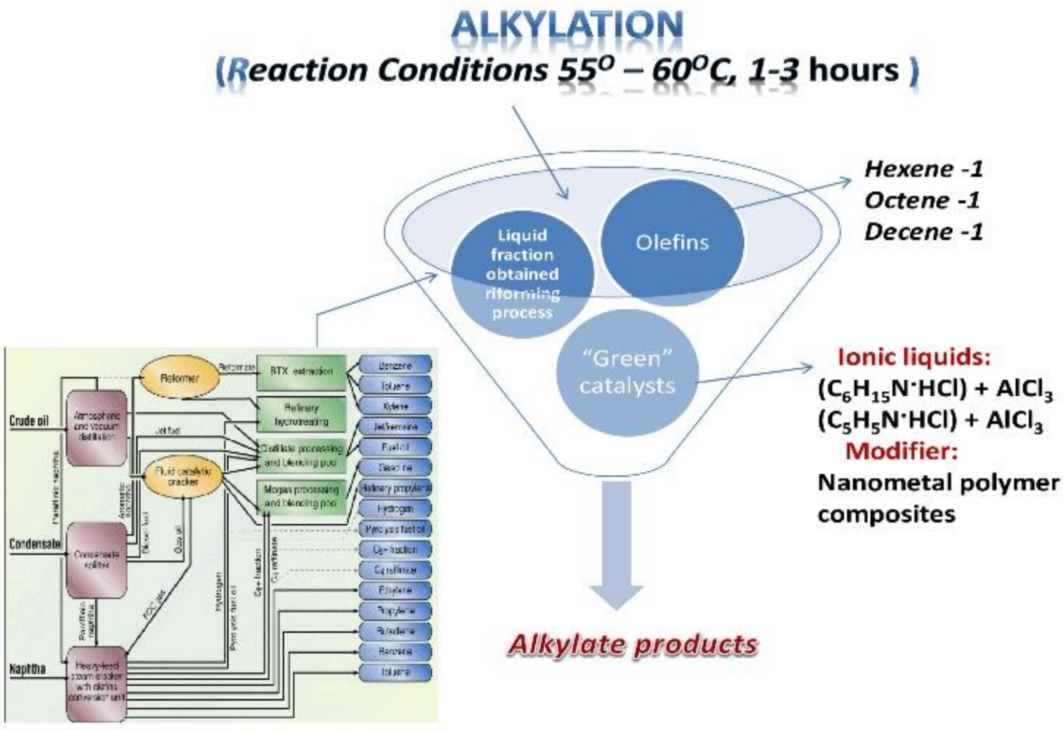
Ionic liquids (IL), which are part of Green Chemistry principles, have drawn much attention in recent years as alternative solvents and catalysts. Ionic liquids are often called as "Green Solvents" or are associated with "Green Chemistry". Ionic liquids (IL) have recently been increasingly employed because of their advantages such as their alternative solvent and catalytic ability, similarity with organic compounds and metal-organic catalysts, and easy separation ability from the reaction product. One of the unique features of IL is that it is compatible with most substances, including (co)polymers. Due to their different structures, polymers can be used in various fields, including carriers. Despite the advantages of IL, a certain amount of halogen atoms can enter to target product. Therefore, to avoid these processes different polymer surfaces were used. These surfaces combine with halogen or other atoms via different physicochemical bonds. This method proves to be valuable not only in the reuse process but also ecologically. The using of IL is very important in alkylation processes because of their (IL) important properties mentioned above.

For many years, extensive research has been conducted on the alkylation of aromatic hydrocarbons with olefins in the presence of ionic liquid catalysts in our laboratory. It is known that the liquid fraction of reforming process (RPLF), which contains 50-60% of aromatic hydrocarbons, is used to obtain individual aromatic hydrocarbons. In our research, we carried out the process of alkylation directly without separating the aromatic hydrocarbons from RPLF with olefins in the presence of ionic liquid catalytic systems. The results were compared with the results obtained by alkylation of individual aromatic hydrocarbons in the presence of IL. The results obtained alkylation processes were analyzed by IR, UV, NMR – spectroscopy, DSC, FIA, chromatographic methods and proved that the alkylation process was going on. A graphical description of the process is presented below.



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ADSORPTION OF Cu(II) BY INTACT AND MODIFIED ACTIVATED CARBON

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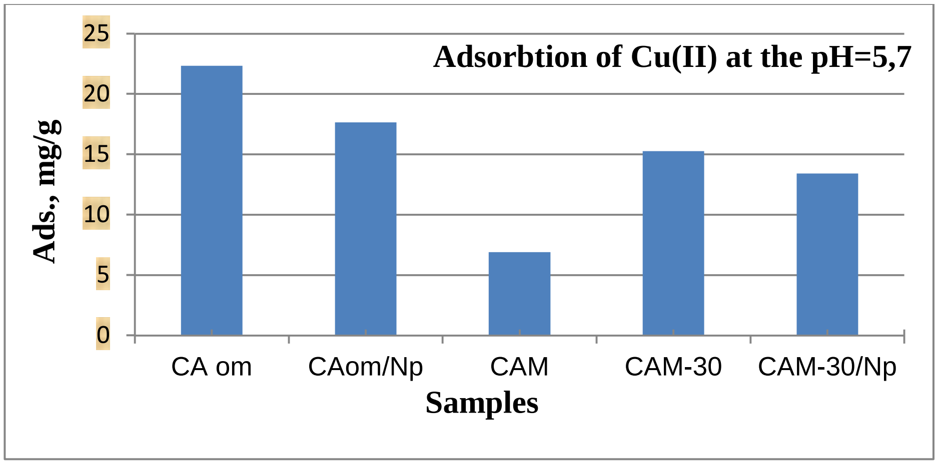
Heavy metal containing wastes are considered to be hazardous to both human life and the environment due to their acute toxicity and non-biodegradability, even when the heavy metals are presented at trace concentrations. A common method for heavy metal removal from water is the ion exchange. One potential application of the adsorbents for heavy metal removal is the treatment with the activated carbon.

Adsorption is a very effective process for a variety of applications, and now it is considered an economical and efficient method for metal ions removal from wastewaters. The most generally used solid adsorbent is the activated carbon, which is used as a very efficient solid adsorbent in many different applications.

The adsorption processes were carried out at room temperature (20±2°C) at the initial metal concentration of 100 mg/L. The process was studied for ions of Cu(II), varying the concentrations of solutions in the limits of 10-180 mg/L. The samples were stirred up on a shaker for 20 h. It was studied the kinetics of the adsorption starting with 0,5 h till 24 h. Then it was continued with the adsorption of Cu(II) at different pH.



Caom *= Activated carbon obtained from Wood coal (to fire up).*

CA-M *= Activated carbon obtained from apple tree wood substance.*

CA-M-30 *= Reactivated sample „CA-M" by heating for 30 min.*

Caom/Np** **and ****CA-M-30/Np* *are samples with nanoparticles.*

The objective of this study was the modification with magnetic nanoparticles of the surface of the activated carbon, for the removal of heavy metals from aqueous media.

In this paper, the adsorption ability of intact or modified activated carbon was investigated for removal of Cu(II) from aqueous systems. Results of the initial screening determined the adsorbents used in further kinetic and isotherm studies, as well as the investigating of the effects on adsorptive performance from pH changes.

Acknowledgments: The research leading to these results has received funding from the international project NanoMed — H2020-MSCA-RISE-2016 and the institutional project 20.80009.7007.21 „Reducing the impact of toxic chemicals on the environment and health by using adsorbents and catalysts obtained from indigenous raw materials".

ALGORITHM OF ANTI-SCIENTIFIC MYTHS REFUTATION BY SCALING OF THE TYPICAL TASKS AND EXPERIMENTS IN CHEMISTRY

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"*Official science would not tell this*" – is an intriguing phrase, widely used by... "modern" promoters of the anti-scientific myths and of the social ignorance. The media space is filled with myths, the absurdity of which is obvious to chemists, but which are easy accepted by significant part of population thanks to simple, attractive and understandable answers. Here are some of them: "*All food additives with the E-code are evil*", "*Palm oil is a poison*", "*Hydrogen peroxide, iodine, soda and lemon-water treat all diseases*", "*The most correct and healthy lifestyle is vegetarian*", "*Well water is always cleaner and safer than tap water*", "*Airplanes specially throw chemical trails with harmful substances*", "*Nuclear energy is not environmentally friendly and should be banned immediately*" and many others.

Modern education process often does not have enough time to raise a barrier to such ignorant aberrations, for several reasons: 1. Volume limited school curriculum does not cover all aspects of modern life. Moreover, curriculum cannot be quickly adapted to all new challenges, since, unfortunately, it is rather inert. 2. Our official scientific agenda is losing ground to a massive flow of false anti-scientific information, since false information is usually less boring and more emotional, and therefore, easier to “enter” the minds. 3. We rarely allow ourselves to go beyond typical tasks and experiments.

And yet, we, teachers of chemistry, can and must systematically demonstrate inconsistency of each new or long-rooted myth or fake. Regardless of whether our students are in school walls or out of it, our routine daily aim is to help them use the richest theoretical and experimental arsenal of chemistry, to think critically, questioning and fact-checking all incoming information, finding its quantitative confirmation or refutation.

The inconsistency of anti-scientific myths cannot be based only on the categoric statement “no, this is all wrong,” that is, it should not be imperative and unsubstantiated. The algorithm for refuting the myth should be based on scientific true and to strength real knowledges, bringing the myth to the point of absurdity, perhaps even to the point of regret that this was initially believed. It can include the following steps:

- **translation of the myth content** into the language of typical chemical task or experiment;
- usually **solving of a chemical task** and/or setting up and realisation of experiment;
- **numerical binding** of the process and of the tasks’ solving results to the myths content;
- **demonstration** of the myth’s inconsistency, **based on numerical and/or experimental data**, that is equal to convincing, reasoned myth’s refutation;
- a brief discussion and conclusion about harm of anti-scientific mythology for the society, economy and for true **understanding of the real picture of the world**.

THE ACYLATION REACTIONS OF CYCLOALKYLPHENOLS WITH ACETIC ACID

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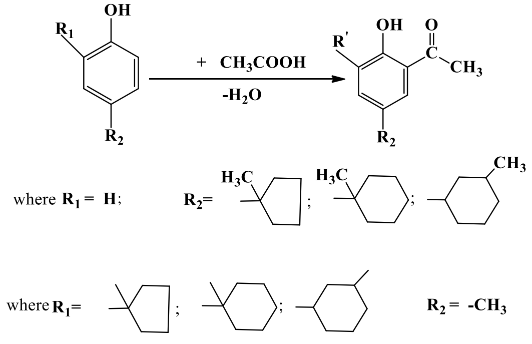
A large amount of C_5-fraction is obtained at the pyrolysis process of low-octane gasoline which has not been determined effective area of utilization. The products of pyrolysis are collected in factories that is the most harmfull for biosphere. The C_5-fractions which is rich with isoprene and piperine is condensed with etilene for getting 1- and 3- methylcyclohexens then it was involved in alkylation reactions with phenol and para cresol.

The acylation reaction of alkylphenols is one the promising area in petroleum chemistry. They are used as the feedstock for the synthesis of high-perpformance thermal and photo stabilizers for polyolefin, additives to oil and fuels.



At the first step, catalytic cycloalkylation reactions occurs phenol and para-cresol with 1-methylcyclopentene and 1(3)-methylcyclohexene in the presence of KY-23 catalyst. According to the results of researches, it was investigated the effects of some parameters (temperature, duration, mol ratio of reagents, amounts of catalyst) on the actual yield of products and selectivity. For each reactions, it was examined the optimal conditions. It was found the the actual yields of products were 71.3-76.7% and selectivity of products were 91.3-96.7.

At the next step, the methylcycloalkylacetophenones were obtained the acylation reaction of para-cycloalkylphenols with acetic acid in the presence of nanosized $ZnCl_2$ as a catalyst and the yield was 51.3-56.7%. The pure products was obtained by rectification at 5 mm Hg and structural formula, element composition, physico-chemical parameters of products were determined.

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THE ROLE OF *INVA*-GENE IN THE DETERMINATION OF *SALMONELLA* SPP. CONTAMINATION OF FOOD

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Key words: *salmonellosis, Salmonella enterica serovar typhimurium, Salmonella enterica serovar enteridis, pathogenesis, primers invA – gene, RT-PCR*

In recent decades, the incidence of salmonellosis has been increasing worldwide. Contamination of food with *Salmonella* spp. And, as a consequence, the development of salmonellosis is a common bacterial disease that affects the intestinal tract and a severe foodborne toxic infection, it is a serious threat that requires great attention to the control of the microbiological purity of food, the development of quick and accurate methods for the detection and identification of *Salmonella* spp. in food in order to ensure their quality in a timely manner and safety, as well as avoidance of economic losses. Currently, *Salmonella* spp. is detected by standard microbiological methods, which are usually laborious and time-consuming. Nowadays, molecular techniques are becoming more and more important for the detection and typing of *Salmonella*.

The modern scientific literature on the mechanisms of development of *Salmonella* infections at the genetic level has been analyzed. The ability of *Salmonella* to penetrate into phagocytes and enterocytes within a few minutes after ingestion of infected food and follow spread throughout the body is provided by a set of effectors whose coordinated expression promotes intracellular survival and replication of bacteria. One of the earliest stages of the pathogenic cycle is the invasion of intestinal epithelial cells. The genetic locus *inv*, which allows *Salmonella* spp. to penetrate intestinal epithelial cells, has been identified. The *invA* gene is a part of this locus and an important component of the inner membrane of the Type III Salmonella Secretion System (T3SS) apparatus, which is responsible for regulation of the export of virulence protein in pathogenic bacteria. Bacterial genome of *Salmonella* includes almost 4.5 thousand genes and consists of one circular chromosome and a number of plasmids. Have been identified the most common genes, and the most detectable gene was the *invA* gene. In the studies of many authors, PCR is used to identify *Salmonella* spp. For this, using special programs, primers are created and implemented that target the *invA* gene, as a conservative and specific indicator of the *Salmonella* genome. These primers are the most selective. The *invA* gene contains unique sequences specific to the genus *Salmonella* and has established itself as a specific target for PCR. To obtain a more accurate profile of the prevalence of *Salmonella* spp, it is appropriate to use the PCR-RT method and to develop primers specific for the *invA* gene. This approach can be considered as a good alternative to the traditional culture method.

GREEN SYNTHESIS OF ZnO NANOPARTICLES USING AQUEOUS PEEL EXTRACTS OF POMEGRANATES AND ITS APPLICATION IN SEED COATING

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The in-depth development of nano-scale and nano-structured materials synthesis methods is due to the need for basic research on size effects and the expansion of their practical applications in modern electronics, medicine and agricultural technology. In recent years, zinc oxide nanoparticles have been used as fertilizers and in seed coating technology. Considering the fact that zinc oxide nanoparticles may promote the yield and growth of food crops. Zinc oxide nanoparticles (Nps ZnO) in practice can be obtained in two basic ways: by chemical means and by “green synthesis”. Green synthesis was used in studies to obtain nano-sized ZnO. This is an efficient, inexpensive, environmentally friendly and easy to apply method. For this experiment, it was used pomegranate peels as a stabilizing agent. The inside of the pomegranate peel contains many substances such as punicalagin, gallic acid, ellagic acid, chlorogenic acid, caffeic acid, punicalin, apigenin, pelargonidin, cyanidin, pomegranate A, and pomegranate B. These compounds are mainly concentrated in the pomegranate peel and have been shown to aid in the green synthesis of a wide variety of nanoparticles [1].

Zinc nitrate hexahydrate [$Zn(NO_3)_2•6H_2O$] was utilized as a forerunner to synthesize zinc oxide nanoparticles. Nanoparticles were synthesized by methodology proposed [2].The synthesized ZnO NPs by this method were characterized by Fourier transform infrared spectroscopy (Varian 3600 FTIR) in the spectral range of 4000 to 400 cm^{-1} were studied.

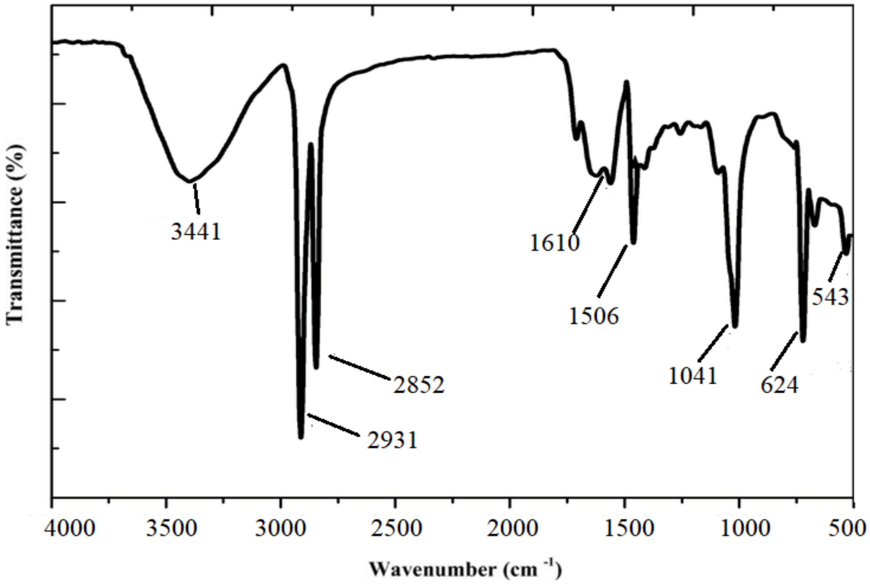

Fig. 1. FTIR spectrum of ZnO nanoparticles

The bands at 543 and 624 cm^{-1} are stretching vibrations of ZnO NPs. The broadband at 3441 cm^{-1} belongs to O-H stretching of organic residues of pomegranate on ZnONPs and the peak at 2931 and 2852 cm^{-1} belongs to C-H stretching vibrations (Fig. 1). This study has shown that ZnO NPs can be prepared at a low cost from pomegranate wastes and obtained ZnO NPs has the potential to be used in agriculture.

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MEDICINAL PLANT PRODUCTS – THE SOURCE OF RAW MATERIALS FOR A SUSTAINABLE PHARMACEUTICAL INDUSTRY

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Phytotherapy and phytopreparations have passed the tests of time and are now used in medicine. Synthesized medicinal preparations are significantly inferior to medicinal plants, since they have natural complexes of biologically active substances, as well as micro- and macroelements. The medicinal plants always, contains a complex of BAS, which is used in medicine and is called an active substance.

Medicinal plant raw materials are widely used in medicine to obtain various medicines in the form of infusions and tinctures, decoctions, extracts, total preparations, etc. Medicinal plant raw materials can be harvested from both wild and cultivated medicinal plants, as well as waste from the food industry.

The reasons why the demand for medicinal plant raw materials is increasing are the relative safety of action, the chemical nature of medicinal plants allows drugs based on them to be easily incorporated into human biochemical processes, providing a multifaceted effect; affordability; favorable attitude of consumers to medicines from plant raw materials, which was formed thanks to centuries-old traditions and vast experience of traditional medicine; the possibility of rational combination of medicinal plants with each other and with synthetic means; is a regenerated raw material.

The development of synthetic chemistry and the chemical industry has ensured the synthetic production of medicinal substances, both obtained from natural materials and completely new ones. The synthesized substances allowed to expand the boundaries in the pharmaceutical industry, however, a number of problems have appeared that have affected the ecological state of the environment. Thus, the pharmaceutical industry is one of the most polluting areas of activity at present.

The use of medicinal plant raw materials in technological processes makes it possible to reduce harmful emissions into the environment that are formed during the synthesis of the pharmaceutical industry. On the other hand, agricultural waste is a condition for the rational use of natural resources. To ensure a prosperous ecological state, it is important to pay attention to environmental education, which affect the learning cycles. Thus, students of the Faculty of Chemistry and Chemical Technology conducted a study, the purpose of which was to detect various types of medicinal plants on the territory of the university. The use of local medicinal plant raw materials can be an ecological alternative to the development of the production of phytopreparations.

The result of the work done showed that there are about 12 medicinal plants on the territory of the University, and the total number in the Republic of Moldova has about 300 species, which indicates a favorable soil and climate for medicinal plants.

In conclusion, we would like to note that the proper use of natural resources, as well as environmental education, are key factors for achieving a sustainable economy and a safe environment.

ANTIBIOTIC RESIDUES IN FOOD

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The presence of antibiotics in foods of animal origin may be due to the mixing of antibiotics from different feeds in order to stimulate growth and improve yield, use for prophylactic or therapeutic purposes, and of course the accidental incorporation of antibiotics into various products. Antibiotics are used in animal husbandry in small quantities to ensure a superior use of feed, guaranteeing a saving of about 5% and a weight gain of about 10%. Identification of antibiotic residues in food of animal origin presence of toxicological interest, as it causes primary and secondary effects on the health of consumers.

In terms of effectiveness, the antibiotics can be 1000 times more active than any other preserving agent. By reason of antibiotics effect is mainly bacteriostatic, for the preservation of food it is necessary that the antibiotic is permanently present in the product, its stability over time being an essential condition.

Antibiotics have a selective action. Antibiotics used as food additives must meet certain characteristics such as: not being related to antibiotics used in human therapy and having little or no absorption after administration. Also these preparations do not must have an impact on the environment or this impact need be reduced.

Sulfadimethoxine, sulfamethoxazole, sulfaquinoxaline and sulfadiazines are the most widely used sulfonamides in veterinary medicine. If the waiting period is not met, products of animal origin may be contaminated with residues of these substances. The interest in detecting these residues is very current. The first, the largest exceedance of the legal level of sulfonamides in tissues was reported in the USA in 1970. In the last 25 years, sulfonamides have produced more overtaking of the maximum permitted limit of residues than any other group, with the highest incidence in pigs, followed by cattle and birds. Actually, exceeding the maximum residues limit for sulfonamides is common for all the world.

Since 2015, the European Center for Prevention and Control and the European Food Safety Agency have published annually the results of research on antimicrobial resistance from all countries of the European Union. In the Republic of Moldova, the problem of the presence of antibiotics in the environment, including food, is little researched, but is a great interest for both research and state institutions.

DEVELOPMENT OF SUSTAINABLE AND COST EFFECTIVE BIOSORBENT FROM HAZELNUT SHELL WASTE FOR LITHIUM EXTRACTION FROM WATER

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Sustainability and green chemistry have been critical for the development of the next generation of materials over the last decade, with the use of bio-based polymer matrices potentially allowing for lower environmental impacts through the use of renewable carbon and more easily biodegradable or reusable materials. On the other hand, energy transition elements are gaining importance due to their ability to provide energy and play an important role as primary energy sources in sustainability as well. To satisfy the enormous growth in worldwide lithium use caused by the rapid adoption of electric vehicles and mobile electronics, researchers are looking for alternate lithium-capable materials and sources. In this study, hazelnut shell waste that is a real cellulose resource that is inexpensive and abundant in Turkey was phosphorylated to develop a novel biosorbent based on natural renewable resource for the recovery of lithium from aqueous solution. Surface morphology and mapping by SEM–EDS, chemical characteristics by FTIR, elemental analysis by XPS, specific surface area by BET, crystallinity by XRD, and thermal properties by TGA were all thoroughly investigated for the synthesized biosorbent. Biosorbent dosage, initial concentration, temperature, contact time, pH, and coexisting ions all had an effect. The equilibrium sorption capacity reached 6.03 mg/g under optimal conditions (i.e., biosorbent dosage of 12.0 g/L, initial Li concentration of 100 mg/L, pH value of 5.8, sorption temperature of 25°C, and sorption time of 6 min). Desorption studies at 25°C revealed that relatively higher desorption efficiency and capacity were achieved at 97.4% and 5.93 mg/g, respectively with a 1.0 M H_2SO_4 among other regenerants (i.e., HCl and NaCl). As a result, because of these unique characteristics, the novel phosphorylated hazelnut shell waste can be valorized for lithium recovery from aqueous solution by contributing sustainability and circular economy.

STUDY OF VITAMIN B_{12} ADSORPTION ACCORDING TO THE NATURE OF THE CARBONIC ADSORBENTS

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Currently, a serious consequence of environmental degradation is the significant deterioration of the health of the population, accompanied by an increase in the number of exogenous poisonings. A simple and effective method of detoxifying the human body is the enterosorption. In the case of enterosorption, endogenous and exogenous metabolites of the digestive tract are subsequently immobilized and eliminated from the digestive tract.

Presently, the method of detoxification of the human body widely used in most of the clinics is the enterosorption and the most applied enterosorbents are made from activated carbon. A special role in this regard belongs to the activated carbons obtained from walnut shells, fruit seeds, grape seeds. Due to the adsorption forces, in the porous structures of activated carbons (in the volume of micropores and mesopores) the adsorption of different types of contaminants takes place. The high adsorption properties of these activated carbons offer wide possibilities for their use, including in the complex treatment of intoxications and pathological conditions.

For research, the activated charcoal obtained in the laboratory was selected from: charcoal (CA-ML), walnut shells (CAN), peach kernels (CA-23), plum kernels (CA-35), intact apple wood and reactivated (CAM and CAM-30), but also a sample of commercially activated carbon (Granucol BI). Vitamin B_{12} (Cyanocobalamin) with MM 1355.38 u.c. was used as a marker substance (fig. 1) which models the situations of intoxication of the human body with toxins with medium molecular weight (MM 500-1500), such as oligopeptides, lipopolysaccharides, etc.

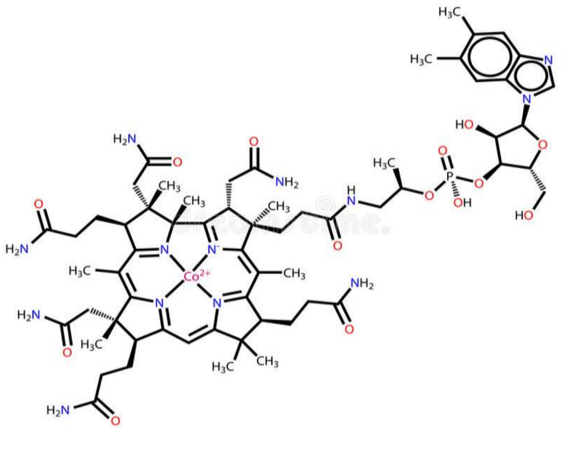

Figure 1. Vitamin B_{12} ($C_{63}H_{88}CoN_{14}O_{14}P$

In this paper, the adsorption of Vitamin B_{12} on several samples of activated carbons mentioned above was studied. The kinetic adsorption curves were determined from 0.5 h to 48 h with the initial concentration of the solutions 200 mg/L, at a temperature of 250°C. The data obtained indicate that the degree of immobilization of Vitamin B_{12} on the activated carbon samples investigated, increases with increasing contact time between the two phases, and the balance is established within 20-24 h.

The adsorption effect of Vitamin B_{12} is obviously different depending on the nature of the adsorbent and there is a big increase in adsorption when reactivated for 30 minutes from 20 mg/g in the case of CAM (activated charcoal obtained from apple wood) to 180 mg/g for CAM-30 sample (same activated carbon with an additional activation of 30 min under the same conditions). The researched carbons show increased immobilization capacities of the marker substances (Vitamin B_{12}), and for the reactivated samples the values are 5-6 times higher than the intact samples.

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NUCLEAR WASTE MANAGEMENT IN KOREA

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The issue of nuclear waste is a global one and its management is important to ensure the safety of water, soil, plants, animals and human health. Worldwide there are *32* countries in which the nuclear power plants operate, where the 441 nuclear reactors generate approximately 10% of global electricity. They must secure the correct management of nuclear waste.

Korea can serve as a good example. There are 24 reactors, which provide about one-third of South Korea's electricity from 23 Gwe of plant. South Korea is among the world's most prominent nuclear energy countries, and exports its technology widely. It is currently involved in the building of the UAE's first nuclear power plant, under a $20 billion contract.

The Korea Radioactive Waste Management Corporation (KRMC) was set up at the beginning of 2009 under the Radioactive Waste Management Act as an umbrella organization to resolve South Korea's waste management issues and waste disposition, and particularly to forge a high-level national consensus on waste. It is accountable to MOTIE. Until then, KHNP had been responsible for managing all its radioactive waste. In mid-2013 KRMC's name changed to the Korea Radioactive Waste Agency (KORAD).

The Atomic Energy Act of 1988 established the principle under which KHNP was levied a fee based on power generated to cover the cost of waste management and disposal. A fee was also levied on Korea Nuclear Fuel. The fees were collected by the Ministry of Education, Science, and Technology (MEST) and paid into the national Nuclear Waste Management Fund. A revised waste programme was drawn up by the Nuclear Environment Technology Institute (NETEC) and approved by the Atomic Energy Commission in 1998. These arrangements are superseded by KORAD, and KHNP now contributes a fee of KRW 900,000 (US$ 705) per kilogram of used fuel to KORAD.

Used fuel is stored on each reactor site pending construction of a centralized interim storage facility, which is planned to be operational by 2035, eventually with 20,000 tonnes capacity. About 14,000 tonnes was stored at the end of 2015, onsite pool capacity being 12,000 tonnes, about half of both figures being for Candu fuel at Wolsong. Dry storage in MACSTOR/KN-400 modules is used for Candu fuel after six years of cooling in pools. Dry storage is also proposed for used fuel at other sites as pools at reactors reach capacity, notably Kori and Hanul/Ulchin.

Reference:

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NON-COVALENT INTERACTIONS – USEFUL TOOLS IN CRYSTAL ENGINEERING

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The search for crystalline molecular materials showing interesting and technologically useful properties is one of the most important challenges of crystal engineering. All the synthetic approaches leading to such systems rely on the directionality of the interactions connecting the building-blocks. Apart from the coordination bonds, largely employed to construct molecular solids, other interactions can be useful too: hydrogen and halogen bonds (both directional), metallophilic and $\pi-\pi$ stacking interactions. Having in mind that “the crystal is a supramolecular entity” (G. R. Desiraju), we currently design new solid-state architectures resulting from the convolution of coordinative and non-covalent interactions. A special emphasis is given to systems containing two different metal ions, as well as to co-crystallization processes.

CURRENT ENVIRONMENTAL CHALLENGES FOR HUMAN SECURITY

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It is necessary to re-conceptualize the national security in the protection of the environment. Let’s turn the traditional Cold War concept into the primary security of the state! The environmental dimension has a major impact on humanity with new threats. Economic decline, environmental degradation, dramatic depletion of natural resources, ecological disasters, increasing pressure on the environment and resources will undermine security and stability. Our political, governmental and security systems must cope with these challenges in order to manage them peacefully.

EXPERIMENTAL SETUP FOR ELEMENTAL ANALYSIS USING PROMPT GAMMA RAYS AT RESEARCH REACTOR IBR-2

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The new experimental setup has been built at the 11b channel of the IBR-2 research reactor at FLNP, JINR, to study the elemental composition of samples by registration of prompt gamma emission during thermal neutron capture. The setup consists of a curved mirror neutron guide and a radiation-resistant HPGe high-purity germanium detector. The detector is surrounded by lead shielding to suppress natural background gamma level. The sample is placed in a vacuum channel and surrounded by a LiF shield to suppress the gamma background generated by scattered neutrons. This work presents characteristics of the experimental setup. An example of hydrogen concentration determining in diamond powder made by detonation synthesis is given and on its basis, the sensitivity of the setup is calculated being ~10μg.

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KETO-ENOL TAUTOMERISM AND GEOMETRICAL ISOMERISM OF DIHYDROXYFUMARIC ACID. A DFT STUDY IN GAS AND WATER

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Dihydroxyfumaric acid (DHF) is an important organic acid found in vegetal and living cells, a proven intermediate in the cycles of di– and tricarboxylic acids, and in the glyoxalic acid cycle via the tartaric acid transformation cycle. Eschenmoser suggested [1] that glyoxylate and its dimer, DHF, could have served as the basic raw material for the synthesis of organic macromolecules in the constraints of prebiotic chemistry, thus leading to the formation of life on Earth. This, in correlation with earlier results that showed that DHF and some of its derivatives may be successfully used for the enhancement and preservation of wines [2], as inhibitors of nitrosoamines formation in vitro [3,4] and in vivo [5], as well as efficient scavengers of DPPH and ABTS free–radicals [6], prompted us to carry on a series of computational studies, using the ORCA software [7].

A total of 45 isomers of DHF, including 23 keto and 22 enediol forms, were identified and their geometrical isomerization was studied at the B3LYP level of theory using the 6–311++G(2df,2p) basis set in the gas phase, and aqueous solution (SMD model). Three most stable enediol structures were identified. Interconversions between the enediol forms and the keto forms proceed through two paths: (1) proton transfer (≈ 135–160 kJ mol^{-1}) and (2) internal rotation (≈ 0.15–75 kJ mol^{-1}). Furthermore, equilibrium constants have been calculated, along with the forward and reverse reaction rates for the isomerization reactions of the three most stable enediol structures, in gas and water.

The DFT method was further used to investigate the keto-enol tautomerism of the most stable three enediol structures of DHF, in the gas phase, and aqueous solution (SMD model). It was found that the activation energy and the free activation energy are in the range of 230–310 kJ mol^{-1} for the gas phase and by 50-80 kJ mol^{-1} lower in water, and transition states structures reveal that the carboxylic oxygen that forms the hydrogen bond in the enediol structure is involved in the mechanism of proton transfer. Furthermore, equilibrium constants have been calculated, along with the forward and reverse reaction rates. This research is important mainly because enols are essential intermediates in many important reactions of carbonyl compounds, as well as in several biological reactions.

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A HYBRID PHOTO CATALYST FOR SOLVING ENVIRONMENTAL PROBLEMS

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Wastewater often contains some toxic organic compounds particularly difficult to clean due to their poor biodegradability and high toxicity. Such type of wastewaters needs careful treatment before discharge into the receiving bodies of water.

Activated carbon adsorption, solvent extraction, chemical oxidation and electrochemical methods are the most widely used ones for removing such compounds from wastewaters. These approaches are often ineffective because they merely transfer the organic pollutants from water to another medium without degrading or mineralizing the organic pollutants.

The method of heterogeneous photocatalysis, one of the measures employed in modern advanced oxidation processes (AOPs), has been used to remove or mineralize a wide range of organic pollutants.

Several semiconductors can act as photocatalysts but TiO_2 stands out as the most effective photocatalyst and has been extensively used in water and wastewater treatment studies because it is cost effective, thermally stable, non-toxic, chemically and biologically inert, strong photoactive and is capable of promoting oxidation of organic compounds.

However the large scale application of this treatment technology is constrained by several factors such as: low adsorption capacity, strong tendency to agglomeration of nano sized TiO_2 particles resulting in reduction or even complete loss of photocatalytic activity; problem of separation of nanosized particle powder in the aqueous media after the photocatalytic process.

Many techniques of immobilization have been developed to attach the TiO_2 powder to simplify the cleaning stage after the photocatalytic process. The dispersion of TiO_2 nanosized particles into porous material is the solution of the problem.

Diatomite is an important porous non-metallic resource with nontoxic and good chemical stability. Application of diatomite as carrier material may enhance the TiO_2 nanosized particles distribution in suspension which enables to adsorb and concentrate the target substances. There are a number of methods for preparing hybrid photocatalysts based on nanosized titanium dioxide and a mineral substrate. Basically, this is a heterogeneous chemical deposition of titanium dioxide from titanium alkoxides or titanium tetrachloride as a precursor of nanosized titanium dioxide. A common disadvantage of the described methods is the use of chemical reagents, the multistage and long duration of the process of obtaining titanium dioxide in the composite.

The electrochemical method developed for the preparation of a hybrid photocatalyst based on nanosized titanium dioxide and local diatomite as a substrate is free of these disadvantages. It is as follows: 2.0 g of purified diatomite dispersed in a solution of $TiCl_4$ of the required concentration in the cathode chamber of the electrolyzer and stirred for 30 minutes. Then a constant current is applied to the electrical contacts of the electrolyzer until a certain pH is reached in the cell. Then the current is turned off, the contents of the cell are filtered, washed with distilled water, dried at room temperature, then in an oven at 100°C, and calcined at 400°C for the development of the anatase phase. The resulting product -NTD- is further stored in a desiccator for further physicochemical and photocatalytic studies.

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