SPI

Symposium on Polymer(s) Innovation

&

Soil Innovation for Regenerative Agriculture

SPI-SIRA 2025

FIEK
MISKOLCI EGYETEM

FACULTY OF MATERIALS AND CHEMICAL ENGINEERING
1735
UNIVERSITY OF MISKOLC

17 35
UNIVERSITAS MISKOLCINENSIS

BorsodChem
Chemistry for generations

University of Miskolc

*Advanced Materials and Intelligent Technologies Higher Education and Industrial Cooperation Centre (**HEICC**)*

Institute of Chemistry

Scientific Advisory Board

Editors

Conference Program

Symposium on Polymer(s) Innovation & Soil Innovation for Regenerative Agriculture

SPI-SIRA 2025

2025.09.22.

12:00 – 13:00	**SOCIAL ACTIVITY AND LUNCH**	
Timeframe	**Speaker**	**LECTURE TITLE, ORGANIZATION**
13:00-13:30	**Prof. Dr. Béla Viskolcz & Prof. Dr. Béla Fiser**	**From Theory to Experiments: Integrated Polymer and Modeling Unit - INPUT** *Opening lecture - University of Miskolc*
Sustainable Pathways in Polymer Science and Green Materials		
13:30 -13:50	**Imen Afdhal**	**Green synthesis of silver nanoparticles using Nigella sativa oil for their biological applications** *(University of Carthage)*
13:50 – 14:10	**Enikő Hornyák-Mester**	**Development of low-VOC flexible polyurethane foams** *(University of Miskolc)*
14:10 - 14:25	**Mohamed El Bakkali**	**Antioxidant activity of Abies marocana essential oil and its application as additive in polyurethane foams** *(Abdelmalek Essaâdi University)*
14:25 – 14:40	**György Marcell Tokaji**	**Investigation of the Chemical Degradation of Model Urethanes – Importance of Industrial Plastic Recycling** *(University of Miskolc)*
14:40-14:55	**Máté Gergő Hatvani-Nagy**	**Isolation of cobalt resistant bacteria from soil** *(University of Miskolc)*
14:55 – 15:10	**Anikó Jordán Csábrádiné**	**Polyurethane biodegradation** *(University of Miskolc)*
15:10 -15:30	**Dr. Tomasz Szmechtyk**	**Epoxy resins with natural co-hardeners from bio-waste** *(University of Lodz)*
15:30	**CLOSING CEREMONY**	

Symposium on Polymer(s) Innovation & Soil Innovation for Regenerative Agriculture

SPI-SIRA 2025

2025.09.23.

Timeframe	Speaker	LECTURE TITLE, ORGANIZATION
10:00 – 10:10	**Prof. Dr. Béla Viskolcz & Prof. Dr. Béla Fiser**	**Opening lecture, *University of Miskolc***
Soil Innovation for Regenerative Agriculture		
10:10 – 10:40	**Prof. Dr. Babak Minofar**	**Computational study of soil enzyme interaction with nano materials** *(University of Miskolc)*
10:40 – 11:00	**Alpár Ferencz Hatvani-Nagy**	**Chemical Invention in Precision Agriculture** *(University of Miskolc)*
Frontiers in Organometallic Chemistry and Noble Metal Catalysis		
11:00 – 11:40	**Prof. Dr. Raluca Septelean**	**Phospha(thioxo)phosphorane, a rich-electron building block for new organometallic and coordination compounds** *(Babes-Bolyai University)*
11:40 – 12:20	**Prof. Dr. Balázs Brém**	**Development of Platinum(IV)-based Anti-Tumour Agents Carrying Anti inflammatori Moieties** *(Babes-Bolyai University)*
12:20 – 12:40	**Bence Benedek Tamás**	**Gas adsorption testing of carbon-based noble metal catalysts** *(BorsodChem)*
12:40 – 13:10	**Dr. Ferenc Kristály**	**Structural changes on nobel metal-based catalysts during hydrogenation** **Crystal structural characteristics of transition metal ferrites for catalyst support** *(BorsodChem)*
13:10-14:10	**LUNCH BREAK**	
Advances in Vacuum Ultraviolet Photoionization Mass Spectrometry		
14:10 – 14:40	**Prof. Dr. Zuoying Wen**	**Ambient volatile organic compounds (VOCs) measured online with a compact VUV photoionization mass spectrometer** *(Chinese Academy of Sciences)*
14:40 – 15:25	**Prof. Dr. Xiaofeng Tang**	**Vacuum ultraviolet photoionization mass spectrometry and its applications** *(Chinese Academy of Sciences)*
15:25 – 16:00	***Laboratory visits within HEICC***	
16:00	**CLOSING CEREMONY**	

Abstracts

Afdhal Imen[1], Sellami Hanen[1]

Green synthesis of silver nanoparticles using *Nigella sativa* oil for their biological applications

[1] Laboratory of Treatment and Valorization of Water Rejectes,Water research and Technology Center (CERTE), Borj Cedria Technopark, University of Carthage, Soliman 8020, Tunisia.

Background: The growing interest in nanoparticles stems from their exceptional surface area and physicochemical properties, which make them valuable in fields like medicine, environmental science, and biomolecular detection. Traditional synthesis methods, however, often involve costly and environmentally harmful processes. To address these limitations, this study adopts a green synthesis approach using *Nigella sativa L.* vegetable oil to produce silver nanoparticles (AgNPs). The research aims to thoroughly assess their physicochemical and biological characteristics, while also investigating their potential use in electrochemical biosensing applications.

Materials/Methods The study employed a structured and multi-step methodology to synthesize and characterize silver nanoparticles (AgNPs-N) using *Nigella sativa L.* oil. Initially, the oil's chemical composition was analyzed via gas chromatography-mass spectrometry (GC-MS). The biosynthesis of AgNPs-N was achieved by mixing the oil with an aqueous silver nitrate solution, with successful nanoparticle formation indicated by a dark brown color change. Comprehensive characterization was conducted using UV-Vis spectroscopy, SEM, DLS, and FTIR to confirm particle morphology, size distribution, and surface chemistry. The biological potential of the AgNPs-N was evaluated through antioxidant (DPPH assay), antibacterial (well diffusion method), and cytotoxicity/biocompatibility tests (MTT assay on T47D and HEK293 cells). Additionally, the nanoparticles were integrated into screen-printed carbon electrodes to develop an electrochemical sensor, whose performance was assessed for catechol detection.

Results The conducted study demonstrated that silver nanoparticles biosynthesized (AgNPs-N) from *Nigella sativa L.* vegetable oil exhibit remarkable physicochemical and biological properties. The oil's composition revealed a high content of unsaturated fatty acids, particularly linoleic acid (56.4%), oleic acid (23.9%), and palmitic acid (12.6%), which play a key role in reducing silver ions and stabilizing the nanoparticles. Characterization techniques such as UV-Vis spectroscopy, FTIR, SEM, and DLS confirmed the formation of spherical, well-dispersed nanoparticles with an average size of 37 nm and a bimodal distribution. The FTIR spectrum revealed additional functional groups, indicating chemical interactions between silver ions and oil constituents. Biologically, the AgNPs-N showed significant antioxidant activity (IC_{50} = 0.189 mg/mL), higher than the oil alone, and strong antibacterial efficacy with MIC values ranging from 145.83 to 229.16 µg/mL and a consistent MBC of 500 µg/mL,

confirming their bactericidal effect. Cytocompatibility tests on HEK293 cells showed good biocompatibility (77.12% viability), while antiproliferative assays on T47D cancer cells revealed strong inhibition (viability reduced to 10.06%), unlike the oil which had no significant effect. Finally, screen-printed carbon electrodes modified with AgNPs-N demonstrated excellent sensitivity and selectivity for catechol detection, due to favorable electrostatic and hydrophobic interactions. The green synthesis method further enhances the biomedical and environmental potential of these nanoparticles.

Conclusion: This study confirms the significant potential of silver nanoparticles (AgNPs) biosynthesized from *Nigella sativa* oil for biological properties. The green synthesis method employed offers an effective and eco-friendly production route.

Enikő Hornyák-Mester[1,2,3,*], Gábor Muránszky[2], Werner Péter Groh[3], Béla Viskolcz[1,2]

Development of low-VOC flexible polyurethane foams

[1] Higher Education and Industrial Cooperation Centre, University of Miskolc, 3515 Miskolc, Hungary
[2] Institute of Chemistry, University of Miskolc, 3515 Miskolc-Egyetemváros, Hungary
[3] MOL Hungarian Oil and Gas Plc., 1117 Budapest, Dombóvári st. 28., Hungary
[*] eniko.hornyak-mester@uni-miskolc.hu

The aim of the research was to investigate the volatile organic compound (VOC) content of flexible polyurethane (PUR) moulded foams and to explore possible reduction strategies. A PUR foam produced with a traditional formulation was selected as a reference, and its volatile emissions (VOC and fog content), as well as its mechanical and acoustic properties, were determined using standardized methods. Measurements revealed that VOC content strongly depends on the ratio of raw materials (NCO-index), with the main emission sources originating from the polyol component formulated with additives. Analysis of the effect of elapsed time after production showed that maximum emission occurred on the 10th day, while significant levels were still detected after 30 days. The predominant emission components were found to originate from additives, including two amine-type catalysts (TEDA and BDMAEE) and polyalkylsiloxane compounds, presumably from the surfactant.

Based on these findings, systematic formulation modifications were carried out by testing different types of low-emission additives. Subsequently, VOC content, mechanical and acoustic properties, and microstructural analyses were determined, followed by additional testing after both dry-aging and autoclave-aging.

The results demonstrated that the application of low-emission additives led to a significant reduction in emissions. Changes in mechanical properties were primarily associated with density differences, while the acoustic properties remained comparable to the reference material. Dry aging resulted in minor cell structure degradation and a decrease in compressive strength, without notable effects on acoustic performance. In contrast, autoclave aging caused significant structural deterioration, which substantially reduced both mechanical and acoustic performance.

Mohamed El Bakkali[1], Amin Bouchfara[1], Hamass Zerrad[2], Badredine Souhail[1], Mounir Nechar[1], Dóra Mentes[4], László Farkas[3], Anikó Csábrádiné Jordán[3], Rehana Bano[3], Béla Viskolcz[3,4], Béla Fiser[4,5]

Abies marocana essential oil and its Application as Additive in Polyurethane Foams

[1] Laboratory of Water, studies and Environmental Analysis, Faculty of Sciences, Tétouan, Abdelmalek Essaâdi University, Morocco

[2] Biotechnologies and Biomolecular Engineering Research Team, Faculty of Sciences and Technologies, Tangier, Abdelmalek Essaâdi University, Morocco

[3] Higher Education and Industrial Cooperation Centre, University of Miskolc, 3515 Miskolc-Egyetemváros, Hungary

[4] Institute of Chemistry, University of Miskolc, 3515 Miskolc-Egyetemváros, Hungary

[5] Department of Physical Chemistry, Faculty of Chemistry, University of Lodz, 90-236 Lodz, Poland

The genus *Abies* is a plant widely known for its medicinal and therapeutic properties, belongs to the family Pinaceae and comprises 51 species, with the majority of them distributed in the temperate and boreal zones of the Northern Hemisphere. Evergreen conifers are found across Europe, Asia, North and Central America, and North Africa [1]. *Abies marocana* is a native tree that grows wild in the calcareous chain of Jebala (northern Morocco), This species is endemic to the high-altitude calcareous peaks of the western Rif Mountains in Morocco, thriving at elevations between 1400 and 2000 m and can reach 50 m in height [2]. It grows in humid and perhumid bioclimates with cold and very cold variants. *Abies marocana* is distributed in two populations Mont Tazaout and Talassemtane, which occupy an area of about 300 ha and approximately 3,760 ha respectively [2].

This study represents the first exploration of the composition, physicochemical properties, total phenolic content and molecular docking simulations to evaluate antioxidant activity of Mont Tazaout *Abies marocana* essential oil (AMEO) and its Application as Additive in Polyurethane Foams. The essential oil was extracted using steam distillation and analyzed with a yield of 0.24%. Then the oil was stored in amber bottles until needed. The composition was investigated using gas chromatography–mass spectrometry (GC-MS). The four major compounds of AMEO were limonene (38.46%), α-Pinene (21.16%), β-Pinene (12.92%) and camphene (11.23%). Physicochemical properties of AMEO were determined, including density (0.888 ± 0.020) g/cm^3, refractive index (1.470 ± 0.010), and optical rotation (-40.52 ± 0.04)°. Furthermore, the total phenolic content (TPC) of the essential oil was found to be (5.07 ± 0.49) mg GAE/g EO. AMEO shows an IC_{50} = (136.28 ± 7.8) mg/mL and IC_{50} = (1.47 ± 0.04) mg/mL in the DPPH and FRAP assays, respectively. Molecular docking used to investigate the mechanism of interaction between the constituents of AMEO and target proteins associated with antioxidant activity. After analyzing the docking results related to the docking of the seven studied compounds (*S*-limonene, *R*-limonene,

camphene, (+)-α-pinene, (-)-α-pinene, (+)-β-pinene and (-)-β-pinene), compounds *R*-limonene and *S*-limonene emerged as the most promising antioxidants. This is due to their favorable binding profiles with both NAD(P)H oxidase and nitric oxide synthase targets. Moreover, the incorporation of AMEO into flexible polyurethane foams was carried out at different concentrations and NCO indices. The addition of the studied essential oil was found to decrease the compressive force and modify the mechanical properties of the foams, while also providing antioxidant protection. Therefore, the use of AMEO as an additive in polyurethane formulations was shown to impart dual benefits, combining mechanical tuning with oxidative stability.

Keywords: *Abies marocana*; Essential oil; physical-chemical characteristics; Chemical compositions; Molecular docking; Antioxidant activity.

References:

1. Marjanovic-Balaban, Z., Cvjetkovic, V. G., Stanojevic, L., Stanojevic, J., Nikolic, L. & Danilovic, B. (2020) Quality Testing of Industrially Produced Essential Oil of Fir (Abies alba L.) from the Republic of Srpska, *Journal of Essential Oil Bearing Plants.* **23**, 503-513.
2. Ben-Said, M. (2022) The taxonomy of Moroccan fir Abies marocana Trab. (Pinaceae): conceptual clarifications from phylogenetic studies, *Mediterranean Botany.* **43**.

György Marcell Tokaji [1,2], Béla Fiser [1,3,4]

Investigation of the Chemical Degradation of Model Urethanes – Importance of Industrial Plastic Recycling –

[1] Chemistry Institute, Miskolci Egyetem, 3515 Miskolc-Egyetemváros, Hungary
[2] Wanhua-BorsodChem Zrt, Bolyai tér 1., 3700 Kazincbarcika, Hungary
[3] Department of Physical Chemistry, Faculty of Chemistry, University of Lodz, 90-236 Lodz, Poland
[4] Ferenc Rakoczi II Transcarpathian Hungarian College of Higher Education, Beregszász 90200, Ukraine

Although plastics have many advantages, they also have one characteristic that makes their use harmful to the environment: their lifespan. It can be said that these materials can persist in our environment for hundreds of years as they wear out. Therefore, plastics can only be used for a certain period of time until their quality deteriorates significantly, at which point they can be considered plastic waste. In most cases, this plastic waste ends up in landfills, which is not an environmentally friendly solution. There are several methods that are suitable for the environmentally friendly treatment of plastic waste, such as chemical decomposition or as know as chemical degradation. With the help of chemical degradation, valuable raw materials can be recovered from plastic waste, which can be used in new plastic production processes. For this, we need specific reaction conditions, catalysts, and, depending on the type of decomposition process, the appropriate decomposition chemical. Based on global market share data, the demand for polyurethane-type plastics is continuously increasing, which is why this research into the treatment of urethane-type plastics has intensified. Although polyurethane waste found in our environment contains several substances (additives) and therefore has a complex structure, it was worthwhile to produce a model diurethane compound in order to investigate the reaction mechanisms and understand them more easily. However, the main question is how to recover the polyol and possibly polyisocyanate raw material from this model compound. The previously mentioned chemical degradation is suitable for this. By performing several different experiments, a reproducible glycolysis process between laboratory levels was developed, which is suitable for recovering the polyol fractions. Furthermore, to understand the molecular mechanism of the degradation reaction, computational chemistry methods were used. Within this framework, the reaction mechanism and activation energy of two catalyst-free, one organometallic, and one DABCO-catalyzed glycolysis processes were determined. This research has enormous potential, as by establishing experimental kinetic/analytical methods, the reaction kinetics of glycolysis can be investigated, which can not only be a validation of computational chemistry results, but also provides an opportunity to save time by relying on the validated computational chemistry methods when investigating the effects of various catalysts and degrading agents on the chemical degradation processes. Furthermore, future plans include the investigation of multi-step chemical degradation mechanisms

linked to the glycolysis process, so that not only the starting alcohol or polyols can be recovered, but also other components of the plastics. Ultimately, the most important thing in the future is to extend the research results to the treatment of plastic waste found in our real environment rather than model compounds, and to scale up this circular polyurethane recycling process to industrial levels.

Keywords: polyurethane, glycolysis, degradation, recycling, plastics

Máté Gergő Hatvani-Nagy[1,2], Péter Koska [1,2], Béla Viskolcz [1,2], Béla Fiser[1,2,3,4]

Isolation of cobalt resistant bacteria from soil

[1] Institute of Chemistry, University of Miskolc, 3515 Miskolc-Egyetemváros, Hungary
[2] Higher Education and Industrial Cooperation Centre, University of Miskolc, 3515 Miskolc-Egyetemváros, Hungary
[3] Ferenc Rakoczi II Transcarpathian Hungarian College of Higher Education, 90200 Beregszász, Transcarpathia, Ukraine
[4] Department of Physical Chemistry, Faculty of Chemistry, University of Lodz, Lodz, Poland

Electronic industries apply several heavy metals to produce batteries, cell phones, and computer parts. Cobalt, nickel, manganese, and copper are ranked as toxic metals which mean a threat to the environment and human health if they are emitted from these factories via their effluents.

Microorganisms offer enormous potential to remove heavy metals from industrial waste waters, via heavy metal biosorption and bioaccumulation. The accumulation of heavy metals is connected to certain types of resistance mechanisms of bacteria.

Therefore, our recent study focused on isolation of cobalt resistant bacteria which are planned to use our cobalt bioremediation studies.

Cobalt resistant bacteria were isolated from garden soil. 1g of garden were suspended in 20ml sterile mineral, and King B medium containing 100mg/L Co^{2+} and were incubated for 48 hours in shaking incubator with parameters of 30°C, 200rpm. The bacterial cultures were subcultures three times with the same parameters as previously described, with 5% inoculation ratio. Pure cultures were obtained with streak cell suspensions on cobalt containing mineral and King B agar. Developed colonies were reisolated until pure cultures were gained.

Pure cultures were tested for cobalt resistance with shake flask fermentation based on evaluation of cell growth, compared to cobalt free medium.

With this process several cobalt resistant pure cultures were isolated, which will be characterized further for cobalt removal efficiency and kinetics. Transcriptome analysis of resistance genes is also planned. Our further plan is to compose a heavy metal resistant microbial consortia which can be efficiently used for heavy metal bioremediation of soil, fresh water, and industrial wastewater.

Anikó Csábrádiné Jordán [1,2], Emma Szőri-Dorogházi [1,*]

Polyurethane biodegradation

[1] Institute of Chemistry, University of Miskolc, 3515 Miskolc, Hungary
[2] Higher Education and Industrial Cooperation Centre, University of Miskolc, 3515 Miskolc, Hungary
[*] emma.szori-doroghazi@uni-miskolc.hu

Polyurethane (PU) and other synthetic polymers are widely used materials that, at the end of their life cycle, can accumulate as waste in aquatic and terrestrial ecosystems, posing serious environmental challenges. Among the various waste management strategies, biodegradation represents a promising option; however, it remains underexploited, as achieving complete mineralization of polyurethane waste requires further knowledge and understanding. What we do know is that microorganisms play a central role in this process through enzyme-mediated depolymerization, mostly involving esterases, lipases, and ureases. These enzyme types have been identified to date as particularly important biocatalysts in polyurethane degradation. To assess the microbial degradability of polymers, model substrates that are chemically similar to plastics are often employed. In the case of polyurethanes, these model compounds are most often Impranil DLN and p-nitrophenyl acetate. In our study, bacterial strains were examined for their ability to degrade Impranil DLN SD. Several *Bacillus* isolates demonstrated degradation potential, with *Bacillus velezensis* CCZ proving to be the most effective. Degradation was assessed by measuring the diameter of the clear zone that appeared around bacterial colonies on agar medium supplemented with the model urethane compound, and by monitoring changes in optical density (OD) at 400–410 nm in liquid fermentation. The presence of esterase activity was confirmed by p-nitrophenyl acetate assays. The increase in bacterial cell concentration and the corresponding changes in OD indicate active enzymatic degradation of Impranil DLN SD. These results highlight the potential of *Bacillus* species in the polyurethane biodegradation and support further research into microbial and enzymatic approaches as sustainable strategies for polymer waste management.

Tomasz Szmechtyk[1]

Epoxy resins with natural co-hardeners from bio-waste

[1] Department of Physical Chemistry, Faculty of Chemistry, University of Lodz, Lodz, Poland

Epoxy resins are common thermosets, but most of commercial compositions are far from being green and harmless. Toxic bisphenol A and curing agents could be released from coatings, dental resins and other everyday object with epoxies. Addition of extract from Scots pine bark as co-hardener could provide more green alternative with additional advantages over common systems.

Extracts obtained using two different methods (conventional and ultrasound-assisted) were evaluated (total phenolic content, total solid content) and best one was selected. Diglycidyl ester bisphenol A epoxy, extract and amine hardener were mixed together and obtained composite was evaluated using DSC, FT-IR, Shore D hardness and mechanical tests (three-point flexural test and Charpy impact test). Obtained results revealed potential of such composites as coatings and their limitations resulting from different cross-linking chemistry.

Babak Minofar[1,2,3]

Computational study of soil enzyme interaction with nano materials

[1] University of Miskolc Institute of Chemistry, H-3515 Miskolc Egyetemváros, Miskolc, Hungary
[2] Department of Physical Chemistry, Faculty of Chemistry, University of Lodz, Pomorska 163/165 90-236, Lodz, Poland
[3] Department of Chemistry, Faculty of Science, University of South Bohemia in České Budějovice, Branišovská 31, 37005 České Budějovice, Czech Republic

The interactions between soil enzymes and nanomaterials are crucial because a wide range of nanomaterials, including metal and non-metal oxides, as well as carbon-based ones like graphene oxide, biochar, and carbon nanotubes, are increasingly present in soil environments, influencing soil health, nutrient cycling, and pollutant degradation.

These interactions are important for all nanoparticles due to their surface chemistry, size, structure, and physicochemical properties. Computational studies, including molecular dynamics, reveal how these nanomaterials affect enzyme performance, where it is shown that carbon-based materials such as biochar enhance soil fertility and bioremediation through stabilization, with strong binding to soil enzymes [1].

In this talk, the machinery of MD simulation will be introduced. After the introduction of MD, its application to different nano-materials applications and their interaction with biomolecules such as proteins and enzymes will be discussed.

Reference

[1] Minofar et al., Soil & Tillage Research 248 (2025) 106405

Alpár Ferencz Hatvani-Nagy[1,2], Anikó Jordán[2], László Vanyorek[1], Béla Fiser[1,3,4], Béla Viskolcz[1,2]

Chemical Invention in Precision Agriculture

[1] Institute of Chemistry, University of Miskolc, 3515 Miskolc-Egyetemváros, Hungary

[2] Higher Education and Industrial Cooperation Centre, University of Miskolc, 3515 Miskolc-Egyetemváros, Hungary

[3] Ferenc Rakoczi II Transcarpathian Hungarian College of Higher Education, 90200 Beregszász, Transcarpathia, Ukraine

[4] Department of Physical Chemistry, Faculty of Chemistry, University of Lodz, Lodz, Poland

The aim of the research is to produce slow-release fertilizers that significantly contribute to the sustainable development of precision agriculture. During the experiments, we fixed urea by surface adsorption on untreated ground lignite and examined the kinetics of the release of the active ingredient. Immobilization was achieved using deep eutectic solvent technology in the presence of glucose. Electron microscopy of the lignite surface revealed active nucleation centers where urea particles concentrate. We examined the dissolution by measuring the amount of ammonia produced on a uniform soil sample under realistic laboratory conditions. We used Bacillus Velezensis strain as a urea-degrading microorganism at the same concentration. The rate of active ingredient decomposition was 20-60% compared to conventional fertilizers. We initially examined the interactions of the lignite-glucose-urea two-phase ternary system using computer modeling, then verified the existence of these interactions using FTIR.

As a result of the research, we succeeded in producing a slow-release fertilizer with precisely controllable dissolution dynamics, which can be successfully applied in precision agriculture. The environmentally friendly materials used reduce the ecological footprint of the product and make the production technologies of agricultural input materials greener.

Raluca A. Septelean[1,*], I. Andreea Aghion[1], Ionut -T. Moraru[1], Gabriela N. Nemes[1]

Phospha(thioxo)phosphorane, a rich-electron building block for new organometallic and coordination compounds

[1] Faculty of Chemistry and Chemical Engineering, Department of Chemistry, Babes-Bolyai University, 11 Arany Janos, Cluj-Napoca 400028, Romania
* raluca.septelean@ubbcluj.ro

Transition metal compounds with organophosphorus ligands containing a RP=CR2 (phosphaalkene) or a RP=C(R)–PR2 (phosphavinylphosphoranes) unit are interesting duet o their possible catalytic activity.[1] Several metal complexes of Ru, Rh, Ir, Ni, Pd and Pt, containing such ligands have shown promising results in various processes.

Due to their multiple coordination possibilities of phosphavinylphosphoranes that have a P(III)=C–P(V)(=S), such as the electron lone pair at the level of the phosphorus or the sulfur atom, as well as the π(P=C) bond, these systems seem very attractive for the preparation of novel metal compounds.

We hereby present a coordination ability study of compounds with the general formula Mes*P═C(Cl)–P(=S)R1,R2 (Mes* = 2,4,6-tri-*t*-butylphenyl; R1 = Cl, R2 = 2,4,6-tri*i*-propylphenyl; R1 = R2 = *i*-propyl) with transition metal fragments containing Au, P, and W, evaluated by means of experimental and theoretical investigations. [2] Targeted compounds were characterized in solution by multinuclear NMR spectroscopy and HRMS, while for several cases, the solid-state structures were measured through X-ray diffraction.

References

1. Ziółkowska A., Doroszuk J., Ponikiewski, Ł., *Organometallics*, 2023, *42*, 505−537.

2. Aghion I.-A., Septelean R., Tomut A.-C, Moraru I.-T., Soran A., Nemes G. , *Organometallics*, 2024, *43*¸ 2062-2076.

Balázs Brém[1,*], Emese Gál[1], Ioana-Luiza Găină[1]

Development of Platinum(IV)-based Anti-Tumour Agents Carrying Anti inflammatori Moieties

[1] Research Center on Fundamental and Applied Heterochemistry, Faculty of Chemistry and Chemical Engineering, Babeş-Bolyai University, 11 Arany Janos str., RO-400028 Cluj-Napoca, România
* balazs.brem@ubbcluj.ro

The development of novel anti-cancer therapies remains a critical area of research, particularly in addressing challenges such as drug resistance and systemic toxicity associated with conventional platinum-based chemotherapy.

Here, we describe the synthesis of new platinum(IV) prodrugs that combine cisplatin with one or two axially coordinated molecules of non-steroidal anti-inflammatory cancer-selective drug. The results suggest that these Pt(IV) complexes exhibit mechanisms of action typical for Pt(II) complex and NSAID, simultaneously. The presence of NSAID ligand(s) in the Pt(IV) complexes promotes the antiproliferative activity and selectivity of cisplatin by inhibiting lactate transporters, resulting in blockage of the glycolytic process and impairment of mitochondrial potential.

References

1. Stefan Richter, Peter Lönnecke, Dijana Bovan, Nicoleta Andrian, Bianca Stoean, Maria Lehene, Radu Silaghi-Dumitrescu, Luiza Gaina, Sanja Mijatović, Danijela Maksimović-Ivanić, Goran N Kaluđerović, Evamarie Hey-Hawkins, Dalton Transactions, 54 (2025) 35970.

2. Philipp Fronik, Isabella Poetsch, Alexander Kastner, Theresa Mendrina, Sonja Hager, Katharina Hohenwallner, Hemma Schueffl, Dietmar Herndler-Brandstetter, Gunda Koellensperger, Evelyn Rampler, Joanna Kopecka, Chiara Riganti, Walter Berger, Bernhard K. Keppler, Petra Heffeter, Christian R. Kowol, Journal of Medicinal Chemistry, 64 (2021) 12132.

Acknowledgements

This work was supported by the project "Targeted Tumor Therapy with multifunctional platinum(iv)-drug conjugates (T3-Pt)" funded by European Union – NextGenerationEU and Romanian Government, PNRR, contract no 760240/28.12.2023, cod PNRR-C9-I8-CF 76/31.07.2023, through the Romanian Ministry of Research, Innovation and Digitalization, within Component 9, "Investment I8".

Bence Tamás[1], Andrea Mihalkó[1], Ferenc Kristály[1,2], László Farkas[1]

Gas adsorption testing of carbon-based noble metal catalysts

[1] Wanhua-BorsodChem Zrt. Bolyai tér 1., 3700 Kazincbarcika, Hungary
[2] University of Miskolc, 3515, Miskolc-Egyetemváros, Hungary

Carbon-supported precious metal catalysts are widely used in hydrogenation reactions, where performance depends strongly on support texture and metal dispersion. Physisorption provides insight into the surface area and porosity of carbon supports, while chemisorption enables quantification of accessible metal sites and dispersion, providing a measure of catalyst manufacturing quality. In this presentation, these complementary methods are demonstrated on carbon black and activated carbon supports, with a focus on palladium-based catalysts. The results highlight how adsorption techniques can link support properties and metal dispersion to catalytic behavior.

Ferenc Kristály[1,2], Andrea Mihalkó[1], Bence Tamás[1], László Farkas[1]

Structural changes on nobel metal-based catalysts during hydrogenation

[1] Wanhua-BorsodChem Zrt. Bolyai tér 1., 3700 Kazincbarcika, Hungary
[2] University of Miskolc, 3515, Miskolc-Egyetemváros, Hungary

Scanning electron microscopy and energy dispersive spectromery (SEM+EDX) investigations indicated that on an active carbon supported Pd/Pt+Fe catalyst undergoes metal mobilization and redistribution associated with structural and/or compositional changes. Several laboratory experiments were performed to test the supposed reorganization under reductive conditions, without active catalysis. The results support the preliminary observations, indicating atomic to nanoscale level diffusion and crystallization, as a necessary step in catalitic processes.

Ferenc Kristály[1,2], Ágnes M. Ilosvai[2], Béla Viskolcz[2], László Vanyorek[2]

Crystal structural characteristics of transition metal ferrites for catalyst support

[1] Wanhua-BorsodChem Zrt. Bolyai tér 1., 3700 Kazincbarcika, Hungary
[2] University of Miskolc, 3515, Miskolc-Egyetemváros, Hungary

Ferrites, the spinel type oxide materials, are a promising solution for catalyst support development, or even catalyzers. The crystal lattice requires the presence of both di- and trivalent cations, thus selective population of atomic sites allows for production of robust and stable materials, or fine tuning of catalytic activity. X-ray powder diffraction, transmission electron microscopy, electron diffraction and X-ray mapping offers valuable insights into the nanoscale characteristics of ferrites crystallization. The present study summarizes recent experiences of ferrite design and crystal structural characterization.

Zuoying Wen[1,*], Ruiqi He[1], XiaoXiao Lin[1], Xuejun Gu[1], Xiaofeng Tang[1,]**

Ambient volatile organic compounds (VOCs) measured online with a compact VUV photoionization mass spectrometer

[1] Hefei Institutes of Physical Science, Chinese Academy of Sciences, Hefei 230031, China.
* zywen@aiofm.ac.cn
** tangxf@aiofm.ac.cn

Volatile organic compounds (VOCs) are key reactive species in the atmospheric environment. They can participate in complex atmospheric chemical reactions and promote the formation of secondary pollutants such as ozone (O_3) and secondary organic aerosols (SOA). However, VOCs in the environment are diverse in species and exhibit distinct regional and temporal characteristics.

In recent years, our group has independently developed a high-sensitivity vacuum ultraviolet photoionization time-of-flight mass spectrometer (VUVPI-TOFMS). It mainly includes a VUV discharge lamp, a low-loss RF quadrupole ion transporter, an electrostatic lens for ion guide, and an orthgonal acceleration reflectron time-of-flight mass analyzer. The overall performance of the mass spectrometer has been characterized with a calibrated standard VOCs samples and shows perfect results, i.e., the limit of detection (LOD) reaching 1 pptv within 1 minute of detection, and the mass resolution ($m/\Delta m$) above 2000. Meanwhile, the VUVPI-TOFMS features a compact structure and low power consumption.

Recently, with the support of the National Key Research and Development Program Project, the VUVPI-TOFMS has been transported and utilized to carry out a comprehensive ambient observation experiment lasting over 40 days at the Longquan Mountain Super Atmospheric Observation Station in Chengdu, at the west of China and almost 2000 km away from Hefei. The VUVPI-TOFMS still worked very well even after a long-term transport. During the observation period, simultaneous data comparison was conducted with commercial gas chromatography-mass spectrometry (GC-MS) and Vocus proton transfer reaction time-of-flight mass spectrometry (Vocus PTR-TOFMS), and the results showed high consistency. A large amount of high-time-resolution VOCs data obtained by this instrument clearly captured the diurnal variation characteristics of biogenic VOCs such as isoprene and monoterpenes, as well as the regional transport characteristics of benzene series. This study indicates that the home-made VUVPI-TOFMS has excellent performances, high portability, and reliable detection results. It can meet the needs of rapid online monitoring of VOCs in complex environments.

Reference

[1] Wen Z, Tang X, Fittschen C, et al. *Review of Scientific Instruments*, 2020, 91(4).

[2] Ma Z, Wen Z, Tang X, et al. *Microchemical Journal*, 2025, 210: 112982.

Zuoying Wen[1], Xuejun Gu[1], Xiaoxiao Lin[1], Xiaofeng Tang[1,*]

Vacuum ultraviolet photoionization mass spectrometry and its applications in atmospheric environment

[1] Hefei Institutes of Physical Science, Chinese Academy of Sciences
* tangxf@aiofm.ac.cn

The origins of atmospheric pollution are complicated and often comprise a series of chemical reactions involving abundant volatile organic compounds (VOCs), free radicals and aerosol particles. How to analyze these species operando is a hot, significant and challenging topic in atmospheric enviroment. In this talk, I will introduce the principle of vacuum ultraviolet (VUV) photoionization mass spectrometry, and present our home-made VUV photoionization time-of-flight mass sepctrometers (VUVPI-TOFMS) as well as photoelectron photoion coincidence (PEPICO) mass spectrometers. Several kinds of light sources, i.e. VUV discharge lamps and synchrotron radiations at Hefei and SOLEIL, have been connected with VUVPI-TOFMS, directly providing mass information of molecular ions benefiting from its “soft” ionization at the threshold ionization energy of molecules. Some novel stratiges have been developed to enhance the detection sensitivity of VUVPI-TOFMS. In combination with synchrotron radiation light sources, mass-selected photoionization spectra or mass-selected threshold photoelectron spectra corresponding to each mass can be obtained by scanning synchrotron photon energy, very powerful to probe the elusive molecular structures and to identify complex isomers. In addition, the applications of VUVPI-TOFMS/PEPICO to analyze atmospheric VOCs, free radicals and their reactions, and the chemical compositions of aerosol particles will be presented.

Abstracts of Posters

Khalida Khalil[1,2], Bela Fiser[1,3], Magdalena Malecka[1]

Harnessing Calix[4]arene for Environmental Remediation: A Supramolecular Approach to Chloro- and Fluorocarbon Removal

[1] University of Lodz, Faculty of Chemistry, Department of Physical Chemistry, Pomorska 163/165, 90-236 Lodz, Poland

[2] Doctoral School of Exact and Natural Sciences, Jana Matejki 21/23, 90-237 Lodz, Poland

[3] Institute of Chemistry, University of Miskolc, 3515 Miskolc-Egyetemváros, Hungary

Chloro- and fluorocarbons are hazardous pollutants that threaten both health and the environment, making their efficient capture a pressing challenge. Calix[4]arene (CX[4]), though widely applied in energy storage and optoelectronics, has received limited attention as a host for pollutant remediation. In this study, the interactions of CX[4] with representative halocarbons (CCl_4, CH_3Cl, CH_2Cl_2, CF_3Cl, CF_4, C_2F_6, and CF_3Br) were explored using theoretical methods. Computational analyses including interaction energy calculations, NBO, FMO, IRI, and QTAIM demonstrate that the cavity of CX[4] provides a favorable binding site stabilized by non-covalent interactions. Chlorinated species, particularly $CHCl_3$ and CCl_4, exhibited the strongest affinities (–61.69 kJ/mol and –60.17 kJ/mol). The computed HOMO–LUMO gaps indicate good kinetic stability of the complexes. These findings establish CX[4] as a promising supramolecular framework for the capture and remediation of toxic halocarbons, with potential applicability under realistic environmental conditions.

Mohd Yasir Al Saif [1], Dr. Richard Cselko[1]

Increasing the Throughput of the Electrospinning Process

[1] Budapest University of Technology and Economics, Budapest, Hungary

Electrospinning is a key technique for producing polymer nanofibers used in drug delivery, filtration, and catalysis. However, conventional DC electrospinning is limited by low throughput and fiber inconsistency. This research focuses on enhancing productivity through alternative high-voltage waveforms, including alternating current (AC) and pulsed voltage (PV). These methods reduce charge accumulation and enable the formation of multiple stable jets, improving fiber yield and uniformity. PV allows control over jet dynamics through adjustable pulse duration and frequency, while AC supports continuous, collectorless spinning. The study emphasizes the chemical stability of polymers under varying electrical conditions, highlighting strategies to maintain functional group integrity and optimize fiber morphology. This approach advances scalable nanofiber production for chemistry-driven applications.

Kumari Neelam[1], Prof. Dr. Hab. Anna Merzec[1], Dr. Noor Haida Mohd. Klaus[1]

Colorants Based on Silane-Silica Hybrids For Polymer Applications

[1] Institute of Polymer and Dye Technology, Łódź University of Technology

The growing demand for high-performance colorants in the textile and polymer industries has led to increased interest in hybrid pigment technologies. This study explores the development of such pigments by functionalizing silica with mono-, di-, and tri-amine silane coupling agents to enhance the immobilization of anthraquinone dyes [1] [2]. The modified silica was reacted with 1,5- and 1,8-dichloroanthraquinone to evaluate the influence of amine group density on dye adsorption, fixation, and surface interaction [1]. Silanization significantly improves the surface reactivity of silica, promoting stronger dye binding through covalent bonding [1] [3]. The resulting pigments exhibited deeper and more uniform coloration, along with enhanced thermal and chemical stability, and reduced dye migration [2] [4]. This approach supports the development of durable, and non-migrating colorant systems for smart textile and polymer applications [4].

References

[1] T. Jesionowski, M. Pokora, W. Tylus, A. Dec and Krysztafkiewicz, "A. Effect of N-2-(Aminoethyl)- 3-Aminopropyltrimethoxysilane Surface Modification and C.I. Acid Red 18 Dye Adsorption on the Physicochemical Properties of Silica Precipitated in an Emulsion Route, Used as a Pigment and a Filler in Acrylic Paints.," Dyes and Pigments, no. 57, p. 29–41, 2003,.

[2] S. B. T. J. Andrzej Krysztafkiewicz, "Adsorption of dyes on a silica surface," Applied Surface Science, vol. 199, no. 1-4, pp. 31-39, 2002.

[3] M. Yang, J. Su, Y. Zheng, C. Fang, W. Lei and Li, "Effect of Different Silane Coupling Agents on Properties of Waste Corrugated Paper Fiber/Polylactic Acid Composites," Polymers, p. 15, 2023.

[4] C. S. D. G. F. R. M. G. F. M. J. Graycyellê R.S. Cavalcanti, "Designing photochromatic pigments based on clay minerals and spiropyran," Dyes and Pigments, vol. 204, 2022.

Sponsors

University of Miskolc

MARIE CURIE ALUMNI

17 35
UNIVERSITAS MISKOLCINENSIS

FACULTY OF MATERIALS AND CHEMICAL ENGINEERING • UNIVERSITY OF MISKOLC •
1735

LIFE
CLIMCOOP

Life

FIEK
MISKOLCI EGYETEM

Széchenyi Terv Plusz
Építsük együtt Magyarországot!

MAGYARORSZÁG KORMÁNYA

Az Európai Unió finanszírozásával
NextGeneration EU

NEMZETI LABORATÓRIUM

NEMZETI KUTATÁSI, FEJLESZTÉSI
ÉS INNOVÁCIÓS HIVATAL

INNOVÁCIÓS ÉS TECHNOLÓGIAI
MINISZTÉRIUM

Nemzeti Kutatási, Fejlesztési
És Innovációs Hivatal

AZ NKFI ALAPBÓL
MEGVALÓSULÓ
PROGRAM