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**Section of
Analytical Chemistry
and
Physical Chemistry**

FTIR SPECTROMETRY MEASUREMENT APPROACHES FOR STUDY OF RADIATION-INDUCED EFFECTS IN ADVANCED CERAMIC BREEDER PEBBLES

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Advanced ceramic breeder (ACB) pebbles consisting of lithium orthosilicate (Li_4SiO_4) and lithium metatitanate (Li_2TiO_3) are considered as candidate material for tritium breeding in future thermonuclear fusion reactors. Alongside the high temperatures and resistance to thermomechanical stresses, the ACB pebbles must also be capable to withstand high neutron flux during expected operational conditions [1]. Fourier transform infrared (FTIR) spectrometry is one of the most frequently used analytical techniques that can be applied for identification of chemical bonds and short-range structures in irradiated Li_4SiO_4 -based ceramic breeder pebbles [2].

In the present work, different approaches for FTIR spectrometry measurements, including absorption, transmission, diffuse reflectance (DR), attenuated total reflectance (ATR) spectrometry and micro-spectrometry, have been compared for their application to study radiation-induced effects in the ACB pebbles. The ACB pebbles have been analysed before and after exposure to various radiation types, i.e., photons, electrons, accelerated ions, and neutrons. The obtained results were also directly compared to data of different thermal analysis methods, e.g., thermogravimetry/differential thermal analysis (TG/DTA) in combination with FTIR spectrometry and thermal desorption-quadrupole mass spectrometry (TD-QMS).

Based on the obtained results, it can be concluded that using selected FTIR spectrometry measurement approaches similar spectra of characteristic bond vibration signals for Li_4SiO_4 and Li_2TiO_3 were recorded between 400 cm^{-1} and 1000 cm^{-1} . The obtained results also clearly showed that handling, storage, and transportation of the irradiated ACB pebbles have a significant influence on sample surface chemical composition and microstructure due to chemisorption processes of water (H_2O) vapour and carbon dioxide (CO_2). The TG/DTA-FTIR and TD-QMS data shows that desorption of chemisorbed H_2O and CO_2 takes place in several stages between 400 °C and 950 °C . During heating, FTIR signal intensity of chemisorption products, i.e., lithium carbonate (Li_2CO_3) and lithium metasilicate (Li_2SiO_3), observed at about 730 , 870 and 1450 cm^{-1} , decreases, while the characteristic bond vibration signals of Li_4SiO_4 , which are observed at 800 , 830 , 900 and 950 cm^{-1} , increases. The formed layer of chemisorption products on the investigated sample surface can affect also correct interpretation of the obtained results for the irradiated ACB pebbles using surface analysis methods, e.g., ATR-FTIR spectrometry and micro-spectrometry.

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POSSIBILITIES TO IMPROVE ELEMENT DETECTION CAPABILITIES IN ICP-MS MEASUREMENT TECHNIQUE

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Inductively Coupled Plasma Mass Spectrometry (ICP-MS) has evolved into a versatile tool for multi-element analysis, offering excellent sensitivity and specificity across various matrices. However, this technique is not without its challenges. One of the most significant drawbacks it faces is spectral interference, a well-documented phenomenon that complicates the analysis of samples with different compositions and origins. Spectral interference occurs when polyatomic (or molecular) ions, generated within the plasma, share the same mass-to-charge (m/z) ratio as the target analyte. This overlap can lead to erroneous results, obscuring the true concentrations of elements within the sample. Such interferences are particularly problematic in complex matrices where various elements and compounds coexist, potentially giving rise to a multitude of interfering species.

To mitigate these interferences, ICP-MS technology has incorporated methods such as collision/reaction cells equipped with gases like helium (He) or oxygen (O_2) to dissociate or react with interfering species, thereby enhancing analytical accuracy. Additionally, the development of high-resolution ICP-MS and the use of tandem mass spectrometry (MS/MS) configurations have further refined the capability to distinguish between analytes and interfering ions.

The role of RF (radio frequency) power adjustments cannot be underestimated. By optimizing the RF power applied to the plasma, it's possible to alter the ionization efficiency and collisional dissociation rates of potential interferences, thereby reducing their impact on the analysis. This adjustment is crucial for achieving lower detection limits and higher specificity, particularly in the analysis of rare earth elements (REEs) and other trace elements in complex environmental, biological, and industrial samples.

In this study, we demonstrate how adjustments in specific measurement parameters impact the detection and quantification limits of various elements, highlighting the critical role of such optimizations in enhancing the analytical performance of ICP-MS. By modulating the RF power, it is possible to fine-tune the ionization efficiency and minimize the effects of spectral interferences, leading to more accurate measurements of trace elements, even in samples with complex matrices. This approach not only improves the specificity and sensitivity of the analysis but also extends the dynamic range of detectable concentrations, enabling the measurement of elements at lower limits of detection.

VARIATION OF CARBON AND NITROGEN STABLE ISOTOPE RATIOS IN CONVENTIONALLY AND ORGANICALLY FERTILIZED WHEAT ROOTS AT DIFFERENT GROWTH STAGES

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Wheat is one of the most grown crops worldwide, with its production reaching 789 million metric tons in the year of 2022 [1]. Research on carbon and nitrogen dynamics in cereals is important for optimizing agricultural productivity. Considering the expanding global population, optimization of agricultural productivity is important for ensuring food security and economic stability worldwide.

In this study samples of wheat roots from conventionally and organically fertilized sample plots, collected at different growth stages (tillering, jointing, booting and milk ripeness) were analysed with Nu Horizon (*Nu Instruments Ltd., UK*) stable isotope mass spectrometer. The $\delta^{13}\text{C}$ values are expressed relative to VPDB and the $\delta^{15}\text{N}$ values relative to AIR.

The results of this study showed that the stable nitrogen isotope ratio values in both conventionally and organically fertilized wheat roots decreased with the growth of wheat crops, with the highest decrease in $\delta^{15}\text{N}_{\text{AIR}}$ values between the booting and milk ripeness stages (Fig. 1.). Meanwhile, the stable carbon isotope ratios in the wheat roots did not show significant changes throughout the development of wheat crops.

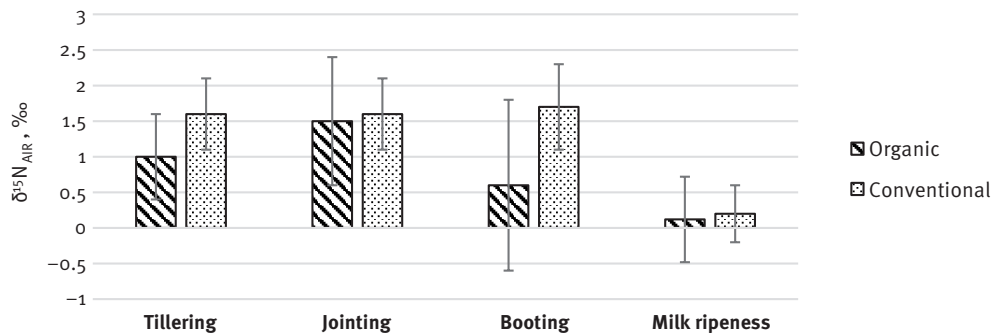


Fig. 1. $\delta^{15}\text{N}_{\text{AIR}}$ values of conventionally and organically fertilized wheat roots at different growth stages

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CONTROL OF CAFFEINE : ANTHRANILIC ACID COCRYSTAL POLYMORPH OBTAINED IN MECHANOCHEMICAL SYNTHESIS

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Many of the compounds in the solid state can exist in a form of different polymorphs, which differ by the arrangement of the molecules or ions in the crystal structure. As polymorphs are different phases, they differ in various properties such as melting point, solubility, stability, etc. Polymorphs can exist both in single-component as well as in multi-component systems, including co-crystals [1, 2].

Co-crystals can be obtained by crystallization from solvent and using solvent-free methods. Lately special attention is paid to co-crystal synthesis using mechanochemical approach by grinding and milling, which are recognized as more environmentally friendly, simpler and faster methods [2, 3].

In this study we employed mechanochemical synthesis of co-crystals, by exploring the possibility to control the obtained crystal form of the caffeine : anthranilic acid (Figure 1) co-crystal.

We observed that the polymorphic form of caffeine : anthranilic acid co-crystal can be controlled by using additives (liquid additives and their specific volume or mass, or together with solids with a specific mass), whereas by milling caffeine and anthranilic acid without additives the co-crystal could not be obtained. Such polymorph control approach correspond to the direction of green chemistry and has a possibility to significantly reduce the volumes of solvent used, thus, creating a smaller impact on the environment, and facilitate and speed-up the preparation of the desired polymorph. In general, understanding the factors allowing mechanochemical polymorph control would be especially useful for the pharmaceutical industry, as it would save financial resources and allow optimization of the drug manufacturing process.

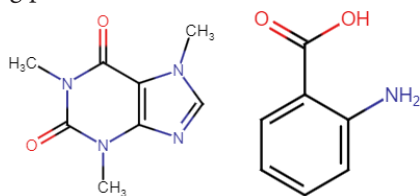


Fig. 1. Molecular structure of caffeine (on the left) and anthranilic acid (on the right)

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EXAFS SPECTROSCOPY STUDIES OF LATTICE DYNAMICS IN METALLIC CHROMIUM

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Solid-solid phase transitions are actively studied in physics and material science. They find applications in modern technologies such as shape memory alloys, high-pressure technologies, etc. These transition can be induced using various techniques [1, 2]. In this study, our focus is on substrate-induced phase transitions.

Two commercially available high-purity metallic chromium foils with the thicknesses of 2 and 5 μm were investigated. The thicker foil was substrate-free, while the thinner one was produced on a polyester substrate.

X-ray diffraction experiments were conducted for the thinner sample using a Rigaku MiniFlex diffractometer before and after substrate removal by thermal heating. X-ray absorption spectroscopy experiments were performed for both samples over a temperature range of 10–300 K at the DESY PETRA III P65 beamline (Hamburg, Germany) in transmission mode at the chromium K-edge. Advanced analysis of the extended X-ray absorption fine structure (EXAFS) spectra was carried out using the reverse Monte Carlo (RMC) method [3].

Our findings indicate that the presence of an organic substrate induces a structural phase transition in the metallic chromium foil from a body-centered cubic (bcc) to a hexagonal close-packed (hcp) phase, presumably due to mechanically induced strain. The atomic coordinates obtained from RMC simulations of EXAFS spectra were utilized to calculate radial distribution functions and mean-square relative displacements (MSRDs) for Cr-Cr atomic pairs. The MSRD values for the thick chromium foil in the bcc phase are consistent with literature data [4]. Furthermore, the analysis of the MSRDs suggests that, unlike bcc chromium, the lattice dynamics of hcp chromium is strongly anisotropic.

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ECO-FRIENDLY SYNTHESIS OF MODIFIED IRON FERROCYANIDE SORBENTS FOR ENHANCED CESIUM SORPTION IN RADIOACTIVE FALLOUT SCENARIOS: ADVANCEMENTS IN WATER PURIFICATION AND PERSONAL PROTECTION MEASURES

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Considering escalating geopolitical tensions, the development of advanced materials to mitigate the risk of nuclear incidents and radioactive contamination has become imperative. This study focused on synthesizing environmentally friendly modified iron ferrocyanide sorbent materials incorporating activated carbon and cotton, which are particularly relevant in scenarios involving radioactive fallout. The specific activity of ¹³⁷Cs, estimated at approximately 3.9×10^{10} Bq/L, underscores the potential impact of radioactive fallout from a nuclear explosion within Latvia's territory.

The primary aim is to develop sustainable and efficient synthesis materials with enhanced sorption capacity for radioactive cesium (Cs⁺) ions, thereby advancing water treatment methods and improving civilian survival rates during metal ion exposure events, especially in cases of radioactive fallout. The synthesis process utilizes a green method to modify the surfaces of activated carbon and cotton fibers, facilitating the synthesis and simultaneous adsorption of iron ferrocyanide on the sorbent surface. This approach ensures controlled synthesis, prevents agglomeration, and promotes a punctate locus for tight binding of ferric ferrocyanide to the adsorbent.

Experimental prototypes of 0.5-liter drinking water bottles were made, each containing different sorbents integrated with iron ferrocyanide, cotton, and activated carbon. The results demonstrate that samples containing ferric ferrocyanide exhibited higher specific sorption of cesium than those without ferric ferrocyanide. Furthermore, experiments conducted over 48 h confirmed that no desorption occurred after sorption within this time frame. Additionally, water contaminated with Cs⁺ ions became safe for consumption within 12 h in the presence of the iron ferrocyanide sorbent, aligning with the derived concentration norm of Cs¹³⁷ radioactivity in drinking water (11 Bq/l).

In conclusion, this study provides valuable insights into the development of materials crucial for addressing the challenges associated with radioactive contamination. Although the modified composite material demonstrated an improved sorption capacity for cesium ions, further experiments are warranted to accurately describe the physicochemical processes between ferric ferrocyanide and cesium and to enhance Cs⁺ ion sorption. These

findings hold promise for application in water treatment and personal protection measures, underscoring the importance of continued research in this domain.

Acknowledgments. This study was facilitated by the generous sharing of knowledge by the esteemed professors and researchers of the University of Latvia (LU). Financial support was provided by the SIA “Mikrotikls” scholarship administered by the LU Foundation.

DETERMINATION OF GLYCOALKALOIDS IN POTATOES IN LATVIA

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Glycoalkaloids are secondary metabolites found in potatoes and other plants of the nightshade family and are highly toxic.

A method for the determination of glycoalkaloids by liquid – chromatography-tandem mass spectrometry was developed, and results on the occurrence of α -solanine and α -chaconine were obtained in 22 potato species grown in Latvia, such as “Levante”, “Aloutte”, “Twister”, “Laura”, “Soraja”, “Adretta”, “Monta”, “Vineta” and “Annuschka”.

The results were compared with the European Commission Recommendation (No 2022/561) [1] on the monitoring of the presence of glycoalkaloids in potatoes and potato-derived products.

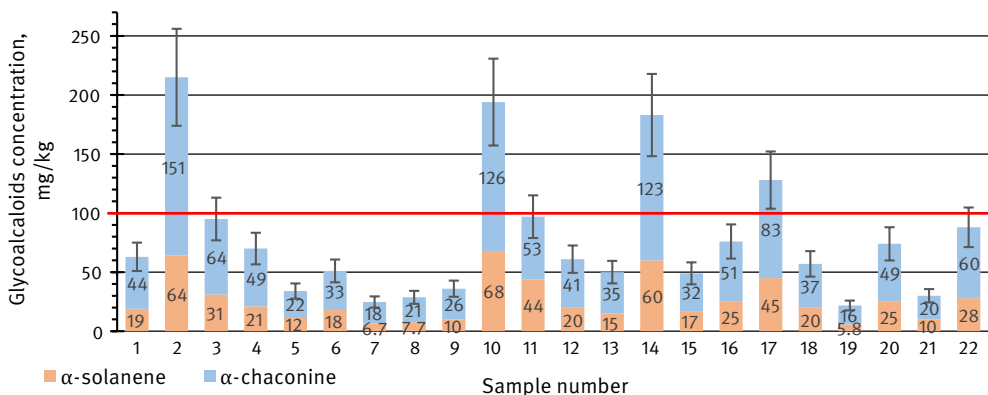


Fig. 1. Glycoalkaloids concentration in Latvian potato samples in comparison to maximum recommended concentration

Seven potatoes have total glycoalkaloid concentrations below half the maximum recommended concentration and four potatoes have total glycoalkaloid concentrations above the maximum recommended concentration.

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GRADUAL THERMAL TREATMENT ANALYSIS OF BENZANTHRONE

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Fluorescent dyes are used to analyze stability of food industry structuring additives [1] and as biological sensors for marking processes, molecules in biological organisms [2–3]. There is a growing interest in developing new biomarkers, characterized by good biocompatibility and photostability [4], because fluorescent molecules possess several characteristics, such as conjugated π -orbitals and luminescent properties, that determine their practicality in various applications [5]. However, the thermal behaviour of fluorescent dyes is still to be characterized.

In the present work, the structure and chemical composition of benzantrone (BZA) and thermally treated BZA is characterized by means of Fourier transform infrared (FTIR) spectrometry and X-ray diffractometry (XRD). FTIR spectra registered with *Bruker Vertex 70v* spectrometer with attenuated total reflection module, range 400–4000 cm^{-1} , resolution $\pm 2 \text{ cm}^{-1}$, in vacuum 2.95 hPa, 20 spectra per measurement, at least 3 measurements per sample.

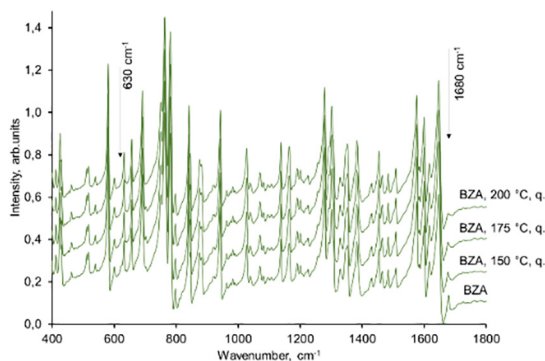


Fig. 1. Infrared spectra on non-treated and thermally treated BZA in quartz (q) tube

The analyses show changes in the -OH liberation bond at 630 cm^{-1} and C = C stretch intensity at 1680 cm^{-1} , while all the other chemical bonds remain stable up to 200 °C. After thermal treatment, no changes were observed in BZA XRD diffractograms.

Acknowledgments. The work is performed within the frames of Latvian Council of Science project No. LZP-2022/1-0436 “Novel fluorescent anthrone-derived functional materials for bioimaging applications”.

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CRYSTALLIZATION CONTROL OF PARA-AMINOBENZOIC ACID USING POLYACRYLIC ACID

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Polymorphism of active pharmaceutical ingredients has been the subject of intense investigation in the drug industry due to its influence on the properties of the drug. A better understanding of the formation of different polymorphic forms and control mechanisms may improve crystallization process efficiency and reduce production costs. [1–2]

In this study, *para*-aminobenzoic acid (*p*ABA) was used as a model substance to investigate the crystallization control approach using additives. *p*ABA has four polymorphic forms, in which there are different types of hydrogen bonding and aromatic interactions (see Fig. 1). [3–4]

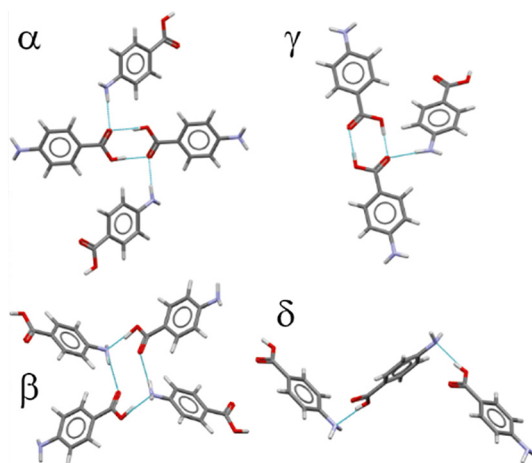


Fig. 1. Hydrogen bonding interactions in the four *p*ABA polymorphs

The polymorphic outcome of crystallization of *p*ABA in the presence of polyacrylic acid was explored under different conditions by performing evaporation and cooling crystallization from water. For the cooling crystallization different cooling rates were used. Solid products obtained in the crystallization were characterized by powder X-ray diffraction. The solubility of different *p*ABA polymorphic forms was determined in pure water and in the presence of polyacrylic acid. Additionally, induction time measurements were performed to determine the effect of the additive on the crystal nucleation rates.

In the crystallization using the fastest cooling rate α or β form or their mixture was obtained, but using the slower cooling rate pure metastable β form was achieved. The solubility of *p*ABA α and β forms in the presence of polyacrylic acid is lower than in the pure water.

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DETERMINATION OF N-(1,3-DIMETHYLBUTYL)-N'-PHENYL-P-PHENYLENEDIAMINE (6PPD) AND ITS DERIVATIVES IN ROAD DUST USING LIQUID CHROMATOGRAPHY – HIGH RESOLUTION MASS SPECTROMETRY

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Substituted p-phenylenediamines (PPDs) are a class of antioxidants widely used in the rubber industry and are recognized as highly effective chemical antiozonants. PPDs have a common structure based on p-phenylenediamine, and their properties depend on the substituent groups attached to the PPD skeleton. [1]

As an antioxidant, 6PPD is designed to reduce the negative effects of ozone on tire rubber, resulting in the formation of transformation products. Other derivatives of these compounds are also known to re-form in road, atmospheric and water environments. These transformation products may have different physicochemical properties and biological effects from the 6PPD compound. The most information can be found specifically on 6PPD-Q because of the toxicological issues reported in several 6PPD studies. [2]

During this study an analytical method with HPLC-Orbitrap-MS for the determination of 6PPD and its derivatives in road dust was developed and optimized.

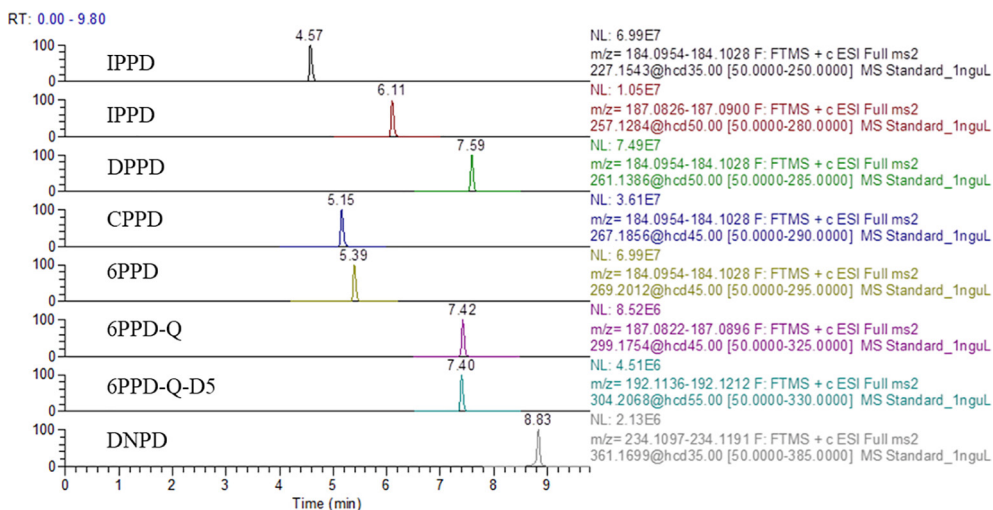


Fig. 1. Chromatogram of PPD compounds

Preliminary investigation revealed that PPD compounds are present in road dust samples from Latvia. Out of the 8 PPD compounds studied, 6PPD and 6PPD-Quinone were most frequently detected and had the highest concentrations.

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ANALYSIS OF GAS RELEASE FROM BIPHASIC LITHIUM CERAMICS PEBBLE BEDS OF VARIOUS PEBBLES SIZES AND CONTENT UNDER NEUTRON IRRADIATION CONDITIONS

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Biphasic lithium ceramics based on lithium orthosilicate Li_4SiO_4 (LOS) and lithium metatitanate Li_2TiO_3 (LMT) are one of the most promising materials for breeder blankets of future fusion reactors.

The results of 4 reactor campaigns on the irradiation of biphasic lithium ceramics containing different ratios of lithium orthosilicate (LOS) and lithium metatitanate (LMT) components (25 and 35 mol% LMT in LOS) are presented. The size distribution of pebbles in pebble beds was 250–1250 μm and 500–710 μm , respectively. The studies were carried out sequentially with each type of ceramics. In experiments carried out using the vacuum extraction method, the composition of gases released from lithium ceramic samples was registered in in-situ mode. The absence of purge gas during the experiments minimized the possibility of T_2O and HTO formation, significantly simplifying processing of the results and providing more opportunities for results analysis. The main goal of the present paper was to identify the general patterns of the release of gases with mass numbers M2 (H_2), M4 ($\text{He} + \text{HT}$), M6 (T_2) and M18 (H_2O) from ceramic samples throughout the entire irradiation experiment in 4 campaigns. Release trends of main gases with mass numbers M2, M4, M6 and M18 for all four campaigns are presented and their comparative analysis was performed. The average partial pressure of tritium release in the form of T_2 and HT molecules for all campaigns was determined as $5.8 \cdot 10^{-7}$ Torr. The dependences of formation rates of helium release peaks on the irradiation time were plotted. The nature of peak emissions does not have a monotonic relationship; upon irradiation, both an increase in the frequency of peaks and a decrease in it are observed. During irradiation, the process of peak helium release does not stop.

The simulation was carried out by the finite element method, assuming that tritium release from the sample is determined by diffusion and desorption processes from the sample surface. The experimental curves are satisfactorily described by a number of sets of desorption and diffusion parameters. One way or another they lie in the range of specified values. The Arrhenius dependences of the effective diffusion coefficient and desorption coefficient obtained for lithium ceramics 35 LMT are equal to:

$$D = 5,2 \times 10^{-11} \left(\frac{\text{m}^2}{\text{s}} \right) \exp \left(\frac{-21 \left(\frac{\text{kJ}}{\text{mole}} \right)}{RT} \right), \quad K = 1,21 \times 10^{-4} \left(\frac{\text{m}^2}{\text{s}} \right) \exp \left(\frac{-64 \left(\frac{\text{kJ}}{\text{mole}} \right)}{RT} \right).$$

The values of the effective diffusion coefficient and tritium desorption coefficient in 25 LMT ceramics were 15 and 20% lower than in 35 LMT ceramics.

BI₂SE₃/SWCNT HETEROSTRUCTURES AS PERSPECTIVE BINDER-FREE ANODE MATERIALS FOR LITHIUM- AND SODIUM-ION BATTERIES

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Graphite is well known as the most common anode material for lithium-ion batteries (LIBs), which has been used since 1991. However, its low theoretical capacity is a major limitation, which is not sufficient to satisfy ever-increasing demands for electrical energy storage. In the meantime, sodium-ion batteries (SIBs) have been extensively studied as an alternative to LIBs. The high abundance of sodium in the Earth's crust makes SIB manufacturing relatively cheaper than LIBs. However, the development of the latest anode materials for SIB does not demonstrate high performance which hinders the progress of SIB system development.

Bismuth selenide (Bi₂Se₃) has already been studied as a perspective anode for LIBs and SIBs. Large volumetric expansion and significant dissolution of selenium are the main drawbacks limiting its performance. A direct nanostructuring of Bi₂Se₃ with single-walled carbon nanotubes (SWCNTs) could remarkably improve its performance. The combination of the active material with a porous SWCNTs network could enhance the anode's mechanical stability, increasing its electrical conductivity and resilience against volume expansion.

The aim of this research was to investigate the electrochemical performance of different ratios of Bi₂Se₃/SWCNTs to demonstrate its perspective use as anodes for LIBs and SIBs. The Bi₂Se₃/SWCNTs were synthesized in a two-step synthesis procedure: i) spray-coating of SWCNTs, ii) physical vapour deposition of Bi₂Se₃ on top of SWCNTs. The performance was tested in coin half-cells (CR2032) by applying different electrochemical techniques. Their morphology and chemical composition were investigated before and after cycling.

The obtained results demonstrated an outstanding performance of Bi₂Se₃/SWCNT heterostructure in both LIBs and SIBs by delivering high capacity and great stability. The main factor for this improvement is the large pseudocapacitive contribution, ensured by a large effective contact area and the Se binding to C which provides additional electron transport pathways and inhibits the dissolution of Se^{1,2}.

Acknowledgments: This research was funded by the European Regional Development Fund (ERDF) Projects No. 1.1.1.1/19/A/139 and 1.1.1.2/VIAA/3/19/522. V.L. acknowledges the support of "Strengthening of the capacity of doctoral studies at the University of Latvia within the framework of the new doctoral model", identification No. 8.2.2.0/20/I/006.

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EVALUATION OF THE CONTENT OF CHEMICAL ELEMENTS IN COMMON BEANS (*PHASEOLUS VULGARIS*) GROWN UNDER CONDITIONS OF DIFFERENT FERTILIZERS

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Beans are widely cultivated and consumed legumes. They stand out as a plant based protein source and can be a good alternative to animal based proteins. [1] Common bean growth and yield can be affected by different kinds of fertilizers – fertilizers are often used to increase the yield and its quality. [2]

As part of the research, 2 variations of common bean (*Phaseolus vulgaris*) – red kidney (*Wavelska*) and yellow wax beans (*Unidor*) – were grown in soil, which had been treated with commercial mineral fertilizers, wood ash, manure or compost. The effect of the used fertilizers on the yield and the content of chemical elements in the beans was mutually evaluated.

Sample were prepared using microwave digestion and sample analysis was carried out by inductively coupled plasma mass spectrometer (Agilent 8900 Triple Quadrupole) at the University of Latvia. The yield results were expressed in tons · ha⁻¹ and chemical element content was expressed in mg/100g or µg/100g.

The results show that fertilization can affect bean yield – in all fertilized fields bean yield was slightly higher than control. There was no significant difference in bean element content between different kinds of fertilizers used on soil.

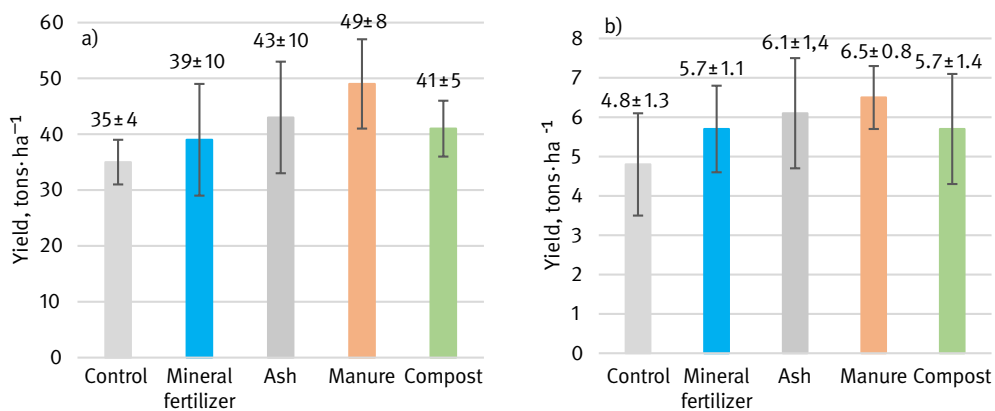


Fig. 1. Fertilizer effect on yield of a) yellow wax beans and b) red kidney beans

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EXPLORING NICKEL OXIDE LATTICE DYNAMICS IN A WIDE TEMPERATURE RANGE USING EXAFS SPECTROSCOPY

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At room temperature, NiO is an antiferromagnetic Mott-Hubbard insulator having the highest temperature ($T_N = 525$ K) of magnetic phase transition from an antiferromagnetic to a paramagnetic state among all transition metal monoxides [1]. The crystal lattice of NiO is slightly rhombohedrally distorted with a space group $R\bar{3}m$ below the Néel temperature T_N and becomes cubic with a space group $Fm\bar{3}m$ upon heating above T_N .

NiO lattice dynamics was investigated over a wide temperature range from 10 K to 900 K. The temperature dependence of the mean square relative displacement (MSRD) values for Ni-O and Ni-Ni atomic pairs was obtained using Ni K-edge X-ray absorption spectroscopy combined with reverse Monte Carlo (RMC) simulations [2]. The obtained MSRD values were approximated using the Einstein model and compared with the literature [3] data.

We found that the MSRD values for Ni-Ni and Ni-O atomic pairs are lower than expected from the theory above the phase transition temperature T_N . Besides, a reduced correlation between the absorbing Ni and O atoms of the 3rd coordination shell was discovered over the whole temperature range.

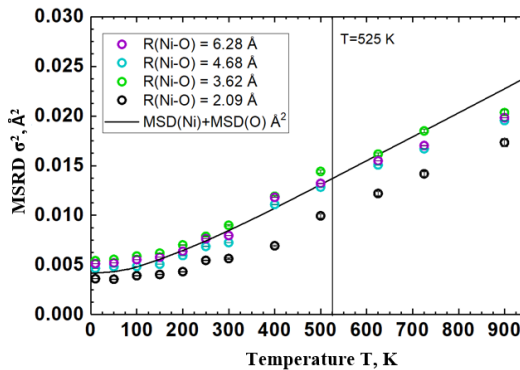


Fig. 1. Temperature dependence of MSRD for different Ni-O atomic pairs obtained by RMC simulations.

Acknowledgments. This study was supported by the Latvian Council of Science project No. LZP-2022/1-0608.

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PREPARATION OF CSPBBR₃ DOPED WITH THIOCYONATES AND ORGANIC BORATE

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In this study we present an innovative approach to improve the photoluminescence quantum yield (PLQY) and long-term stability of CsPbBr₃ nanoparticles, a promising material for green light-emitting diodes (LEDs). The method involves a post-synthetic treatment of the nanoparticles using oleylammonium thiocyanate and organic borate salt solutions, derived from ethylene glycol, and oleylamine. The treated nanoparticles exhibit near unity PLQY and remain stable for at least 53 days under ambient conditions. We characterize the nanoparticles using various techniques, including PLQY measurements, electroluminescence, photoluminescence spectroscopies, X-ray diffraction, absorption spectroscopy, and transmission electron microscopy. Additionally, the study demonstrates the successful fabrication of quantum dot LEDs from the nanoparticle solutions, with electroluminescence spectra comparable to the photoluminescence spectra of the nanocrystal solutions. The proposed post-treatment strategy is applicable to both freshly synthesized and aged CsPbBr₃ nanoparticle samples, highlighting the effectiveness of both the organic borate and thiocyanates as a dopants for perovskite nanocrystals.

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TRITIUM DIFFUSION THROUGH THE WALLS OF THE PIPE

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Radioactive hydrogen isotope, tritium, a nuclear fuel in fusion reactors, could cause an air contamination if permeated or leaked from its carrier pipes. Therefore, its diffusion through the pipe walls must be assessed in order to estimate risks [1]. For the description of diffusion in objects of cylindrical symmetry, the second Fick's law in cylindrical coordinates must be used under the condition that the concentration $c = \partial c / \partial \varphi = 0$:

$$\frac{\partial c}{\partial t} = D \left(\frac{\partial^2 c}{\partial r^2} + \frac{1}{r} \frac{\partial c}{\partial r} \right)$$

when doing variable separation $c = T \cdot R$ $T = k \cdot \exp(-\lambda^2 \cdot Dt)$

$$\frac{d^2 R}{dr^2} + \frac{1}{r} \frac{dR}{dr} + \lambda^2 R = 0$$

The general solution is

$$c = \exp(-\lambda^2 Dt) \cdot [A \cdot J_0(\lambda \cdot r) + B \cdot Y_0(\lambda \cdot r)] + c_0 \left(\ln \left(\frac{r}{R_2} \right) / \ln \left(\frac{R_1}{R_2} \right) \right),$$

where J_0 and Y_0 Bessel functions of first and second order.

By fulfilling the initial and boundary conditions $c_{t=0} = 0$ $c_{R_1} = c_0$ $c_{R_2} = 0$

$$C_{(r,t)} = \sum_{\alpha} \frac{2C_0 R_1 M e^{-\frac{\alpha^2 Dt}{R_2^2}} \left[J_0 \left(\alpha \cdot \frac{r}{R_2} \right) - \frac{J_0(\alpha)}{Y_0(\alpha)} Y_0 \left(\alpha \cdot \frac{r}{R_2} \right) \right]}{\alpha R_2 \left\{ \left[J_1(\alpha) - \frac{J_0(\alpha)}{Y_0(\alpha)} Y_1(\alpha) \right]^2 - \left(\frac{R_1}{R_2} \right)^2 M^2 \right\}} + C_0 \frac{\ln \frac{r}{R_2}}{\ln \frac{R_1}{R_2}}$$

where $M = J_1 \left(\alpha \frac{R_1}{R_2} \right) - \frac{J_0(\alpha)}{Y_0(\alpha)} \cdot Y_1 \left(\alpha \frac{R_1}{R_2} \right)$,

α – eigenvalues of

$$J_0 \left(\alpha \frac{R_1}{R_2} \right) - \frac{J_0(\alpha)}{Y_0(\alpha)} Y_0 \left(\alpha \frac{R_1}{R_2} \right) = 0$$

The total diffusant flux through the boundary surface $r = R_2$ is calculated according to the equation

$$j = -2\pi R_2 D \left(\frac{\partial c}{\partial r} \right)_{r=R_2}$$

The time dependence of the flow is shown in the Fig. 1., where it is compared with calculations through an area of an infinite plate $2\pi \frac{R_1 + R_2}{2}$ of the thickness $R_2 - R_1$.

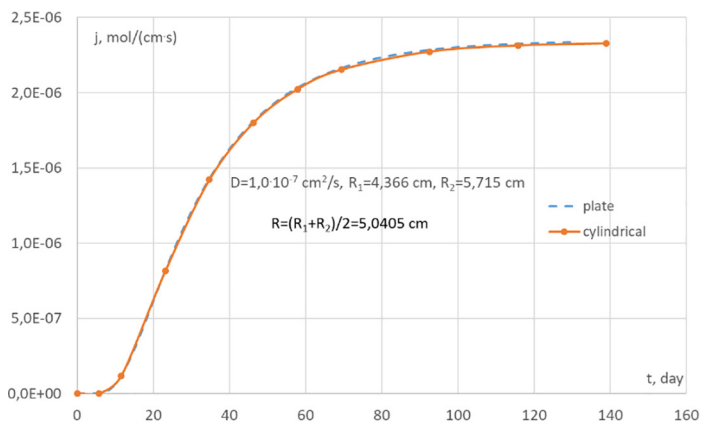


Fig. 1. The time dependence of the flow

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AN OCCURRENCE STUDY OF MYCOTOXINS IN PLANT-BASED BEVERAGES USING LIQUID CHROMATOGRAPHY–MASS SPECTROMETRY

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Mycotoxins are toxic mold metabolites that can adversely affect human and animal health. More than 400 mycotoxins have been identified so far. Cereals and nuts are the predominant mycotoxin-contaminated foodstuffs [1]. Plant-based drinks produced from cereals, nuts, and legumes have grown in popularity. The mycotoxins accumulated in these crops may transfer to these beverages.

A liquid chromatography–tandem mass spectrometry method was developed and optimized for the assessment of 22 mycotoxins in commercially available plant-based drinks in Latvia and Lithuania. A total of 64% of the seventy-two analyzed beverages were positive for one to sixteen mycotoxins, with deoxynivalenol, beauvericin, enniatins A, B, B1, T-2, and HT-2 toxins detected most frequently.

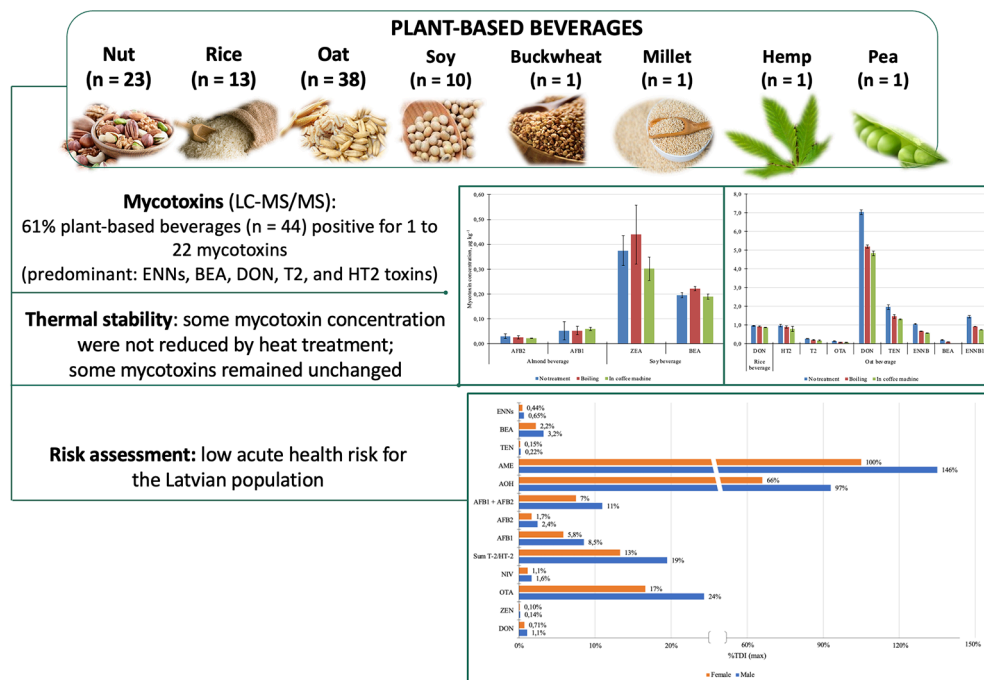


Fig. 1. The results of mycotoxin occurrence in plant drinks, thermal stability, and risk assessment

The European Commission and the European Food Safety Authority have not established guidelines for mycotoxin levels in plant-based drinks, leaving a regulatory gap. To assess safety, acute exposure studies in Latvia assumed a switch from dairy to plant-based beverages. The results suggest that the tested plant-based drinks are relatively safe, but emerging mycotoxins should be monitored [1].

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A NEW SOLVATES OF ISONICOTINAMIDE AND ALKYL CARBOXYLIC ACIDS

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Active pharmaceutical ingredients (APIs) can form different crystalline solid forms. [1] These include single component solid forms (polymorphs) and different types of two and multi component systems such as solvates, co-crystals etc. Solvates and co-crystals usually have physicochemical properties different from those of the pure API. These properties have an impact on the drug dosage form and the manufacturing route. [2] Therefore, crystal engineering opens new opportunities to obtain APIs with better physicochemical properties. [3,4]

In the research we present an investigation of solvate formation of isonicotinamide (INA) with linear monocarboxylic acids and several other solvents. The obtained phase structures were determined using SCXRD and PXRD and characterized using thermal analysis, but their crystal structures were analyzed using theoretical calculations.

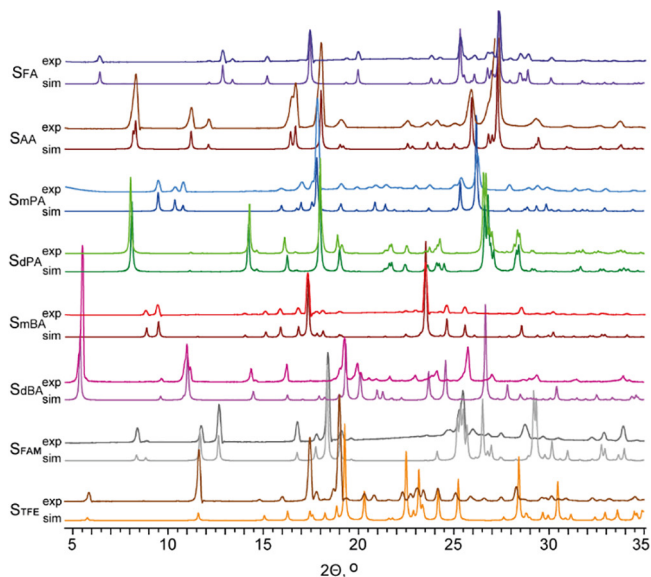


Fig. 1. Experimental and simulated PXRD patterns (obtained from crystal structures) of INA solvates

Four new INA solvates were obtained and crystallographic analysis of in total eight solvates were performed. Similar hydrogen bond patterns can be observed in all eight solvates. Based on the hydrogen bond motif present almost all solvates can be divided in

two distinct types: type A (containing tetramer formed from two solvent molecules and an INA dimer) and type B (containing trimer formed from a solvent: INA dimer and an additional solvent molecule), except for the formamide solvate which does not belong to any of these types.

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PER- AND POLYFLUOROALKYL SUBSTANCES (PFAS) AND HIGH-RESOLUTION MASS SPECTROMETRY (HRMS) BASED STRATEGIES FOR NON-TARGET SCREENING OF PFAS

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Per- and poly- fluoroalkyl substances (PFAS) consist of a fluorinated alkyl chain and a polar head group. Due to the strength of the C-F bond, these chemicals are extremely resistant to thermal and chemical degradation and are commonly referred to as "forever chemicals". Because of their hydrophobic and lipophobic properties, as well as their ability to withstand high temperatures, PFAS have a lot of uses as surfactants and surface protectors in fire-fighting foams, foodcontact materials, medical devices, textiles, cosmetics, etc [1].

Although the properties of PFAS have made them widely used compounds, legacy PFAS health hazards, toxicity and tendency to accumulate through the food chains are wellknown. Typically, laboratories monitor four long-chain PFAS – perfluorooctanoic acid (PFOA), perfluorooctane sulfonate (PFOS), perfluorononanoic acid (PFNA), and perfluorohexane sulfonic acid (PFHxS) – in food (regulated by the European Union) and other legacy PFAS using target methods. To minimize the use of legacy PFAS, they are being replaced with shorter-chain or less fluorinated compounds, so called emerging PFAS. With more than 5000 different PFAS, monitoring all of them becomes challenging. To understand the extent of environmental pollution caused by emerging PFAS, whose health hazards are not fully understood, and to determine appropriate mitigation strategies, researchers are using suspect screening and non-target analysis based on high-resolution mass spectrometry. Most researchers use Time of Flight (TOF) and Orbitrap mass spectrometry, while some opt for Fourier-Transform Ion Cyclotron Resonance (FT ICR) mass spectrometry.

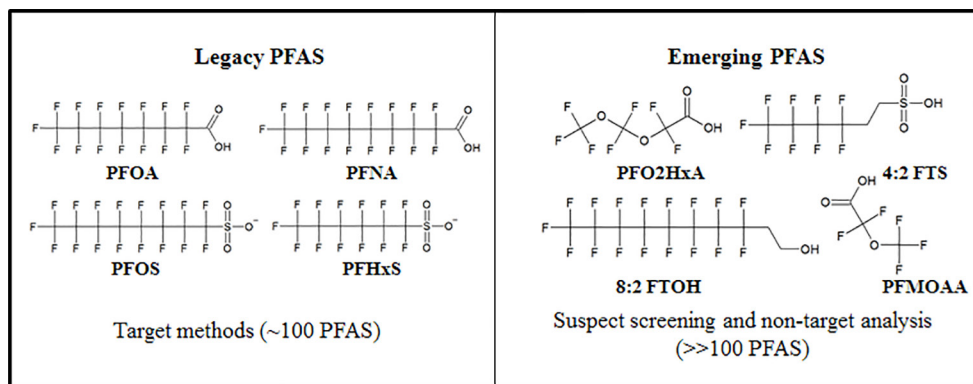


Fig. 1. Examples of legacy and emerging PFAS

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ELECTROCONDUCTIVITY OF SULFONATED POLY(ETHER ETHER KETONE) COMPOSITE MEMBRANES CONTAINING R-IMIDAZOLIUM DIMETHYLPHOSPHATE IONIC LIQUIDS

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The need to decrease the reliance on fossil fuels is ever more important with the consensus in the scientific community on the global climate change. This requires widespread deployment of renewable energy sources, which isn't feasible without various options for energy storage, including batteries. Sodium batteries are proposed as a suitable option for economic and safe stationary energy storage [1]. In this work, several ionic liquid (IL)/polymer (SPEEK) composite materials for use as solid state electrolytes in sodium batteries were developed. Results for one type of composite are shown in Fig. 1.

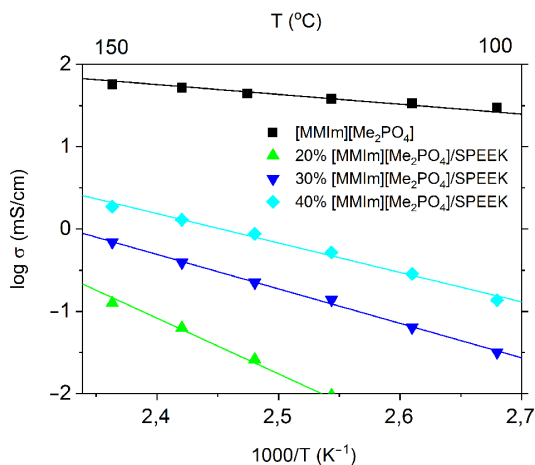


Fig. 1. Arrhenius plots of conductivity for IL and IL/SPEEK composites at various IL concentrations

Proton conductivity values reached 1,9 mS/cm at 150 °C for [MMIm][Me₂PO₄]/SPEEK composite membrane with 40 w% IL content. At these conditions the material still retained a stable solid state, making it potentially suitable for use in sodium batteries at elevated temperatures. Also, the chemical structure of different ILs had significant impact on the conductivity of these composites.

Acknowledgments. This work was supported by Latvian Council of Science (project No. LZP-2020/1-0391).

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A COMPARATIVE STUDY ON THE IMPACT OF ARGININE PHOSPHATE FERTILIZATION ON ISOTOPE RATIOS AND ELEMENTAL COMPOSITION IN SCOTS PINE WITHIN LATVIA'S FOREST ECOSYSTEMS

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Latvia's extensive forested landscapes, covering over half of the country's territory with approximately 3.4 million hectares, are experiencing a steady increase in forested areas. This expansion is largely driven by afforestation on previously unused agricultural lands and rehabilitated mining sites, as well as natural forest regeneration. A key strategy in forest ecosystem productivity is soil fertilization, which involves adding essential nutrients, notably nitrogen, to enhance plant growth.

The research was conducted in four distinct pedological settings, specifically focusing on *Vacciniosa mel.* and *Myrtillosa* forest types, both characterized by dry conditions and improved mineral soil drainage. The study aimed to evaluate the impact of arginine phosphate-infused fertilizers on the growth of Scots pine (*Pinus sylvestris* L.), examining changes in isotope ratios and elemental contents in the needles, branches, roots, and soil of treated and control specimens [1].

Advanced analytical techniques were used to assess the effects of fertilization, including isotopically labeled nitrogen fertilizers, light-stable isotope ratio mass spectrometry (Euro EA-Nu Horizon IRMS), and inductively coupled plasma mass spectrometry (Agilent 8900 ICPMS QQQ). The data analysis was conducted using the R statistical software, providing a thorough evaluation of the fertilizer's impact on Scots pine.

In conclusion, the investigation reveals that Scots pine seedlings planted in podzolic soil forests displayed the most significant nitrogen uptake, likely due to the nutrient-poor soil in these areas, which leads to an increased reliance on supplemental fertilization. All plants, regardless of fertilization, tended to decrease their nitrogen uptake in the first year after planting, which is attributed to the stress of transplantation and the time required for acclimatization. Analysis of the data also indicated that the fertilized samples from podzolic soil forests in 2022 were closely associated with the $\delta^{15}\text{N}$ content, suggesting a distinct isotopic nitrogen signature as a result of fertilization. These findings contribute to the field of sustainable forest management by providing insights into effective nutrient management practices for forest vegetation.

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Section of Organic Chemistry

MELDRUM'S ACID BASED ANTIOXIDANT SYNTHESIS AND ANTIRADICAL ACTIVITY EVALUATION

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Antioxidants are molecules which inhibit oxidation processes, consequently improving the longevity of various products and, in the case of living organisms, preventing illnesses associated with oxidative stress [1].

Our work is focused on carbon-centered 1,3-dicarbonyl type antioxidants [2], more specifically arylmethyl Meldrum's acids – compounds which have shown promising radical scavenging ability [3]. Previously we have found that dendrimeric structures containing multiple Meldrum's acid moieties show consistently high antiradical activity [4]. In this work we have synthesized dendrimers which contain 1,2,3-triazole linkers between the core and surface groups.

The key steps of the synthesis are cycloaddition of azide **1** with alkynes **2a** and **2b**, Knoevenagel condensation of the resulting aldehydes **3** with Meldrum's acid (**4**), and the reduction of the arylidenes **5** to the final products **6**.

The obtained products have higher radical scavenging ability (inhibition at a 100 μ M concentration AA = 88% and 83%, respectively) in the DPPH assay than commercial antioxidants ascorbic acid (AA = 14%) and BHT (AA = 16%) under the same experimental conditions.

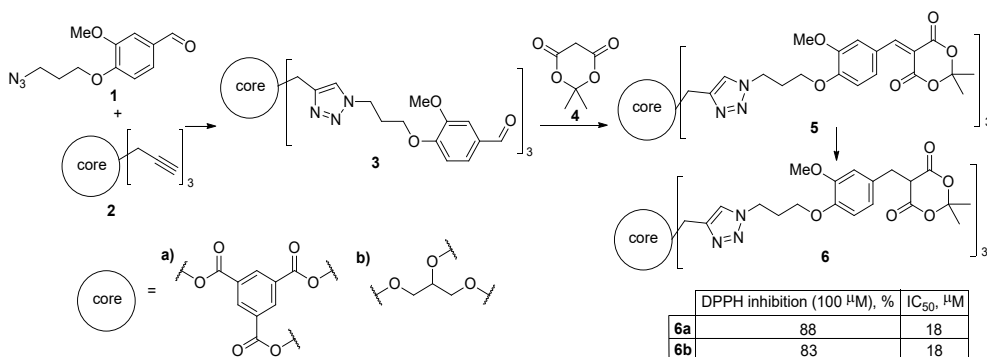


Fig. 1. Synthesis and antiradical activity of dendrimers **6**

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SYNTHESIS OF ORGANIC LIGANDS FOR DEVELOPMENT OF METAL ION SENSORS

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In recent years, significant attention has been directed towards environmental pollution and its monitoring. With the development of industrialization, heavy metals have emerged as one of the primary pollutants capable of accumulating in various living organisms [1]. However, the most widely used methods for the determination of heavy metal concentration, such as ICP-MS, entail significant costs and are only available in specialized laboratories. Consequently, in collaboration with the Institute of Atomic Physics and Spectroscopy, we are developing an organic ligand sensor, that could enable on-field analysis of metal ion concentration.

The Salen-type ligand **1** is employed in coordination chemistry due to its ability to form stable metal complexes [2]. Additionally, the inherent properties of the ligand structure often impart selectivity towards particular metal ions. In this report, we delve into the structural patterns of ligand **1** and explore its potential applications in metal ion detection (Fig. 1).

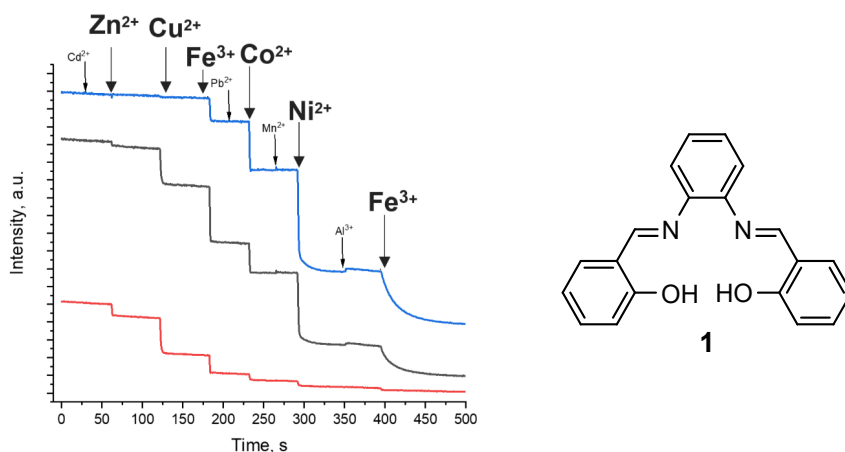


Fig. 1. Preliminary transmittance test with metal ions for ligand **1**.

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INVESTIGATION OF RETRO-BROOK REACTION ON PROTECTED 2PROPARGYL PHENOL

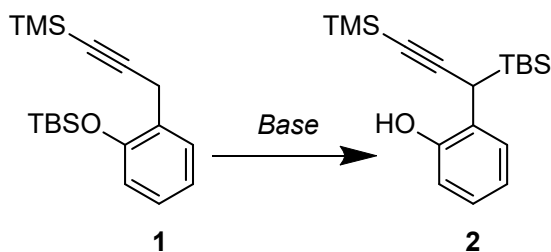
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We report a new use of retro-Brook rearrangement in protected 2-propargyl phenols to yield propargyl silanes **2**. In 2014, benzylic retroBrook [1,4]-rearrangements were investigated in substituted o-cresols with LDA in refluxing THF [1]. Five years later, retroBrook rearrangement was reported for TBS-protected terminal alkynols using 2 equivalents of butyllithium [2]. In this work, we aim to examine the utility of base-promoted retro-Brook [1,4]-rearrangement in 2-propargyl phenols.

We also propose a convenient synthetic pathway to protected propargyl phenol **1** from commercially available *o*-cresol, which can be carried out in 3 steps involving silylation, bromination and alkylation.



Scheme. 1. Retro-Brook rearrangement in 2-propargyl phenol

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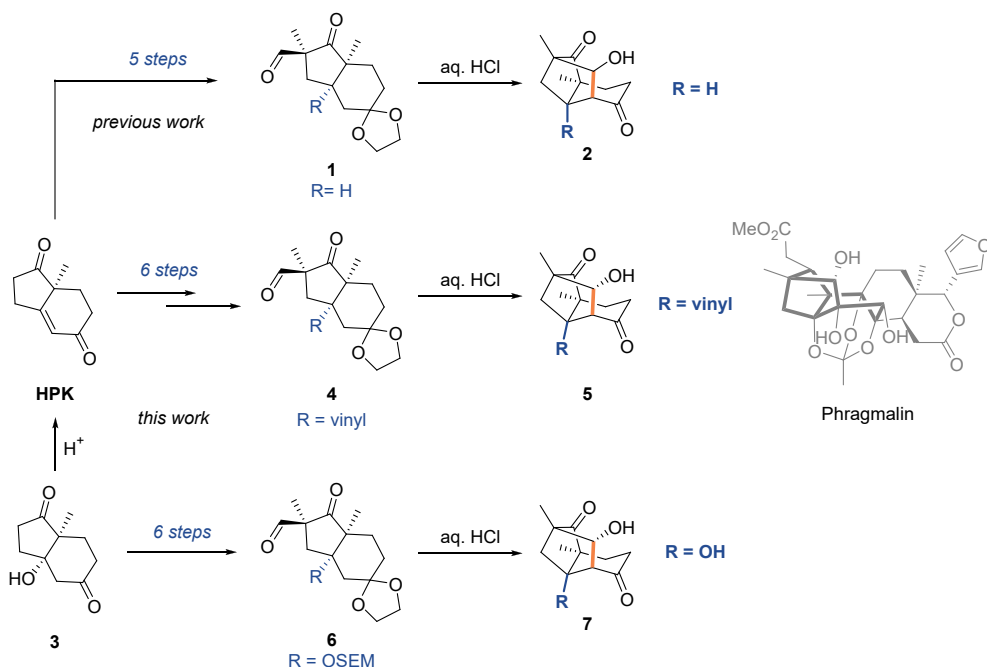
ELABORATING THE NEW ROUTE TOWARD METHANOINDENE CAGE KEY INTERMEDIATE

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Phragmalin-type limonoids stand out as intricate natural compounds, showcasing a diverse array of biological activities including anti-cancer, anti-bacterial, and anti-inflammatory properties [1]. These compounds feature an unconventional octa-hydro-1*H*-2,4-methanoindene cage structure (Scheme 1, bolded), whose synthetic approaches prior to this work were limited to racemic versions [2]. To construct this scaffold, the Hajos–Parrish ketone (HPK) has been chosen as the readily available starting material for the synthesis of key intermediate **1**. Subsequently, through the strategic aldol reaction (Scheme 1), aldehyde **1** can be transformed into the product **2** with distinctive cage framework [3].

Herein, we focused on the installation of the hydroxy group or its precursor (vinyl moiety) at the bridgehead position in order to construct the target methanoindene frameworks (Scheme 1). Therefore, the HPK and Hajos–Parrish ketol (**3**) were used as affordable optically pure starting materials in proposed synthetic approaches, yielding the desired products **5** and **7** in 7 steps. Further work will be devoted to the synthesis of phragmalin-type limonoids employing compounds **5** and **7** as key building blocks.



Scheme 1. The new routes toward the methanoindene derivatives.

Acknowledgments. This work was supported by ESIF project Nr.1.1.1.2/VIAA/4/20/752 and LIOS internal student grant IG202406. We thank *Dr. chem.* M. Skvorcova for theoretical and practical consultation.

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ETHER-FUNCTIONALIZED IMIDAZOLIUM IONIC LIQUIDS

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Ionic liquids (ILs) are ambient-temperature liquid salts composed entirely of ions. The combination of organic cations and inorganic anions allows for the creation of ILs with desirable physical properties such as low melting points, tunable viscosities, increased electrochemical stability, and relatively high ionic conductivity. The first known IL was reported by the Latvian chemist Paul Walden in 1914 [1].

Fluorinated anions produce ILs of low melting points and viscosities, and high electrochemical stability. Ether functionalization has demonstrated to significantly reduce pure IL viscosities and densities [2].

In this work, we have developed multigram synthetic routes to novel PEG-monomeric and PEG-dimeric imidazolium ILs based on bis-(trifluoromethanesulfonyl)imide [NTf₂]⁻ anion (**Figure 1**) for energy storage applications. Density and viscosity analysis has been carried out using rolling ball viscometry and vibrating tube densimetry.

To understand the role of connectivity between the PEG chain and the ionic core, the linker length in cations has been varied from one (**1**, **2**, **3**) to two (**4**) carbon atoms. To facilitate cooperative interactions of the two chains with plausible solute ions, the chains have been placed in a parallel (1,2-substituted) fashion (**3**). Controls (1,3-substituted) have also been prepared (**1**, **2**, **3**).

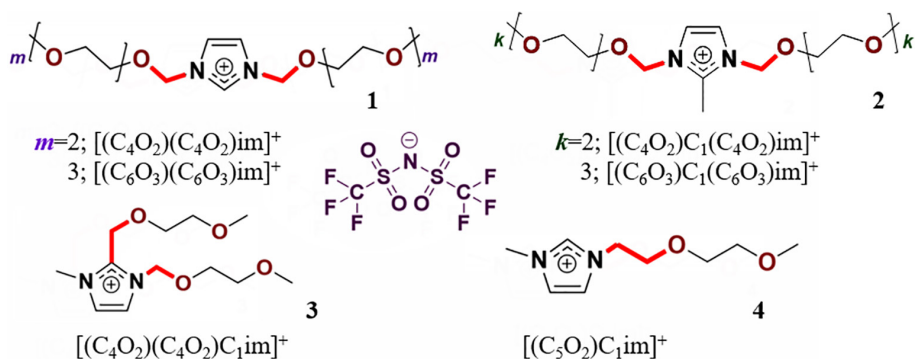


Figure 1. Structures of the cations of intermediates and [NTf₂]⁻ ILs prepared

Acknowledgments. This work was supported by the Latvian Council of Science (Grant No. lzp-2020/1-0391)

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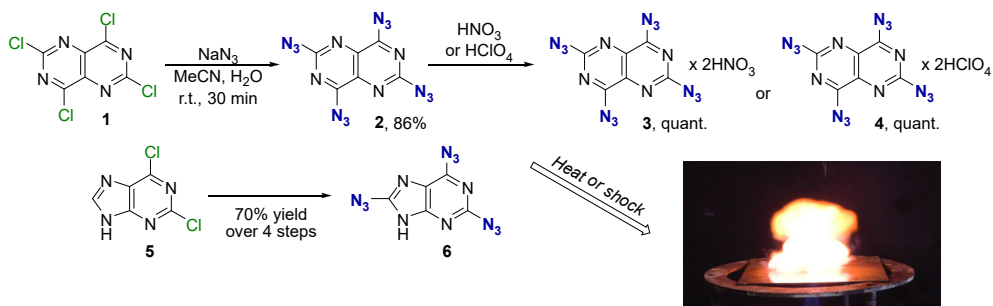
SYNTHESIS AND ENERGETIC PROPERTIES OF NOVEL ANNULATED POLYAZIDOPYRIMIDINES AND THEIR SOLVATES

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Binary C_xN_y organic compounds are impact-sensitive and possess explosive properties due to the high nitrogen content. The performance of nitrogen-rich compounds is attributed to the high heat of formation. Moreover, the main combustion product of such nitrogen-rich compounds is nontoxic nitrogen gas rather than the CO₂ from oxidation of a carbon backbone as in traditionally used explosives (TNT, RDX). Hence, nitrogen-rich compounds are currently the most promising candidates for the next-generation “green” explosives [1].

To the best of our knowledge, purine and its homologue – pyrimido[5,4*d*]pyrimidine have not been used in the synthesis of energetic materials before. However, the nitrogen-rich backbone presents excellent features for application such as high energy density materials. Recently, we have designed an approach towards binary C₆N₁₆ compound **2**, triazidopurine (**6**), and their solvates. Also, energetic properties of these compounds have been tested (**Scheme 1**) [2].



Scheme 1. Synthesis of polyazidopyrimidines and their solvates

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C2 MODIFICATION OF QUINAZOLINE DERIVATIVES VIA AZIDE-TETRAZOLE TAUTOMERISM

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Quinazoline derivatives exhibit a broad range of biological activities, finding use as anticancer, antimicrobial, antimalarial, and antiviral agents. Numerous 2-amino-6,7-dimethoxyquinazoline analogs are extensively employed as α_1 -adrenoreceptor blockers and in recent years quinazoline-based OLED materials have also gained attention [1–3].

Several methods of selective C4 position modification are known, but the modification of the C2 position is still challenging[4].

In this research, we employ the sulfonyl group dance[5] to achieve 4-azido-2-sulfonylquinazolines, which inverse the regioselectivity and further undergo C2 substitution, yielding 2-amino-4-azidoquinazolines. The regioselectivity of the transformation was proven by chemical synthesis, NMR, and X-ray crystallography.

Furthermore, we show the applications for these products in the synthesis of phosphonylidenes, fluorescent 4-triazolyquinazolines, and the development of a novel synthesis pathway toward α_1 -adrenoreceptor blockers terazosin and prazosin.

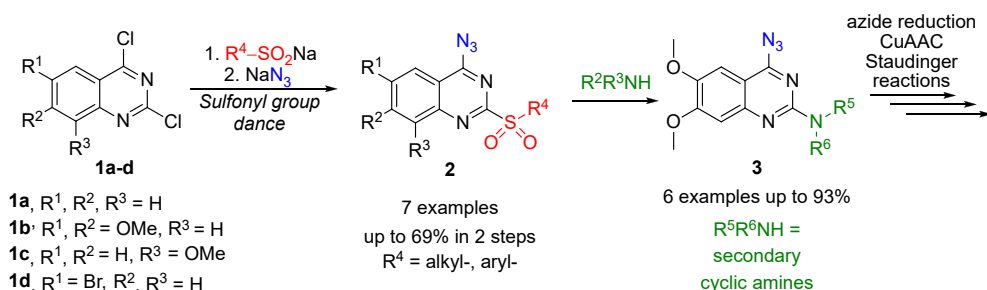


Fig. 1. Inversion of the regioselectivity of the quinazoline core via sulfonyl group dance

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SARS-CoV-2 METHYLTRANSFERASE INHIBITORS CONTAINING (ADENOSYLTHIO) METHYL BENZOIC ACID ANALOGUES

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Considering the recent global COVID-19 pandemic, it is important to develop new SARS-CoV-2 antiviral drugs and it is vital to study them to prevent future possible spreading of coronavirus. Coronaviral methyltransferases NSP14 and NSP16 are considered valid antiviral targets.

Recently we have discovered 3-phenyl benzoic acid containing adenosine derivative **1** as a bisubstrate inhibitor of SARS-CoV-2 methyltransferase NSP14. Here we report the development of new coronavirus methyltransferase inhibitors based on structure **1**. We explored 3-phenyl benzoic acid scaffold of the structure to complement the structure-activity relationship of adenosylthiobenzoic acid derivatives. Another approach is the fragmentation of the structure **1**. We prepared several analogs of compound **1** without the adenine moiety resulting in a new class of coronavirus methyltransferase inhibitors [1].

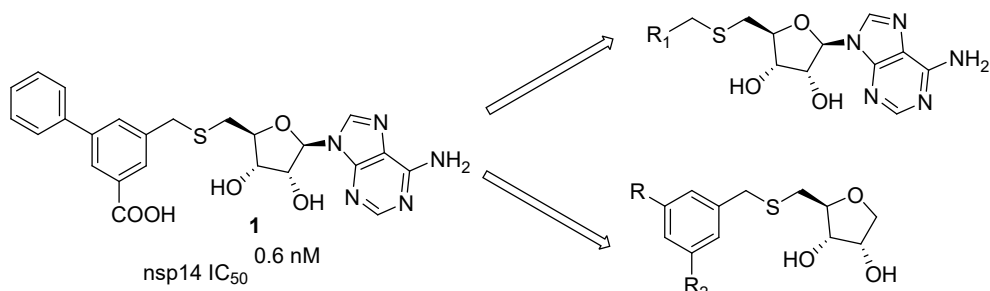


Fig. 1. Design of SARS-CoV-2 methyltransferase inhibitors

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SYNTHETIC APPLICATION OF 2-FLUOROCYCLOPROPYL-1-SULFINATE

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Fluoroalkyl containing compounds (e.g. $-\text{CF}_3$, $-\text{CF}_2\text{H}$, $-\text{CFH}_2$) are of high significance in research of pharmaceuticals [1], agrochemicals [2] and advanced materials [3] as fluoroalkyl groups can alter physiochemical properties of a molecule, for example, metabolic stability and bioavailability [4]. Monofluorocyclopropyl group is an intriguing moiety with potential application in medicinal chemistry, therefore, monofluorocyclopropylsulfinate **1**, being similar to Langlois reagent [5], could be an attractive, yet little explored, source of this moiety in fluorine chemistry.

Herein, we demonstrate application of little explored monofluorocyclopropylsulfinate **1** to access monofluorocyclopropanes via reaction with primary or secondary alkyl halides **2**. This strategy significantly complements our group's developed approach to monofluorocyclopropylsulfones **3** using the Johnson-Corey-Chaykovsky reaction [6], since now not only aromatic, but also aliphatic monofluorocyclopropylsulfones **3** can be obtained.

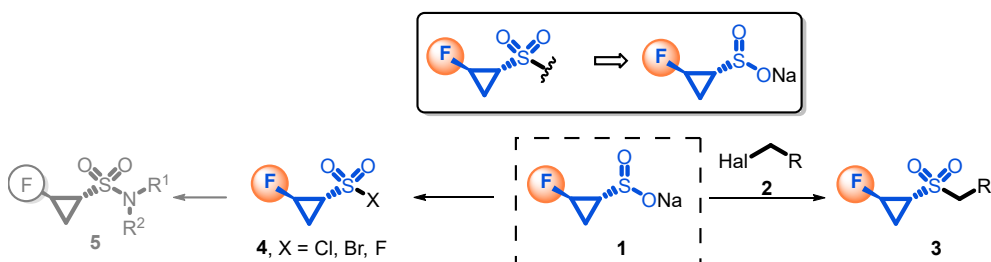


Fig. 1. Synthetic application of 2-fluorocyclopropyl-1-sulfinate **1**.

Acknowledgments. This work has been supported by the Latvian Council of Science project lzp-2022/1-0335.

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ORGANO-PHOTOREDOX CATALYZED RADICAL FLUOROMETHYLATION-CASCADE CYCLIZATION OF ARYL N-ACRYLAMIDES

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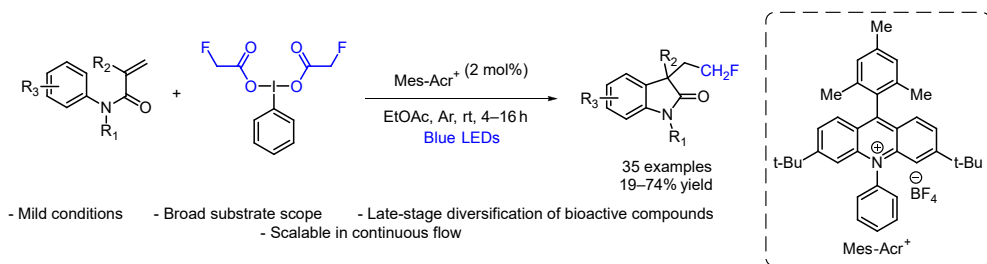
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2-Indolones are common motifs in many natural products and some commercially available drugs. Currently researchers are focusing on developing methods for accessing bioactive 3,3-disubstituted 2-indolones with diverse substitution patterns. Incorporation of fluorine atoms or fluoroalkyl groups into organic compounds has been shown to improve physicochemical and biological properties such as conformation, lipophilicity, potency etc. [1]. Introduction of trifluoromethyl group is well developed, however methods for incorporating monofluoromethyl group are less explored.

Herein, we report a method for accessing monofluoromethylated 2-indolones using an iodine (III) reagent as a fluoromethyl radical source under visible-light photoredox catalysis [2]. Contrary to the previous reports employing metal-photocatalysts for this process [3,4], our method uses an organophotocatalyst – 9-mesityl 10-phenylacridinium (a metal-free approach). This protocol is also applicable to synthesis of other polycyclic nitrogen heterocycles containing fluoromethyl group.



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ELECTROCHEMICAL SYNTHESIS OF PYRROLIDINE AND PIPERIDINE FRAGMENT-CONTAINING COMPOUNDS BY UTILIZING THE INTRAMOLECULAR HOFER-MOEST REACTION

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Pyrrolidine and piperidine fragment-containing molecules play a vital role in drug research due to their versatile pharmacological properties and structural diversity, making these heterocycles valuable scaffolds for drug discovery and development. Pyrrolidines and piperidines have been integrated into various pharmaceuticals, including anticancer, antibacterial, and anti-inflammatory drugs, which renders these compounds attractive targets for medicinal chemistry studies [1].

Recently, the synthesis of tetrahydropyran and tetrahydrofuran fragment-containing unnatural amino acids was achieved via the electrochemical decarboxylation/oxidation of readily available *N*-acetyl amino malonic acid monoesters followed by the intramolecular cyclization with a tethered *O*-nucleophile [2]. In the current research, the scope of tethered nucleophiles has been expanded by introducing *N*-tethered nucleophiles to afford pyrrolidine and piperidine fragment-containing compounds.

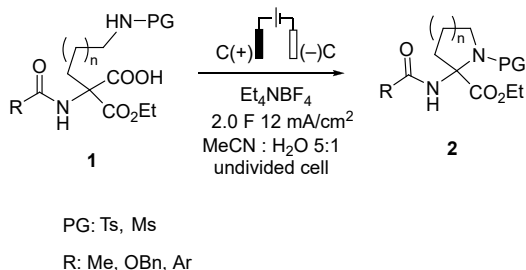


Fig. 1. Electrochemical synthesis of *N*-heterocycles **2**.

The developed electrochemical method provides access to pyrrolidine and piperidine fragment-containing amino acid derivatives. These novel compounds hold significant promise for drug discovery efforts, particularly in the development of bioactive molecules.

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SYNTHESIS AND USE OF BIFUNCTIONAL NON-COVALENT MOLECULARLY IMPRINTED POLYMERS (MIPS) FOR SELECTIVE EXTRACTION OF CATECHOLAMINES AND THEIR METABOLITES

Artūrs Šilaks¹, Antons Podjava¹

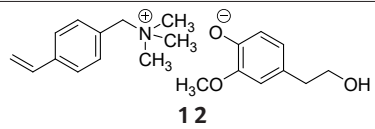
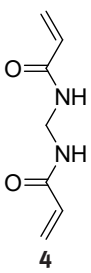
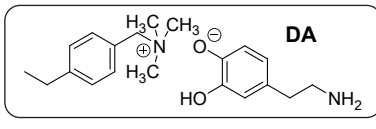
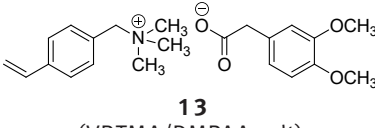
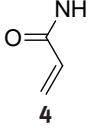
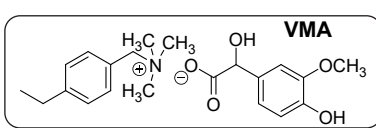
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Catecholamines (CAs) are an important group of hormones and neurotransmitters. Abnormal CA levels in bodily fluids can be linked to neurodegenerative diseases as well as adrenogenic tumors (e.g. neuroblastoma). Simultaneous determination of both CAs and their metabolites in biological fluids is an efficient way of reliably diagnosing the aforementioned diseases. Molecularly imprinted polymers (MIPs) are slowly replacing conventional sorbents for use in solid-phase extraction (SPE) to achieve superior selectivity for target analyte isolation from biological matrices. Simultaneous isolation of CAs and their acidic metabolites using MIPs is a novel and potentially viable approach that is being studied by our group [1].

To provide better recovery and molecular recognition for both CAs and their metabolites, the MIP is synthesized using a non-covalent approach. Methylenebisacrylamide (MBAA, cross-linker 4) is polymerized in the presence of a salt of (4-vinylbenzyl)trimethylammonium (VBTMA, 1) and homovanillyl alkoxide (2) and a salt formed by homoveratric acid (3) and 2, which act as dual-purpose templates/monomers for CAs and their metabolites, respectively.

Non-covalent MIP sorbents and non-imprinted polymers (NIPs) with variable cross-linker/monomer ratios were synthesized and packed into cartridges. Standard analyte mixture was passed through. The imprinting factor (IF) and recovery for each compound were calculated and compared to the NIPs. Preliminary results show that two MIPs show better retention and IF of CAs compared to the NIPs. These polymers will be used for further studies.

Table 1. Structural formulas of the compounds chosen for synthesis of the MIPs

Analyte	Combined Functional Monomer/ Template	Cross-linker	Analyte Binding Site
CAs, MN and NM	 <p>12 (VBTMA/Homovanillyl alcohol salt)</p>	 <p>4</p>	 <p>DA</p>
HVA and VMA	 <p>13 (VBTMA/DMPAA salt)</p>	 <p>4</p>	 <p>VMA</p>

Acknowledgments. This work is supported by the Fundamental and Applied Research Project lzp-2022/1-0141.

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TRIMETHYLENEMETHANE CYCLOADDITION TO SULFUR DIOXIDE AS A NEW METHOD FOR SULTINE SYNTHESIS

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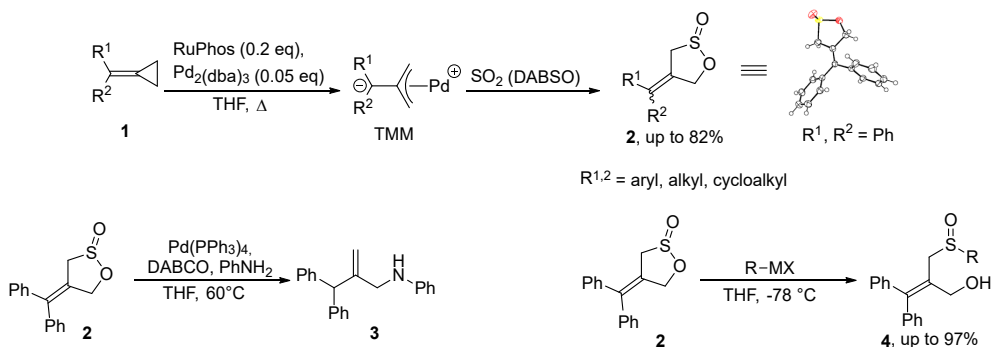
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Sultines (cyclic sulfinate esters) are largely unexplored class of compounds, even though they have been known since late 19th century, which is mostly attributed to difficult and wasteful synthesis. For the past 20 years, research into novel synthetic methods has not ceased, since sultines are potentially versatile building blocks for preparation of biologically active molecules as they undergo ring opening, alkylation, reduction and oxidation reactions yielding variety of useful products. [1, 2]

Experimental research yielded new synthetic method for γ -sultine synthesis through trimethylenemethane intermediates reaction with sulfur dioxide. Optimization of reaction conditions and catalytical system allowed yields up to 82% of various γ -sultines.

Further investigation into synthetic utility of the obtained products uncovered possibility to practically “regenerate” trimethylenemethane from these γ -sultines and sequentially form adduct to aniline. Additionally, ring opening reactions with carbon nucleophiles were performed achieving various sulfoxides with allyl alcohol moiety.



Scheme 1. New method for γ -sultine synthesis and explored derivatization pathways

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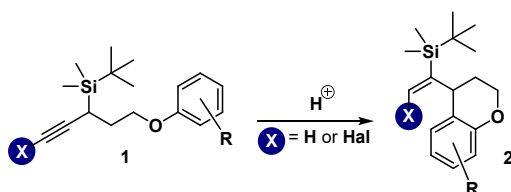
SYNTHESIS OF SUBSTITUTED CHROMANES VIA TANDEM 1,2-SILYL SHIFT – FRIEDEL–CRAFTS CYCLIZATION

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Previously our scientific group has found 1,2-silyl shift approach to be a powerful tool to the formation of 5-membered cycles, both carbocycles [1] (indenes) and heterocycles [2] (tetrahydrofuranes, pyrrolidines, tetrahydrothiophenes and isoxazolidines).

In this work, we apply acid-induced 1,2-silyl shift for the formation of 6-membered rings. We have developed a convenient synthetic pathway to substituted chromanes. Key synthetic step (Scheme 1) to substituted chromane **2** involves protonation of alkynes **1** and 1,2-silyl shift with consequent Friedel–Crafts cyclization with yields up to 99 %.



Scheme 1. Chromane synthesis via tandem 1,2-silyl shift – Friedel–Crafts cyclization.

The starting material **1** can be obtained in 70–80 % yield from commercially available pent-4-yn-1-ol in 3 or 4 steps: O-silylation, retro-Brook rearrangement [3] under Schlosser conditions and modified Mitsunobu reaction [4] with corresponding phenols. In the additional step, haloalkyne (Hal = Cl, Br, I) synthesis was conducted, and the resulting aryl ether **1** undergoes acid-catalyzed cyclization in the same fashion yielding chromane with *E*-selective alkene side chain.

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**Section of
Institute of Chemical Physics**

INVESTIGATION OF RADIATION-INDUCED EFFECTS IN LITHIUM ORTHOSILICATE-BASED CERAMIC BREEDER MATERIALS USING FOURIER TRANSFORM INFRARED SPECTROMETRY

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Biphasic ceramic pebbles, consisting of lithium orthosilicate (Li_4SiO_4) and lithium metatitanate (Li_2TiO_3) referred also as advanced ceramic breeder (ACB) material, are being developed in the European Union (EU) for tritium breeding in future thermonuclear reactors [1]. Under operational conditions, tritium breeding material must withstand high neutron flux and high temperatures. It is already known that the interaction mechanism of radiation with matter depends on the mass, electric charge, and energy of the incident particles. Therefore, it is necessary to investigate radiation-induced effects and the induced changes in Li_4SiO_4 -based ceramic breeder materials under actions of various radiation types and high temperature.

In this study, Li_4SiO_4 -based ceramic breeder materials were characterised before and after irradiation with accelerated ions in order to simulate neutron-induced effects, while avoiding nuclear transmutation reactions and consequently the formation of radioactive atomic nuclei [2]. The radiation-induced structural changes were investigated using attenuated total reflection – Fourier transform infrared (ATR-FTIR) spectrometry. Alongside ATR-FTIR spectrometry, various thermal and evolved gas analysis methods, e.g., thermogravimetry/differential thermal analysis (TG/DTA), differential scanning calorimetry/thermogravimetry (DSC/TG) and thermal desorption – quadrupole mass spectrometry (TD-QMS), were used in order to study thermal processes in the unirradiated and irradiated samples during heating.

Previously, it has been showed that after exposure to simultaneous action of accelerated electrons and high temperature, crystalline phase transitions and formation of new phases were not observed in irradiated Li_4SiO_4 -based ceramic breeder materials [3]. After irradiation with neutrons, it was detected that the increasing lithium loss due to nuclear transmutation processes during the irradiation leads to the formation of lithium metasilicate (Li_2SiO_3) [2]. After irradiation with accelerated ions, the formation of chemisorption product layer, which mainly consists of lithium carbonate (Li_2CO_3), was detected on the sample surface using ATR-FTIR spectrometry. During heating up to 1000 °C, the intensity decreases of the bond vibrations at about 1450 cm^{-1} , which were attributed to Li_2CO_3 , was detected. Using thermal and evolved gas analysis methods, gradual release of chemisorbed water (H_2O) and carbon dioxide (CO_2) from the sample surface before and after irradiation were detected in temperatures between 150 and 800 °C.

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INFRARED SPECTROMETRY ANALYSIS OF THERMALLY TREATED SILICON FOR FABRICATION OF NANOCAPACITORS

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Silicon nitride nanocapacitors have an important role in micro- and nano-electronical devices to be employed under action of ionizing radiation. Infrared spectrometry has been applied for monitoring the product radiation stability [1]. However, additionally to the impact of ionizing radiation, the thermal effects need to be taken into account. The impact of thermal effects on the chemical bonds has been recently estimated for the thin films on the Si containing surfaces, however, the estimation of the substrate long term stability is still required. Therefore, in the present research the stability of the chemical bonds in Si substrates was analysed.

The selected Si wafers, as satellite samples were treated analogous to the ones used in the fabrication process of the thin films [3]. After preparation Si samples were heated up to 150 °C at a rate of 10 °C/min, held at 150 °C for 8 hours and allowed to cool down to room temperature (one heating cycle). After each of the heating cycles, the Fourier transform infrared (FTIR) spectra were measured. Up to 3 FTIR measurements for each sample. A total of 33 heating cycles were performed. The FTIR measurements were performed with a Bruker Vertex 70v spectrometer equipped with an attenuated total reflection module.

In the FTIR spectra the main signal occurs at 600–630 cm⁻¹, corresponding to Si-Si asymmetric vibrations [4]. The variations of the signal intensity are used to determine the thermal stability of the Si structures. The slope of the signal at 610 cm⁻¹ shows to less than 0.1% changes over the 264 h cyclic heating tests, signifying the stability of the thin films. The obtained results will be used for further development of the nanocapacitors with improved dielectric layers.

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NEW FUNCTIONAL AEROGELS FOR ELECTROCHEMICAL APPLICATIONS

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Carbon aerogels (CAs) with three-dimensional porous networks are promising materials for electrochemical energy storage applications [1]. Recent efforts have focused on the modification of CAs using dopants. One area of significant interest is the incorporation of metal species into the carbon framework to modify the structure, conductivity, and catalytic activity of the aerogel [2].

This research proposes a simple, fast, and cost-effective synthesis of copper doped-carbon aerogels (Cu-CAs). The synthesis consists of sol-gel polycondensation of resorcinol with formaldehyde in a basic aqueous solution followed by drying at ambient pressure, and carbonization.

The X-ray diffraction measurements (XRD) reveal the presence of metallic copper in the sample (Fig. 1), and the scanning electron microscopy (SEM) images show a porous structure with copper particles (Fig. 2).

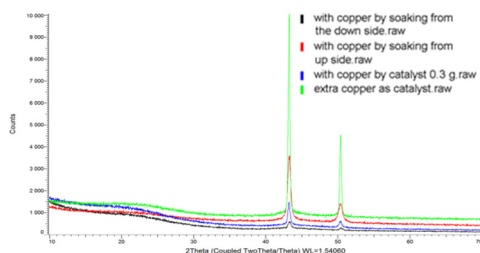


Fig. 1. XRD patterns for (Cu-CAs)

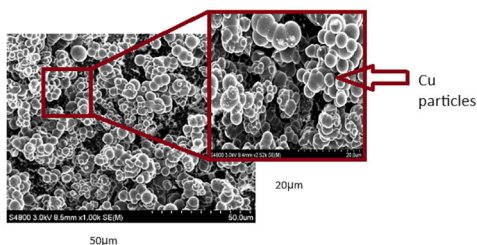


Fig. 2. SEM images for (Cu-CAs)

The potential use of this material in storage devices was investigated by preparing numerous electrodes using Cu-CAs and testing its applicability as electrodes in Zn-air batteries, lithium-ion batteries, sodium-ion batteries, and supercapacitors. Electrochemical impedance spectroscopy, cyclic voltammetry, and charge/discharge measurements indicated that Cu-CAs could be as a prospective material for the use as an electrode for a supercapacitor.

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ANALYSIS OF HUMAN LUNG TISSUE BIOPSY MATERIAL USING ATOMIC FORCE MICROSCOPY

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The study of human lung cancer is important as it is one of the leading causes of cancer-related mortality worldwide, if categorising cancers by the origination organ, with diverse subtypes exhibiting distinct pathological and molecular characteristics.¹ Understanding the morphological features and mechanical properties of lung cancer tissues can provide crucial insights into disease progression, metastasis, and treatment response. Atomic Force Microscopy (AFM) offers several advantageous properties for studying human lung cancer tissues. AFM offers high-resolution imaging of biological samples at the nanoscale, revealing cellular and subcellular structures with exceptional detail, and it can measure tissue mechanical properties like stiffness, elasticity, and adhesion, which can indicate cancer development and progression.

While human breast cancer biopsies, human liver cancer tissues, and even small human pulmonary arteries from tissue have been studied with AFM, to the authors' knowledge, no analysis of human lung cancer tissues with AFM has been conducted. AFM presents a promising yet underexplored field for such investigations, potentially unveiling novel characteristics of different cancer types. As lung cancer is relatively common and there is urgent need for more effective diagnostic and characterization methods, it is important to explore AFM's applicability with histologically relevant sample preparation techniques for practical implementation.

In this work, the potential application of atomic force microscopy (AFM) methods in the analysis of human lung cancer tissue biopsies was investigated. Human lung adenocarcinoma and squamous cell carcinoma tissue samples, prepared as histological samples by cryotomography tissue sections and as cytological samples using liquid-based cytology methods, were studied. The tumour tissue sections were prepared for tissue and cell morphology imaging, and AFM tapping mode was considered as the best, so that the probe-sample adhesive forces are small enough to get good quality AFM images. Good AFM image quality was achieved for 5–20 µm thick tissue sections with scan areas from 2x2 to 60x60 µm², and scan speeds ranging from 0.17 to 1.35 Hz. For these samples also stability of structures vs time was examined. The cytological samples were prepared for cell surface morphology and viscoelasticity studies with AFM, and these samples were measured in contact mode. In this mode AFM images can be acquired and then the areas of interest, e.g. specific locations on the cell can be selected to measure force-displacement curves. For AFM method testing also different cell chemical fixation methods were compared by using A549 cell culture and ASC52telo stem cell culture.

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ARTIFICIAL INTELLIGENCE, HUMAN VALUES AND NANOTECHNOLOGIES

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The rapid development of Large language models (LLM) shows that the emergence of more powerful than human artificial consciousness (AGI) and high-level machine intelligence or superintelligence (ASI) is a matter of near future [1]. To ensure sufficient artificial intelligence (AI) safety, the two main routes are Representation Engineering (RepE) [2] and Mechanistic Interpretability (Mechinterp or MI) [3]. Both options require a better understanding and modelling of natural and artificial consciousness. If the AI is close to biological consciousness, then it will be possible to ensure ASI friendliness and goodwill for humanity and build successful cooperation between ASI and people. Many facts suggest a potential significant role of quantum effects in the functioning of consciousness. Key functions of biological consciousness can be repeated without direct use of quantum effects through artificial neural networks. However, the question of the importance of quantum effects remains open and the principles of consciousness and the comparative aspects of the functioning of natural and artificial neuronal networks should be thoroughly investigated.

A useful model of mind action can be built using analytical psychology and emotional informative theory. According to the model, used in analytical psychology, psyche can be divided into four main parts: present, future, logic, emotion [4]. Present and future model assessments and pathways (logic) for achieving the future from the present are created by the emotional system based on four key criteria. During the evaluation process, combinations of emotions in the psyche are formed on the basis of four main criteria. The main, basic emotions are 16. Emotions help to understand and classify human values and virtues.

The question of the role of quantum effects in natural and artificial intelligence research is becoming even more pressing as quantum computer building begins. The AI must be based on programming a human value system into AI-forming elements (chips). Understanding the structure of a value system and commitment to emotion allows you to create a human-friendly AGI and ASI. Bringing artificial neuronal networks and artificial intelligence closer to nature makes it possible to deal more effectively with RepE and Mechinterp challenges and at the same time build the optimum human collaboration with AI. Quantum effects studies make it possible to understand the relationship between free will and spontaneous loss of symmetry, to clarify the possibilities for modelling by LLM in light of Heisenberg's principle of uncertainty, and to understand the role of non-locality and quantum entanglement in consciousness and in quantum computers.

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USE OF Sb_2Te_3 AND SINGLE-WALL NANOTUBE HETEROSTRUCTURES IN THE FORMATION OF THERMOELECTRIC SAMPLES BY ENCAPSULATING THEM IN DIFFERENT POLYMERS

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The need to reduce CO_2 emissions, which are mainly caused by different sources of energy production, poses a significant challenge to researchers working on the development of thermoelectric (TE) materials. As industrialization intensifies and the population grows, the demand for heat and electricity will continue to grow. More efficient use of heat and energy is very important, as more than half of the heat currently produced is dissipated into the atmosphere in an unused form [1].

Encapsulation of Sb_2Te_3 and p-type SWCNT samples in various polymers provides their protection from environmental influences, and it is also possible to obtain thermoelectric samples. Both before and after the encapsulation of the samples in polymers, their resistance and Seebeck coefficient were measured, which are one of the most important quantities characterizing thermoelectric materials.

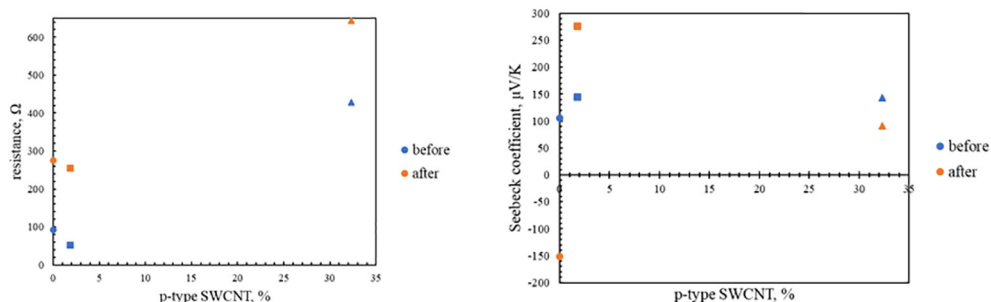


Fig. 1. Resistance and Seebeck coefficient as a function of p-type SWCNT concentration before and after Sb_2Te_3 on p-type SWCNT sample encapsulation in nylon 6/12, PMMA and PS

After all the samples were encapsulated in the different polymers, their resistance increased, and their Seebeck coefficient decreased in the case of nylon 6/12 and PS, while it increased in the case of PMMA.

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EFFECT OF SYNTHESIS PARAMETERS ON THE MORPHOLOGY AND THERMOELECTRIC PROPERTIES OF HYBRID METAL OXIDE NANOWIRE ARRAYS

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Thermoelectric generators (TEGs) are devices made for generating an electrical current by applying a temperature difference. This is achieved by connecting thermoelectric elements in a series of alternating p-type and n-type materials [1]. Previous research has shown that Cu₂O and ZnO nanowires are a relatively cheap and non-toxic option for the p-type semiconductor and the n-type semiconductor, respectively [2,3]. In order to decrease sample size, a hybrid material is proposed by adding an oxidized zinc layer on top of Cu₂O nanowires. Synthesis parameters and morphology of the material must be studied to maximize the efficiency of the hybrid metal oxide nanowire array.

In this work, CuO nanowires were synthesized by thermal oxidation of copper foil at different temperatures and annealed in a vacuum to produce Cu₂O nanowires [2]. A layer of zinc was deposited on the surface of Cu₂O nanowires via physical vapour deposition and then oxidized. Morphology of the nanowires was characterized using scanning electron microscopy (SEM). Electrical and thermoelectric properties were measured using Keithley 6430 sourcemeter and HP 34401A multimeter. A temperature difference was applied using Peltier's element and measured using a thermocouple. The optimal copper foil oxidation temperature was investigated for use in further experiments and the effect of ZnO thickness on the thermoelectric properties of the hybrid metal oxide nanowire array was also researched.

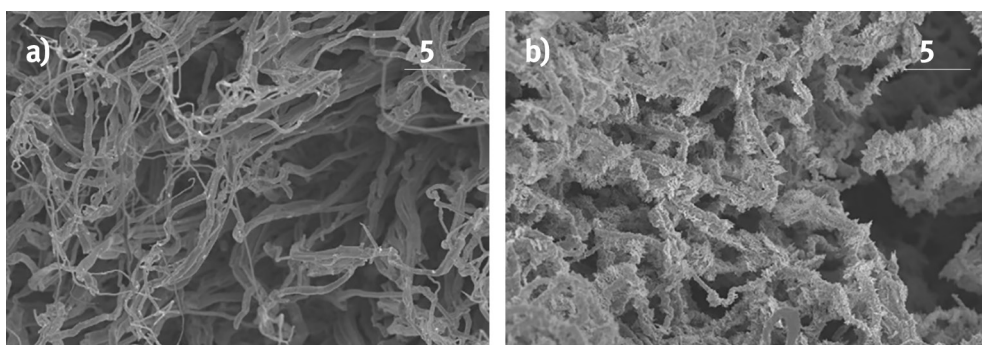


Fig. 1. SEM images of a) Cu₂O nanowires on copper foil; b) ZnO on Cu₂O nanowires

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OCCUPATIONAL SAFETY IN WORKING WITH TRITIUM IN RESEARCH LABORATORIES: DEVELOPMENT OF AN ALGORITHM USING MODEL EXPERIMENTS

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Tritium (T) is a radioactive isotope of hydrogen with a half-life of 12.33 years, and it is a low energy beta emitter. It is found in several forms such as HT, HTO and it tends to replace stable hydrogen in water molecules in the human body [1]. Tritium is widely used in laboratories in the labelled atom method, and many reagents and reactions have been developed to tritiate both single molecules and various materials [2].

This experimental study was dedicated for the qualitative assessment of tritium contamination in the laboratory processes. Model experiments were carried out at the University of Latvia Laboratory of Radiation Chemistry of Solids of the Institute of Chemical Physics (UoL ICP LRCS). This study involved the evaluation of the tritium contamination on the surfaces at workplace, exposure from air and deposition in urine after the work with tritium rich sources. Tritiated water ($2 \cdot 10^{-6}$ – 0,1 ppm) was used measure evaporation rate and provide a mathematical formula for exposure assessment and development of description/procedure for safety management during the work with T sources. Urine samples for tritium determination were collected from employees every 3 days for 1 weekend prepared according to procedure reported in literature [3]. At least 3 parallel measurements were made for each sample. Liquid form T measurements were performed by liquid scintillator (*PerkinElmer* TriCarb TR-2900) and air measurements using a proportional gas flow counter (*MabSolutions* TEM 2100A).

Results for the surface assessment indicated no detectable levels of tritium, however, inadequate airflow in 2 out of 6 fume hoods was determined. At the completion of this study fume hood airflow was remedied. Screening of tritium deposition indicated that employees at the UoL ICP LRCS do not have an elevated level of tritium in their organisms. The determined T levels in urine were below the Republic of Latvia established limit for tritium compounds in drinking water of 0.1 Bq/L [4]. A complete algorithm for establishing risks in research laboratories working with tritium was developed during this study.

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IMPLEMENTATION OF SHEEP WOOL FIBERS IN AIR FILTRATING SYSTEMS FOR ABSORPTION OF VOLATILE ORGANIC COMPOUNDS

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Sheep wool fibers have been recognized as natural, local, self-sustainable, renewable and biodegradable source, that can be applied in various fields such as building materials [1], composites [2], water [3] and air filtrating systems [4]. Surface structure and polar bonds in the chemical composition of sheep wool fibers allow to apply it in non-modified way as physical and chemical filter, analogous to other materials from bio-fibers. However, in order to expand the application field and improve the properties of the filters, various modification methods can be applied. Thermal treatment of sheep wool fibers allows to create carbon and activated carbon with large surface area, that changes the filtrating properties.

In conditions, where it is necessary to exclude presence of volatile organic compounds in airflow, the sheep wool and thermally modified sheep wool filters may be introduced. In the present research, the sheep wool fibers and thermally modified fibers from Latvian Darkhead sheeps were used as filtrating material. The filtrating efficiency was monitored by employing infrared spectrometer Bruker Vertex 70v with gas analysing unit cell, 400–4000 cm⁻¹, ±4 cm⁻¹. Airflow with additions of volatile organic compounds, such as acetone vapour, was guided through wool and wool-carbon combined filters.

The results show to decrease in the content of the organic molecules, that is comparable with the commercially available synthetic filters.

Acknowledgments. The Research performed within the European Regional Development Fund (ERDF) 1.1.1.1 Practical Orientation Research 4th round project No. 1.1.1.1/20/A/155 “Development of novel and innovative composite materials with enhanced sorption properties from renewable biological natural resources available in the Republic of Latvia for commercial air purification filtration systems”.

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DIFFERENT APPROACHES TO OBTAINING NANOPOROUS ANODIC ALUMINA MEMBRANES WITH AAO LAYER THICKNESS OVER 60 μm BY ANODISATION IN SULFURIC ACID ELECTROLYTE

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Nanoporous anodic aluminum oxide (AAO) is one of the most popular and cost-effective platforms for various applications: from templates and molecular separation to drug delivery and energy generation. Its unique optical and electrochemical properties have been extensively explored as a platform for developing biosensing and energy-harvesting nanodevices.

Membranes with a small pore diameter (<25 nm) are of particular importance, since their integration in nanodevices is often preferable. The thickness of such membranes usually does not exceed 60 μm . The reason is that much thinner inter-pore walls in *sulfuric*-AAO membranes, compared to *oxalic*-AAO or *phosphoric*-AAO, after long anodisation in the sulfuric acid electrolyte are turning into Al_2O_3 nanowires, that are blocking the pores.

In this work three different approaches have been used to solve this problem:

- 1) direct anodisation in 0.3M sulfuric acid electrolyte – maximum thickness obtained is 65 μm ;
- 2) step-by-step anodisation in oxalic and sulfuric acid – the attempts to increase the *sulfuric*-AAO layer thickness above 50 microns leads to delamination of the *oxalic*-AAO layer;
- 3) pulse anodisation in 0.3M sulfuric acid electrolyte – appeared to be the most promising method for obtaining membranes that consist of alternating highly ordered nanoporous sulfuric-AAO layers with pore diameters $d_{\text{pore}} = 20$ nm and 40 nm and the total thicknesses of 80 – 100 microns.

All anodisation and postanodisation treatment conditions (concentration and type of electrolyte, applied potential between electrodes, temperature and time of anodisation, the way of aluminum layer dissolution, and time of barrier layer etching) were optimized for fabricating robust AAO membranes. The morphology of the AAO membranes was characterized by the means of scanning electron microscopy (SEM).

MODERNIZATION OF LEGACY SCIENTIFIC EQUIPMENT VIA REMOTELY CONTROLLED ADAPTER

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Many well equipped laboratories over time start to suffer from growing technical difficulties, having to retrofit existing equipment or integrate newly acquired instruments to the current research infrastructure. Automation of experiments is often done using general purpose computers, however, the complexity is highly dependent on the specific equipment and modern computers may not have the required hardware interfaces.

With this research, a prototype (Fig. 1) was developed for an adapter capable of receiving and sending commands via standard wireless interface and converting the data to RS-232 protocol through the DE-9 communications port.

If multiple such adapters were to be connected to the same network, they could be linked together with an IoT (Internet of Things) protocol and organized to send simultaneous commands with tens of milliseconds accuracy. The current prototype utilizes a battery, meaning it is able to operate without external power and could be used for instruments that are galvanically isolated. This prototype shows potential for simultaneous synchronized data acquisition at remote locations, allowing to accurately control experiments and monitor processes at different time scales.

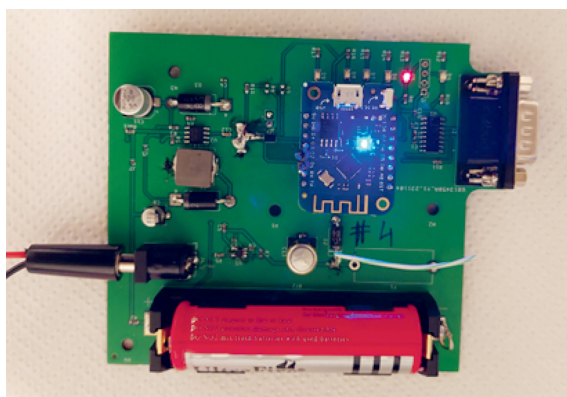


Fig. 1. Prototype for the wireless device adapter

BISMUTH SELENIDE AND NITROGEN-DOPED MWCNT HETEROSTRUCTURES FOR USE IN FLEXIBLE THERMOELECTRICS

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With an increasing demand for efficiency and greener power, the field of thermoelectrics has seen a rising number of researchers and scientific publications. A well-known material with great thermoelectrical properties is bismuth selenide (Bi_2Se_3), however, for thermoelectrics, it's thermal and electrical conductivity left much to be desired. Attempts of improvement have turned to nanostructured materials, for example, using carbon nanotube (CNTs) networks which helped increasing the electrical conductivity and reducing the thermal conductivity, allowing for greater efficiency thermoelectric materials [1].

In this work Bi_2Se_3 is deposited on to Nitrogen-doped MWCNT network, which have been shown to exhibit n-type behaviour [2]. Seebeck coefficient and electrical resistance is measured before and after encapsulation with PVA, which allows for separation from synthesis substrate for further application in flexible thermoelectric devices.

The MWCNT networks are prepared on a 2.5×2.5 cm glass substrate via spray-coating technique and subsequent Bi_2Se_3 deposition is carried out by a catalyst-free vapour-solid deposition method. Non-stoichiometric region is removed, leaving around 1 cm wide strip. Copper wire strands are attached to the samples with low-viscosity silver conductive paint. Electrical and thermoelectrical measurements are carried out on a lab-made setup using commercial Peltier modules, heating-cooling controller. Keithley6487 picoammeter, HP34401A desktop multimeter and K-type thermocouples.

Results show a negative Seebeck value though-out the concentration range, as well as greater absolute values below 5 wt%. (Fig 1.)

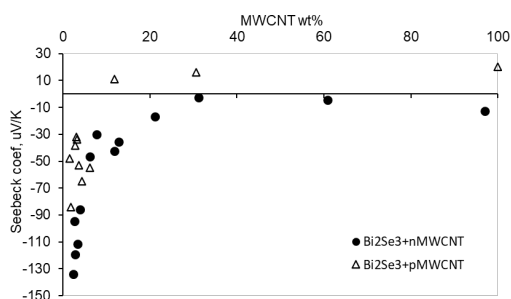


Fig 1. Seebeck coefficient depending on CNT concentration in sample

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THERMAL STABILITY AND DECOMPOSITION PROCESSES OF FLUORESCENT BENZANTHRONE-BASED DYES

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The implementation of luminescence effect into biological and medical investigations plays a crucial role in understanding the behaviour of the cells and microorganisms [1]. Benzanthrone (BZA)-based compounds have various industrial and scientific application possibilities, including innovative approaches in forensic sciences [2] and as fluorescent dyes for microscopic visualization of biological objects [3]. Previously, various BZA derivatives have been synthesised and their spectroscopic properties have been characterised [4–6]. However, the thermal stability and decomposition processes of synthesised BZA derivatives have not been described in detail, which is important for technological applications in various fields when the samples may be heated.

In the present work, thermal stability and decomposition processes of three BZA derivatives containing substituted bromo, nitro and amino groups were investigated and compared to non-substituted BZA using isochronal annealing and attenuated total reflectance-Fourier transform infrared (ATR-FTIR) spectrometry. The obtained results of ATR-FTIR spectrometry were also directly compared with other relevant methods, e.g., powder X-ray diffractometry (PXRD), differential scanning calorimetry/thermogravimetry (DSC/TG), etc.

The obtained results of ATR-FTIR spectrometry show that introduction of functional groups affects the thermal stability of BZA derivatives, that reflects as changes in the FTIR spectra signal intensities after thermal treatment. The ATR-FTIR results fit well with the DSC/TG results, where substituted BZA derivatives show more complex decomposition processes in comparison to non-substituted BZA.

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