YOUNGCHEM

18th International Congress of Young Chemists

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19-22.05.2025

Hotel Senator****
Kołobrzeg - Dźwirzyno, Poland

Book of Abstracts

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Dear Participants, Honorable Guests

It is my great pleasure to welcome you to the 18th International Congress of Young Chemists YoungChem in Dźwirzyno. I am very glad to see that we have managed to attract such a great number of young scientists, reviving the tradition of the annual Congress after several years of its absence.

YoungChem is an excellent place to share the experience of young researchers of diverse backgrounds, exchange ideas and to integrate the forthcoming generation of chemists. The participants will have a chance to enjoy lectures prepared by scientists from various fields of chemistry. The invited keynote speakers will present their recent research and share their enormous experience in our common passion – chemistry. I am truly honored and thankful that our guests, top-class researchers, want to share their time, knowledge, and experience with so many young scientists.

The Organizing Committee would also like to express their thanks to all the sponsors. It would not be possible to reach such a high organizational standard without their help. We also wish to thank the authorities of the Faculty of Chemistry at Warsaw University of Technology, for their support and trust in our organizing of YoungChem. Last but not least, we thank all the participants of the Conference, for having come even from distant places.

Personally, I would like to thank the members of the Chemical Scientific Society Flogiston, for their great effort in preparations. Thanks to their hard work throughout the last months, and the atmosphere of friendship that we all create, the YoungChem Conference would not be possible.

We wish all the participants success in their presentations, exciting discussions, lots of new experience and knowledge, plentiful new contacts, and a lovely, unforgettable time in Poland.

Bruno Skoczeń

President of Organizing Committee

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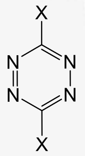
NEW ADVANCES IN TETRAZINES AND HEPTAZINES CHEMISTRY. FLUORESCENCE, PHOTOCATALYSIS AND APPLICATIONS TO OPV

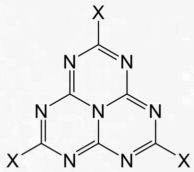
Pierre Audebert, PPSM, ENS Paris Saclay, XLIM, U. Limoges.

audebert@ppsm.ens-cachan.fr

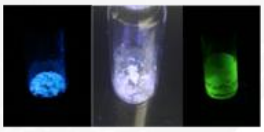
s-Tetrazines[1], and the more enigmatic heptazines[2,3], which count much less described examples, are among the most electron deficient stable aromatic heterocycles, due to their high-nitrogen content, while purely organic (Fig. 1). This situation confers them original physico-chemical characteristics, among which a high electrochemical reduction potential, and especially a strong oxidation potential in the excited state, which is e.g. highly desired for organic photocatalysis. In addition, heptazines display delayed fluorescence and can trigger enhanced electron transport in OPV devices[4]. However, their synthetic approach, for heptazines, is still in its beginning. We will present original applications o tetrazines, eg fingerprints revelation, and new strategic synthetic procedures to produce heptazines, as well as recent results obtained with new derivatives of these families.



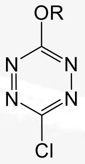
s-tetrazines



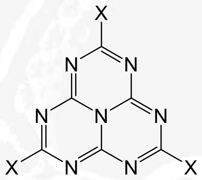
heptazines



This lecture will therefore recall new original results on tetrazines, and heptazines, obtained in our group over the last 15 years. In the case of tetrazines, the accent will be put on new applications rather than on long-known syntheses. The original delayed fluorescence of original heptazines, substituted by thiols, will be presented. We will also describe new heptazines presenting a singlet-triplet inversion, along with first results in photocatalysis. Examples featuring the molecules concerned are gathered in the Scheme below. Finally, the synthesis and properties of a new type of heptazine-porphyrin dyad will also be described.

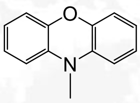


s-tetrazines for electrofluorochromism



heptazines

X = Pyrazoles, Imidazoles, thioaryls and alcohols.



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NMR CRYSTALLOGRAPHY OF ORGANIC SOLIDS AT HIGH MAGNETIC FIELDS

Marta K. Dudek

Centre of Molecular and Macromolecular Studies, Polish Academy of Sciences, Sienkiewicza 112, 90-363 Łódź, Poland, e-mail: marta.dudek@cbmm.lodz.pl

NMR crystallography, combining solid-state NMR, powder X-ray diffraction and theoretical calculations offers a real possibility of solving a crystal structure of a molecule when single crystal X-ray diffraction cannot be used (for example because the crystals large enough could not be obtained). It is not, however, a straight-forward techique, not least because of the fact that solid-state NMR spectra are often quite crowded and difficult to assign, even when advanced 2D techniques are applied [1, 2]. As a result it can be immensely difficult to build a reliable structural model from the experimental data, which can be further refined through calculations. This lecture will showcase the application of NMR crystallography to solve several structural puzzels, the answer to which is impossible to find using other experimental techniques. In particular, it will be shown how this method can be used to reveal hidden disroder in the crystals of meloxicam:pyrazole cocrystal polymorphs, to establish a tautomeric form present in a crystal of meloxicam:pyrazine cocrystal, especially through the use of ^{1}H-^{1}H BaBa and ^{1}H-^{14}N T-HMQC spectra registered at 1GHz NMR spectrometer (Fig.1), and to unambiguously differentiate between salts and cocrystals in meloxicam:imidazol binary crystals.

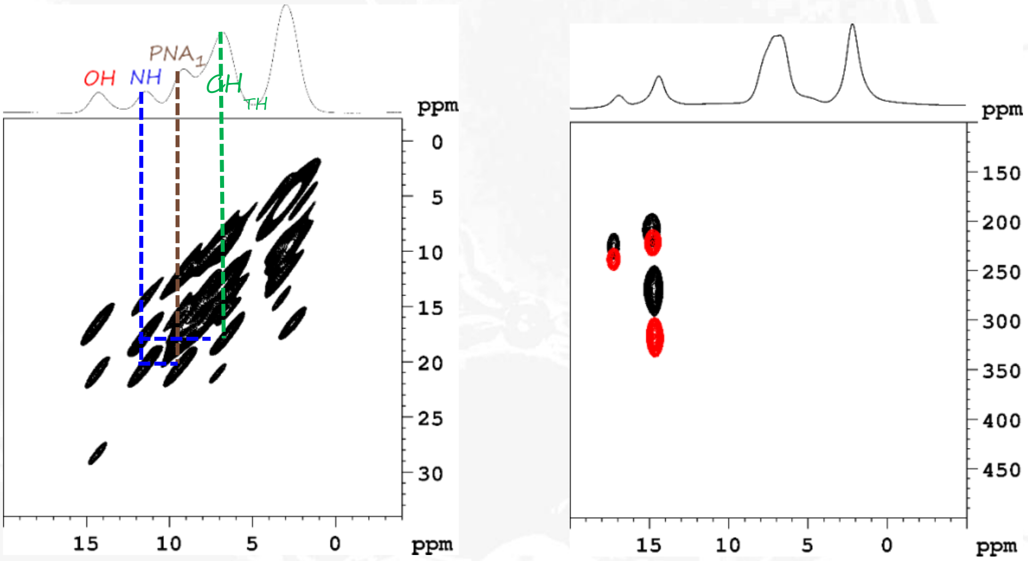

Figure 1. ^{1}H-^{1}H DQ-SQ Back-to-Back spectrum of meloxicam:pyrazine system (left) registered at 1GHz spectrometer and an overlay of two ^{1}H-^{14}N T-HMQC spectra registered at 1GHz and 850 MHz for meloxicam:imidazole system (right).

Acknowledgements

This work was financially support of the Polish National Science Centre under Sonata Bis grant No 2022/46/E/ST4/00392. We gratefully acknowledge Polish high-performance computing infrastructure PLGrid (ACK Cyfronet AGH) grant no. PLG/2024/017624

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METAL DOPED MAPbBr$_3$ SINGLE CRYSTAL P-N JUNCTION PHOTODIODE FOR SELF-POWERED PHOTO DETECTION

Vishnu Anilkumar[1], Daniel Prochowicz[1]

[1] Institute of Physical Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, 01-224 Warsaw, Poland

vanilkumar@ichf.edu.pl

Organic-Inorganic Metal Halide Perovskites (OIMHP) single crystal photodetectors have gained attention for their tunable band gap, high absorption coefficient, long carrier diffusion length, and high mobility. Lead halide perovskite is particularly promising in this field. However, most of the reported lead halide-based Photodetectors require an external power source. To overcome this drawback, a planar photodetector using metal-doped p-type and n-type MAPbBr$_3$ single crystals is introduced, demonstrating impressive self-powered photodetection properties. A p-n junction is formed by epitaxial growth of Ag$^+$-doped MAPbBr$_3$ (p-type) on Sb^{3+}-doped MAPbBr$_3$ (n-type). The device exhibits typical photovoltaic behaviour with a high open-circuit voltage of 0.95 V and sensitivity to 530 nm light, achieving a responsivity of 0.41 A W^{-1} and a specific detectivity of 6.39×10^{11} Jones. [1] The rise and fall times are 14 ms and 10 ms, respectively. [1] These findings support the development of self-powered perovskite-based photodiodes, with potential applications in advanced photodetection and optoelectronic devices.

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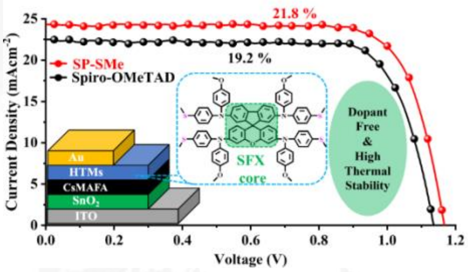
DEVELOPMENT OF HOLE TRANSPORT MATERIALS FOR STABLE AND EFFICIENT PEROVSKITE SOLAR CELLS

Muhammad Ans[1], Daniel Prochowicz[1]

[1] Institute of Physical Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, Warsaw, 01–224 Poland
mans@ichf.edu.pl

Perovskite solar cells (PSCs) have seen explosive development in power conversion efficiency (PCE) over 26%, reaching the level of classical crystalline silicon solar cells. As an absorbing material, lead halide perovskites (LHPs) possess unique and excellent optical properties, including low production cost, tuneable band gap, broad absorption, low exciton binding energy, and high charge-carrier mobility. However, their stability is the main obstacle to the commercialization of PSCs. So far, much effort has been devoted to tackling the stability of PSCs by interfacial engineering (passivating the main layers) as well as compositional engineering (development of each major layer and the metal electrode). Recently, developing low-cost hole transport materials (HTMs) that make PSCs more efficient and stable has become a more important direction. Despite the existence of various potential HTMs, to date, the 2,2′,7,7′-tetrakis-(N,N-di-p-methoxyphenylamine)-9,9′-spirobifluorene (spiro-OMeTAD) remains the only benchmark HTM for highly efficient PSCs. However, spiro-OMeTAD suffers from expensive and tedious synthesis steps and low stability under thermal stress. In addition, the hygroscopic dopants, 4-tert-butylpyridine (t-BP), lithium bis (Trifluoromethanesulfonyl) imide (LiTFSI), and tris(2-(1H -pyrazol-1-yl)-4- tert-butylpyridine) cobalt(III) tri[hexafluorophosphate] (FK209) required for increasing spiro-OMeTAD conductivity play a negative role in the long-term durability of PSCs.

In this presentation, I will discuss promising alternatives of spiro-OMeTAD: spiroxanthene-based SFX core materials and metal phthalocyanine-based HTMs. SFX derivatives offer tunable electronic properties, improved hole mobility, and the potential for structural modification with diphenylamine units[1]. Meanwhile, metal phthalocyanines (MPcs) have received a great attention as potential HTMs due to their low-cost synthesis, high carrier mobility and high thermal stability making them suitable for scalable solar cell applications[2]. Together, these materials represent viable pathways to replace spiro-OMeTAD in the next generation of efficient and stable perovskite solar cells.



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INTERCALATED IRON CHALCOGENIDES – SYNTHESIS, PROPERTIES AND APPLICATIONS

Tomasz Chabło, Anna Krztoń-Maziopa

Wydział Chemiczny, Politechnika Warszawska, ul. Noakowskiego 3, 00-664 Warszawa
tomasz.chablo.dokt@pw.edu.pl

Transition metal chalcogenides are large family of materials exhibiting various properties and applications. Among them, the tetragonal phase of non-stoichiometric iron selenide (β-$FeSe_{1-x}$) with its layered structure and big van der Waals gaps (~3 Å), capable to host foreign ions and/or larger organic molecules. This is especially promising in the field of electrochemical energy generation and storage, electrocatalysis, superconducting and magnetic materials engineering through fine tuning of band structure via structural and electronic tuning being the result of intercalation and doping. So far there have been scientific reports about intercalation of β-$FeSe_{1-x}$ with various species including alkali metal ions, Lewis base adducts or organic ammonium ions[1][2]. Intercalated β-$FeSe_{1-x}$ is studied as a way to synthetize materials for energy production and conversion (including potential catalysts and absorbers in dye sensitized solar cells[3] or electrode material in lithium-sulphur batteries[4]).

For preparation of these functional materials, mainly chemical intercalation is utilized, however due to strong reducing environment during the intercalation reaction, the host material itself may decompose, leading to formation of unwanted phases, changing the properties of the material. To overcome these obstacles, a novel method of electrochemical intercalation of β-$FeSe_{1-x}$ is being developed. So far, using the electrointercalation methods, intercalants with tetramethylammonium (TMA^+) and cetyltrimethylammonium (CTA^+) ions were synthesized[2][5]. Here we will discuss the morphology and crystal structure of different intercalated β-$FeSe_{1-x}$ and potential modifications of β-$FeSe_{1-x}$ structure, in view of its application in the electrochemical energy generation

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Ca-TEMPO COMPLEXES AS MODEL SYSTEMS IN MOLECULAR OXYGEN ACTIVATION

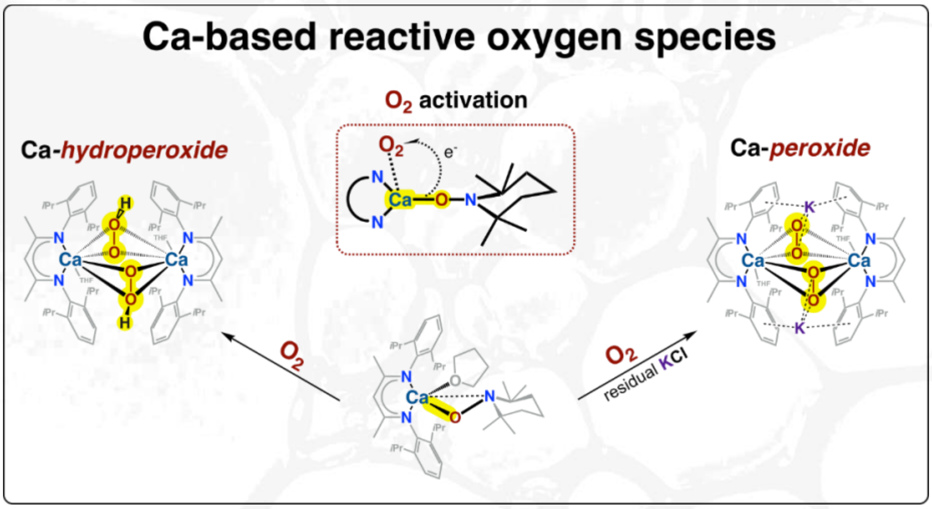
Jakub Chmurski,[1] **Arkadiusz Kornowicz,**[2] **Tomasz Pietrzak,**[1] **Krzesimir Korona,**[1] **Michał Terlecki,**[1] **Iwona Justyniak,**[2] **Adam Kubas**[2] **i Janusz Lewiński**[1,2]

[1] Wydział Chemii, Politechnika Warszawska, ul. Noakowskiego 3, 00-664 Warszawa
[2]Instytut Chemii Fizycznej Polskiej Akademii Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa
jakub.chmurski.dokt@pw.edu.pl

Redox-inactive metal ions, including Ca^{2+} cations, are essential modulators of the reactivity of many metal–oxygen complexes and metalloenzymes, such as the reactivity of reactive oxygen species (ROS) based on transition metals or the oxidation of water to dioxygen catalyzed by the oxygen-evolving complex (OEC) in photosystem II (PSII). The mechanism of O–O bond formation in the short-lived S4 state of the Kok cycle remains a subject of intense debate, and current reports suggest that the redox-inactive Ca^{2+} ion is necessary for stabilizing reactive intermediates, although its exact role has not yet been elucidated. A detailed understanding of how Ca^{2+} ions facilitate O_2 formation requires an in-depth explanation of the interactions between the Ca^{2+} center and the reactive oxygen species.

Synthetic structural models of the OEC are an effective way to understand nature-driven processes, and two main approaches have been used to clarify the role of Mn and Ca centers: (i) modeling the reactivity of previously designed heterometallic Mn/Ca clusters, and (ii) using cubane-like MnxOy cluster structures. However, despite recent advances in modeling the OEC, studies on Ca-based ROS systems remain scarce.

In our research, we describe the reactivity of a model Ca–TEMPO complex (TEMPO – the 2,2,6,6-tetramethylpiperidin-1-oxyl anion) supported by a β-diketiminate ligand toward O_2, leading to the first structurally characterized Ca hydroperoxide and a heterometallic Ca/K peroxide.[1] O_2 activation on Ca–TEMPO and the resulting Ca peroxide directly relate to the proposed S4 transition state in the water-splitting process in PSII at the heterometallic Mn_4CaO_5 cluster.



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ORGANOMETALLIC METHODS FOR THE PRODUCTION OF ZINC OXIDE NANOCRYSTALS USING ZWITTERIONIC STABILISING COMPOUNDS AND EXTENSION OF THE METHOD TO INCLUDE SELECTED IMIDAZOLIUM IONIC LIQUIDS

Z. Drużyński[1], **M. Wolska-Pietkiewicz**[1], **J. Lewiński**[1,2]

[1] Wydział Chemiczny, Politechnika Warszawska, ul. Noakowskiego 3, 00-664 Warszawa
[2] Instytut Chemii Fizycznej Polskiej Akademii Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa
zygmunt.druzynski@pw.edu.pl

Nanocrystalline zinc oxide (ZnO NCs) is one of the most versatile semiconductor materials and the fifth most used nanomaterial in consumer products [1]. The reproducible fabrication of zinc oxide nanocrystals (ZnO NCs) of appropriate quality, stable in polar environments (including water and alcohols), characterised by time-invariant physicochemical properties and optical parameters and high homogeneity, is still a considerable challenge. Despite its simplicity, the common wet-chemical method, sol-gel, has several disadvantages, such as a lack of repeatability, the inherent presence of alkali metal ion admixtures, and instability [2]. The presented results continue research to obtain high-quality ZnO quantum dots (ZnO QDs) by controlled hydrolysis and oxidation of organometallic precursors [3,4]. The presented results concern the development of an original method for producing ZnO NCs using organozinc precursors and a new class of stabilising compounds, i.e., compounds containing separated fragments with a positive and negative charge (betaines) [5], not considered in this context so far, as well as the extension of the organometallic method by applying selected imidazolium ionic liquids and salts with organic cation [6]. The use of organic ligands of the mentioned type was aimed at producing solution-stable, luminescent inorganic-organic hybrid ZnO systems with a small core diameter in the so-called "*quantum size regime*" which form colloidal solutions in both non-polar and polar solvents (such as H_2O, MeOH, EtOH, 1-PrOH).

One of the materials was successfully tested as an electron transport layer in a planar *n-i-p* perovskite solar cell architecture. The ZnO/perovskite interface passivation by NH_4F enabled a record-breaking power conversion efficiency factor for this type of construction (PCE = 21.9%) and competitive stability, retaining ~78% of its initial PCE under 1 Sun illumination with maximum power tracking for 250 hours [7].

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PHYSICOCHEMICAL CHARACTERISTICS OF DIBROMOBENZIMIDAZOLE DERIVATIVES

A. Pobudkowska-Mirecka[1], K. Duranc[1]

[1] Wydział Chemiczny, Politechnika Warszawska, ul. Noakowskiego 3, 00-664 Warszawa

The continuous discovery and refinement of therapeutic agents necessitates rigorous evaluation prior to their market introduction. A comprehensive investigation into their physicochemical characteristics serves as an invaluable starting point for exploring potential medicinal substances.

A notable compound within the structural framework of medicinal substances is benzimidazole, whose structural characteristics underpin the formation of significant and complex structures, exemplified by vitamin B_{12}.

The present engineering thesis focuses on the physicochemical properties of four compounds based on the benzimidazole structure from the group of N-phenacyl-dibromobenzimidazoles.

The thesis incorporates a comprehensive literature review on benzimidazoles and their derivatives, which is essential for the acquisition of the necessary information for the analysis of the studied structures and the facilitation of the interpretation of research results.

The methods of synthesising N-phenacyl-dibromobenzimidazoles and their anticancer properties against various cell lines are reviewed.

The theoretical section of the chapter sets out the concepts underpinning the research, with the chapter itself describing the differential scanning calorimetry (DSC) employed for thermal analysis and the phase equilibria of the binary solid-liquid system. In addition, the chapter presents three correlation equations based on the theory of local concentration.

The experimental section is pivotal in presenting the determined phase diagrams, which necessitate the theoretical underpinnings concerning phase equilibria and correlation equations. This chapter delineates the methodologies employed to ascertain the phase diagrams within the binary solid-liquid system across three distinct solvents: water, ethanol, and 1-octanol. The experimental points were correlated using three equations: Wilson, NRTL, and UNIQUAC.Phase diagrams could only be determined for two solvents.In water, due to the low solubility of N-phenacyl-dibromobenzimidazoles, this was not possible. Thermal analysis provided information about the purity and physical transformations of the studied substances. DSC graphs were obtained, along with the melting points and enthalpies.

The results obtained from these analyses were then subjected to detailed scrutiny and interpretation, leading to the formulation of conclusions based on the physicochemical studies. A pivotal aspect of the discussion pertained to the observed disparities, which were attributed to the nature and positioning of the substituent. This segment of the thesis furthermore engaged in a comparative analysis of N-phenacyl-dibromobenzimidazoles that differed in their substituent with chlorine, as well as in the positioning of bromine within the benzimidazole ring.

The findings of this study, when considered in conjunction with the conclusions that were formulated, can be regarded as a significant foundation for further research and development of new pharmaceutical agents derived from N-phenacyl-dibromobenzimidazoles. It is anticipated that these agents will have a substantial and positive impact on the ongoing efforts to combat severe and debilitating diseases, such as cancer.

HOW FAR CAN BATTERIES GO? BIVALENT-METAL BATTERIES AS RUNNER-UPS FOR BEST NOVEL BATTERY TECHNOLOGY

Natalia Izdebska[1], Klaudia Kierepka[1], Maciej Marczewski[1], Władysław Wieczorek[1]

[1]Faculty of Chemistry, Warsaw University of Technology, Noakowskiego 3, 00-664 Warsaw, Poland

Natalia.izdebska.dokt@pw.edu.pl

Despite their widespread use and popularity, lithium-ion batteries in Europe face significant challenges related to limited raw material availability and continuously rising costs. These issues are especially evident in the increasing prices of consumer electronics. Against this backdrop, there is a growing interest in novel battery technologies that promise improved performance and more sustainable solutions. Among these emerging technologies, bivalent metal-organic batteries represent a cutting-edge and still relatively underexplored area of research. These batteries are considered promising candidates for next-generation energy storage systems due to their high energy density, cost-effectiveness, and environmental benefits. However, despite their potential, these technologies encounter several critical obstacles that impede their practical application and commercial viability. Key challenges include poor cycling stability and limited electrode kinetics, which directly impact battery efficiency and lifespan. For rechargeable magnesium (RMB) and calcium batteries (RCB), a major issue lies in electrolyte speciation, which leads to ion pair formation and hampers the desolvation of multivalent ions. Additionally, anode materials suffer from inefficient metal plating and stripping processes, resulting in the formation of passive layers with poor electrical conductivity.

To address these challenges, electrolyte additives have been developed to act as ion pair scavengers, effectively capturing cations or anions to prevent ion pair formation and facilitate the desolvation of multivalent ions. Our research focuses not only on the interactions between bivalent metal cations and chelating additives but also on the interactions between salt anions and anion receptor additives. By carefully designing additive molecules, it is possible to partially immobilize anions, promoting salt dissociation and improving electrolyte properties. In this work, we present a comprehensive roadmap for the development of electrolyte additives, which play a crucial role in enhancing the performance of multivalent metal-organic batteries. We propose a systematic approach to designing and optimizing these additives, taking into account their solubility, redox potential, stability, and compatibility with the components of RMB and RCB systems. We discuss key strategies aimed at improving cycling stability, suppressing side reactions, and enhancing ion transport kinetics. Recent advances in additive synthesis and characterization methods are also highlighted, providing a foundation for future improvements.

Moreover, we emphasize the importance of advanced analytical techniques and comprehensive electrochemical testing in evaluating additive performance, which is vital for their practical implementation. The role of computational modeling is also discussed, as it accelerates the discovery and optimization of electrolyte additives by enabling precise and efficient molecular design.

IORGANIC METAL CHLORIDE PEROVSKITE AS ARTIFICAL SOLID ELECTROLYTE INTERFACE FOR ENHANCED ANODE PROTECTION IN LITHIUM METAL BATTERIES

Juhi Juhi[a,b,*], Mariana Vargas Ordaz[b], Sara Drvarič Talian[b], Wladyslaw Wieczorek[a], Robert Dominko[b,c],

[a]Faculty of Chemistry, Warsaw University of Technology, Noakowskiego 3, 00-664
Warsaw, Poland
[b]National Institute of Chemistry, Hajdrihova Ulica 19, 1000 Ljubljana, Slovenia
[c]ALISTORE - European Research Institute, CNRS FR 3104, 15 Rue Baudelocque, Amiens
80039 Cedex, France

juhi.juhi@pw.edu.pl

Lithium metal is widely regarded as the "Holy Grail" anode for next-generation high-energy-density rechargeable batteries due to its exceptionally high theoretical specific capacity and low electrochemical potential [1]. However, its practical application has been significantly hindered by its intrinsic instability in conventional liquid electrolytes, which leads to uncontrolled dendritic growth, continuous electrolyte decomposition, and poor coulombic efficiency [2]. To address these challenges, we present a facile and cost-effective drop-casting approach to fabricate an artificial solid electrolyte interphase (SEI) on the lithium surface using cesium lead chloride ($CsPbCl_3$), an inorganic metal halide perovskite.

The $CsPbCl_3$-based coating effectively stabilizes the lithium–electrolyte interface by suppressing parasitic side reactions and promoting uniform lithium ion flux during plating and stripping. Symmetric Li|Li cells incorporating the $CsPbCl_3$-protected lithium anodes exhibit excellent cycling stability over 600 hours at a current density of 1 mA cm^{-2} with an areal capacity of 1 mAh cm^{-2}. Furthermore, full-cell configurations employing $LiFePO_4$ (LFP) cathodes with a high mass loading of 7.5 mg cm^{-2} demonstrate superior electrochemical performance, retaining 99.46% of their initial capacity over 250 cycles at 1C when paired with $CsPbCl_3$-coated lithium anodes. In contrast, cells with bare lithium anodes exhibit pronounced capacity fading under identical conditions.

This work highlights the potential of $CsPbCl_3$ as an effective artificial SEI material for lithium metal protection. The proposed strategy offers a scalable and efficient pathway toward enhancing the long-term stability of lithium metal and graphite anodes, thereby advancing the practical realization of high-energy-density rechargeable batteries.

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PREPARATION, MODIFICATION AND CHARACTERIZATION OF LINEAR POLYAMINES WITH ANTIMICROBIAL PROPERTIES

Aleksandra Kowalska, Julita Pachla, Dominik Jańczewski

Faculty of Chemistry, Warsaw University of Technology, ul. Noakowskiego 3, 00-664 Warsaw
aleksandra.kowalska6.stud@pw.edu.pl

The growing problem of antibiotic resistance highlights the need for new antimicrobial compounds with alternative mechanisms of action [1]. Cationic polymers have emerged as a promising class of agents, as they can disrupt bacterial membranes, leading to rapid cell death while minimizing the risk of resistance development [2].

This study presents the synthesis of linear polyethylenimine (PEI) and polytrimethylenimine (PTMI) derivatives bearing alkyl groups incorporated into the polymer backbone. The materials were obtained via cationic ring-opening polymerization (CROP) of substituted 2-oxazoline and 2-oxazine monomers. Three types of polymers with varying molecular weights were synthesized: poly(5-ethyl-2-methyloxazoline), poly(2,4-dimethyloxazoline), and poly(2,4-dimethyloxazine).

Polymerization kinetics were investigated, and propagation rate constants were determined for each system. Subsequent hydrolysis yielded the corresponding PEI and PTMI derivatives with alkyl side chains. The synthesized polymers represent a step toward the development of new antimicrobial materials with tunable properties and reduced risk of resistance development.

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EXPLORING THE SOLID-STATE FORMS OF METACETAMOL: POLYMORPHS AND CO-CRYSTALS WITH SULFONIC ACIDS

Kamil Krzemiński[1] , **Izabela Madura**[1], **Anna Hoser**[2], **Maura Malińska**[2], **Marta Dudek**[3]

[1] Faculty of Chemistry, Warsaw University of Technology, ul. Noakowskiego 3,
00-664 Warszawa, kamil.krzeminski.stud@pw.edu.pl, izabela.madura@pw.edu.pl
[2] Faculty of Chemistry, University of Warsaw, ul. Pasteura 1, 02-093 Warszawa
a.hoser@uw.edu.pl, m.malinska@uw.edu.pl
[3] Centre of Molecular and Macromolecular Studies Polish Academy of Sciences,
ul. Sienkiewicza 112, 90-363 Łódź, marta.dudek@cbmm.lodz.pl

Metacetamol is a structural isomer of paracetamol that also exhibits analgesic properties. However, it is not yet utilized in the pharmaceutical industry due to the limited number of studies conducted to date. Currently, two polymorphic forms of metacetamol are known: form I, which is stable, and form II, which is difficult to obtain.

As part of the research, tools such as Mercury and ConQuest, along with the Cambridge Structural Database (CSD), were used to analyze existing structures of metacetamol and paracetamol, as well as to design new model systems. In addition to synthesizing form II of metacetamol under mild ~~melting~~ conditions and from solution, a significant achievement was the successful formation of a metacetamol co-crystal with p-toluenesulfonic acid, inspired by analogous systems known for paracetamol. Subsequently, three new co-crystals were synthesized using other sulfonic acid derivatives.

The results clearly demonstrate that metacetamol possesses a high capacity for forming multicomponent crystalline structures with sulfonic acids. Considering their strong donor-acceptor properties and ability to form stable hydrogen bonds, sulfonic acids represent a particularly promising group of coformers.

Importantly, the use of mechanochemical methods, such as grinding in a mortar or ball mill which enable the synthesis of co-crystals without the need for solvents aligns with the principles of green chemistry. Grinding with sulfonic acids can not only simplify and accelerate the co-crystal formation process but also allow for rapid screening of various combinations of metacetamol with novel coformers. This approach may lead to the discovery of new, stable forms with improved pharmacokinetic and physicochemical properties, such as enhanced solubility, bioavailability, or thermal stability.

In conclusion, further research should focus on expanding the range of sulfonic acids used as coformers, optimizing grinding conditions (e.g., time, humidity, presence of additives), and investigating the properties of the obtained systems in terms of their potential pharmaceutical applications.

APPLICATION OF ECOLOGICAL SOLVENTS IN SINGLE-DROP MICROEXTRACTION TO LIQUID PHASE OF AROMATIC EXPLOSIVE SUBSTANCES FROM THE WATER SAMPLES

dr hab. Waldemar Tomaszewski[1], inż. Katarzyna Niedośpiał[1]

[1] Wydział Chemiczny, Politechnika Warszawska, ul. Noakowskiego 3, 00-664 Warszawa
katarzyna.niedospial.stud@pw.edu.pl

Aromatic explosive substances are classified as hazardous environmental pollutions, that are generated during their production, storage and use. An effective method for preparing samples for chromatographic analysis, can be liquid-phase microextraction.

The term microextraction refers to the use of small amounts of organic solvents. There are several variations of this method. In microextraction techniques, the selection of the solvent is crucial - the solvent should be ecologically, non-toxic and the most important - ensure high recovery of the target substances of the substances.

The aim of this study was exploring and defining the applicability of various environmentally friendly solvents in single-drop microextraction of aromatic explosive substances from water samples.

In the presented study investigated substances: decanoic acid (HBD-hydrogen bond donor) and tetrabutylammonium bromide, camphor, menthol (HBA-hydrogen bond acceptor). The conducted research proved that the obtained substances were successfully synthesized and can be used as deep eutectic solvents. Tetrabutylammonium bromide did not form a hydrogen bond with decanoic acid and therefore cannot be used as a hydrogen bond acceptor. On the other hand, camphor and menthol can act as acceptors. They form hydrogen bonds with decanoic acid, which was confirmed by FT-IR analysis. The described deep eutectic solvents can be obtained by using an excess of the hydrogen bond donor, but not the acceptor.

Differential scanning calorimetry (DSC) analysis enabled to determinate melting points-mixtures of the used components in various molar ratios could formed during the analysis (as evidenced duplicate signals on thermograms). None of the tested liquids showed signals indicating a solid–solid phase transition.

High-performance liquid chromatography (HPLC) analysis confirmed that the applied single-drop microextraction was successful. During the extraction droplet of solvent was stable. Analysed deep eutectic solvents based on the described chemical compounds in various molar ratios can be used as extractants. An increase in stirring speed during extraction leads to higher extraction efficiency.

STRUCTURE AND PROPERTIES OF SELECTED Fe(II) COMPLEXES STABILIZED BY N,N'- AND N,O,N'-DONOR LIGANDS

A. Podobas,[1, 2] K. Korona,[2] M. Terlecki,[2] I. Justyniak,[1] M. Magott,[3] J. Żukrowski,[4] A. Kornowicz,[2] D. Pinkowicz,[3] A. Kubas,[2] J. Lewiński[1, 2]

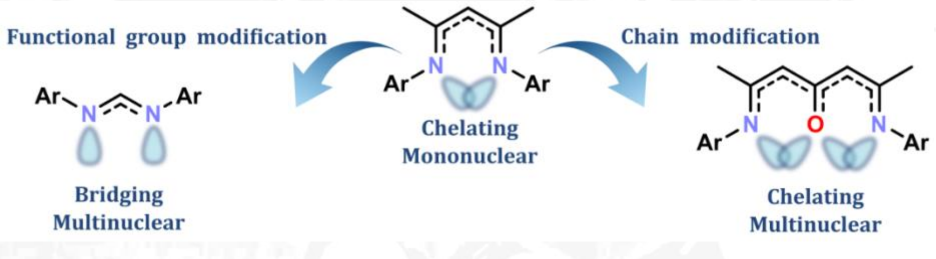
[1]Wydział Chemiczny, Politechnika Warszawska, Noakowskiego 3, 00-664 Warszawa
[2] Instytut Chemii Fizycznej, Polska Akademia Nauk, Kasprzaka 44/52, 01-224 Warszawa
[3] Wydział Chemiczny, Uniwersytet Jagielloński, Gronostajowa 2, 30-387 Kraków
[4] Akademickie Centrum Materiałów i Nanotechnologii, Akademia Górniczo-Hutnicza, A. Mickiewicza 30, 30-059 Kraków

email: anna.podobas.stud@pw.edu.pl

The coordination chemistry of iron compounds plays a significant role in many scientific fields. Due to its low cost and occurrence of this element in numerous enzymes, Fe(II) is considered as a promising metal center for the development of next-generation catalysts capable of activating small molecules such as N_2 and CO_2[1, 2].

A major challenge in contemporary coordination chemistry is the rational design of ligands that can stabilize metal centers with defined spatial arrangements and electronic structures, allowing for the formation of Fe(II) compounds with specific properties and functions, e.g., as catalysts or magnetic materials. Particular attention is given to N,N'- and N,O,N' donor ligands, which allow access to a wide variety of Fe(II) complexes with diverse numbers and metal center geometries. Moreover, an appropriate choice of ligand steric factors and reaction conditions offers additional possibilities for influencing the structure of the stabilized complexes[3]. However, these aspects of Fe(II) coordination chemistry still incompletely understood.

In this work, we present the synthesis and characterization of a series of Fe(II) compounds stabilized by N,N'- and N,O,N'-donor ligands. The obtained compounds were characterized by Mössbauer spectroscopy, single-crystal X-ray diffraction and theoretical calculations, which allowed for the analysis of the electronic structure of the studied complexes.



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SUPRAMOLECULAR ELECTROLYTE ADDITIVES FOR LI-ION BATTERIES - INSIGHTS INTO ANION-ADDITIVE INTERACTIONS

L.Ramotowska[1], D.Kurek[2], N.Izdebska[1]

[1] Faculty of Chemistry, Warsaw University of Technology, Noakowskiego 3, 00-664 Warsaw [2] Medical University of Warsaw, 61 Zwirki i Wigury Street, 02-091 Warsaw laura.ramotowska.stud@pw.edu.pl

Due to the increasing share of renewable energy in final energy consumption and the European Union’s ambitious goal of achieving climate neutrality by 2050, the development of efficient and safe energy storage systems has become a key research priority. As energy systems become more dependent on intermittent renewable sources, such as solar and wind power, the need for advanced batteries with high capacity, long cycle life, and improved safety grows accordingly. In this context, metallic anodes—especially lithium, sodium, and potassium—are attracting increasing attention from the scientific community due to their extremely high volumetric and gravimetric capacities. However, their practical implementation faces significant challenges, including the tendency for passivation in electrolyte environments, as well as the potential risk of thermal runaway and self-ignition.

To address these limitations, researchers are focusing on innovative solutions, such as the use of functional electrolyte additives that can enhance the stability, safety, and overall performance of the battery cell. A promising class of such additives includes supramolecular compounds, particularly calix[n]arenes, such as calix[4]arenes and calix[6]arenes. These macrocyclic compounds possess a unique cup-like structure with a central cavity capable of selectively binding anions from the electrolyte. This anion immobilization can contribute to suppressing unwanted side reactions and dendrite formation by directing charge transfer processes toward the more stable and controlled movement of metal cations.

Moreover, calixarenes are highly tunable via chemical modification, which significantly broadens their application potential. The presence of unsubstituted aromatic rings allows for facile functionalization through standard organic synthesis techniques. Introducing bulky substituents like tert-butyl groups increases the hydrophobicity and effective surface area of the molecule, further enhancing its anion-trapping capabilities. Alternatively, the introduction of electron-withdrawing substituents, such as hydroxyl or carboxyl groups, enhances hydrophilicity, which is particularly beneficial for the development of water-based electrolyte systems—an increasingly important area of research due to safety and environmental considerations.

In summary, the integration of functionalized supramolecular compounds into electrolyte formulations represents a forward-looking strategy in the design of safer and more efficient battery technologies. As such, the continued exploration of calix[n]arene derivatives holds great promise for overcoming the limitations of metallic anodes and advancing the performance of modern energy storage systems aligned with sustainable development goals. We present our research focused on addition calix[4]arene and calix[6]arene to battery electrolytes and their impact on cells capacity during long-term cycling.

THE PAST AND FUTURE OF HG (II) CARBIDES AND THEIR APPLICATION IN COORDINATION CHEMISTRY

Kornel Sacharczuk[1], Michał Terlecki[1], Arkadiusz Kornowicz[2], Janusz Lewiński[12]

[1]Wydział Chemii, Politechnika Warszawska, ul. Noakowskiego 3, 00-664 Warszawa
[2] Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Marcina Kasprzaka 44/52, 01-224 Warszawa
kornel.sach@gmail.com

Despite their toxicity, mercury-organic derivatives are still widely used by chemists. The popularity of this class of organometallic compounds is due to their unique ability to mediate organic transformations - as a large soft Lewis acid or in coordination chemistry due to the unique properties of mercury. The history of work with the cation CHg_4^{4+} began 127 years ago[1] - K. A. Hoffman conducted research in search of a better substitute for the much-used mercury fulminate $Hg(CNO)_2$. In an incomprehensible reaction of mercuric oxide with ethanol, he isolated a new material described as per mercuric ethane. The resulting substance proved to be an inferior explosive and work on it was abandoned. In the 1960s, possible ion exchange was discovered in these compounds[2] which motivated structural chemists to study them[3]. In 1974, Prof. Grdenic's group obtained the first non-ionic derivative, and importantly isolated the monocrystal and solved the structure-core of CHg_4^{4+} . Our interest was drawn by the remarkable stability of these mercury derivatives, the geometry of this cation and possible applications (MOF, coordination polymers) or the linearity of the bonds formed by mercury. Our research work has addressed the synthesis and characterization of CHg_4^{4+} carbide clusters containing trifluoroacetate or hexamethyldisilazane counterions with heterocyclic ligands. The use of the multimetal cation CHg_4^{4+} in coordination chemistry opens up entirely new synthetic possibilities.

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SYNTHESIS AND REACTIVITY OF ALKYLALUMINIUM DERIVATIVES SUPPORTED BY *O,O*-CHELATING MONOANIONIC LIGANDS

Bruno Skoczeń[1], **Vadim Szejko**[1], **Iwona Justyniak**[2], **Janusz Lewiński**[1,2]

[1] Faculty of Chemistry, Warsaw University of Technology, Noakowskiego 3; 00-664 Warsaw
bruno.skoczen.stud@pw.edu.pl
[2] Institute of Physical Chemistry, Polish Academy of Sciences, Kasprzaka 44/52;
01-224 Warsaw

Knowledge and understanding of the factors influencing the structure and reactivity of organometallic aluminium compounds is of great importance for the design of reaction systems with broad applications in the polymer industry and in organic synthesis [1]. This work further investigates the role of the ligand in the structure and properties of alkylaluminium complexes, focusing on *O*,*O*-chelating monoanionic ligands, in particular derivatives of hydroxyketones featuring a conjugated unsaturated bond system [2,3], such as 2-hydroxybenzophenone (2-*hybzp*-H). A diethylaluminium derivative of 2-hydroxybenzophenone, Et_2Al(2-*hybzp*) and its reaction product with molecular oxygen, i.e. the corresponding dimeric ethyl(ethoxy)aluminium derivative, [Et(EtO)Al(2-*hybzp*)]$_2$, were obtained. It was also shown that while the oxidation of Et_2Al(2-*hybzp*) yields the alkoxy compound with high selectivity, its reactions with alcohols such as ethanol and benzyl alcohol lead to an intractable mixture of appropriate alcoholysis products instead, and therefore could not be isolated and characterized in details. The product of the reaction of Et_2Al(2-*hybzp*) with O_2 and products of alcoholysis were used as initiators for the ring-opening polymerization of *rac*-lactide. This demonstrated the potential of oxidising organoaluminum complexes to generate well-defined catalytic systems that allow for the production of biodegradable polyesters with lower dispersity compared to classical methods based on organoaluminium-alcohol systems, while preserving similar catalytic activity. The carried out studies extend the knowledge on the structure and reactivity of alkyl and alkylalkoxy chelates of aluminium and provide additional data for the rational design of catalytic systems for ring-opening polymerization.

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CHARACTERISATION OF AQUEOUS SOLUTIONS OF IONIC LIQUIDS FOR APPLICATION IN ABSORPTION CHILLERS

Marta Skorupa[1], Marta Królikowska[1], Michał Skonieczny[1]

[1] Wydział Chemii, Politechnika Warszawska, ul. Noakowskiego 3, 00-664 Warszawa
marta.skorupa.stud@pw.edu.pl

The subject of this work is „Characterisation of aqueous solutions of ionic liquids for application in absorption chillers”. The objective of this work was to synthesize and test physicochemical properties of two aqueous solutions of ionic liquids, and then to determine their possible application as working pairs in absorption refrigeration technology. Such systems should show a higher cooling efficiency than {LiBr + H2O}, which is currently used commercially. Crystallization of lithium bromide inside the chiller limits the usage of this device with its full efficiency. Application of ionic liquids as absorbents in working pairs will enable a continuous work of the device due to low melting points of these substances.

As part of this work, two dimethyl phosphates were synthesized – one with a methyl pyridinium cation [C1Py][DMP] and one with a N,N,N-triethyl-N-methylammonium cation [N1,2,2,2][DMP]. After purification of the products and spectroscopic identification, their aqueous solutions of different concentrations were prepared. Density and viscosity of each solution was tested, obtaining their dependency on concentration and temperature. Next step was to measure isothermal (vapor-liquid) phase equilibria diagrams as function of pressure and concentration of each aqueous system. Based on abroad literature review and obtained VLE results, simulations of a model refrigeration circuit was prepared, enabling to obtain values of coefficient of performance COP. This value was then compared with different working pairs using ionic liquids (both aqueous and ethanolic) and with a commercially used system, enabling to determine structural elements’ influence on obtained values and possibilities of applying tested systems in absorption refrigeration technology.

Obtained results enable comparison of efficiencies of both tested systems with other {IL + H2O} working pairs, enabling drawing conclusions about favourable structure of ionic liquids’ cations and anions used in absorption chillers. Moreover, results enable determining absorbate affecting the working pair efficiency, because both ionic liquids were previously tested with ethanol in terms of this possible application.

SUSTAINABLE AND SOLVENT-FREE ELECTRODES FOR LITHIUM-ION BATTERY CELLS CONTAINING NOVEL ELECTROLYTE COMPOSITIONS

Maciej Smoliński[a]*, Natalia Izdebska[a], Wojciech Bardziński[a], Maciej Marczewski[a], Marek Marcinek[a]

[a] – Warsaw University of Technology, Faculty of Chemistry, Noakowskiego 3, 00-664 Warsaw, Poland

*- corresponding authors: maciej.smolinski.dokt@pw.edu.pl

For many years, it has been evident that as the world continues to develop, the global demand for energy is steadily increasing. Back in the second half of the 20th century, when the use of portable electronic devices was rapidly growing, it was already foreseeable that advancements in battery technology would play a vital role in the future. As a result, research into new battery materials has been accelerating in recent years.

The production of lithium-ion batteries requires large quantities of solvents, which are not only hazardous to human health and the environment but also essential in the conventional process of electrode fabrication. Beyond their environmental impact, the use of solvents necessitates their evaporation - a process that consumes a substantial amount of energy. Presented research focus on improving two key components of the battery: The electrode and the electrolyte. We propose a solvent-free method for electrode fabrication. By adopting a dry process, we significantly lower the energy demand associated with cell manufacturing. Traditional electrode production involves a drying phase that is both energy-intensive and technically complex, typically requiring high-temperature vacuum ovens. Moreover, solvents like *N*-methylpyrrolidone, which are commonly used in cathode manufacturing, present serious health, safety, and environmental hazards and demand sophisticated and costly recovery systems. Studies have indicated that the steps involving wet electrode preparation, drying, and solvent recovery can account for up to half of the total energy consumption in battery production. **As for the electrolyte,** we are actively developing a new lithium salt as an alternative to the widely used $LiPF_6$, which is not only toxic and expensive but can also lead to the generation of hydrofluoric acid, a corrosive substance that damages the battery from within. Our objective is to design electrolytes with no fluorine or a reduced fluorine content. Alongside the new salt, we are also creating performance-enhancing additives to improve the overall efficiency of the battery.

Our efforts[a] aim to support more cost-effective, environmentally friendly, and energy-efficient battery production in Europe and globally, aligning with the sustainability objectives of the European Green Deal.

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IN VITRO SKIN MODELS AS TOOLS FOR ASSESSING THE BIOLOGICAL EFFECTS OF CHEMICAL SUBSTANCES

Anna Sobiepanek, Ph.D.[1]

[1] Faculty of Chemistry, Warsaw University of Technology, Noakowskiego 3; 00-664 Warsaw

The human skin is a complex, multilayered organ composed of diverse cell types and structural proteins that play essential roles in barrier function, immune response, and tissue integrity. Understanding its architecture is crucial for developing reliable *in vitro* models capable of mimicking its biological and physiological properties. This presentation explores the current strategies in constructing 2D and 3D *in vitro* skin models, including a variety of different cultures, and their application in evaluating the biological effects of chemical substances.

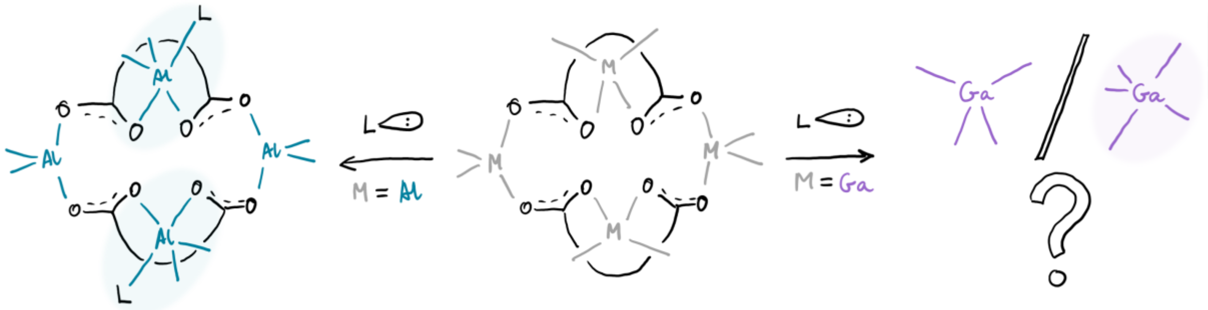
During the lecture, key cellular components such as skin cells (keratinocytes, fibroblasts, etc.) along with extracellular matrix proteins (like collagen and elastin) will be discussed in the context of a model design. The creation of multicellular spheres and skin equivalents will be introduced. Moreover, various methods for evaluating model functionality will be presented, with a focus on biological assays such as cytotoxicity (MTT, LDH), assessment of apoptotic processes, morphological characterization, and analysis of mechanical properties. The advantages and limitations of different model types will be also addressed, highlighting their relevance as alternatives to animal testing and their growing importance in regulatory and industrial settings.

STRUCTURAL DIVERSITY OF ORGANOGALLIUM CARBOXYLATES IN PRESENCE OF LEWIS BASES

Maksymilian Solka,[1] Michał Terlecki,[2] Iwona Justyniak,[1] Janusz Lewiński[1,2]

[1] Instytut Chemii Fizycznej Polskiej Akademii Nauk, Kasprzaka 44/52, 01-224 Warszawa
[2] Wydział Chemiczny, Politechnika Warszawska, Noakowskiego 3, 00-664 Warszawa
email: msolka@ichf.edu.pl

The coordination chemistry of Group 13 elements (B, Al, Ga, In) is vital for basic chemistry, mainly because of the use of organoaluminum compounds in the polymerization of olefins. Nevertheless, it is still not comprehensively understood. Carboxylates enable facile studies of Lewis acidity, which is an important part of the investigations on Group 13 chemistry. A few years ago, studies on the reactivity of dimethylgallium naphthalene-2,3-dicarboxylates towards selected Lewis bases (derivatives of pyridine) were carried out. They showed that the aluminum centers of the studied complexes can form five-coordinated acid-base adducts and appear to disobey the octet rule.[1, 2]



The present study showed the effect of changing the coordination center from aluminum to gallium, using the identical carboxylate ligands and analogous Lewis bases. The studies carried out illuminate aspects of Group 13 chemistry, such as the tendency of the coordination center to form five-coordination complexes, the affinity of the acidic center for different Lewis bases with the π-electron system, the difference in the structure of the coordination centers (differences in atomic, ionic, van der Waals radii; electronegativity or electron configuration).

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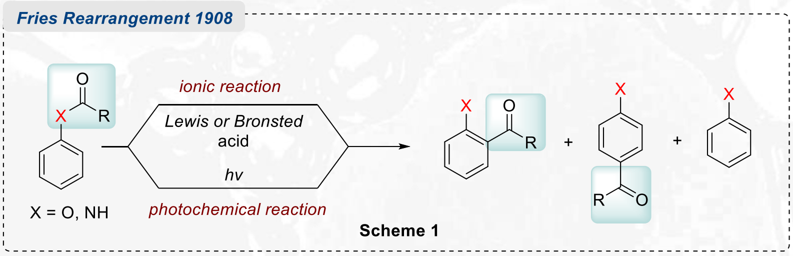
PHOTOCHEMICAL FRIES REARRANGEMENT IN THE SYNTHESIS OF HIGH VALUE-ADDED NITROGEN-BASED HETEROCYCLES.

Piotr Szcześniak

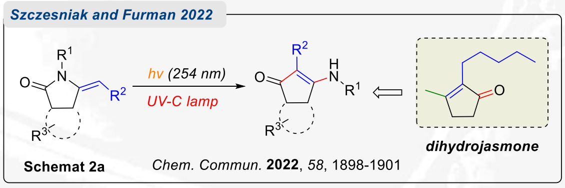
Instytut Chemii Organicznej PAN, ul. Kasprzaka 44/52, 01-224 Warszawa
piotr.szczesniak@icho.edu.pl

The Fries rearrangement involves the transformation of aromatic esters or amides into *ortho*- and *para*-substituted phenols or anilines. First described by Karl Fries in 1908, the reaction proceeds *via* a 1,3- or 1,5-acyl migration catalyzed by either Lewis or Brønsted acids, and a photochemical variant of this process is also known (Scheme 1).



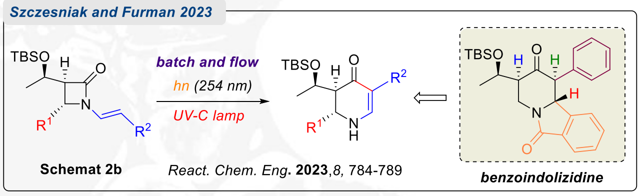
Scheme 1

We present three intramolecular variants of the Fries rearrangement that lead to nitrogen-containing heterocyclic compounds. The first is a photo-induced transformation of five-membered enamides into enaminones (Scheme 2a).[2] The second involves the photochemical rearrangement of optically pure *N*-vinylazetidinones into non-racemic six-membered enaminones (Scheme 2b).[3] Lastly, we describe a photochemical Fries rearrangement of *N*-aryllactams, resulting in the formation of *ortho*- and *para*-cyclophanes (Scheme 2c).[4]



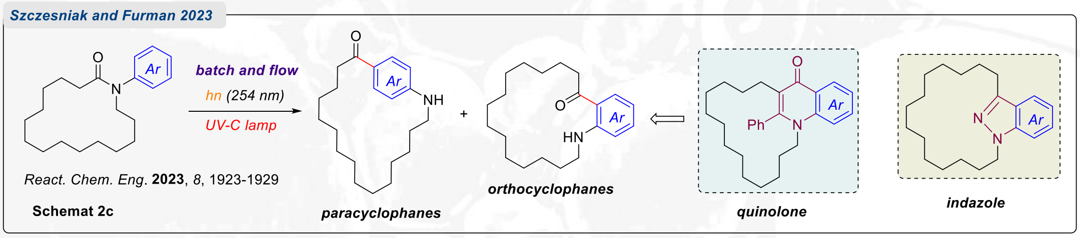
Schemat 2a

Chem. Commun. **2022**, *58*, 1898-1901



Schemat 2b

React. Chem. Eng. **2023**,*8*, 784-789



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Schemat 2c

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FISCHER-TROPSCH SYNTHESIS FOR ADVANCED FUEL PRODUCTION

Urszula Ulkowska[1], **Michał Młotek**[1], **Hubert Ronduda**[1], **Wioletta Raróg-Pilecka**[1]

[1] Wydział Chemiczny, Politechnika Warszawska, ul. Noakowskiego 3, 00-664 Warszawa
urszula.ulkowska@pw.edu.pl

Fischer-Tropsch Synthesis (FTS) is a catalytic process that converts syngas (a mixture of CO and H_2) into hydrocarbons, which can be further processed into fuels and chemicals. Developed nearly a century ago, FTS remains a key technology for the production of synthetic fuels, particularly in scenarios where conventional oil sources are scarce or strategically impractical. Recent advancements focus on optimizing catalyst performance, enhancing reaction efficiency, and integrating renewable syngas sources, including CO_2-derived carbon.

This presentation reviews the most commonly used catalysts in Fischer-Tropsch synthesis, primarily iron (Fe) and cobalt (Co) catalysts, along with the less frequently applied nickel (Ni). Examples of catalyst formulations, support materials, and promoters will be presented, highlighting what makes a catalyst highly active and selective in FTS processes.

In the experimental part of the research, tests have been initiated using a fixed-bed flow reactor under controlled conditions (200–300°C, 20–40 bar), with gas mixtures (H_2 + CO + CO_2) derived from a co-electrolyzer. The primary goal is to optimize product selectivity towards long-chain hydrocarbons (C_{5+}) while minimizing methane formation and unwanted side reactions. Special attention is given to the effect of syngas composition and process parameters on the distribution of hydrocarbons.

Additionally, plasma-assisted FTS is proposed as an innovative method to enhance conversion rates and catalyst regeneration. The integration of dielectric barrier discharge (DBD) reactors under mild conditions (150–200°C, atmospheric pressure) shows promising results for in-situ reduction of CoO to Co and sustained CO conversion above 99%. Future experiments are planned to extend this research to a spark discharge reactor, with the aim of further improving efficiency and stability in FTS operations.

The findings are expected to contribute to the development of efficient, sustainable production pathways for e-fuels and advanced synthetic hydrocarbons, supporting global energy transitions and carbon neutrality initiatives.

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DETERMINATION OF THE EFFECT OF RUTHENIUM CRYSTALLITE SIZE ON CO_2 METHANATION

K. Ziobro, A. Ostrowski, E. Truszkiewicz

Wydział Chemii, Politechnika Warszawska, ul. Noakowskiego 3, 00-664 Warszawa
*corresponding author: kacper.ziobro.stud@pw.edu.pl

The catalytic reaction of carbon dioxide with hydrogen leads to methane and water. This reaction is called methanation [1]. It is a process used in industry to purify a gas mixture for ammonia synthesis from trace amounts of carbon oxides. What is more, the process can be used to obtain synthetic natural gas (SNG), which is a promising method for reducing CO_2 emissions into the atmosphere [2].

The aim of the study was to obtain ruthenium catalysts with a low active phase content (2 wt.%) deposited on carbon supports with different specific surface areas (S_{BET}). The effect of ruthenium crystallite size on the activity in carbon dioxide methanation reaction was studied. Three catalysts containing the same amount of ruthenium (2 wt.%) deposited on carbon supports (C1, C2, C3) differing in specific surface area – 16, 23, 572 m^2/g, respectively – were obtained. The precursor of the active phase was $RuCl_3 \cdot 0{,}5H_2O$, introduced onto the carbon support using a wet impregnation method.

Study showed that larger ruthenium particles formed on C1 (73,3 nm) and C2 (62,9 nm) supports, and the smallest on C3 (2,4 nm). X-ray powder diffraction studies clearly indicate the presence of crystalline phases of ruthenium and carbon in the catalyst samples. It was found that the addition of ruthenium results in the formation of new active sites of basic nature. Such sites are considered to be particularly active in the studied reaction [3].

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