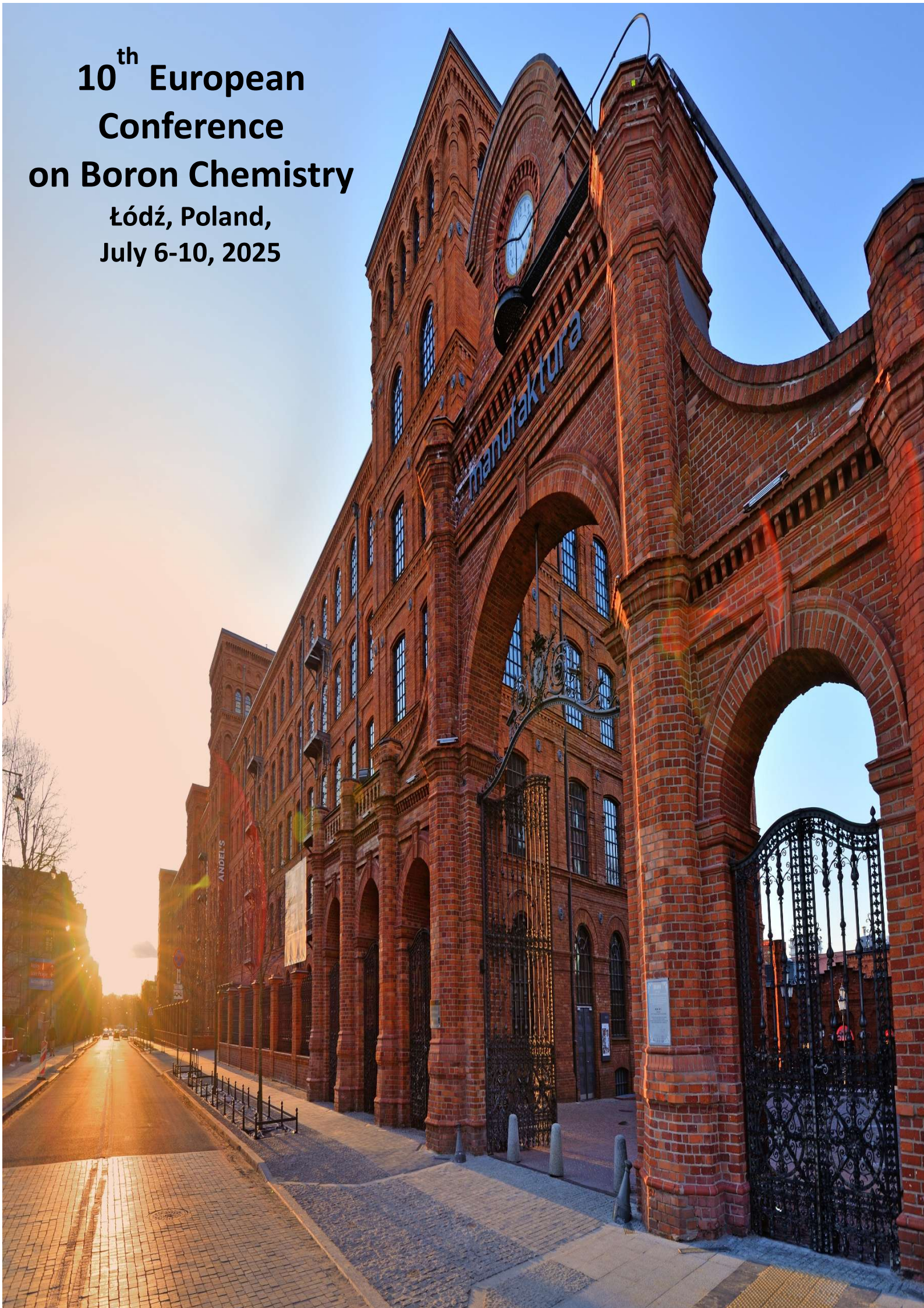
10th European Conference on Boron Chemistry

Łódź, Poland,
July 6-10, 2025



10th European Conference on Boron Chemistry

6-10 July 2025 Łódź, Poland

BOOK OF ABSTRACTS

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The project was co-financed by funds from the state budget awarded by the Minister of Science within the framework of the Excellent Science II (Poland) programme.

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Dear Colleagues and Friends,

It is our pleasure to welcome you to Euroboron10 Conference. On behalf of the Scientific and Organizing Committees we invite you to Lodz. We are proud that the International Euroboron Committee has entrusted us with the organization of the 10th anniversary Conference in our city.

Over the past almost three decades, the scope of the Conference has gradually evolved, but Euroboron has consistently brought together researchers from various fields of boron chemistry and its applications, with a key feature of interdisciplinarity. It is worth emphasizing too, that the meeting has always been open to guests from outside Europe.

The Conference offers a creative environment and forum for presentations and discussions, benefiting both professionals and students alike. We hope you will enjoy the symposium, which will feature reports on exciting scientific discoveries, discussions, and numerous opportunities to meet old friends and make new ones.

The meeting is held on the campus of the University of Lodz in the modern building of the Faculty of Philology, which has been made available for our Conference.

Social activities, including a welcome banquet, a gala dinner, an Industria String Quartet performance, and an excursion, will accompany the scientific program.

We wish you a wonderful time at Euroboron10 and also in Łódź!

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Program

July 6, 2025 Sunday	July 7, 2025 Monday	July 8, 2025 Tuesday	July 9, 2025 Wednesday	July 10, 2025 Thursday
Registration 10:00-15:00	Keynote Lecture 9:00-9:55	Keynote Lecture 9:00-9:55	Keynote Lecture 9:00-9:55	Keynote Lecture 9:00-9:55
	Invited lectures (panels A and B) 10:00-10:40	Invited lectures (panels A and B) 10:00-10:40	Invited lectures (panels A and B) 10:00-10:40	Invited lectures (panels A and B) 10:00-10:40
	Coffee break 10:40-11:10	Coffee break 10:40-11:10	Coffee break 10:40-11:10	Coffee break 10:40-11:10
	Oral communications (panels A and B) 11:10-12:00	Oral communications (panels A and B) 11:10-12:00	Oral communications (panels A and B) 11:10-12:00	Oral communications (panels A and B) 11:10-12:00
Opening ceremony 15:00-15:15	Poster Session 1 12:00-13:30	Poster Session 2 12:00-13:30	Oral communications (panels A and B) 12:00-13:15	Oral communications 12:00-12:50
Historical lecture 15:15-15:45	Lunch break 13:30-15:00	Lunch break 13:30-15:00	Lunch break 13:15-14:45	Lunch break 12:50-13:50
Industria String Quartet performance 15:45-16:15	Invited lectures (panels A and B) 15:00-15:40	Invited lectures (panels A and B) 15:00-15:40	Excursion 15:00-18:00	Poster Awards Congress closing 14:00-14:30
	Oral communications (panels A and B) 15:40-16:30	Oral communications (panels A and B) 15:40-16:30		
	Coffee break 16:30-17:00	Coffee break 16:30-17:00		**Plenary lecture** – 45 min + 15 min discussion **Keynote lecture**–45 min + 10 min discussion **Invited lecture** – 35 min + 5 min discussion **Oral communication** – 20 min + 5 min discussion
Plenary lecture 16:15-17:15	Oral communications 17:00-17:50	Elsevier training courses 17:00-19:15	Gala Dinner 19:00-22:00	
Welcoming buffet 17:15-19:00				

Historical Lecture

‘Polish Manchester’ or ‘Polish Detroit’? The rise and fall of industrial Łódź

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The origins of industrial Łódź can be traced back to 1821, when the New Town was demarcated to the south of a settlement that had been granted city rights by King Władysław Jagiełło (but was in reality no different from a village). Between 1824 and 1828 a new settlement, Łódka, was established south of the New Town. Wooden houses with pitched roofs, built on long narrow lots with gardens at the back, were inhabited by craftsmen: cotton weavers and flax spinners. In addition, in the valley of the small river Jasień, land was designated for the construction of large industrial plants. It was there that the great industry of Lodz was born.

By the mid-1880s, the population of Lodz exceeded 100,000, and the center of the city took on a metropolitan character. The city's development was closely linked to the construction of new factories and residential buildings, as well as splendid tenement houses modeled on the architecture of Vienna and Berlin. The planned development of the city was interrupted by the revolution of 1905 and then by the First World War. The new reality after 1918 brought independence to Poland and the coveted status of a provincial city to Lodz. At the same time, the clearly industrial center of half a million inhabitants suffered from a serious lack of public facilities, inner-city greenery, or infrastructure. The new municipal authorities faced serious challenges in their attempt to make up for the backwardness caused by the indolence of the Russian administration. Unfortunately, by the outbreak of the Second World War, Lodz had not gotten rid of all the problems it had inherited from the earlier period. The problem of housing for the poorer part of the population was not solved. Despite all efforts, it was not possible to establish a university in the city.

The years 1945-1989 were a unique period in the history of Lodz, which not only maintained its pre-war status, but also became an important academic center. The city's long-term development plan included the construction of new housing estates, the development of light industry and the construction of new public buildings associated with the metropolitan character of post-war Lodz. The political transformation of 1989 thwarted these ambitious plans and contributed to the city's decline. The closure of factories, high unemployment and lack of new investments made the early 1990s a difficult period in the city's history. It took several years for Lodz to recover from the collapse.

Paradoxically, in an almost hopeless situation, the people of Łódź saw the potential that helped the city recover from its decline. The growing popularity of post-industrial aesthetics meant that more and more people began to see the unobvious beauty of Łódź. Step by step, factory by factory, tenement by tenement, the city began to revive - no longer as an industrial center, but as a "mixed-use" zone, where decapitalized parts of the city underwent comprehensive revitalization, modern services coexisted with creative industries, and the headquarters of large corporations with universities.

Elsevier Author Workshop

Paulina Milewska, Piotr Gołkiewicz

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1. Author Workshop (Paulina Milewska)

The workshop devoted to Publishing Scientific Articles will be held during the EuroBoron10 conference. The content of the workshop will consist of the following topic:

Publishing Scientific Articles: A Pathway to Academic Success

This focused 45-minute workshop provides early-career researchers and authors with essential strategies for successful scientific publishing. Participants will learn how to effectively select the appropriate journal, understand the critical stages of the publication process, and develop high-quality manuscripts that meet peer review standards. The session offers practical insights to improve publication outcomes, along with a curated set of tools and resources designed to support authors at every step. An interactive Q&A will allow attendees to address their specific publishing challenges and enhance their academic and professional development.

2. Systematic Reviews of Biomedical Literature using Embase (Piotr Gołkiewicz)

Embase is the world's largest biomedical database of published, peer-reviewed literature, press publications, and conference abstracts. The Embase database contains manually indexed information from over 8,500 biomedical journals from more than 5,000 publishers, over 40 million records including 2.4 million conference abstracts. The database indexes full texts based on the EMTREE biomedical thesaurus.
Users have access to functionalities and tools that assist in research and educational work.
During the training, we will demonstrate the benefits that the Embase database provides for research and education in biomedical fields and review all of its functionalities.

3. Reaxys as an Essential Tool for Research and Education in the Broad Field of Chemical Sciences (Piotr Gołkiewicz)

Reaxys is a comprehensive, carefully curated database in the field of chemistry and related sciences, providing chemists with access to over 260 million substances, 60 million reactions, 500 million experimental data points, 45 million patents from 105 patent offices worldwide, manually translated by experts in the field. Additionally, Reaxys contains information on the biological activity of chemical substances, including interactive bioactivity tables... and more!
During the training, we will demonstrate the main functionalities of the database and its content.

Plenary Lecture

Advances and Prospects in Boron Chemistry and Compounds for BNCT

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Boron chemistry has been experiencing increasing interest in recent decades. Since the introduction around the middle of the last century of both the chemistry of compounds containing single boron atoms and the chemistry of boron clusters, there has been an increasing development of methodologies using this element. In addition to the use of boron in various forms as a reagent for the interconversion of functional groups, compounds in which boron is retained within the structure to exploit its properties have grown, taking advantage of boron's ability to form stable bonds with carbon and other elements commonly found in organic molecules, culminating in the development of boronic acid-containing drugs. [1,2]

Boron neutron capture therapy is contributing to the development of a significant number of new structures, especially after the introduction of so-called AB-BNCT, namely BNCT based on the use of accelerators as neutron sources. [3]

In this context, the presentation will focus primarily on boron-containing carbohydrate derivatives, either in single-atom form or as clusters.

The introduction of boron into carbohydrates is based on the use of different biological mechanisms for preferential transport of the boronate compound to cancer cells. In particular, sugars bound to carboranes or dodecaborates, sugars containing boronic acids, conjugates between carboranes and polysaccharides and nanoparticles loaded with boron compounds will be discussed.

An emerging aspect of relevant importance in BNCT is the possibility of monitoring boron-containing compounds in vivo, ideally in perspective during the therapy. Some of our results in this respect will be shown.

In addition to the chemical part, the physico-chemical and biological properties of the different compounds, where available, will be discussed.

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Keynote Lectures

Chirality – Appealing Phenomenon in Boron Cluster Chemistry

Bohumír Grűner,[a,*] Ece Zeynep Tüzün,[a] Miroslava Litecká,[a] Dmytro Bavol,[a] Lucia Pazderová,[a] Jan Nekvinda,[a] Drahomír Hnyk,[a] Ondřej Horáček,[b] Radim Kučera[b]

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Chirality belongs to ubiquitous properties of natural systems where the lock-key principle given by chiral interactions enables an evolutionary advantage. Although the structures of the most studied boranes, carboranes and metallacarboranes are derived from highly symmetric icosahedron, the asymmetry of the whole molecule can be easily induced using simple synthetic transformations.[1,2] However, compared e.g. to unfailing interest in chiral ferrocenes, the chemistry of chiral boron cluster compounds remains considerably feeble.

This presentation focuses specifically on creating chiral cobalt bis(dicarbollide) ions, presumably via modifications of carbon atoms with a variety of groups. Depending on substitution, different types of chirality can be introduced and these features are discussed in context of synthesis and structural and physicochemical properties of the new compounds. The chiral structures include substitutions of one or two carbon atoms with a series of groups producing compounds of general formulae [(1-X-(1,2-$C_2B_9H_{10}$)(1,2-$C_2B_9H_{11}$)-3,3'-Co]- (planar chirality) and *rac*-[(1,1'-X-(1,2-$C_2B_9H_{10}$)2-3,3'-Co]- (X= BPin, Ph, N_2, NH_2, CN, OH, Br, I, etc.),[3,4] compounds that contain a symmetric bridge and asymmetric substitution,[5] or asymmetrically located bridges in *rac*-[(1,1'-Y-(1,2-$C_2B_9H_{10}$)$_2$-3,3'-Co]- (Y= CH_2, arylene) (axial chirality). These are accompanied with new di-*ansa* and tri-*ansa*-substituted compounds that contain ethylene or arylene substituents interconnecting carbon-carbon and boron-boron, or carbon-boron positions,[6] which leads to a propeller shape (axial or helical chirality).

We believe, this knowledge may contribute to applications in medical chemistry where space orientation of the groups plays a key role in attaining specific intramolecular interactions, or in other fields where the preorganization of functional groups is essential.

Acknowledgment: Support from Czech Science Foundation, project No. 25-16216S.

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KL2

Boracyclic compounds as effective light emitters and their use in OLEDs

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Luminescent organoboron compounds have been intensively investigated for many years as promising materials for applications in various fields including optoelectronics, photocatalysis and biomedical engineering. Among them, boracyclic compounds are an interesting subject of research in this respect as their rigidified molecular structure often results in reduced non-radiative relaxation consistent with boosted emission properties.

The ongoing interest in our group is focused on investigation of structure-properties relationships for selected three- and four-coordinate boracyclic emitters. We have paid special attention to compounds comprising highly electron-deficient boracyclic cores as we observed that the presence of a strong Lewis acid boron centre is a key factor responsible for improvement of stability of respective complexes with aromatic chelating (N,O) and (O,O) ligands. We have considered various molecular architectures of 5- and 6-membered boracyclic scaffolds including 5,10-dihydroboranthrene,[1] naphtho[1,8-*cd*][1,2]oxaborinin-3-one,[2] and dibenzo[*b*,*e*][1,4]thiaborinine 5,5-dioxide (SO2B).[3] The inherent electron-acceptor character of such systems can be further enhanced by appropriate structural modifications, e.g,, in diazaborafluorenes the central borole ring is fused with two electron-deficient pyridine rings replacing two benzene ones.[4] Installation of peripheral fluoro and heavier halogen substituents at the boracyclic scaffold is a simple yet effective tool for achieving the latter goal.[1,4]

Our recent findings indicate a significant practical potential of three-coordinate SO2B derivatives featuring D-π-A architecture where various simple or more structurally extended moieties serve as donor fragments. In those systems, low values of the singlet-triplet energy gap (ΔE_{ST}) are observed, favoring the occurrence of thermally activated delayed fluorescence (TADF). As a proof of concept, selected derivatives were tested as emitters in 3rd generation organic light-emitting diodes (OLEDs): some of them exhibit high external quantum efficiency (EQE) exceeding 20% and luminance of nearly 20,000 $cd \cdot m^{-2}$,[3a] which ranks them among the best organoboron emitters known to date.

The research is supported by the National Science Centre (Poland) within the framework of the project DEC-UMO-2023/49/B/ST5/00824.

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New Frontiers in Boron Clusters: Challenges Toward Next-Generation Therapeutics

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Boron clusters exhibit unique chemical properties that transcend conventional boundaries between inorganic and organic chemistry, owing to their unique multicenter bonding structures. These structural features underlie their exceptional thermal stability and oxidative resistance, attracting growing interest in both materials science and drug discovery.

Focusing on representative icosahedral cluster compounds—carboranes ($C_2B_{10}H_{12}$) and dodecaborates ($[B_{12}H_{12}]^{2-}$)—we have identified several steric and electronic features from an organic chemistry perspective.[1] In the context of drug design targeting protein–protein interactions (PPIs), we have employed carboranes as a three-dimensional scaffold to explore novel chemical space, thereby enabling unique molecular recognition and bioactivity beyond the reach of conventional organic molecules.[2,3]

Furthermore, leveraging the high hydrophobicity of carboranes, we demonstrated that their incorporation as hydrophobic tags can induce degradation of target proteins via the ubiquitin–proteasome system by exploiting chaperone-mediated recognition. This mechanism, distinct from the traditional PROTAC strategy that relies on ligands for E3 ubiquitin ligases, presents a new paradigm for intracellular protein regulation.[4]

In parallel, we are developing next-generation boron carriers for boron neutron capture therapy (BNCT) by integrating the water-soluble inorganic ion cluster dodecaborate into organic molecules. One such multifunctional boron carrier, *pteroyl closo-dodecaborate conjugated with iodophenyl* (PBC-IP), combines a lysine-based platform with an iodophenyl moiety for albumin binding, a pteroyl group targeting folate receptors overexpressed in many cancer cells, and a *closo*-dodecaborate core as a ^{10}B source essential for BNCT. PBC-IP has shown high affinity toward glioma cells and has demonstrated potent BNCT effects. Preclinical studies targeting glioblastoma, a treatment-resistant brain tumor, are currently underway.[5]

This presentation will highlight our recent progress in developing innovative applications of boron cluster chemistry in medicine.

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KL4

Nanostructured boron nitride-based ceramics - Synthesis, properties and applications

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Among nanostructured materials, the interest for boron nitride BN-based materials has progressively increased because of their high chemical stability, mechanical strength, resistance to oxidation, thermal conductivity, and electrical insulation. BN exists in four crystalline forms: hexagonal BN (h-BN), cubic BN (c-BN), rhombohedral BN (r-BN), and wurtzite BN (w-BN), in which the main difference among them is the hybridization: h-BN and r-BN are dense phases with sp2 hybridization, whereas c-BN and w-BN are low-density phases with sp3 hybridized B-N bonds. Among them, h-BN is particularly interesting because of its structural analogy with graphite. Therefore, h-BN nanomaterials can be zero-dimensional (0D; e.g. nanospheres), one-dimensional (1D; e.g. nanotubes, nanofibers, and nanoribbons), two-dimensional (2D; e.g. thin films and nanosheets), and three-dimensional (3D; e.g. nanostructured porous materials). Unique physical and chemical properties, such as wide band gap (~5.5 eV), high chemical and thermal stability, and excellent electric insulation, can be obtained by combining the low-dimensional quantum confinement and surface effects of BN.

Therefore, h-BN is a promising scaffold for functional materials and for many potential applications, in energy, health and environment applications at various scales.

In our works, we used different synthesis techniques such as the so-called Polymer-Derived Ceramics route suitable leading to various materials through a molecule-to-ceramic conversion with a controlled chemical composition and in complex shapes, atomic layer deposition (ALD) for the obtaining of atomic thickness layers, electrospinning for the fabrication of nanofibers, polymer-derived ceramic/Pickering emulsions hybrid method for the preparation of porous materials, exfoliation for the synthesis of two-dimensional BN nanosheets etc. as the main tools for the creation of specific (nano)boron nitride-based materials for intended applications.

In this presentation, we will show examples of how these methods can be used to create fibers for composite materials, coatings, porous materials and membranes for osmotic energy harvesting, water treatment or gas storage, bio-nanocomposites materials for packaging, nanofibers for catalysis devices, etc… illustrating a part of the work carried out by our group over more than twenty years.

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euIOBoron

10th European Conference on Boron Chemistry

Łódź, Poland, July 6 - 10, 2025

CREATES

Invited Lectures

Invited Lectures

Nau Werner M.	Boron Clusters as Superchaotropic Anions for Supramolecular Chemistry and Drug Delivery	**INV1**
Matějíček Pavel	*Closo*-Dodecaborate-Based Dianionic Surfactants: Role of Counterions and Linkers to Micellization in Water	**INV2**
Smietana Michael	Merging boron and nucleic acid chemistries	**INV3**
Rosario Núñez	Icosahedral Boron Clusters: From Antimicrobials to Cancer Therapy and Optoelectronics	**INV4**
Viñas Clara	Revolutionizing Nanomedicine: Harnessing Amphiphilic Nanomolecules for Multimodal, Carrier-Free Synergies	**INV5**
Nowak-Król Agnieszka	Synthetic Methods for the Preparation of Chiral Azaborole Compounds and Their Application in the Synthesis of Photoresponsive Materials	**INV6**
Gabel Detlef	Dodecaborate – Not just an innocent bystander in synthesis	**INV7**
Fanfrlík Jindřich	Exo-Substituted *Closo* Thiaborane Clusters: On the Road From Isolated Molecules to Crystals	**INV8**
Teixidor Francesc	From Boron Hydrides to Aromatic Hydrocarbons: Bridging 2D and 3D Aromaticity	**INV9**
Geninatti Crich Simonetta	Enhancing Neutron Capture Therapy Using Gadolinium and Boron-Integrated and Targeted Delivery Systems	**INV10**
Planas José Giner	“Complexity within Order” in Metal-Organic Frameworks Incorporating Carborane Ligands: A Multivariate Approach	**INV11**
Hey-Hawkins Evamarie	Carborane-Containing Drugs: New Keys for Old Locks	**INV12**

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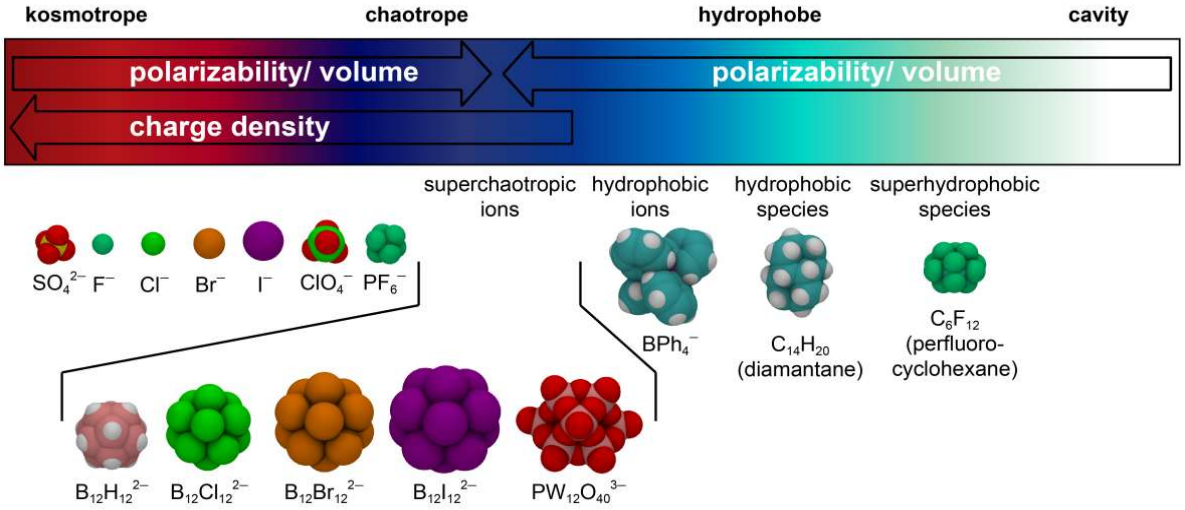
Following up on scattered reports about interactions of conventional chaotropic ions (e.g., I^-, SCN^-, ClO_4^-) with macrocyclic host molecules, biomolecules, and hydrophobic neutral surfaces in aqueous solution, the chaotropic effect has emerged as a generic driving force for supramolecular assembly, orthogonal to the hydrophobic effect. The chaotropic effect becomes most effective for very large ions that extend beyond the classical Hofmeister scale, and that can be referred to as superchaotropic ions among which borate cluster anions are the prototypes. We present a continuous scale of water-solute interactions (Scheme below) which includes the solvation of kosmotropic, chaotropic, and hydrophobic solutes.[1] Recent examples for the soft-matter association of chaotropic anions to hydrophobic macrocyclic binding sites,[2,3] lipid bilayers,[4-6] peptides,[7] and proteins[8] as well as a new application line will be described. Namely, we describe the use of superchaotropic anions as transmembrane transporters in cell biology and medicinal chemistry, including borate clusters[6-9] and metallacarborane ions.[10]



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Closo-Dodecaborate-Based Dianionic Surfactants: Role of Counterions and Linkers to Micellization in Water

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Anionic boron cluster compounds are prominent tools in supramolecular chemistry due to their unique physicochemical properties.[1,2] They have a 3D cage-like nanometer-sized structure and delocalized charge, making them attractive building blocks for the development of novel amphiphilic nanostructures.

In this context, we synthesized novel boron cluster-containing surfactants of very high cationic purity.[3] They consist of a bulky dianionic head formed by *closo*-dodecaborate, and alkyl tail, connected to the head via short linkers created by opening of cyclic oxonium conjugates. The aim of this study was to investigate the micellization behavior of unique surfactants with di-anionic superchaotropic[2] head, and to understand the impact of alkaline counterions on their self-assembly. We used diverse experimental techniques such as tensiometry, isothermal titration calorimetry (ITC), and NMR spectroscopy, completed by all-atom MD simulations.

The study revealed an unconventional micellization process where size and counterion binding of the micelles is related in unusual way to the surfactant concentration. The study challenges the traditional concept of step-like micellization in ionic surfactants, offering new insights into their behavior.

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Merging boron and nucleic acid chemistries

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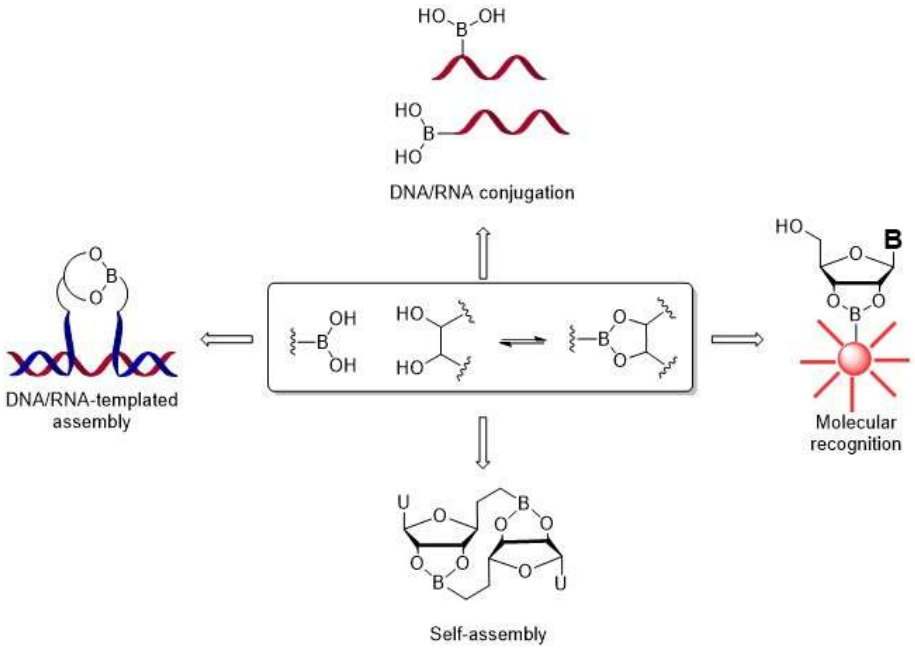
Over the past few decades, boron and nucleic acid chemistries have attracted significant attention for their applications in biology, medicine, and analytical sciences. Our laboratory has maintained a long-standing interest in both fields. Leveraging the unique ability of boronic acids to interact with cis-diol functions in aqueous media, we have developed a wide range of applications—from molecular recognition and sensing to the design of reversible dynamic systems where the natural phosphodiester linkage is replaced with a boronate. The reversible formation of boronate esters occurs in a templated manner and has been shown to restore the activity of split DNA and RNA enzymes, as well as a split fluorescent light-up aptamer. This reversibility is a crucial feature for biological self-assembly. In this discussion, we will explore the fundamental concept of stimuli-responsive boronate formation applied to nuclei acids, highlighting its potential for future research and innovation.[1-3]



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Icosahedral Boron Clusters: From Antimicrobials to Cancer Therapy and Optoelectronics

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This presentation will show recent advancements in boron cluster chemistry, focusing on the applications of carboranes and metallacarboranes in antimicrobial therapy, cancer treatment, and optoelectronic materials. A major focus will be the antimicrobial properties of cobaltabisdicarbollide (COSAN) derivatives. COSAN's stability, hydrophobicity, and low nucleophilicity make it a promising platform to address antimicrobial resistance, particularly *Stenotrophomonas maltophilia* and *Pseudomonas aeruginosa*.[1] Our studies show that COSAN enhances colistin's efficacy, significantly lowering the minimum inhibitory concentration (MIC) for both pathogens. *In vivo* testing with the Galleria mellonella model shows improved survival, supporting COSAN as a valuable adjuvant for treating MDR infections.[2] I also present COSAN-functionalized nanoparticles in Boron Neutron Capture Therapy (BNCT) for cancer treatment. These nanoparticles demonstrate excellent biocompatibility, efficient cellular uptake, and prolonged intracellular retention, significantly enhancing BNCT's efficacy even at lower boron concentrations compared to conventional agents.[3] This makes them strong candidates for advanced cancer therapies. Additionally, the nonlinear optical properties of *o*-carborane compounds will be discussed, particularly in two- photon absorption (TPA) systems. Advances in quadrupolar and octupolar carborane architectures have revealed unique photophysical behaviors, making them suitable for applications in microfabrication and optical data storage. These compounds also exhibit reversible luminescence switching under thermal and light stimuli, potentially aiding in rewritable optical memory systems.[4] By integrating chemistry, nanotechnology, and biomedicine, boron clusters-based materials are poised to drive significant innovations in healthcare and advanced materials science.

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Revolutionizing Nanomedicine: Harnessing Amphiphilic Nanomolecules for Multimodal, Carrier-Free Synergies

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Aromatic compounds that play important roles in biochemistry found numerous applications from drug delivery to nanotechnology or biological markers. We met an major achievement demonstrating experimentally/theoretically that icosahedral boron clusters display global aromaticity.[1] Based on the relationship between stability-aromaticity, we have opened new applications of boron clusters as key components in the field of biological chemistry. Our research has been focused on the development of nanoparticles and, purely inorganic nanovesicles/micelles as vehicles of cancer drugs or as anticancer drugs that, exhibiting desirable in vitro antitumor activities, offer the possibility of multimodal-action, which may result in significant clinical benefits for glioblastoma, breast cancer treatment, and head and neck cancer treatment.

The interaction of 3D aromatic[1] metallabis(dicarbollides) with biomolecules (proteins and ds-DNA)[2] as well as their translocation through bilayer membranes that have been experimentally studied will be presented.[3] Molecular dynamic simulations were employed to investigate the translocation mechanism of metallabis(dicarbollide) nano-anions across membranes, which is the result of a flip-flop translocation mechanism with the formation of a transient, elongated structure inside the membrane.

Biodistribution studies of (metalla)carboranes in cancer cells and *in vivo* will be reported.[2a,b,5] Finally, but not least, taking advantage of their outstanding chemical and biological properties and their retention in tumors, we explored the suitability of this small molecules for multimodal (BNCT, PBFT, gamma radiation, X ray, Mössbauer) cancer therapy.[4]

Parallel to their use as anticancer agents, boron clusters have been found to be very good scaffolds for diagnostic and therapeutic labelling,[5] opening the door to a wide range of biomedical applications.

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Synthetic Methods for the Preparation of Chiral Azaborole Compounds and Their Application in the Synthesis of Photoresponsive Materials

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In recent years, boron-containing polycyclic aromatic hydrocarbons (PAHs) have emerged as a prominent class of aromatic compounds due to their attractive photophysical properties.[1-3] Incorporation of boron, often with other heteroatoms, can significantly modulate the electron density of PAHs, resulting in materials with desirable properties for a range of applications in technology and biology. The development of more complex boron-doped architectures is inextricably linked to advances in synthetic methodology. Our group has contributed to progress in this field through the synthesis of chiral strained systems, such as azaborahelicenes and multihelicenes, and the elaboration of new synthetic methodologies.[4-9]

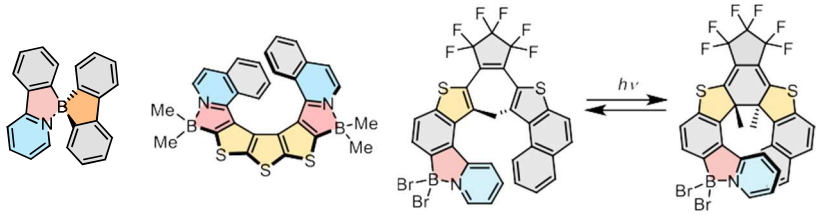

Fig. *Molecular structures of a selected boron-centered spiro compound, an azaborathiahelicene and a boron-containing photoswitch.*

In this talk, we will present the synthesis of boron-centered spiro compounds and azaborathiahelicenes via our new protocols that proved critical in the synthesis of boron-containing photoresponsive materials. The unusual behavior of the latter systems will be briefly discussed.

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Dodecaborate – Not just an innocent bystander in synthesis

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Introduction: The dodecaborate cluster is a very electron-rich unit. This manifests itself in the elevated pKA values of OH, SH, and NH_3 substituents, in the stability of trivalent oxonium and sulfonium salts, the change in chemical shift of F attached to substituents,[1] and in the large bathochromic shift in push-pull chromophores. With the possibility to attach, in a facile manner, organic substituents to the cluster,[2-3] the goal was to utilize the electron-donating power for reactions on substituents.

Results: Reactions of a phenyl substituent under Friedel-Crafts condition with alkyl halides failed consistently; halogenation of the cluster was observed instead. Reaction under acidic conditions with carbocations produced from tertiary alcohols could not differentiate between the cluster and the phenyl group. Acidic conditions led to reaction with solvent if no other reaction partner was present. Diazonium salts reacted with the cluster in a manner which so far could not yet been identified. Examples for such reactions will be given.

Summary: The reactivity of the dodecaborate cluster under conditions suitable for reacting electron-rich aromatic compounds is higher than that of an aromatic substituent. No reaction could be found that differentiated between cluster and substituent.

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Exo-Substituted *Closo* Thiaborane Clusters: On the Road From Isolated Molecules to Crystals

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Closo thiaboranes represent an interesting group of compounds with diverse shapes and properties that have recently attracted attention due to unconventional non-covalent interactions.[1-4] The sulfur heterovertices in thiaborane clusters is generally the center of the partial positive charge of the cluster, although exceptions exemplified with SB_4Cl_4 are known.[2] Since the sulfur vertices have highly positive ESP molecular surface, in the the crystal packing of thiaborane clusters chalcogen bonding with prevails. Again, there exist exceptions, such as SB_5Br_5, whose crystal packing is dictated by the formation of dihalogen bonds.[3] A typical example of crystal packing dominated by chalcogen bonding is the crystal structure of 12-Ph-$SB_{11}H_{10}$ with the S···π type chalcogen bonds.[3] The strength of the chalcogen bond and consequently the properties of the materials made from the phenylated thiaboranes can be modulated by introducing substituents on the phenyl ring.[4]

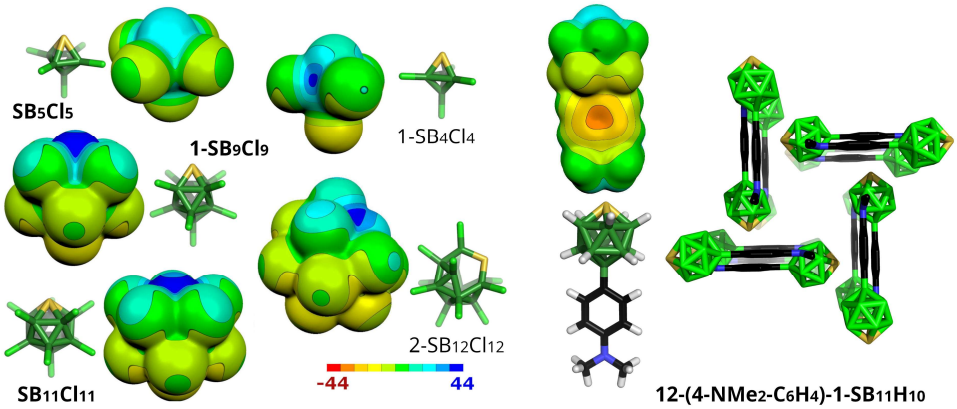

Figure 1. Computed ESP molecular surface of various closo thiaboranes. In casec when respective experimental structures were determined by 11B NMR are labeled in bold, others were determined by HRMS. ESP range in kcal/mol.

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From Boron Hydrides to Aromatic Hydrocarbons: Bridging 2D and 3D Aromaticity

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Looking for molecules that are isoelectronic with already existing ones is a useful strategy to design a new molecule because their electronic structures are known to be stable. For example, molecules with 10 electrons include N_2, CO, CN^-, NO^+ and their existence suggest that B_2H_4 could exist, [1] and was made, although in tiny amounts. In contrast, benzene (C_6H_6) is a highly stable molecule that is planar, with a cyclic structure that adheres to Hückel's rule. It contains 6 π-electrons, like the $[B_6H_6]^{6-}$ anion, which is also planar when Li counterions are considered. [2] However, its high charge precludes a high stability. To design molecules with improved stability than $[B_6H_6]^{6-}$, one possibility is to incorporate neutral atoms. To say by substituting a negative boron atom (B^-) by a carbon atom (C). Hence, $[B_6H_6]^{6-}$ is isoelectronic to borabenzene ($[C_5H_5BH]^-$), or diborabenzene ($[C_4H_4B_2H_2]^{2-}$)[3] and ultimately with C_6H_6. Any of the last three will be more stable than $[B_6H_6]^{6-}$. Alternatively, negative charges can be transformed into fragments; for example, 4 electrons (4e−) are isoelectronic to a BH unit. Therefore, $[B_6H_6]^{6-}$ is isoelectronic to $[B_7H_7]^{2-}$, as C_6H_6 is isoelectronic to $[B_7H_7]^{2-}$. These transformations are explained using the Electronically Confined Space Analogy (ECSA). Indeed, π aromaticity and three-dimensional aromaticity are the two sides of the same coin. [4a-d] We have moved from the Hückel's 4n+2 rule to the Wade's 2n+2 rule.

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Enhancing Neutron Capture Therapy Using Gadolinium and Boron-Integrated and Targeted Delivery Systems

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Non-invasive diagnostic imaging plays a key role in advancing precision medicine, particularly in scenarios where achieving a minimum drug concentration threshold is critical for therapeutic efficacy. Boron Neutron Capture Therapy (BNCT) is a pre-targeting technique that involves the injection of a non-radioactive, non-toxic chemical containing ^{10}B, which is only triggered by neutron irradiation after accumulation at the tumour site. The main advantage of this approach is that by administering ^{10}B and producing alpha radiation selectively in diseased cells, it can kill the pathological cells while sparing the surrounding healthy tissue.[1] However, the expected efficacy has been compromised by the non-specific and non-sufficient biodistribution and rapid metabolism of clinically used BNCT agents. By incorporating a magnetic resonance imaging (MRI) probe into the NCT agent, it is possible to assess the amount of ^{10}B nuclei that have reached the tumour region, thus offering the possibility of personalised therapy thanks to direct observation of biodistribution. In addition, the non-radioactive isotope ^{157}Gd can also react with neutrons to produce high LET Auger electrons, further enhancing the therapeutic power. Therefore, our research is focused on the development of theranostic agents based on closo-carboranes, with high boron content and in vivo stability, acting as a platform linked to a suitable biological vector and an MRI agent. These agents were administered alone or formulated into nanoparticles capable of improving pharmacokinetics and achieving an appropriate tumour-to-blood ratio.[2] To avoid tumour cell relapse and increase the efficacy of the boron agents, a synergistic strategy was also adopted by coupling the enzymatic inhibition of carbonic anhydrase IX to BNCT.[3] (Figure 1) More recently, our group has envisaged the use of BNCT as a powerful and innovative technique for the treatment of Alzheimer's disease as a means of disaggregating β-amyloid plaques.

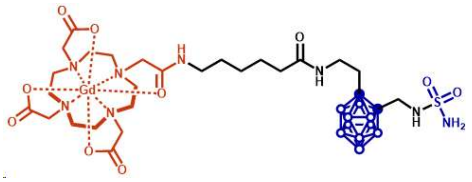

Figure 1: Theranostic agent Gd-B-CA-SF

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"Complexity within Order" in Metal-Organic Frameworks Incorporating Carborane Ligands: A Multivariate Approach

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Carboranes have emerged as a fascinating class of compounds for the synthesis of 3D ligands and the construction of metal-organic frameworks (MOFs).[1] The unique properties of these polyhedral boron clusters—such as thermal stability, chemical inertness, hydrophobicity, tunable electronic and steric characteristics—are highly valuable for addressing the challenges associated with carbon-based MOFs. In recent years, we have reported carborane-based MOFs as promising materials for various applications.[2-4]

We are currently exploring the integration of lanthanide or transition metal ions with carborane ligands to create a range of innovative multifunctional materials. Our recent work demonstrated that the bulkiness and acidity of carborane linkers enables the synthesis of multi-metallic multivariate (MTV) MOFs incorporating flexible combinations of multiple lanthanides. This strategy has produced Tb/Eu MOFs for anticounterfeiting,[5] GdLn (Ln = Dy, Tb, Tb/Eu) MOFs with magnetocaloric and luminescent properties,[6] and the first-ever MOF containing eight different lanthanides.[7] Leveraging the multivariate approach, we are currently synthesizing carborane-based MOFs with strategically selected lanthanide combinations and exploring our approach to transition metals. This strategy allows us to explore the properties of complex multifunctional materials and develop novel materials with tailored functionalities.

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Carborane-Containing Drugs: New Keys for Old Locks

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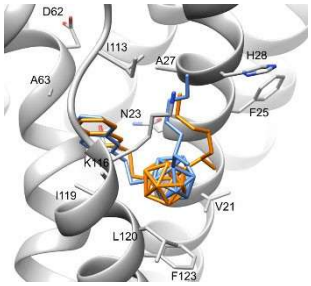
Since the discovery of polyhedral carboranes more than fifty years ago, their potential for various applications has been unlocked. Mainly, their use as pharmacophores is due to their remarkable biological stability and hydrophobicity. The cage framework of these clusters can be easily modified with a variety of substituents both at the carbon and at the boron atoms. It has been shown that the implementation of the carboranyl moiety, as a phenyl mimetic, in biologically active molecules results in compounds that can exhibit improved biological stability and activity in comparison to their generic paradigms. However, up to now, the use of carboranes as pharmacophores is limited to just a few examples.[1] Our research focuses on several types of enzyme inhibitors, such as cyclooxygenase (COX),[2] lipoxygenase (LOX)[3] or ABCG2 inhibitors[4] as well as cannabinoid receptor Type 2 (CB2R) ligands[5].

A highly coveted approach in the design of novel nonsteroidal anti-inflammatory drugs that are applied in the treatment of various inflammatory processes is achieving cyclooxygenase (COX) 2 selectivity. By implementing a carboranyl moiety in the structures of known COX inhibitors more selective and robust COX-2 inhibitors were obtained.[2]

5-Lipoxygenase (5-LOX) is an enzyme of the extracellular matrix and plays a role in increased metastasis and angiogenesis. Numerous reports show the overexpression of 5-LOX in several cancer cell lines. For the activation of 5-LOX, the 5-LOX-activating protein (FLAP) is necessary. Therefore, inhibition of 5-LOX or FLAP could inhibit tumour growth and angiogenesis. Replacement of phenyl rings in selected 5-LOX inhibitors by carboranes resulted in a similar enzymatic inhibitory behaviour but markedly increased cytotoxicity against several melanoma and colon cancer cell lines.[3]



Selected examples also for other biological targets[4,5] will also be presented.

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Oral Communications

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Building blocks containing boryl and silyl groups dedicated to the controlled synthesis of unsaturated organic compounds

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The presentation aims to determine the importance of borylsilyl-functionalized unsaturated reagents in the synthesis of organic molecules containing conjugated carbon-carbon double (C=C) and triple (C≡C) bonds. Such motifs are present in the structures of natural products (with therapeutic or toxic effects), drugs, dyes, different types of components dedicated to materials science, etc.[1,2] Our research is focused on developing highly effective, simple, and easily accessible methods for synthesizing silicon-based building blocks and transforming them into valuable products. Developed protocols will allow control over the type, number, order, and substitution of conjugated C-C bonds in the structure of molecules. As a result of the studies, areas of application of the obtained building blocks and methods for their modification will be established.[3-10]

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Synthesis of Boron-doped Carbon via Ethynyl-Containing Boron Precursor

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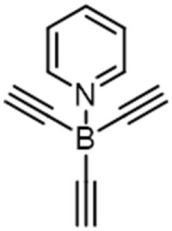
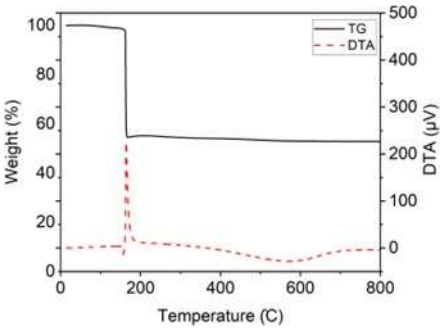
Boron-doped carbon (BDC) has attracted attention as an alkali-ion storage as an anode material.[1] Previous studies have reported the synthesis of BDC materials using boric acid or boron oxide as starting materials.[2] These molecules have stable B-O bonds. It is difficult to cleave these bonds and reform the B-C bonds. Therefore, it is challenging to control the bonding states of boron. Thermal treatments of ethynyl groups are effective ways to build 3D carbon frameworks. Ogoshi *et al.* reported constructing 3D carbon structures from organic compounds including ethynyl groups.[3] For BDC synthesis, no example exists to build the carbon from ethynyl groups. In this study, we designed ethynyl-containing boron molecules as building blocks for the BDCs. We focused on triethynylborane pyridine complex (**TEB-Py**) as an ethynyl-containing boron molecule (Figure 1). We observed the thermal behavior of **TEB-Py** by TG-DTA. As a result, we confirmed the endothermic peak at 157 °C. It indicated the desorption of pyridine. After desorbing the pyridine, we confirmed the exothermic peak (160 °C) indicating the polymerization of ethynyl groups. Based on the TGA analysis, we found that the ethynyl groups needed 160 °C to polymerize. Then we synthesized the BDC at three different temperatures (200, 600, 900 °C) and named them as **TEB-C**$_{\textbf{temperature}}$. We confirmed **TEB-C**s have amorphous carbon peaks in the XRD analysis. In the **TEB- C**$_{\textbf{200}}$, we confirmed two sharp peaks. We compared XRD simulation of **TEB-Py** molecule and **TEB-C**$_{\textbf{200}}$. It is evidence for carbonization proceeding by desorption of pyridine.

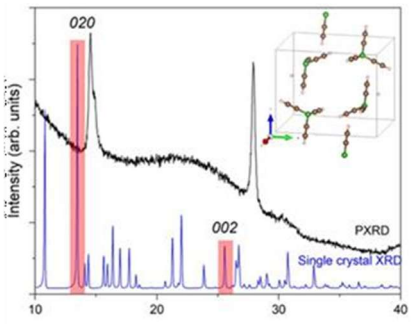
Finally, we evaluated their potential for lithium and sodium ion storage.



(Figure 1) Precursor of boron- doped carbon (**TEB-Py**)



(Figure 2) TG-DTA analysis of **TEB-Py**



(Figure 3) XRD patterns of **TEB-Py** simulated (blue) and **TEB-C**$_{\textbf{200}}$ measured (black).

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[3] Ogoshi, T.; Nishina, Y. et al. *Commun Chem*. **2021**, *4*, 75(Figure 1) Precursor of boron-doped carbon (**TEB-Py**)

Metallacarborane-peptide hybrids with antimicrobial activity

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The rapid rise of multi-drug resistant infections coupled with the slow development of new antibiotics, presents a significant danger to public health. Despite the rise of resistant strains, few new antibiotic classes have been introduced in the past two decades, with most being derivatives of existing ones. The overuse of established scaffolds has exhausted current antibiotic options, necessitating innovative approaches. A promising strategy is to shift beyond traditional organic compounds to explore the vast potential of inorganic and organometallic chemistry.[1]

Metallacarboranes show the potential to be new chemical leads for antibiotic design as they are abiotic and resistant to enzymatic degradation, interact with biomolecules such as lipid membranes and proteins, and their structure, as well as physicochemical properties, are different from organic compounds.[2] Additionally, metallacarborane derivatives showed high antimicrobial activity, including against multidrug-resistant (MDR) strains.[3] For further development of metallacarborane-based antimicrobials innovations in organofunctionalization methods of metallacarboranes are essential.

We propose the conjugation of metallacarboranes with ultrashort peptides, which provide enormous structural diversity, selectivity, and biocompatibility, as a promising strategy for the development of metallacarborane-based biologically active compounds. We synthesized metallacarborane-peptide hybrids consisting of cationic di- and tripeptides conjugated with 3,3'-cobalt bis(dicarbollide) (COSAN) or its iodinated derivative I-COSAN. By modulating the lipophilicity and charge of the hybrids, we optimized them for high antibacterial activity and biocompatibility. Synthesis, biological activity, and mechanism of action will be presented.

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The Boron Buckyball—A Milestone in Fullerene Chemistry and Nanomaterials Science

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The discovery of the boron buckyball, a cage-like molecule composed entirely of boron atoms, represents a transformative milestone in nanomaterials science. Theoretical predictions dating back to 2007 first proposed the existence of a stable, highly symmetric B_{80} fullerene, analogous to the carbon buckyball (C_{60}) but featuring an additional boron atom at the center of each hexagonal face [1]. This theoretical insight catalyzed extensive investigations into the structural, electronic, and energetic properties of boron-based nanomaterials, ultimately leading to the experimental confirmation of smaller boron fullerenes such as B_{40} through photoelectron spectroscopy [2].

Despite its predicted stability, the synthesis of B_{80} remained a formidable challenge due to boron's electron deficiency and its preference for multicenter bonding configurations [3]. Unlike carbon, which readily forms highly symmetric sp^2-hybridized structures, boron exhibits a more complex bonding landscape that complicates the formation of hollow, fullerene-like architectures. However, recent advancements in experimental methodologies, including precision cluster deposition and refined spectroscopic techniques, have at last enabled the successful synthesis of the long-sought B_{80} boron buckyball, as reported in a landmark 2024 study [4]. This breakthrough not only validates decades of theoretical models but also unlocks new opportunities in boron-based nanotechnology, particularly in molecular electronics, catalysis, and next-generation photodetectors.

This presentation will offer a comprehensive analysis of the theoretical framework, experimental realization, and prospective applications of boron fullerenes. Emphasis will be placed on the structural and electronic properties of experimentally confirmed boron fullerenes, their potential integration into optoelectronic devices, and the broader implications for materials science. The successful synthesis of the boron buckyball marks a pivotal moment in fullerene chemistry, paving the way for the exploration of novel boron-based nanostructures with unprecedented electronic, optical, and mechanical properties.

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Synthesis of boron-containing drug candidates as potential PARP inhibitors

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The 18 members of the poly (ADP-Ribose) Polymerase (PARP) family of enzymes are involved in a variety of biological processes, such as apoptosis and DNA repair. [1] The PARP enzyme consumes NAD^+ as a substrate, and competitive inhibitors are used to mimic the natural NAD^+ substrate to prevent PARylation. Inhibiting PARP is clinically utilized in cancer treatment. These inhibitors also have the potential to function as sensitizers, so they can increase the effectiveness of anticancer therapies, including radiation therapy and chemotherapy medications. Since PARP inhibitors cause synthetic lethality in homologous recombination-dysfunction cells, they are also used as single-agent treatments in individuals with BRCA-deficient breast, ovarian, or prostate cancer. [2] Organoboron compounds can be described as Lewis acids due to their empty p-orbital, which accepts lone pair electrons (Lewis Base) and changes hybridization. This unique feature makes organoboron compounds preferred drug candidates, leading to an increase in the number of functional groups, including boronic acid, in medicinal chemistry. [3] Boron-containing heterocyclic rigid structures improve drug-enzyme interactions based on forming tertiary complexes between boronic acids and responsible amino acids such as serine. For this reason, we created a boron-containing heterocyclic library that includes 19 benzoxazaborinin derivatives, with yields ranging from 20% to 99%. The synthesized compounds were characterized by NMR spectroscopy and HRMS and tested for their inhibitory activity using a PARP-1 screening assay. The assay quantified leftover NAD^+ substrate by converting it to a fluorophore group that enabled excitation at 372 nm and emission at 444 nm. Overall, various benzoxazaborinin-based PARP inhibitors were synthesized, with the lowest IC_{50} value of 31 μM obtained for structure 15A.

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Borohydrides as Synthetic Platform for Large *B,N*-doped Aromatics

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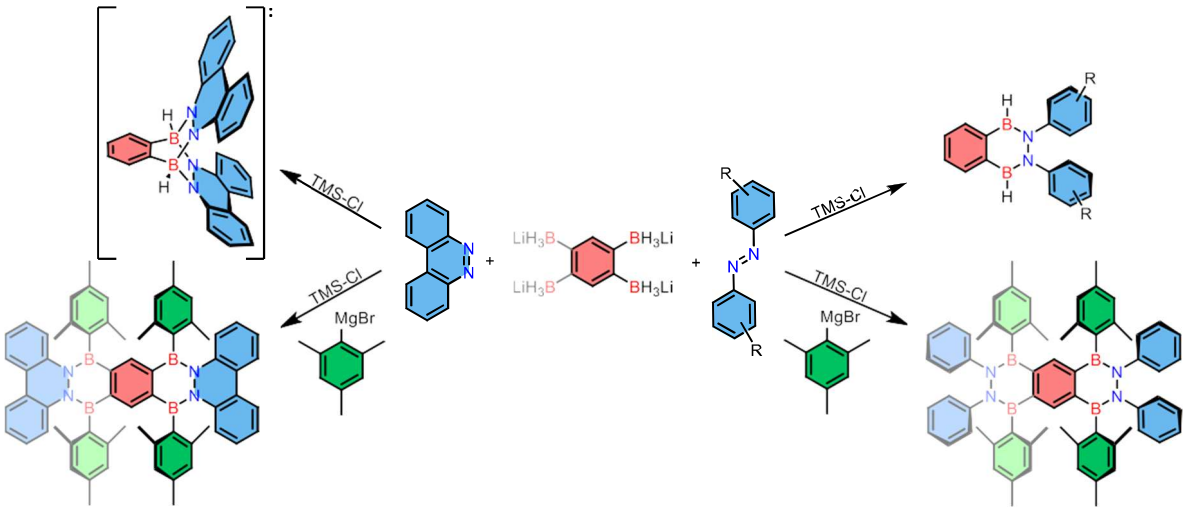
Boron-Nitrogen doped acenes have become a central focus in materials chemistry, with one central application being organic electronics.[1] A central advantage over classic acenes is hereby the improved stability of the B,N-derivatives compared to their carbon counterparts.[2] In order to develop new materials for organic electronics, our group has utilized phenylenebistrihydridoborate as precursor for both B,N-radicals and B,N-acenes.[3] Herein, we present the extension of our methodology to phenylenetetratri(hydridoborate) to target a variety of large and complex B,N-acenes. Furthermore, we extended the scope of our azobenzene-based B,N-acenes to air-stable derivatives and gained access to octa-aryl substituted B,N-anthracenes.



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DNA-boron cluster composites and their assembly into nanoparticle carriers of therapeutic nucleic acids

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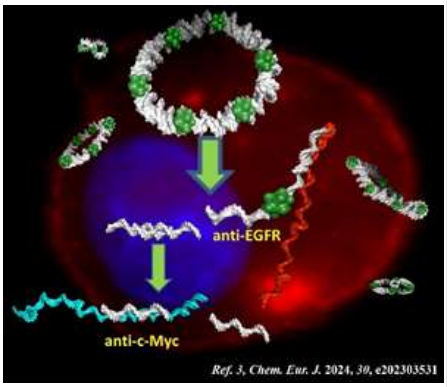
In the Laboratory of Medicinal Chemistry of the Institute of Medical Biology several methods of oligofunctionalization of carboranes and metallacarboranes have been developed and some of them were used to synthesize conjugates of boron clusters and DNA-oligonucleotides [1-5].



Nanoparticle with dual EGFR and c-MYC silencing activity. A hypothetical mechanism of action.

Specifically designed types of the conjugates were used as building blocks in construction of new class of bionanoparticles capable of silencing the expression of selected target genes such as Epidermal Growth Factor Receptor (EGFR) [2, 4] or EGFR and c-MYC (myelocytomatosis oncogene) genes simultaneously [3]. Herein we present methods developed in our laboratories for the synthesis of these novel bioinorganic composites and their application for the construction of functional nanoparticles with therapeutic potential as gene silencing agents.

Acknowledgement: This work was supported by the National Science Center, Poland, grant No 2015/16/W/ST5/00413; the Bio-Med-Chem Doctoral School of the University of Łódź support and contribution from the Statutory Fund of IMB PAS is also appreciated.

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Isolating ideal one-dimensional large-spin chains in Carborane-Based Metal-Organic Frameworks

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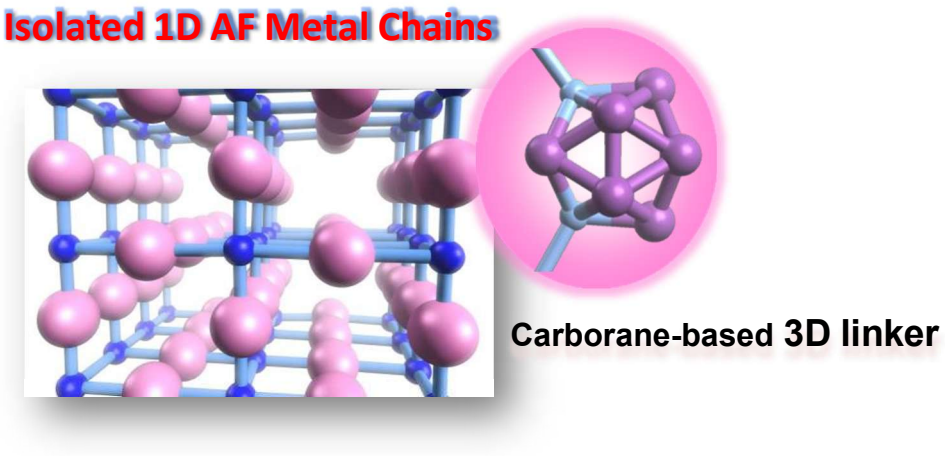
Metal-organic frameworks (MOFs) link simple organic and inorganic building blocks through strong bonds to form extended, porous crystalline solids. By selecting specific magnetic cations, tailoring their coordination environment, and designing both intrachain and interchain linkers, MOFs can host different types of spin chains with precise control over magnetic interactions.[1] One-dimensional (1D) antiferromagnetic chains are fascinating because of their exotic quantum phenomena.[2] Currently, despite some progress in creating and working on integer and half-integer large *S* Heisenberg antiferromagnetic (AFM) chain formations in hybrid inorganic-organic materials, isolating large-spin *S* chains remains challenging as even minimal interchain interaction *J'* tends to drive unwanted long-range ordering.[3]

In this work, we present two new *m*CB-MOFs that feature water-bridged Co ($S = 3/2$) or Ni ($S = 1$) spin chains that are effectively separated by bulky carborane linkers. This behavior highlights *m*CB-Co and *m*CB-Ni as promising high-spin one-dimensional antiferromagnetic chains, offering a unique platform for exploring quantum effects in well-isolated spin chains.



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Selective Synthesis of Some Phenyl-Substituted Aliyclic β-Amino Esters and β-Lactams

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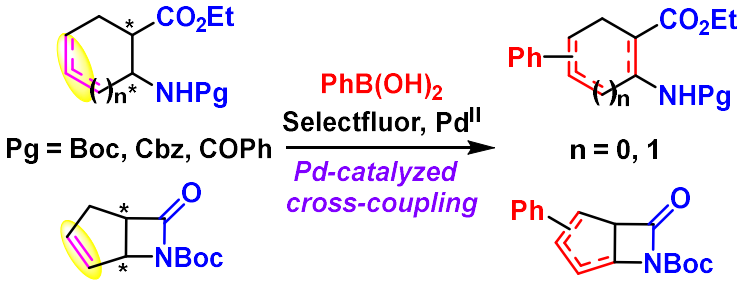
Cylic β-amino acids are interesting molecular elements in medicinal chemistry, being components of natural products and vrious bioactive compounds. Some representative small-molecular entities of this class of compounds are known as antifungal or antibacterial agents, while the phenyl-substituted cyclohexene amino ester Tilidine is an analgesic drug.[1,2] Conformationally rigid alicyclic β-amino acids are valuable building elements for the synthesis of novel type of oligopeptides with important pharmaceutical potential, with significant relevance in drug design. The aromatic–aromatic (π–π) and CH–π interactions in and between various helix-type structures might have significant effect on the secondary or tertiary arrangements of oligopeptides.[3,4]

A convenient synthetic protocol has been developed for the preparation of several phenyl-substituted alicyclic β-amino acid derivatives. The substrate-dependent palladium-catalyzed cross-coupling of phenylboronic acid with five- or six-membered cycloalkene β-amino esters and unsaturated bicyclic β-lactams in the presence of Selectfluor as oxidant furnished some phenyl-substituted alicyclic β-amino esters and azetidin-2-ones. The phenylations were investigated under various experimental conditions with different ligands and solvent systems. The structural architecture of the starting compounds and the position of their ring C-C double bond predetermined the structure of the products.



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New Anthracenyl and Pyrenyl Derivatives of ortho-Carborane. Synthesis and Properties

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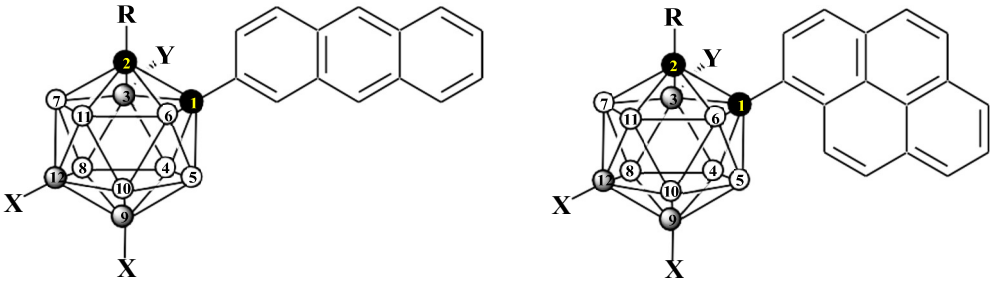
The *ortho*-carborane derivatives containing luminophoric polycyclic aryl groups are known to demonstrate intense solid-state emission due to the suppression of luminescence quenching caused by the restriction of intramolecular rotation of the aryl groups in the aggregate state.[1] In turn, the electron-acceptor effect of the carborane fragment can be regulated by introducing substituents of various natures,[2] which makes it possible to control the luminescence wavelength and opens up good prospects for the development of stimuli- responsive luminochromic materials.

A series of *ortho*-carborane derivatives containing luminophoric anthracenyl and pyrenyl substituents at carbon atoms and various substituents of electron-releasing and electron-withdrawing nature at boron atoms 1-L-2-R-9,12-X_2-1,2-$C_2B_{10}H_8$, 1,2-L_2-9,12-X_2-1,2-$C_2B_{10}H_8$, 1-L-3-X-1,2-$C_2B_{10}H_{10}$ and 1-L-3,6-X_2-1,2-$C_2B_{10}H_9$ were synthesized by Ni-catalysed microwave-assisted cross-coupling of the carboranyl Grignard reagents with the corresponding aryl bromides.



Derivatives with anthracenyl and pyrenyl substituents at the boron atoms in positions 6 and 9 of the *ortho*-carborane cage were synthesized by Pd-catalyzed cross-coupling of the corresponding carboranyl iodides with the *in situ* prepared aryl zinc bromides, similarly to that described previously for the synthesis of functionalized phenyl derivatives [3,4].

The crystal structures of the synthesized compounds were determined and their luminescent properties both in solution and in the solid state were studied. The relationship between their structure (the presence of additional substituents of various natures and their position) and luminescent properties will be discussed.

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Nonmetallic Frustrated Cations – An Innovative Concept for Small Molecule Activation

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Is it possible to combine coordinative unsaturation and intrinsic electron deficiency within a single molecule while still retaining frustrated Lewis pair-like behavior? Indeed, it is. Building on our research in the chemistry of low-coordinate B–P bond systems with ambiphilic properties, we recently introduced the concept of nonmetallic frustrated cations (NFCs), in which a Lewis acidic low-coordinate boron atom is directly bonded with a Lewis basic phosphorus atom. This novel class of reactive species, generated *in situ* via heterolytic cleavage of the boron-bromide bond in bromophosphinoborane, exhibits remarkable activation potential toward small molecules (Figure 1).[1, 2] A close proximity of B and P centers, along with ineffective side-by-side overlapping of empty and filled valence B and P orbitals, promotes reactions that lead to thermodynamically stable cyclic single-, double- and double-mixed activation products under mild conditions without any catalyst. Moreover, their strong Lewis acidic properties manifest in reactions with Lewis bases, such as *N*-heterocyclic carbenes, resulting in the formation of phosphinoborenium cations.[3, 4]

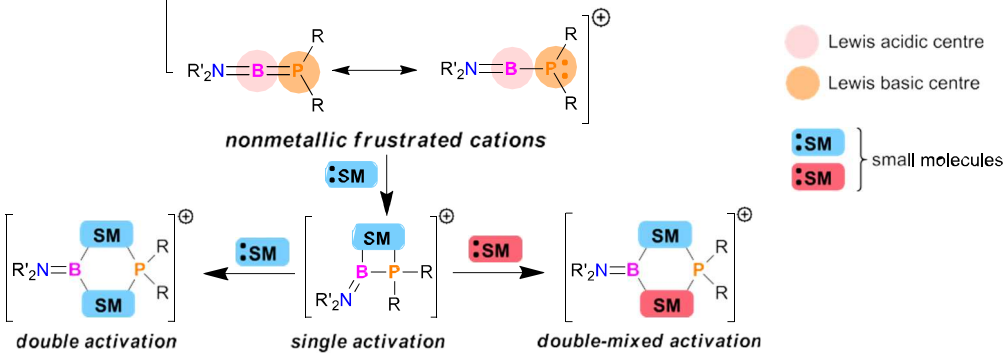

Figure 1. Small molecule activation via nonmetallic frustrated cations[1, 2]

Financial support of these studies from Gdańsk University of Technology by the DEC-20/2021/IDUB/I.3.3 grant under the ARGENTUM – 'Excellence Initiative – Research University' program is gratefully acknowledged.

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Triplet Photosensitizers Derived from Rigid Organoboron Scaffolds: From Molecular Design to Applications

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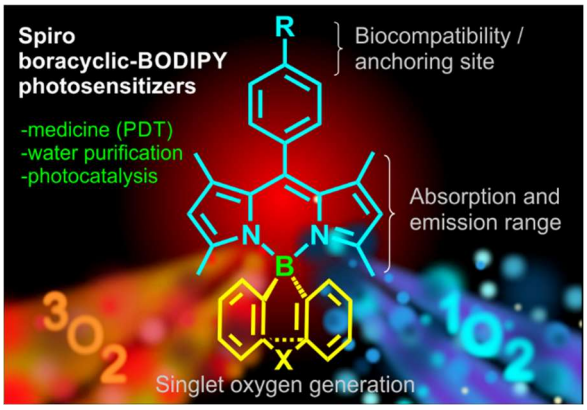
Herein we present a new strategy for the development of efficient heavy-atom free singlet oxygen BODIPY photosensitizers (PS) based on rigid boracyclic scaffolds.[1-4] The proposed conception benefits from the natural separation of the ligand and organoboron species through boron node. The photophysical behaviour of boracyclic-BODIPY PS mostly results from the electronic features of organoboron donor moiety and orthogonal alignment of donor and acceptor sites, altogether enhancing intersystem crossing to local triplet state via SOCT-ISC mechanism. The practical implications of the proposed molecular design are of high significance. Now the generation of ROS can be controlled by the organoboron moiety, while the other physicochemical properties can be easily tailored by the modification of the BODIPY frame. This was used for shifting the absorption wavelength to red or NIR regions of the spectra or connecting to another organic moiety with specific predestined functionality (eg. to enhance biocompatibility by cationic quaternary amine, PEG, nucleotide or sterol groups). The measured singlet oxygen quantum yields for these systems reach up to 85%. They show high hydrolytic (also in acidic conditions), photolytic and oxidative stability making them suitable for subsequent post-synthetic functionalization. Biological studies showed that boracyclic-BODIPY complexes are efficient in photoinactivation of microbes, biofilms and cancerous cells with negligible dark cytotoxicity. Furthermore, we have incorporated selected boracyclic-BODIPY derivatives in polymeric nanoparticles, composites of silica nanograins coated with polymeric shell, chemically bonded PSt molecules with TMS-based aerogels and on the surface of SiO_2-nanopallets. All of these materials exhibit photocatalytic and antimicrobial properties upon irradiation with white light.



This work was supported by National Science Centre (Poland) within the framework of the OPUS project "*Efficient triplet photosensitizers derived from rigid organoboron structures as singlet oxygen generators*" UMO-2020/39/B/ST4/02370.

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Metallacarboranes alter cellular metabolism at single micromolar concentrations

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Since their synthesis in the 1960s by Hawthorne, inorganic metallacarboranes, including cobalt bis(dicarbollide) ([COSAN]$^-$), have attracted attention not only from chemists, but also biologists and clinicians. [COSAN]$^-$'s remarkable physicochemical properties such as 3D aromaticity, delocalized negative charge and superchaotropic character place it beyond the scope of conventional organic pharmacophores.[1] Recent reports describe [COSAN]$^-$ derivatives' utility as atypical antimicrobials toward Gram-positive bacteria and fungi,[2] carriers for otherwise impermeable cationic peptides[3] and boron source in experimental anticancer therapies (BNCT and PBCT). Despite its potential, little is known about [COSAN]$^-$'s activity in a cellular environment and its molecular mechanism of action.[4] To bridge that gap, we have selected three simple derivatives of the iodinated [I-COSAN]$^-$ and studied their effects on the viability and metabolic state of exemplary A549 lung adenocarcinoma cells. We show that [I-COSAN]$^-$'s derivatives at low micromolar concentrations are not cytotoxic, however boost the mitochondrial functions and lead to the NAD^+/NADH ratio shift and increase in the ROS production. Such results suggest that [COSAN]$^-$-based molecules could affect cellular physiology at as low as single micromolar concentrations. This study enhances the understanding of metallacarboranes' interactions in biological systems, aiding the design of novel bioactive compounds with potential medical applications.

Acknowledgements:
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Synthesis of boron doped p-conjugated polymers by cyclotrimerization of alkynyl boranes

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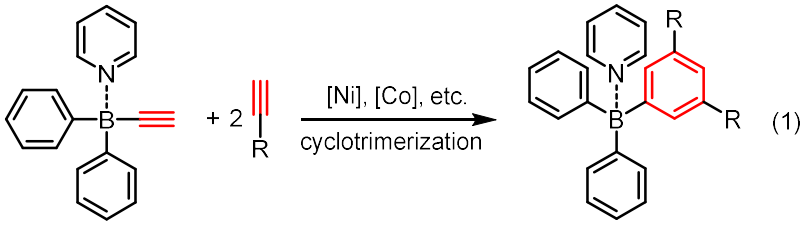
Boron-doped polymers, which are applied in various fields such as sensors, gas separation, and catalysts, have been synthesized using a variety of methods.[1-3] These polymer structures can be classified into two types: those containing boron in their backbone and those with boron-containing compounds in their side chains. In this study, we synthesized a polymer containing boron atoms in its backbone through the alkyne cyclotrimerization. We expected that a large number of Lewis acid sites and a high surface area of the material would improve the performance in the applications. For the polymer synthesis, triethynylborane·pyridine complex was used as a raw material. Firstly, ethynyldiphenylborane pyridine complex was designed to optimize the reaction condition for the cyclotrimerization of alkynes (eq. 1). Commonly known catalysts for this reactions, such as Ni(0), Co(0), and other catalysts[4] were investigated to establish the optimal conditions. Then, triethynylborane·pyridine complex was reacted under the optimized conditions (eq. 2). The polymer produced by Ni(0) catalyst exhibited the release of pyridine (boiling point 115 °C) at 300 °C in TG-MS measurement. This phenomenon was attributed to the strong interaction between Lewis acid sites in the polymer and pyridine as a Lewis base.



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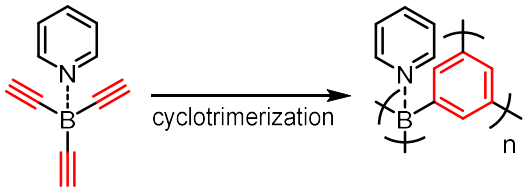

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Exploration of new tools for the chiral separation of anionic boron clusters

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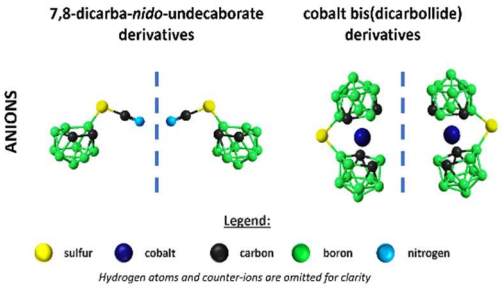
Introduction - anionic boron clusters (see the schema) have recently made their way not only into medicinal chemistry due to their favourable physical-chemical properties. These compounds possess either their own biological activity or are studied as nonclassical bioisosteres of a phenyl ring in pharmacophores [1]. Although lots of these compounds exhibit chirality, this feature has been grossly overlooked. However, the different spatial arrangement of the functional groups in drugs acquired high attention since the thalidomide affair. Naturally, the regulation authorities require a detailed description of the fate and activity of both enantiomers. Thus, chiral analytical methods are of the utmost importance during the pharmacokinetic studies of new drug candidates or for the evaluation of enantiomeric purity.



Results –our group has recently explored the possibilities of fast and reliable chiral method development for the anionic boron clusters. We aimed at a systematic investigation of the main effect responsible for the absence of successful chiral separations of especially anionic carboranes in HPLC. The cyclodextrin-based stationary phases have been shown to separate enantiomers of anionic carboranes. Moreover, the enantioseparation of 7,8-dicarba-nido-undecaborate(1-) ions was achieved for the first time in HPLC. [2] Our results further revealed that it is also possible to use polysaccharide-based chiral selectors under RPLC conditions for the chiral separation of anionic species. [3] Additionally, SFC has been proven as a useful tool for rapid baseline separations within 10 minutes, exceeding significantly HPLC in the number of separated chiral carboranes, resolution and analysis time. [4]

Summary – our work brings new and useful observations concerning the chiral method development strategy for the anionic carboranes for the purposes of drug development. Moreover, the results may be used in any area, where the chirality of these interesting molecules is of concern.

Acknowledgment - the Czech Science Foundation, Project No. 25-16216S.

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Opening a new library for MR-TADF molecules; introducing heterocycles with Nitrogen atom to amplify MR-TADF behavior

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Organic light-emitting diodes (OLEDs) have revolutionized display and lighting technologies due to their efficiency, flexibility, and potential for producing vivid colors. Despite their advantages, achieving high efficiency while maintaining long operational lifetimes remains a challenge. [1] Thermally Activated Delayed Fluorescence (TADF) materials have emerged as a promising solution, offering high efficiency without the need for heavy metals by utilizing reverse intersystem crossing (RISC) to harvest triplet excitons. [2] Recently, Multi-Resonance TADF (MR-TADF) materials have garnered significant attention due to their superior color purity and efficiency. These materials leverage a unique multi-resonance effect that results in narrow emission spectra and high color purity, which is crucial for display applications. Incorporating boron atoms into TADF and MR-TADF materials has shown to further enhance their properties, providing a pathway to highly efficient and stable OLEDs.[3] This study explores how to expand the library of the potential of boron-containing MR-TADF materials with introducing new moieties as heterocycles. We investigate the computational energy levels of these advanced materials. Our findings highlight the advantages of MR-TADF materials, such as minimal structural relaxation, small Stokes shifts, narrow electroluminescence peaks, higher color purity, and potential enhanced device performance, making them highly suitable for advanced optoelectronic applications.

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Boron Cluster-Derived Photoluminescent Dyes: A New Approach to Antimicrobial Photodynamic Therapy

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The rising prevalence of antimicrobial resistance (AMR) poses a significant global threat by diminishing the effectiveness of traditional antibiotic treatments. This situation has prompted the need for alternative strategies. One such promising approach is Antimicrobial Photodynamic Therapy (aPDT), which employs light-activated photosensitizers (PSs) to produce reactive oxygen species (ROS) that can inactivate bacteria without leading to resistance [1]. Unlike traditional antimicrobial agents, the significant advantage of aPDT lies in its low likelihood of inducing microbial resistance [2]. The main objective of this project is to develop efficient biocompatible boron cluster-containing BODIPY-based photosensitizers as promising agents for aPDT [3]. This approach takes advantage of the boron clusters´ ability to prevent molecular aggregation, their antimicrobial properties [4], and the PSs' capability to generate singlet oxygen. The most effective antibacterial photosensitizers could help to fight nosocomial diseases by inactivating microorganisms in sanitary instruments and medical devices. We have synthesized two novel families of photosensitizers based on boron cluster-BODIPY. The first family consists of two neutral PSs. Both compounds include a *meso*phenolyl-BODIPY core with two *ortho* or *meta* carborane units. The second family consists of three ionic PSs. These compounds are based on a *meso*pyridyl- BODIPY core linked to metallacarborane and dodecaborate anions through an ethylene glycol chain. **All compounds exhibited efficient $^1O_2$ production, making them promising candidates for aPDT**. Currently, we are evaluating the **aPDT properties** *in vitro* and *in vivo* of photosensitizers activated by visible light against **gram-positive and gram-negative bacteria** commonly associated with antimicrobial resistance. Ongoing research focuses on exploring their antimicrobial potential, with these findings paving the way for **designing even more efficient photosensitizers.**

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Sustainable Photocatalytic Oxidation with Cobaltabis(dicarbollide): from Alkanes to Aromatic Hydrocarbons

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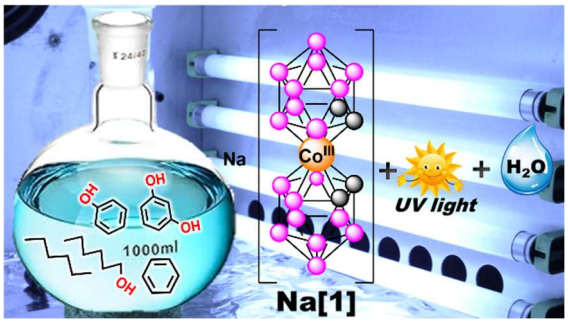

In recent decades, numerous homogeneous catalysts have been developed for photoredox oxidation reactions. We demonstrate that the cobaltabis(dicarbollide) θ-shaped complex, Na[3,3′-Co(1,2-$C_2B_9H_{11}$)$_2$] (Na[1]), is an efficient and sustainable photosensitizer for alcohol oxidation,[1] alkene epoxidation,[2] and hydroxylation in aqueous media. Operating via a single-electron transfer (SET) mechanism, Na[1] enables fast reactions with low catalyst loading. Its efficiency stems from unique properties such as water solubility,[3] surfactant behavior,[4] molecular compactness, and the strong oxidizing power of the $Co^{4+/3+}$ redox couple.[5] This sustainable approach offers a highly efficient, green alternative for the hydroxylating alkanes and aromatic hydrocarbons, surpassing conventional oxidation methods by avoiding harsh conditions while maintaining high selectivity. We developed a cutting-edge photooxidation process using Na[1] as a photoredox catalyst, operating in water at room temperature under UV light-completely avoiding organic solvents and extreme reaction conditions. Notable results include 92 % cyclohexanol yield from cyclohexane and 98% phenol yield from benzene and highly selective alkane hydroxylation.

By leveraging metallacarborane photocatalysts, this study introduces a scalable, eco-friendly, and cost-effective approach to hydrocarbon oxidation method using metallacarborane photocatalysts, with transformative potential for fine chemical synthesis and sustainable fuel production.

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Dual Reactivity of Diborane(4): Substrate Coordination And Reduction Through Stimulated Diborane-Substrate Electron Transfer

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The selective coordination and reduction of substrates within the coordination sphere represent a reactivity pattern typically linked to late transition metals in low oxidation states.[1] Recently we were able to show that electron rich diborane compounds can also exhibit such reactivity by acting as both Lewis acid and electron donor. In our group, doubly guanidinate-stabilized diborane(4) compounds have successfully been applied in such reactions.[2,3]
The ditriflato- and dibromo-diboranes(4) $[XB(hpp)]_2$ (X = OTf, Br)[4] readily undergo triflate/bromide elimination to form cationic diboranes stabilized by neutral organic bases.[3,5]
In this study, we present reaction sequences in which pyrazine derivatives are first coordinated to the diborane. Subsequently, electron transfer is initiated through pyrazine methylation by adding MeOTf in a second, separate step. This process enhances the acceptor strength of the coordinated pyrazine unit, leading to oxidative B-B bond cleavage and reduction of the pyrazine.

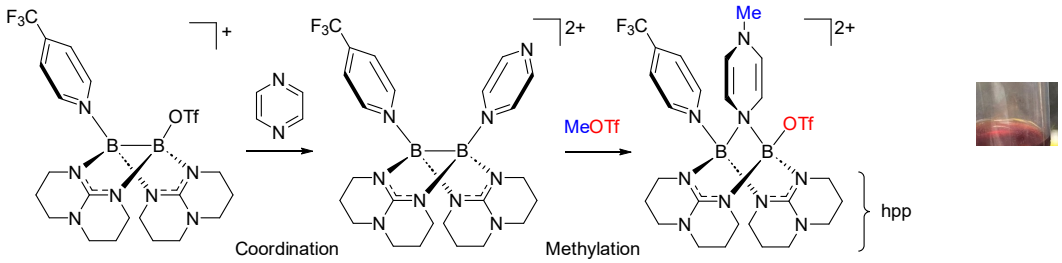

Figure: Coordination of pyrazine by a monocationic diborane and addition of methyl triflate, triggering pyrazine reduction and oxidative B-B bond cleavage.

We carry out a systematic study to investigate this stimulated electron transfer in mono- and dicationic diboranes. Moreover, we showed electron transfer could also be triggered by an excess of pyrazine, leading to cyclic compounds with reduced pyrazine units and non-reduced.

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LIBS – an alternative sensitive method for low boron determination

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The precise determination of low concentrations of elements (at levels of single ppm or less) presents a significant analytical challenge. Commonly used methods involve various physical-chemical techniques, but these typically require sophisticated and expensive equipment. Among the most prevalent methods are ICP-MS (Inductively Coupled Plasma Mass Spectrometry) and micro-XRF (X-Ray Fluorescence). However, these techniques are complex and necessitate specialized laboratories, which limits their mobility and potential applications.

Boron is a particularly promising candidate, especially in the context of BNCT (Boron Neutron Capture Therapy), where the selective capture of thermal neutrons by ^{10}B isotope atoms produces the desired therapeutic effect. An additional challenge lies in the isotopic differentiation of the two stable boron isotopes, ^{10}B and ^{11}B, even during laboratory studies using single test cell lines to determine the concentration (uptake) of boron and its carrier by cells.

To facilitate rapid and user-friendly boron quantification, we propose implementing an alternative spectroscopic technique with very high sensitivity, namely LIBS (Laser-Induced Breakdown Spectroscopy), instead of relying on mass spectrometric methods. As part of this project, we are developing this optical spectroscopy method, which will enable us to economically and quickly measure the concentrations of selected elements of interest. Additionally, we are utilizing NAA (Neutron Activation Analysis) as a supporting analytical method. A system is planned to be constructed in the Neutron Activation Analysis Laboratory, located at SOLARIS NSRC, to measure the uptake of new boron carriers in biological samples irradiated with thermal neutrons.

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Transformation of carboranes by carbenes: From isomerization to positively charged clusters

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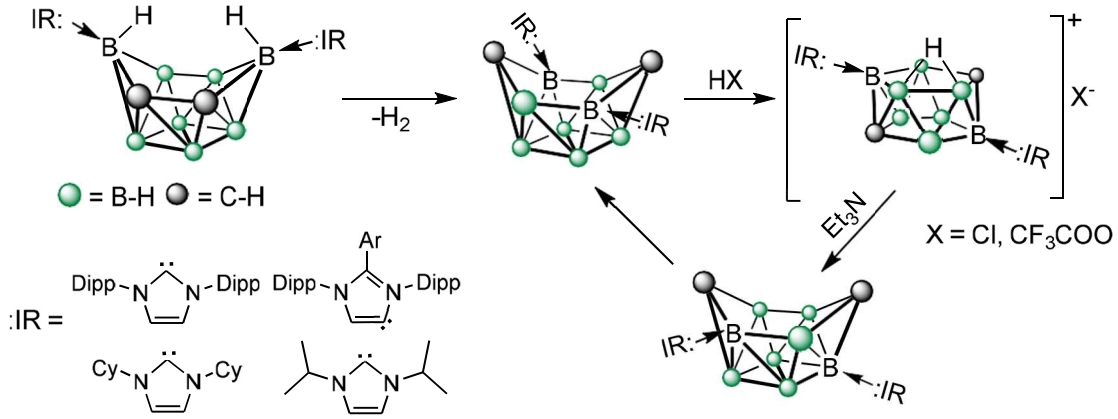
The chemistry of heteroborane clusters is a well known and developed branch of inorganic chemistry.[1] The polyhedral boranes are typically neutral or negatively charged species, which is not surprising considering they are built of electron-deficient boron atoms bound by multicentered two-electron bonds. Our group demonstrated that coordination of N-heterocyclic carbene leads to umpolung of the carborane, which acted subsequently as a base and enabled the synthesis of the first thermally robust positively charged heteroboranes.[2] Recently, we have demonstrated that similar approach can be used for chalcogenaboranes.[3]

In this work, we present reactivity of carboranes with several types of carbenes. These complexes easily undergo various transformations (isomerization or hydrogen elimination, Scheme 1) yielding unprecedented cluster shapes and can be used as ligands for a broad range of main group and transition metals. Their reactivity with acids will be presented as well.



Scheme 1. Transformations of carborane-carbene complexes.

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LabsinLove: a company ''targeted'' in BNCT

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LabsinLove is a spin-off company founded in 2023, as a joint venture between ICMAB-CSIC and the University of Granada. The company is devoted to achieving improvements in BNCT treatments in the different elements that are necessary to carry out this therapy, in order to take advantage of the new neutron beam facilities that are planned worldwide.[1] Regarding the drugs for BNCT it is known that an improvement in targeting is needed.[2] Therefore, our synthetic research is focused on obtaining molecules with high boron content that would be able to target cancer cells, by means of linking analogs of ligands for receptors that are overexpressed in cancer cells to one or many icosahedral boron clusters (Figure 1). The architecture of the molecules also allows the presence of imaging groups such as DOTA, which means they will be able to selectively perform BNCT while we are able to locate them in the body.

COSAN has shown promise as a boron carrier in cell studies.[3] Based on this, two new drugs were synthesized by linking COSAN to Tyr_3-octreotate, a Somatostatin analog. These drugs have been tested in cell cultures and in animals with triple-negative breast cancer for imaging, with promising results. The patent for these new drugs has been submitted.[4]

Regarding drug administration, LabsinLove is also performing studies with BPA-mannitol conjugate, which is an alternative to BPA-fructose for fructose-allergic patients. Furthermore, the company also offers its expertise for the characterization of new neutron beams and radiobiological studies.

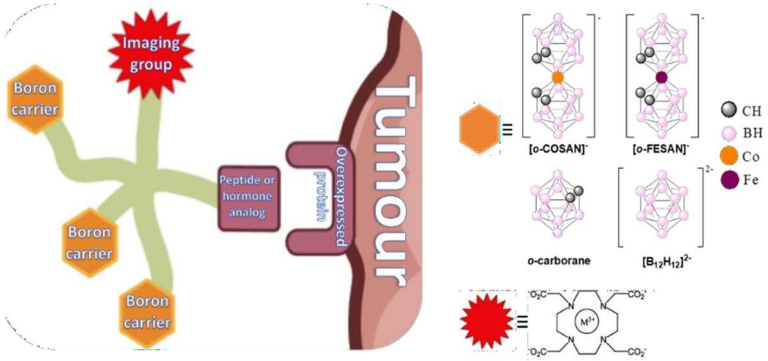

Figure 1 Left: Architecture of new drugs for BNCT. Right: Chart for boron clusters and imaging groups.

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Can the Relationship Between 3D and 2D Aromatic Systems Be Reconciled? The Possible Conjugation via the Different Edges of Borane Clusters

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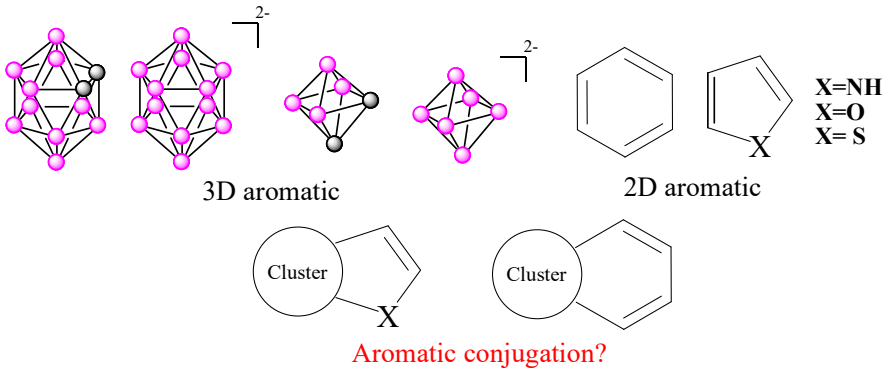
The potential aromatic conjugation between 3D and 2D aromatic units has been a topic of interest since the synthesis of benzocarborane. It has been demonstrated that in 3D aromatic icosahedral 1,2-dicarba-closo-dodecaborane systems fused with 2D aromatic rings, a global 3D/2D aromaticity does not exist.[1,2] Nevertheless, in recent years, several studies have suggested interactions between 2D and 3D aromaticmoieties. Therefore, we have computationally studied various systems,[2] focusing on different aromatic descriptors. However, there are several pitfalls that may lead to an overestimation of the 2D aromatic character of these compounds. The magnetic field of the carborane has a significant impact over a large radius around the cluster and it can be solely responsible for distinguishing between the nuclear independent chemicals shift values., which were widely used for estimation of aromatic character. Moreover, ring strain is depend on the type of the cluster, strongly influencing the overall stability of these systems, which may attributed to their global aromatic characters. Certain conjugative properties can be attributed to the well-known effect of negative hyperconjugation, [3] which is rather a local effect. [4]



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Novel boron-based Arginase 1/2 Inhibitor OATD-02: From Discovery to Clinical Trials in Cancer Immunotherapy

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Over the past decade, the range of boron-based drug candidates has grown significantly, particularly in the area of boronic acid-based arginase inhibitors. Arginases (ARG1 and ARG2) are manganese-dependent metalloenzymes that catalyze the conversion of L-arginine to L-ornithine and urea. Elevated levels of ARG1/2, released by immunosuppressive cells (e.g., MDSCs, TAMs, CAFs) or cancer cells, deplete arginine in the tumor microenvironment, thereby inhibiting the immune response and promoting tumor progression. Arginase inhibitors have the potential to enhance cancer immunotherapy.[1]

Here, we report the discovery and development of **OATD-02**, a first-in-class, low nanomolar dual ARG1/2 inhibitor with high intracellular activity. **OATD-02** has demonstrated a unique pharmacokinetic profile (PK) in animal models and favorable PK predictions in humans. It has also shown strong pharmacodynamic effects correlating with antitumor efficacy. **OATD-02** is currently in a late-stage Phase 1 dose-escalation clinical trials for cancer immunotherapy.[2]

Additionally, we present two backup series of peptide-like boronic acid-based arginase inhibitors. The first one consists of piperidine derivatives with low intracellular activity, primarily targeting extracellular arginase. These compounds have shown good *in vitro* inhibitory potential, favorable pharmacokinetics, and moderate-to-high oral bioavailability.[3]

The second series includes peptide-like boronic acids designed as derivatives of the clinical candidate **OATD-02**. These compounds have demonstrated high *in vitro* activity and antitumor efficacy in a murine model of colorectal carcinoma without safety concerns.

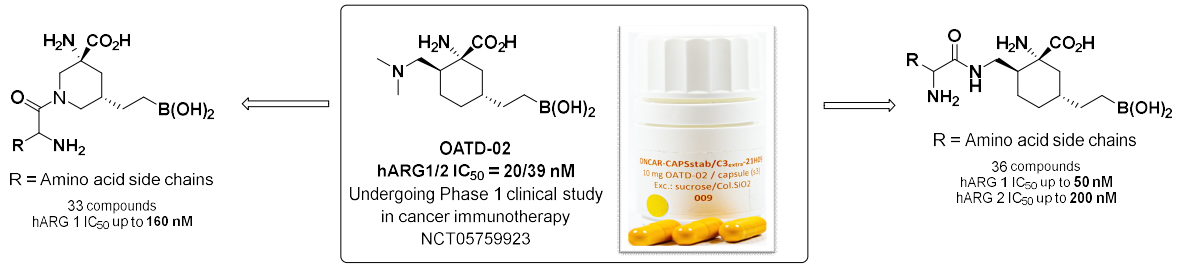

Fig. 1. OATD-02 clinical candidate and its backup series

This study was supported by the project: Pre-clinical and clinical development of arginase inhibitor for application in anti-cancer immunotherapy (POIR.01.01.01-00 0415/17), acronym ARG- co-financed by the National Centre for Research and Development in the framework of the European Funds Smart Growth and European Regional Development Funds.

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Gold(I) and Platinum(II) Complexes Bearing Direct P-B Bonds

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Metal complexes that contain both a Lewis acid and a Lewis base as ligands exhibit intriguing ambiphilic properties.[1] Since boron acts as an electrophile and phosphorus as a nucleophile, we found bromo(phosphino)boranes, **R(Br)BPR'$_2$** (R = amino, alkyl, aryl; R' = alkyl, aryl), particularly interesting to investigate as ligand precursors for transition metal complexes.

The exploration of bromo(phosphino)boranes as precursors has led to the development of novel gold(I) and platinum(II) complexes featuring direct phosphorus–boron (P–B) bonds (Figure 1). Reactions between bromo(phosphino)boranes and N-heterocyclic carbenes (NHCs) yielded stable phosphinoborenium cations, characterized by a planar trigonal boron center bonded to a pyramidal phosphanyl group. These cations demonstrated the ability to act as phosphido group donors, undergoing heterolytic P–B bond cleavage upon reaction with AuCl·SMe$_2$, resulting in gold(I) complexes.[2]

Additionally, the oxidative addition of bromo(phosphino)boranes to platinum(0) compounds facilitated the formation of platinum(II) complexes with unprecedented side-on coordination of the phosphinoboryl ligand.[3]

These findings highlight the versatility of bromo(phosphino)boranes in constructing metal complexes with direct P–B bonds. Moreover, depending on the reactants, either B-P or B-Br bond activation occurred.

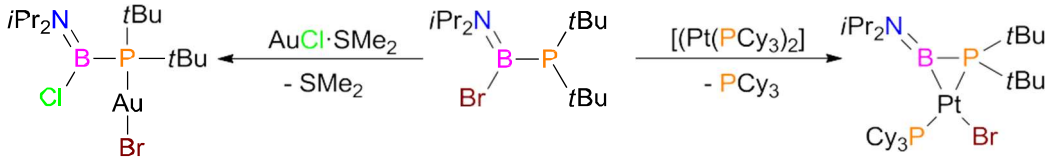

Figure 1. Selected reactivity patterns of *i*Pr$_2$N(Br)BP*t*Bu$_2$ with Au(I) and Pt(0) metal centers.

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Novel Boronated Monocarbonyl Analogues of Curcumin (BMAC) to access Boron Neutron Capture Therapy (BNCT) in the treatment of Alzheimer's disease

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Alzheimer's disease (AD) is the most common form of dementia. Currently, over 55 million people worldwide live with dementia and the number is expected to grow to 139 million by 2050. Despite the ongoing debate on AD pathogenesis, the central role of the misfolded β- amyloid (Aβ) is still widely accepted. Studies identified Aβ oligomers as the most neurotoxic species.[1] Curcumin is currently being investigated for its capability of preventing the neuronal damage observed in AD.[2] However, its clinical use is limited due to its low stability, therefore Monocarbonyl Analogues of Curcumin (MAC) were investigated thanks to their improved features.[3] Pivoting on our long standing research in BNCT and theranostics,[4] we recently began to study the application of NCT against AD. In accordance with the amyloid hypothesis, we present the synthesis and biological investigations on novel carboranyl derivatives with high affinity for Aβ plaques, aiming at triggering the disaggregation process upon BNCT.

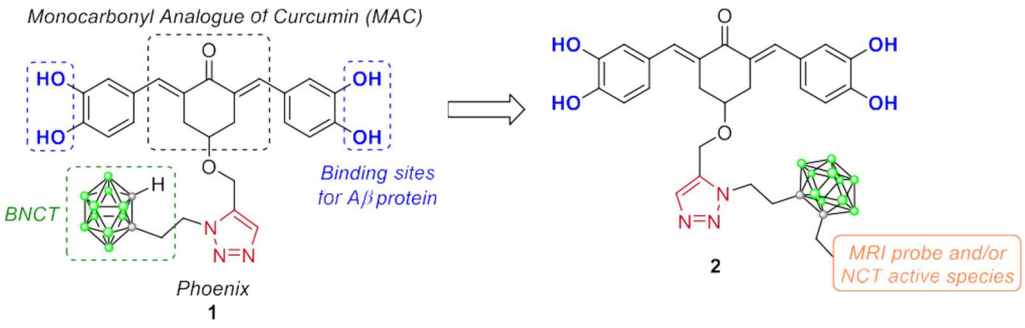

Figure 1 Left: Structure of the BMAC Phoenix **1**; Right: target theranostic agent bearing a MRI probe **2**.

The boronated MAC **1** was synthesized in order to have a strong binding to Aβ protein, thanks to the four OH groups, then a *o*-carborane was introduced to access BNCT. *In vitro* and *in vivo* investigations have been carried out. Our ongoing research is focusing on the introduction of a suitable moiety which can act as MRI probe (**2**), to monitor the biodistribution of the agent, and/or as NCT active species, to improve the therapeutic efficiency.

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Unexpectedly Efficient CO2 Binding in Phosphine Borane Anions

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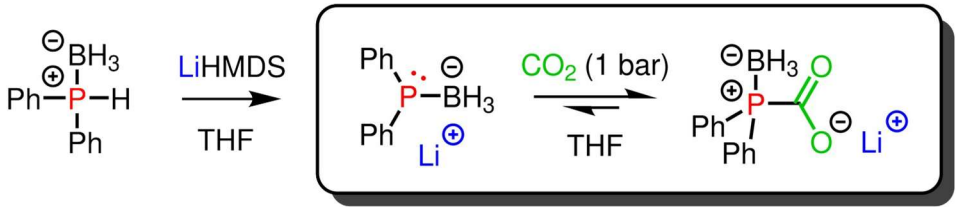
Finding efficient approaches for scavenging CO_2 from dilute sources presents a substantial challenge on the path to zero-carbon economy. While many amines possess excellent ability to bind CO_2, phosphines generally do not form stable CO_2 adducts with the notable exception of a few phosphorus superbases.

Here we report a rare case of a moderately basic phosphorus compound exhibiting unusually strong CO_2 binding. We demonstrate that anionic phosphine BH_3 complexes prepared by deprotonation of secondary phosphine boranes have CO_2 binding ΔG of −8.2 to −23.1 kcal/mol in THF depending on the counterion and the substituents at the P atom. At the same time, these phosphine borane anions are considerably less basic than other CO_2-binding phosphines. Brønsted basicity of our phosphine borane anions is no less than 15 pK_b units lower than that of the previously reported P superbases displaying similar CO_2 affinity, and is comparable to that of the *tert*-butoxide anion.



Anionic phosphine borane CO_2 complexes prepared in this work have been fully characterized by multinuclear NMR spectroscopy, single crystal X-ray diffraction, IR spectroscopy and TGA. Furthermore, ^{13}C labeling studies were used to confirm that the P-COO^- unit in the adduct is indeed derived from the CO_2 introduced into the reaction vessel. Work is underway to develop a new generation of more robust CO_2-binding phosphine borane systems by shutting down decomposition pathways such as P–B bond cleavage.

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Boroxazolidones as safe active agents in mice brain

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Boron-containing compounds are bioactive compounds with increasing potential as drugs for humans [1]. Effects induced by administration of some boroxazolidones (adducts of amino acids and borinic acids) have shown diverse activity in the brain [2]. Among these actions are decreasing of parkinsonism in drug-induced murine models of Parkinson disease [3], limiting the memory loss observed after gonadectomy (and hormones depletion) [4], as well as activity in the neuron excitation [5].

In this work, the effects of boroxazolidones on the motor symptoms induced by MPTP administration, associated with Parkinson's Disease are presented. But also, the toxicity of these compounds in vitro for astrocytes and neurons is described. Two tested compounds induced amelioration of MPTP-induced parkinsonism, judged by performance in open field, grasp and rotarod tests, difference is in dependence of the structure of compound. The toxicity of these compounds in astrocytes and neurons cell cultures showed that induced damage was observed just at concentrations ≥200 μM. These data support the potential of these compounds as promissory tools for neurodegenerative motor diseases.

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Carborane-decorated siloles with highly efficient solid-state emissions – what drives the photophysical properties?

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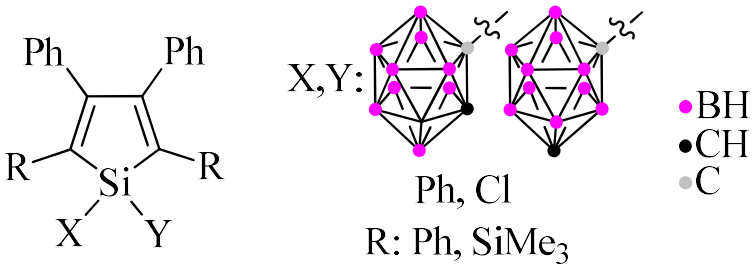
Aggregation-induced emission (AIE) is a unique photophysical phenomenon where compounds are found to be weakly or not fluorescent in diluted solution but highly fluorescent when aggregated. This unique behavior was first described in the case of siloles.[1] Most of these compounds do not show significant fluorescence in diluted solution because nonradiative relaxation occurs due to the rotation of the different substituents of the silole ring. These rotational motions are hindered in the aggregate state; the fluorescence could be recovered in the aggregate or solid state. Later, the same behavior was described in the case of the 3-dimensional *o*-carborane compounds. Still, unlike siloles, the AIE behavior could be attributed to C-C bond vibration within the cluster framework.[2] Questions arise about how the system derived from combining the two types of AIE active compounds behaves.



In our work[3], we have synthesized and structurally characterized a series of air-stable compounds by linking carboranes and siloles, both of which are known as aggregation-induced emission active units. Although most of the newly synthesized systems do not display notable quantum yield either in solution or in the aggregated state, they emit strongly in the solid-state, and a quantum yield of up to 100% can be achieved. The tailorable quantum yield can be attributed to the packing of the molecules in the crystal lattice ruled by the carborane and phenyl moieties according to the SC-XRD data. Our experimental results, complemented by density functional theory calculations, show that the silole moiety primarily influences the photophysical properties. At the same time, the carborane serves as a steric building block without direct responsibility for the aggregation-induced emission property. The patterns of substituents can alter the absorption and emission properties.

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Advances in Diclofenac Derivatives: Exploring Carborane-Substituted N-Methyl, Nitrile, Amidine and Lactam Analogs for Anti-Cancer Therapy

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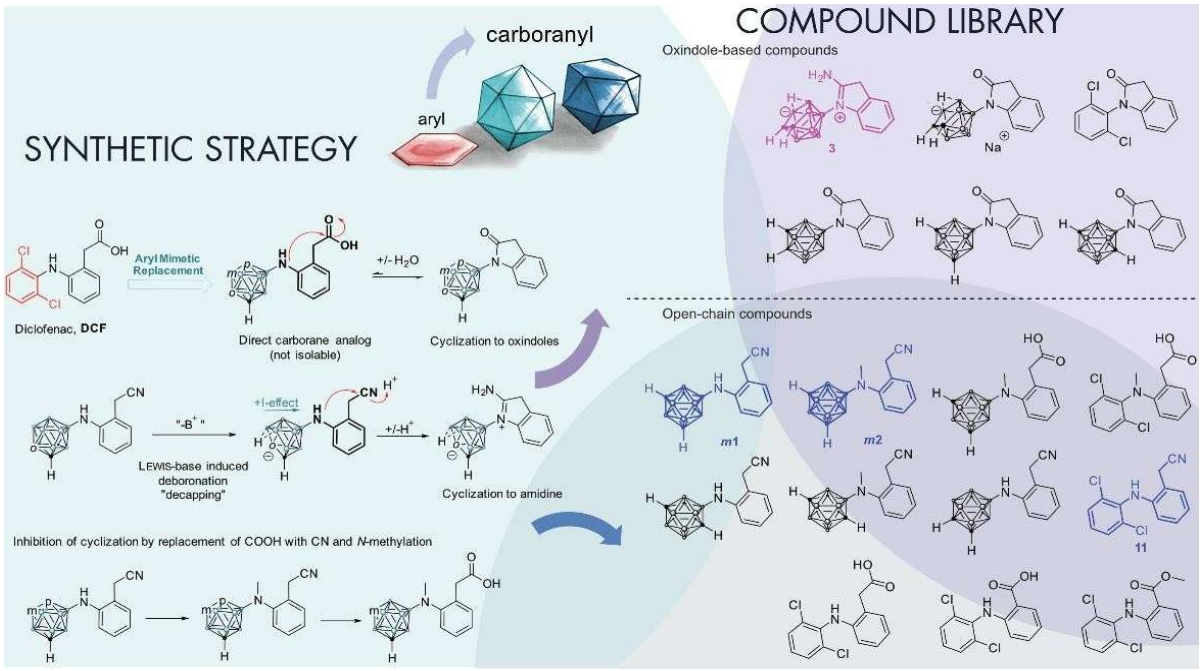

Figure 1. Overview of design concept, synthetic strategy and compound library of the phenyl- and carboranyl-based analogs of diclofenac.

We herein present our recent research efforts to design novel anti-cancer agents based on the well-established diclofenac framework fused with carborane clusters. Our studies focused on synthesizing and testing a range of carborane-substituted (pro)drug analogs of diclofenac featuring cyclic lactams and amidines as well as *N*-methylated open-ring derivatives. These compounds were evaluated for their anti-cancer potential against various colorectal cancer cell lines, including murine colon adenocarcinoma (MC38) and human colorectal carcinoma (HCT116, HT29). The redesigned molecules demonstrated a spectrum of anti-cancer activities, with one zwitterionic amidine species showing particularly strong cell division inhibition and selective cytotoxicity in MC38 cells, likely through both, COX-dependent and independent pathways. Our findings highlight the potential of carborane-based prodrugs as innovative cancer therapeutics, offering insights into their mechanisms and applications.

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Direct B-H xanthylation of closo-carboranes via photoinduced Hydrogen Atom Transfer

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Icosahedral carboranes (i.e., $C_2B_{10}H_{12}$) are polyhedral boranes which, owing to their chemical stability and synthetic versatility, find unique applications ranging from medicine, as promising Boron Neutron Capture Therapy (BNCT) agents, to smart materials.[1] Currently, the heterolytic activations of B-H sites generally require costly transition metal-based catalysts and pre- installed moieties acting as directing groups.[2] Meanwhile, visible light-mediated processes have attracted increasingly high interest from the scientific community in recent years, allowing the generation of versatile radical intermediates in a controlled fashion under mild reaction conditions. In this context, *N*-xanthylamides have displayed valuable synthetic applications as precursors of highly reactive Hydrogen Atom Transfer (HAT) agents, allowing direct C-H xanthylations.[3] Furthermore, the installment of the xanthyl moiety represents a valuable synthetic handle for further functionalizations, such as thioetherification, azidation and alkylation.[4]

Despite the great potential of photoinduced HAT strategies for B-H derivatizations in the field of carborane chemistry, only few examples have been reported in the literature so far.[6]

In this work, we disclose our ongoing efforts in the direct activation of B-H sites among ten chemically similar vertices on *closo*-carborane clusters, accessing xanthyl carboranes as novel synthetic platforms.

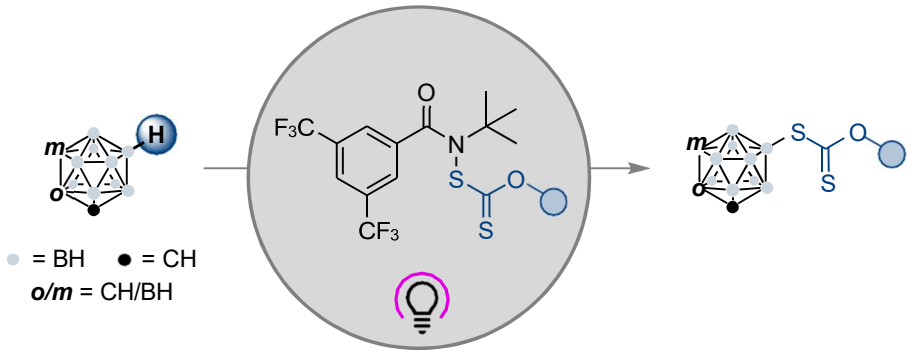

Figure 1. Photoinduced xanthylation of *closo*-carboranes.

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The “chemical tug-of-war” in carborane clusters: distinct tuning on different sides of the cluster

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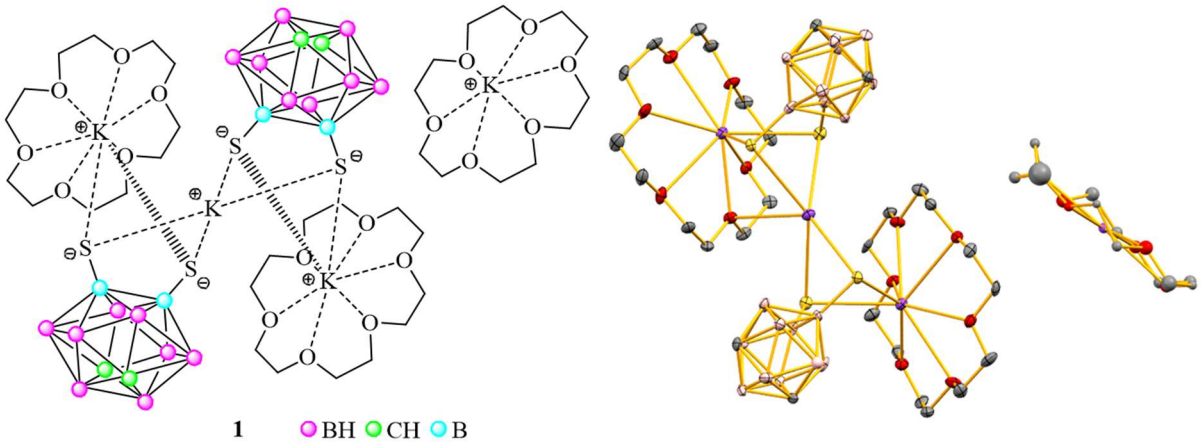
The special C–C bond in icosahedral *closo*-dicarbadodecaboranes has high plasticity, which has been investigated several times using different substituents.[1-3] In the case of other bonds within the carborane clusters have not been investigated yet.

In our work, DFT calculations demonstrated that stretching of B–B generally requires more energy, however the elongation is ruled by the same effects as the well-investigated C–C bond. The most promising derivatives were synthesized, and the effects of the variation of π-donor substituents were examined to the length of the B–B bond. In the case of the 9,10-*m*-carboranyl-disulfanide derivatives (**1**), the B9–B10 bond distance is elongated up to 1.92(2) Å. [4]



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Transition metal vs. orrganocatalyzed hydrometallation reactions

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Organoboron compounds are key reagents in modern organic chemistry due to their high stability, low toxicity, and unique reactivity.[1] Transition metal (TM) catalyzed processes still dominate this branch of chemistry, but main group elements catalysts or organocatalysts start to play an important role as well, often leading to different products compared to traditionally TM-catalyzed hydrometallation reactions.

Our research focuses on the practical and highly selective methods of the synthesis of organoboron compounds based on the hydroboration, and coupling reactions of olefins, alkynes, conjugated 1,3-diynes, carbonyl compounds, imines, and nitriles.[1-7] The communication will discuss the new methods for the functionalization of these compounds using practical and straightforward catalytic systems based on TM and organocatalysts. We will prove that the proper selection of readily available catalysts might significantly influence or change the process regio- and stereoselecitivity.[1-9]

Acknowledgments: Financial Support from the National Science Centre (Poland), no. UMO-2019/34/E/ST4/00068.

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Boracyclic cores as acceptors within extended CT TADF emitters

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Thermally activated delayed fluorescence (TADF) phenomenon is of broad interest to researchers thanks to applicability of TADF emitters in OLED displays and possibility to expand correlation between molecule structure and its photophysics. This effect comprise RISC from triplet to singlet excited state and subsequent fluorescence, allowing to harvest triplet excitons in electroluminescence process. TADF emitters should be characterized by separation of frontier molecular orbitals. This separation is usually achieved upon introducing strong donor and acceptor fragments. The latter often contain boron atom, which enhances electron deficiency of the fragment.

A series of borole-fused cores was synthesized by sequence of organometallic reactions. As a consequence of both antiaromaticity of borole ring and presence of electron withdrawing groups, boron centers show strong Lewis acidity, existing in the water complex form, as confirmed by ^{11}B NMR analysis and theoretical calculations. In reactions with aromatic proligands under mild conditions, it forms chelate complexes. Boracyclic cores have been functionalized with ligands based on donor-acceptor and donor-acceptor-donor architectures to achieve TADF materials.

The compounds show intense emission, with color strongly dependent on solvent polarity, indicating the formation of a charge-transfer excited state. Transient photoluminescence decay characteristics, as expected, show delayed fluorescence. Furthermore, quantum calculations of the energy and nature of the excited states of the studied emitters provide an argument for attributing the experimentally observed delayed fluorescence to TADF.

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Cobaltabis(dicarbollide) ([*o*-COSAN]$^-$) loaded APOFERRITIN: An innovative high-capacity boron delivery system to target tumour cells for BNCT applications.

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This study describes an innovative apoferritin-based nanohybrid, Apo:[o-COSAN]$^-$, as a high-capacity boron delivery system for potential application in Boron Neutron Capture Therapy (BNCT)[1]. The nanohybrid is characterized by an high boron content, stability, and promoting biological interactions of cobaltabis(dicarbollide) ([o-COSAN]$^-$)[2], encapsulated within the apoferritin protein cavity through an acid-induced dissociation and reassembly process. The Apo:[o-COSAN]$^-$ nanohybrid demonstrated enhanced boron uptake in MCF7 breast cancer [3] and AB22 mesothelioma cell lines [4], with superior stability and biocompatibility under physiological conditions. Notably, AB22 cells treated with Apo:[o-COSAN]$^-$ showed significant cytotoxic effects following neutron irradiation, highlighting the potential of this system in BNCT. These findings underscore the versatility of apoferritin as a multifunctional nanocarrier for targeted cancer therapy, combining high boron payloads with selective tumor cell uptake.

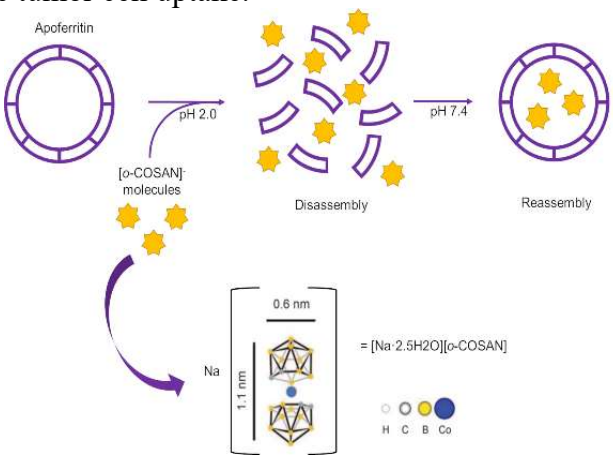

Figure 1: Schematic representation of [*o*-COSAN]$^-$ molecules encapsulation strategy in the Apoferritin cavity using the pH changing method.

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Boron Clusters for Protein Delivery

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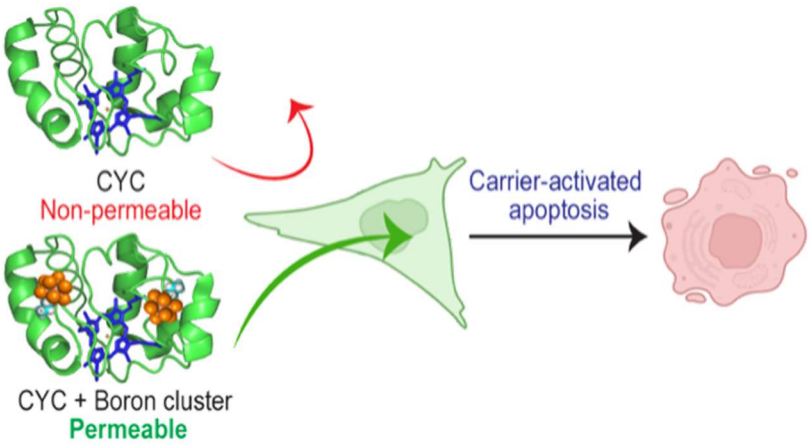
Intracellular protein delivery is a transformative strategy in biological and pharmaceutical research. The delivery of intrinsically impermeable proteins into living cells can replace poorly expressed, dysfunctional, and missing proteins, or regulate key intracellular metabolic or signaling pathways.[1] The direct delivery of proteins into the cytosol is highly desirable to achieve biological activity, as it allows a continuous, endocytosis-independent migration into the subcellular organelles or nucleus.[2] Molecular carrier approaches, which exploit small-molecule additives to activate intracellular uptake, present an appealing method with long-term therapeutic potential.

Inorganic boron clusters of the icosahedral dodecaborate[3] and cobalt bis(dicarbollide) type[4] have been introduced as an unconventional class of molecular carriers; these inorganic anions draw their carrier potential from their superchaotropic ionic nature.[5] Most recently, we have applied the boron cluster approach to the intracellular delivery of a functional membrane-impermeable protein, cytochrome c,[6] which was internalized into cells through a direct permeation pathway into the cytoplasm. Most importantly, cytochrome c retained its bioactivity, reflected by an induced apoptosis. We now report the cluster-mediated transport of other proteins which have been difficult to transport – with largely varying molecular weight (4.6-170 kDa) and *p*I values (0-12) – confirming the potential of boron cluster anions as protein transport vehicles with an extensive potential for biomedical applications.



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L-Cystine diphenylborinic-adduct as Fatty Acid Amide Hydrolase inhibitor

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The endocannabinoid system has been recognized as novel therapeutical target for some neurodegenerative diseases such as Parkinson, Alzheimer, neuropathic pain and depression [1,2]. The main receptors expressed in this system are the type 1 (CB1) and the type 2 (CB2), recently it has been demonstrated that the neurotransmitter modulation through the activation of cannabinoid receptors, CB1 and CB2, exhibit neuroprotective effects [3]. These effects can be reached by the endocannabinoids but their hydrolysis pathway mediated by enzymes reduce the availability of this substances. On the other hand, the use of boron compounds has demonstrated neuroprotective effects, enzyme inhibition [4] and improvement in the cognitive function in animal models [5]. The present work includes the design and in silico evaluation of L-cystine diphenylborinic-adduct as inhibitor of the fatty acid amide hydrolase as an alternative for maintain the synaptic concentrations of endoccanabinoids and modulate the neurotransmission through activation of cannabinoid receptors.

The in silico evaluation was performed using different databases available online, SwissAdme was used for elucidate the apparent pharmacokinetics and physicochemical properties of the compound. BindingDB was used for select more than 100 ligands that exhibit non-covalent inhibition in the enzyme and validate their affinity in the catalytic site by Docking simulations (PDB: 6MRG). As complementary in this study, DFT calculations were performed to predict the antioxidant mechanism of the precursor of the main boron containing compound, L-cisteine diphenylborinic adduct.

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In silico evaluation of boron containing compounds as Histaminergic modulators

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The histaminergic system is a therapeutical target to treat some diseases involving the central nervous system, cardiovascular system and gastrointestinal system. The main receptors expressed in this system are the H1, H2 and H3[1]. The effects exhibited when these receptors are activated are the neuromodulation (only H1 and H3 receptors) and the gastric acid secretion (H2 receptor). The neuromodulation effect associated to these receptors could be a novel treatment for some neurodegenerative diseases [2]. The neuromodulation is the main objective in the present work than includes the design and in silico evaluation of different boron containing compounds derived from L-amino acids.

The in silico evaluation was performed using the FASTA sequence of the human H3 receptor and a new model was created using the Swiss Model server [3]. The IUPHAR database [4] was employed to obtain the main ligands active in the histaminergic system and then, these structures were coupled in the H3 receptor model to obtain the free energy of binding and correlate the calculated affinity with the reported (experimental) pKi available in the database. The possible binding sites in the model were predicted with the FTmap server [5]. All boron containing compounds reach the orthosteric binding site in the H3 receptor model as predicted with the mapping and exhibit free energy of binding in ranges from -8.0 to -9.9 kcal mol^{-1}.

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High Resolution Mass Spectrometry as a Tool For Distinguishing the Different Substituted Cobalt Bis(Dicarbollide) Ions

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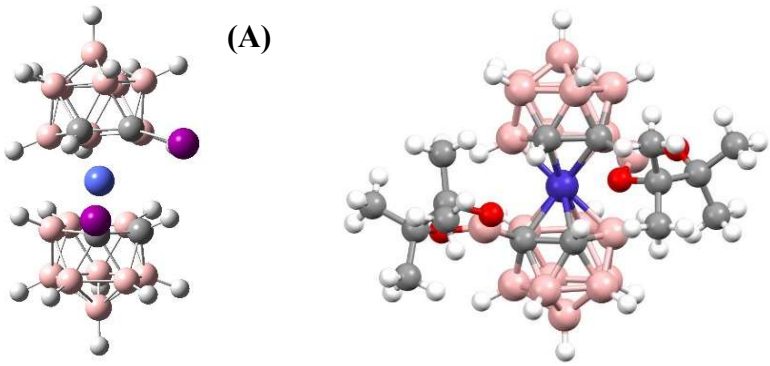
High resolution mass spectrometry (HRMS) has undergone a thrilling phase of technological evolution. HRMS is used in analytical chemistry to measure ions' mass-to-charge ratio (*m/z*) with high precision and accuracy. Unlike standard MS, which typically provides a lower resolution, HRMS offers much more detailed information about the analyzed compounds. HRMS can discriminate compounds with the same nominal mass by precisely measuring their specific mass defect, which is the difference between the exact and nominal mass. This technique is particularly valuable for identifying compounds and analyzing complex samples in research settings, as we show here, also in boron cluster chemistry. In this post, we would like to show some examples of HRMS measurements using direct sample infusion, from the perspective of a qualitative tool in measuring variously substituted cobalt bis(dicarbollide) ion ($COSAN^-$).[1] With the main focus on scenarios where the results show overlapping or matching nominal masses between the analyte being analyzed and its minor products, starting materials, or unexpected products (see an example below). We show here that MS with the direct introduction of a sample into the mass spectrometer's ionization source, leads to a more streamlined process, and enables reliable identification of anionic boron species, especially when the complexity of the sample does not require detailed separation or fractionation.

(A) **(B)**



	Peak Maximum (*m/z*)		Isotopic Mass (*m/z*)	
	Calculated	Experimental	Calculated	Experimental
rac-I_2-$COSAN^-$ (**A**)	576.0778	576.0773 (100%)	579.0678	579.0673 (M^-, 12%)
rac-$Bpin_2$-$COSAN^-$ (**B**)	576.4559	576.4553 (100%)	579.4484	579.4477 (M^-, 12%)

Acknowledgment: Support from Czech Science Foundation, project No. 25-16216S

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Laterally Extended Azaborole Helicenes Containing a Five-Membered Carbocyclic Ring

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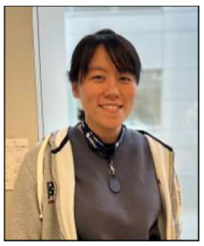

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Polycyclic aromatic hydrocarbons (PAHs), which are composed of six-membered rings of sp^2-hybridized carbon atoms leading to fully planar structures and extended π-conjunction systems, are commonly studied in organic electronics and optoelectronics.[1-3] Boron atoms incorporated into PAH scaffolds can be stabilized by donation of electron density from the lone electron pair of the heteroatom to the unoccupied p_z orbital of boron, which enhances the charge-transport characteristics of the molecules.[4] Our group has shown that the lateral extension of the pristine azabora[7]helicene has led to enhanced quantum yield and luminescence dissymmetry factor.[5,6] Further modulation of optical properties can be achieved by introducing five-membered carbocyclic rings into the system.

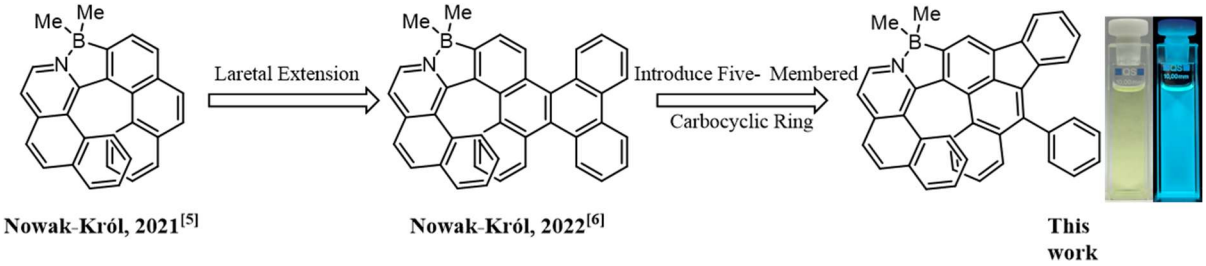

Figure 1. Structural changes leading to enhanced fluorescence quantum yields of the azaborahelicenes developed by our group.

In this work, we introduced a five-membered carbocyclic ring into the laterally extended part of our π-extended azabora[7]helicene. The resulting compound showed blue fluorescence with maximum at 469 nm, and an improved fluorescence quantum yield. The attractive optical properties of the new compound indicate its potential for application in chiral optoelectronic devices.

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Molecular dynamics simulations of a boroxazolidone on D2 dopamine receptor and probable relationship to motor performance of C57BL/6 mice

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Parkinson's disease is a progressive neurodegenerative disorder characterized by the loss of dopaminergic neurons in the substantia nigra, resulting in decreased dopamine levels in some basal nuclei. As a result of this deficiency, some classic motor symptoms are observed, such as tremors at rest, rigidity, bradykinesia, and postural instability. Although conventional pharmacological treatment, based on levodopa and dopamine D2 dopamine receptor (D2DR) agonists, continues to be considered the therapeutic standard, the search for efficient and safe compounds is ongoing [1].

Thus, boron-containing compounds are presented as compounds with unique properties, such as the ability to form reversible bonds with diol groups and increase selectivity towards certain biological targets, but also with probable action modulators of inflammatory pathways and antioxidants [2]. Among these, borolatonin, a boroxazolidone derived from tryptophan has attracted attention for its effects as a neuroprotector and modulator of cognitive processes, but also for probable interaction with monoamine receptors [3,4].

In this work, molecular dynamics on D2DR were carried out as it is considered a key target in the treatment of Parkinson's motor symptoms, comparatively to the endogenous ligand dopamine. Still, rotarod tests and grip tests were performed on C57BL/6 mice previously induced to the parkinsonian syndrome by intoxication with 1-methyl-4-phenyl-1,2,3,6 tetrahydropyridine (MPTP) and compared with healthy mice, and intoxicated treated with levodopa. Molecular dynamics showed increased movements in D2DR when borolatonin was added, while improved performance in C57BL/6 subjects treated with borolatonin was observed; it was notable in regards of the coordination, balance, and motor skills in the tests, compared to conventional levodopa treatment. In conclusion, borolatonin could be an option in motor disturbances in mice, its effect could involve enhanced interactions and activity on D2DR.

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Merging Pyrrole with Boron: p-π*-Conjugated Di-(2-pyrryl)boranes

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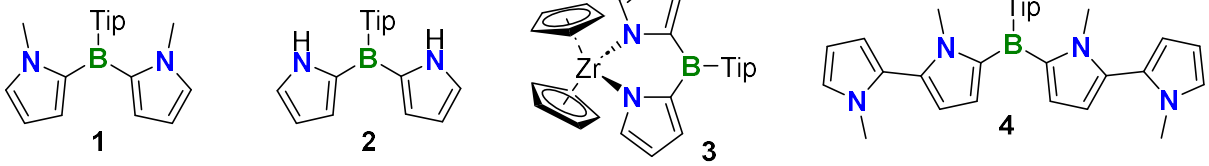
During the last decades, π-conjugated materials in which electron-rich organic building blocks are combined with electron-deficient borane moieties have received tremendous attention due to their applications in organic optoelectronics, sensors, and bioimaging.[1,2] Thiophene derivatives have been extensively studied in recent years in this regard.[3-5] Our group has also introduced furan units into boron-doped conjugated materials, which in combination with our Si/B exchange protocol enabled a sustainable approach to strongly luminescent hybrid materials.[3,6,7] Pyrrole congeners thereof, on the other hand, have scarcely been studied.

We developed a multigram scale synthesis of a dipyrryl(tri-*iso*-propylphenyl)borane with methyl groups on the nitrogen atom (**1**) as well as an unprotected derivative (**2**). The structures of both compounds were determined by single-crystal X-ray diffraction, revealing an almost planar structure of the dipyrrylborane unit in **2** and only a slightly twisted one for **1**. The new compounds are intense blue-light emitters due to a TICT character of the excited state structure, as confirmed by TD-DFT calculations. We also investigated the formation of a transition metal complex (**3**) and further extended π-systems such as **4**.[8]



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Production of New Boron Citrate Ester Compounds as Nutritional Supplementation Agents

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Boron is an essential element for animal and human biology. Studies on boron have shown that it plays an important role in bone development, particularly due to its ability to activate calcium and magnesium metabolism in animal cells. It has been found to help prevent the development of osteoporosis and, when regularly consumed by postmenopausal women, to reduce the excretion of calcium, magnesium, and phosphorus from the body. It is also known to potentially play a role in wound healing. Additionally, recent studies have suggested that boron may be effective in preventing the development of certain types of cancer.[1,2] However, known boron supplement forms have begun to be questioned after some time due to reasons such as accumulation in tissues instead of bone marrow. For this reason, the presence of boron complexes similar to natural boron esters on the market has been increasing day by day. This trend started with calcium fructoborate, the first compound whose molecular structure was characterized.[3] Since then, the synthesis and commercialization of esters of new sugar molecules and other biologically active ligands have become an area of interest.[4] In particular, fructoborates have been used as dietary supplements to support healthy bones and joints. More recently, they have also been used in vitamin D metabolism, prostate health, and the regulation of steroid hormone levels.[4,5] In this study, mono-and di-esters of fructose ligand, which are not produced in Türkiye but are approved as food supplements in the USA (by FDA) and Europe (by EFSA), and used in markets of the USA and many other countries, have been synthesized. The structural properties of the synthesized compounds—molecules obtained in solid form from aqueous solutions using a spray dryer—were analyzed using elemental analysis, melting point determination, infrared spectroscopy (FT-IR), thermal analysis (TGA/DTA), mass spectrometry (GC-MS), and single crystal X-ray diffraction (SC-XRD). Compliance studies with the food codex were conducted for the structurally analyzed molecules, and their inclusion in the Turkish Food Codex was achieved. Following structural characterization and codex compliance studies of the synthesized boron ester compounds, they were produced in micron-sized form for commercial use at laboratory and pilot scales. Subsequently, these molecules were introduced to the market as boron-containing dietary supplements.

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Synthesis and characterization of chiral organoboron PAHs for bioimaging application

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Fluorophores are essential for imaging cells, tissues, and living organisms, significantly advancing biological and biomedical research. Ideal fluorophores must possess several key qualities, including long absorption and emission wavelengths, large Stokes shifts, high brightness and stability.[1-4] Although many commercially available and known fluorophores have high molar extinction coefficients and strong fluorescence quantum yields suitable for bioimaging, they often suffer from small Stokes shifts. This limitation leads to poor signal-to-noise ratios and self-quenching in advanced imaging techniques.[2-4] Additionally, small Stokes shifts restrict their use in complex imaging methods, such as single-excitation multicolor imaging.[2] To overcome this limitation, we have developed and synthesized novel chiral boron complexes based on azinylcarbazoles[3, 4] and azabora[*n*]helicene substructures,[5] starting from carbazole.

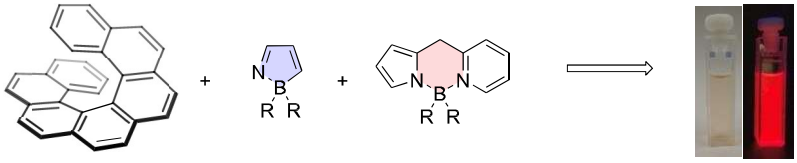

Figure 1. The design of novel chiral boron complexes with NIR emission.

In this poster, we report on the photophysical studies (absorption and emission spectra, CD and CPL measurements) and electrochemical properties (cyclic voltammetry) of these new compounds.

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Silver(I) Salts of the Chlorinated 1-Carba-*closo*-dodecaborate

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Silver(I) salts of weakly coordinating anions are useful one-electron oxidation agents and can be applied for halide abstraction reactions.[1, 2] They also have the ability to coordinate solvents, which leads to polymeric structures in the solid state.[2-4] The chlorinated 1-carba-*closo*-dodecaborate $[HCB_{11}Cl_{11}]^-$ is a versatile and very weakly coordination anion, which has a higher stability compared to the parent $[HCB_{11}H_{11}]^-$ anion.[5]

We report the syntheses and crystal structures of new silver(I) complexes of the chlorinated 1-carba-*closo*-dodecaborate $[HCB_{11}Cl_{11}]^-$ containing various ligands (e.g. C_6H_6, C_4H_8O, CH_2Cl_2). As an example, Figure 1 shows the structure of $[Ag(C_4H_8O)][HCB_{11}Cl_{11}]$. The solvent-free salt $Ag[HCB_{11}Cl_{11}]$ could be obtained as well.

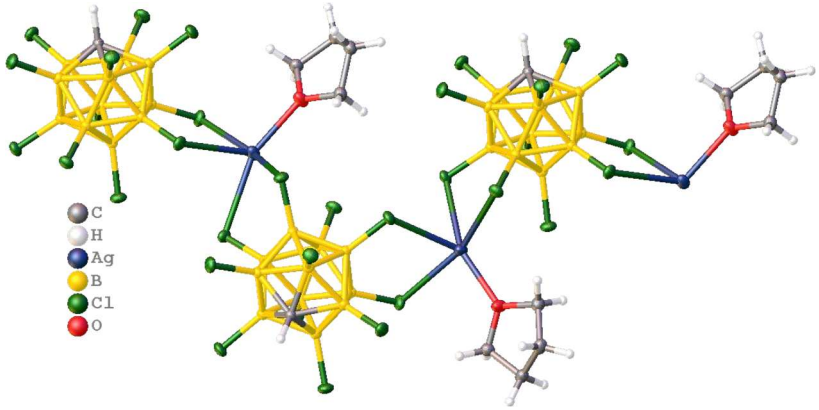

Figure 1: Part of the crystal structure of [Ag(C4H8O)][HCB11Cl11].

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DFT Surface Confirms Experimental Availability of Dianionic and Dicationic Boron Clusters from Neutral Tetrahedral and Octahedral Precursors

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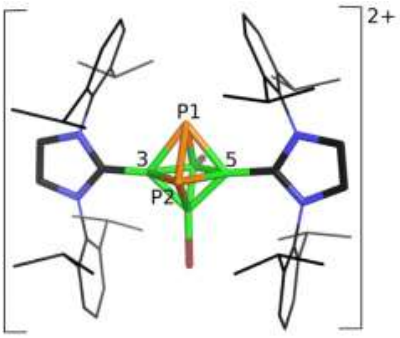
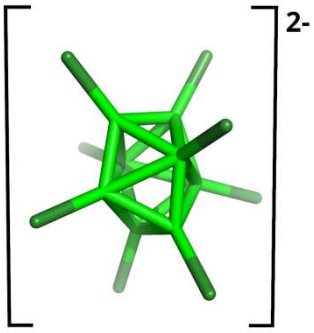
Neutral octahedral heteroboranes, exemplified with *closo*-1,2-Pn_2B$_4$Br$_4$ (Pn = P, As), undergo a reaction with *N*-heterocyclic carbenes (exemplified with *I*dip) to get the monocationic [4-Idip-*closo*-1,2-As$_2$B$_4$Br$_3$]$^+$ and the first **dicationic** motif, i.e. **[3,5-Idip$_2$-*closo*-1,2-P$_2$B$_4$Br$_2$]$^{2+}$**, in this area, with the octahedral molecular shapes retained. In contrast, a neutral tetrahedral B$_4$Cl$_4$ with a symmetry of T$_d$ is reduced with an iodide to yield the **dianionic [B$_8$Cl$_8$]$^{2-}$** of a symmetry of D$_{2d}$. The Jahn-Teller distortion of T$_d$-symmetrical B$_4$Cl$_4$ to D$_{2d}$-symmetrical anionradical [B$_4$Cl$_4$]$^{\bullet -}$ is the driving force of the entire pathway.

The experimental ^{11}B NMR spectra of the both products were verified in terms of applying the DFT (*ab initio*)/GIAO/NMR method. A modern computational protocol examined these two reactions computationally, a few transition states and intermediates having been located in each process. Interestingly, the second reaction may be viewed as of the "1+1=2" type, i.e. no extra product/byproduct originated during this simple reduction.



[3,5-Idip$_2$-*closo*-1,2-P$_2$B$_4$Br$_2$]$^{2+}$



[B$_8$Cl$_8$]$^{2-}$

Supported by the Czech Science Foundation (project no. 25-15887S)

REACTIONS OF *NIDO*-TRICARBOLLIDES WITH VARIOUS ORGANIC AND INORGANIC AGENTS: ORIGINATION OF NEUTRAL AND CATIONIC DERIVATIVES BASED ON 7-Me_3N-*nido*-7,8,9-$C_3B_8H_{10}$

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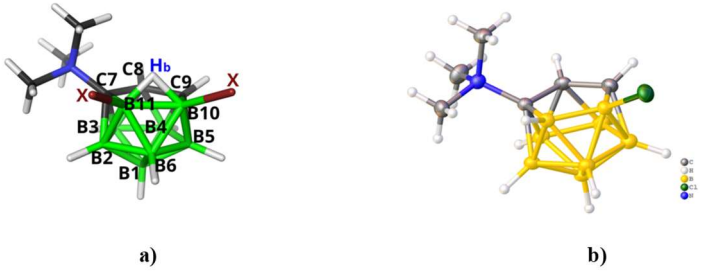
Four pairs of neutral vs. cationic systems based on 10,11-X_2-7-Me_3N-*nido*-7,8,9-$C_3B_8H_{8+q}^q$ (X=H, Cl, Br, I; q = 0,1+, respectively) have been prepared by reacting the parent tricarbollide[1] (Figure 1a) with *N*-chlorosuccinimide, with tetrabutylammonium tribromide and very slowly with iodine in acetonitrile.[2] All these compounds were structurally characterized by the joint experimental/computational DFT/ZORA/NMR method as well as by MS spectroscopy and partly by X-ray diffraction techniques. The chlorination has been attempted in a greater detail, i.e. apart from N-chlorosuccinimide, $PdCl_2$ and $RhCl_3$ were employed (Figure 1b). The last inorganic chlorides have been shown to be more specific and, consequently, provided "only" 10-Cl-7-Me_3N-*nido*-7,8,9-$C_3B_8H_9$, the latter being prone to its protonation as well. The iodination has also been tackled computationally and two "iodonium" cations have been detected. In the form of the electronic structure, the B10-B11 bond in the open pentagonal belt in the neutral species is prevailingly of the classical 2c-2e nature; in the cation, on the other hand, this separation is a part of several 3c-2e bonds, which is also partly true for one of the "iodonium" cations. Interestingly, attempts to fluorinate the parent tricarbollide have failed and different structural patterns have been spotted.



a) b)

Figure 1 a) Molecular diagram of 7-Me_3N-*nido*-7,8,9-$C_3B_8H_{10}$ and its protonized form with H_b with the atomic numbering of the whole cage; b) crystal structure of 10-Cl-7-Me_3N-*nido*-7,8,9-$C_3B_8H_9$.

Acknowledgement
This work was supported by the Czech Science Foundation (project no. 25-15887S).

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Chiral separations of *nido*-[7,8-$C_2B_9H_{12}$]$^-$ and [$Co(C_2B_9H_{11})_2$]$^-$ derivatives

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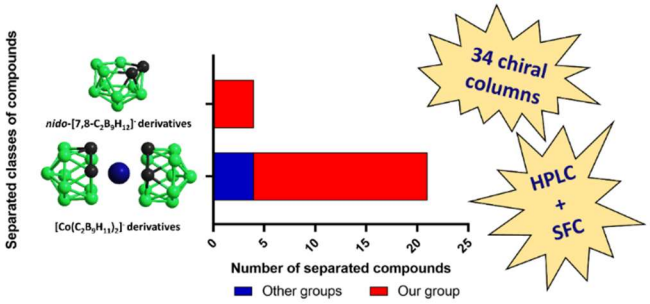
Nido-[7,8-$C_2B_9H_{12}$]$^-$ and [$Co(C_2B_9H_{11})_2$]$^-$ derivatives, are currently under extensive investigation in medicinal chemistry due to their high stability, solubility of their salts in water, and low toxicity.[1] However, some derivatives of *nido*-[7,8-$C_2B_9H_{12}$]$^-$ and [$Co(C_2B_9H_{11})_2$]$^-$ are chiral compounds. Therefore, as it is known since thalidomide affair, the activity and toxicity of individual enantiomers must be examined well before introducing the potential drugs to the clinical trials. The somewhat underdeveloped chiral separations of carboranes hinder the progress of new potential pharmaceuticals based on *nido*-[7,8-$C_2B_9H_{12}$]$^-$ and [$Co(C_2B_9H_{11})_2$]$^-$ that have potential to address the antimicrobial, anticancer, and anti-inflammatory effects.[1] For example, the enhancement of the activity of indomethacin towards COX-2 by "simply" substituting phenyl ring with *nido*-carborane.[2]

In this work, more than 20 different chiral *nido*-[7,8-$C_2B_9H_{12}$]$^-$ and [$Co(C_2B_9H_{11})_2$]$^-$ derivatives were separated into enantiomers using HPLC and SFC. We explored quinine-, cyclodextrin-, polysaccharide-based, and Pirkle type chiral stationary phases in HPLC and SFC. SFC methods with polysaccharide-based columns are superior for [$Co(C_2B_9H_{11})_2$]$^-$ and zwitterionic *nido*-[7,8-$C_2B_9H_{12}$]$^-$ derivatives.[3] HPLC employing 2-hydroxypropyl-β-cyclodextrin can be also used for fast enantioseparations of dihydroxyalkyl-, oxygen bridged hydroxyalkyl-, and bisphenylene bridged derivatives of [$Co(C_2B_9H_{11})_2$]$^-$.[4] The anionic *nido*-[7,8-$C_2B_9H_{12}$]$^-$ derivatives were not previously separated in HPLC and attempts in SFC were also unsuccessful. We developed a method separating anionic *nido*-[7,8-$C_2B_9H_{12}$]$^-$ derivatives in HPLC using native β-cyclodextrin.[5]

All developed methods provide a foundation for chiral separations of [$Co(C_2B_9H_{11})_2$]$^-$ and *nido*-[7,8-$C_2B_9H_{12}$]$^-$ derivatives allowing progress in development of chiral drugs based on these compounds.



Acknowledgment: Czech Science Foundation, project No. 25-16216S.

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Functional ligands based on *closo*-decaborate anion for metal complexes

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The electronic and steric properties of carboranes[1] and *closo*-boranes are attractive factors in designing functional ligands[2-4] for transition metal complexes acting as catalysts, luminescent materials, molecular objects, functional grids or MOFs (metal-organic frameworks). The latter materials typically use homoditopic carborane carboxylic acids as ligands. Among *closo*-boranes, the [*closo*-$B_{10}H_{10}]^{2-}$ anion[5,6] is exceptional due to its D_{4d} symmetry and high lying HOMO with large amplitudes at the apical positions. Despite these features, it received little attention as a structural element of functional ligands.

Herein, we present two new classes of functional ligands for metal-ion complexes based on [*closo*-$B_{10}H_{10}]^{2-}$ anion.

Firstly, a potentially general intermediate [*closo*-$B_{10}H_8$-10-IPh-1-COOH]$^-$ was converted to the pyridinium derivative, an example of a class of functional anionic carboxylic acids, [*closo*-$B_{10}H_8$-10-X-1-COOH]$^{2-}$, and subsequently to coordination complexes with $(phen)_2Cu^{2+}$ and $(phen)_2Zn^{2+}$ ions. The availability of such acids opens access to functional metal-ion complexes with compensated charges.

Secondly, a new class of rigid, photoactive heteroditopic anionic ligands based on the 1,10-disubstituted [closo-$B_{10}H_{10}]^{2-}$ anion was obtained. The design includes two apical substituents, a metal coordinating cyano group and an azinium (4-cyanopyridinium, 4,4′-bipyridynium, pyrazinium, pyrimidinium, and pyridazinium), which provides a secondary binding site. Two of the ligands were converted to (η5-Cp)(dppe)Fe complexes and one of them was used to obtain a heterodinuclear complex with Cu(pdc)$(H_2O)_3$ to demonstrate the ditopic function of the ligand. All three iron complexes were characterized by the XRD method.

ACKNOWLEDGEMENTS

This work was supported by the National Science Foundation (DMR-1611250 and XRD facility CHE-1626549 grants).

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POLYBORAZLENE:
Advanced Epoxy Composites with Borane Compounds

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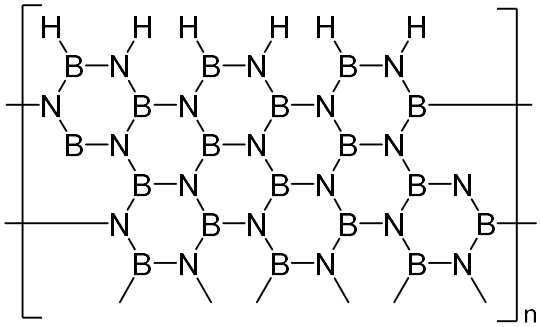
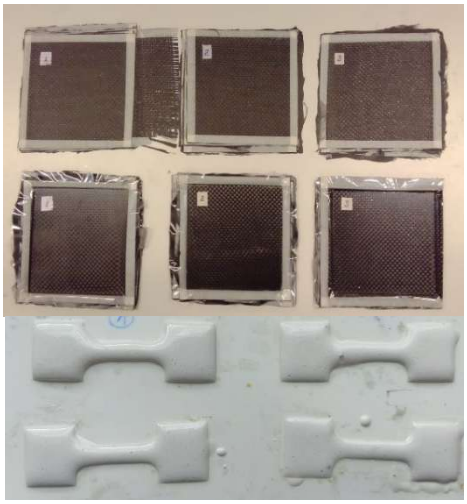
Polyborazylene is a fine white powder and an oligomer, with a molecular structure that lies between monomeric borazine and the final polymeric structure of hexagonal boron nitride. Its molecular structure and physical properties depend on the synthesis method, particularly the reaction temperature and duration.[1,2] We focused on the development and production of composite coatings and modified matrices for fiber-reinforced composites, specifically GFRP (glass fiber-reinforced polymers) and CFRP (carbon fiber-reinforced polymers), with improved properties due to the incorporation of boron compounds into the polymer matrix.





It was found that the addition of polyborazylene prepared from ammonia borane complex by its calcination to 700-900 °C does not significantly change the properties of the polymeric matrix and allows preparation of laminates with carbon cloth (see Figure).

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Investigation of Phenyloboronic Compounds' Interactions With AMP in Aqueous Solutions Using NMR Techniques

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Benzoxaboroles, similarly to other phenylboronic compounds, are characterized by Lewis acidity and affinity to vicinal diols. Some benzoxaboroles are biologically active. Two drugs featuring benzoxaborole skeleton (Tavaborole and Crisaborole) were approved by FDA. Benzoxaboroles with antibacterial, antifungal or antiviral properties are being researched. Biological activity of benzoxaboroles is the result of their interactions with enzyme binding sites. Recent studies suggest that benzoxaboroles could be prodrugs that bind to enzymes only after forming adducts with AMP (adenosine 5'-monophosphate).[1]

In this work, interactions of benzoxaboroles with AMP were studied in aqueous solutions in broad pH range (pH 3-10). NMR techniques (^{1}H, ^{11}B and ^{19}F NMR were used). Five model benzoxaboroles were studied to determine the influence of substituents on the pH in which AMP is bound by benzoxaborole. Interactions of Tavaborole with AMP in aqueous solution were studied for the first time. Additionally, acidity constants of benzoxaboroles were determined using NMR and the influence of cosolvent on acidity constants of benzoxaboroles was researched.

All the studied benzoxaboroles interacted with AMP forming two or more diastereoisomeric adducts (Figure 1). These observations were in accordance with the structure of adducts postulated in the literature. The research conducted revealed that benzoxaboroles with fluorine atom in position 5 (Figure 1) were more acidic than their non¬-fluorinated counterparts. Alkyl substituent in position 3 (Figure 1) had little influence on the acidity of benzoxaboroles and their affinity to AMP. This can be advantageous from the point of view of obtaining biologically active benzoxaboroles functionalized in this position. The benzoxaborole with a hydroxyl group in position 3 (a tautomer of 5-fluoro-2-formyloboronic acid) displayed particularly high acidity and interacted with AMP in the lowest pH of all studied benzoxaboroles.

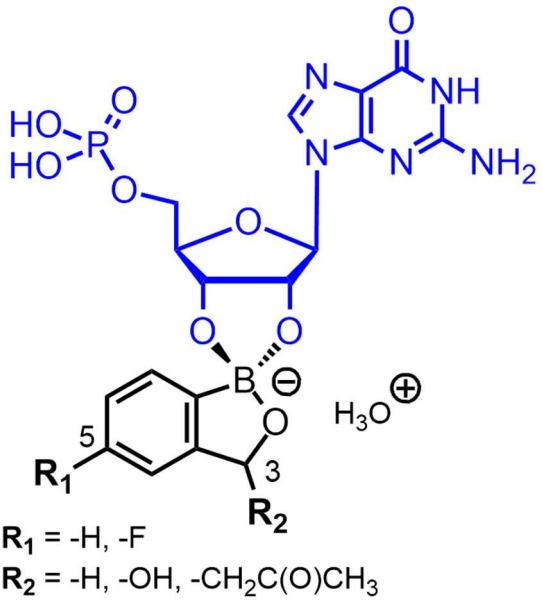

Figure 2. Adduct of benzoxaborole (black) and adenosine 5'-monophosphate (blue).

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Lanthanide-Based Carborane MOFs: Multifunctional Applications via Multivariate Design

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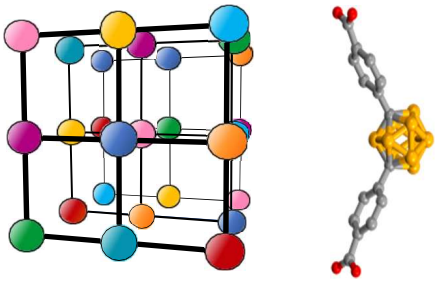
Metal-Organic Frameworks (MOFs), composed of organic linkers and metal ions arranged in crystalline, porous structures, have gained widespread attention due to their versatility in applications such as catalysis, gas storage, and sensing. Lanthanide-based MOFs, in particular, stand out for their unique magnetic, electronic, and optical properties, making them attractive for advanced technologies including information storage and processing, magnetic refrigeration, or luminescence. In this study we are exploring the integration of lanthanide ions with carborane ligands to create a range of innovative multifunctional materials. Our recent work demonstrated that the bulkiness and acidity of carborane linkers enables the synthesis of multivariate MOFs incorporating flexible combinations of multiple lanthanides. This strategy has produced Tb/Eu MOFs for anticounterfeiting,[1] GdLn MOFs with magnetocaloric and luminescent properties,[2] and the first-ever MOF containing eight different lanthanides.[3] Leveraging the multivariate approach, we are currently synthesizing carborane- based MOFs with strategically selected lanthanide combinations. This strategy allows us to explore the properties of "complex magnetic materials" and develop novel materials with tailored functionalities, with exciting possibilities in quantum computing and luminescence applications. Expanding the library of multi-lanthanide MOFs could also pave the way for AI-driven discovery of materials with novel or selected properties.



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Development of Theranostic Silica Nanoparticles Combining Quantitative ^{19}F MRI and Boron Neutron Capture Therapy. (BNCT)

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Melanoma is an aggressive cancer, known for its resistance to conventional therapies. Indeed, most melanoma cells exhibit radio- and chemoresistance and rapidly adapt to targeted therapies. **[1]** Boron Neutron Capture Therapy (BNCT) is a promising alternative, as it selectively destroys cancer cells through neutron irradiation of ^{10}B accumulated in the tumor. However, due to the low intra-tumor concentration of the currently approved compounds, there is a need to develop trackable boron-based drugs that can reach higher tumoral concentrations. **[2]**

To meet these objectives, we propose a nanoplatform (NP) based on mesoporous silica nanoparticles (MSN) with a core-shell structure encapsulating a PFCE emulsion (Perfluoro crown-ether), which provides the ^{19}F MRI quantitative signal. The NP is tailored to BNCT through its functionalization with borocaptate (BSH) modified organosilane synthesized in our laboratory. The currently optimized nanoparticles are stabilized by polyethylene glycol (PEG) coating which stabilizes the NP in physiological fluids and culture media.

Their physicochemical properties were evaluated using various characterization techniques, including dynamic light scattering (DLS), transmission electron microscopy (TEM), ^{1}H and ^{19}F NMR/MRI, inductively coupled plasma (ICP) analysis, and Fourier-transform infrared (FT-IR) spectroscopy. The cytotoxicity of the NP was also evaluated using MTT assays on the A375 melanoma cell line. To improve their specificity, the nanoparticles will be functionalized with a RGD peptide targeting integrins, known to be frequently overexpressed on cancer cells. **[3]** The next steps of the project also include *in vitro* studies of nanoparticle internalization pathways and accumulation in 2D and 3D melanoma (A375) and fibroblasts (HDF) cell models, followed by *in vitro* neutron irradiation tests, and *in vivo* biodistribution analysis on murine models.

In summary, this project aims to demonstrate the feasibility of using our nanoparticles for BNCT, offering a promising approach to cancer treatment with quantifiable boron intra-tumour accumulation and fewer side effects.

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The Reactivity of Electron-rich 10-vertex Carborane Clusters

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The chemistry of borane and heteroborane clusters are a part of modern inorganic chemistry. They appear almost exclusively as neutral or anionic species, while the cationic ones are protonated at exoskeletal heteroatoms, or they are unstable at room temperature. [1] In 2021, we described the first thermally robust cationic carboranes supported by bulky *N*-heterocyclic carbenes.[2] In this work, the reactivity of 10-vertex *closo*-dicarbaboranes with different *N*-heterocyclic and mesoionic carbenes (NHC^{Dipp}, NHC^{Cy}, NHC^{iPr}, MIC^{NNN}, MIC^{CMe}) to 10-vertex *nido*-dicarboranes-bis-carbene adducts will be discussed as along with their structural rearrangements to thermodynamically stable products. The reactivity of such electron-rich clusters with various acids, transition metal complexes, and main group compounds will be presented as well.

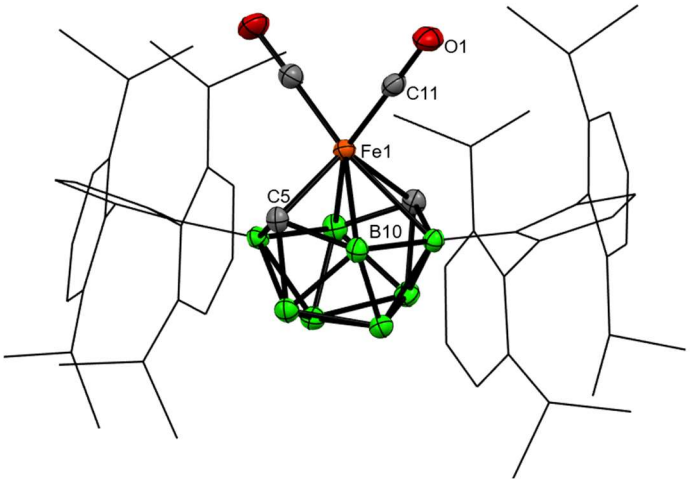

Figure 3. The molecular structure of [*closo*-(3,6-NHC^{Dipp}-2,5-$C_2B_8H_8$)$Fe(CO)_2$]

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Fluorinative Olefin Bond Difunctionalization of Selected Cycloalkene-Fused beta-Lactams and beta-Amino Esters

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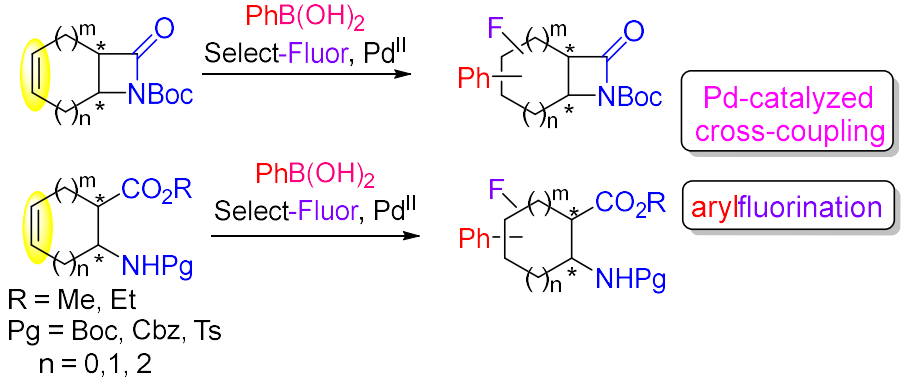
Organofluorine chemistry is considered a hot topic of organic chemistry and drug research, since around 25% of the newly introduced small-molecular based drugs approved by FDA contain fluorinated active ingredient.[1] Development of synthetic methods for the incorporation of a fluorine atom into the structure of an organic molecule has generated increasing significance.[2] Among the fluorinative olefin bond difunctionalizations the Pd-catalyzed arylfluorination have emerged high attention during past years.[3,4]

Investigations on Pd-catalyzed arylfluorination of the ring olefin bond of cycloalkene-fused azetidine-2-one and beta-amino esters were performed under versatile experimental conditions. The arylfluorinative difunctionalization of cycloalkene-fused β-lactam, performed with phenylboronic acid, in the presence of Selectfluor, azacyclic ligands, solvents afforded a separable mixture of various fluorinated and non-fluorinated products, while arylfluorination of cycloalkene-β-amino esters proceeded, under similar conditions, regio- and stereoselectively providing a single phenyl-fluorinated compound. Possible synthetic pathways related to the outcome of these types of transformation were also proposed.



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Synthesis of Boron-Containing Conjugated Polymers via Sonogashira Coupling

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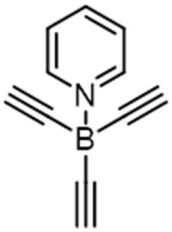
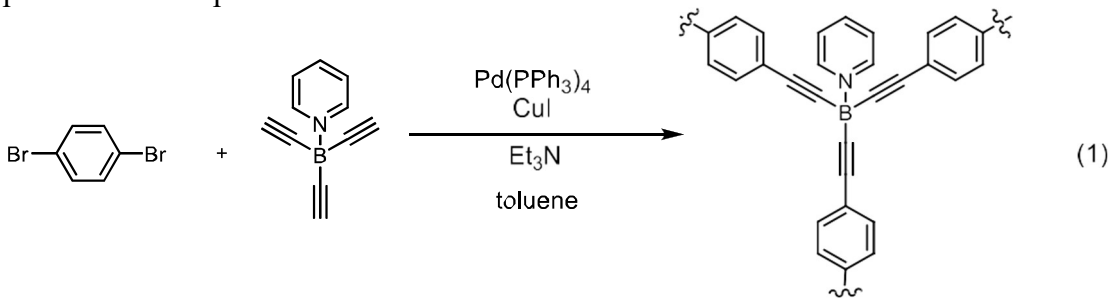
Boron-containing polymers have attracted attention as multifunctional catalysts and sensors.[1] However, due to the high reactivity of boron, bulky substituents are essential for polymer synthesis.[2] Consequently, most reported boron-containing polymers have incorporated bulky substituents. In this study, we aimed to synthesize boron-containing polymers without bulky substituents. We focused on the triethynylborane pyridine complex (**TEB-Py**) as a boron-containing monomer (Figure 1). We stabilized the triethynylborane by coordinating Lewis base (Pyridine) to the boron center. We successfully synthesized polymers by reacting **TEB-Py** with aryl halides via Sonogashira coupling (eq. 1).

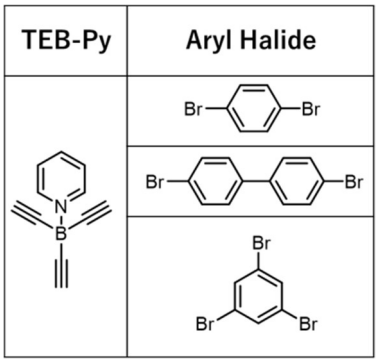


(Figure 1)
Boron-containing monomer (**TEB-Py**)

The aryl halides investigated for polymerization included 1,4- dibromobenzene, 4,4'-dibromobiphenyl, and 1,3,5-tribromobenzene (Figure 2). The molecular weights of the obtained polymers were measured using MALDI-TOF MS, revealing structures with a maximum molecular weight of approximately 4000.Furthermore, ESR measurements of the synthesized polymers confirmed the presence of carbon radicals. Detailed findings will be presented in the poster session.



(1)



(Figure 2) The combination of starting materials

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Production Technology of Anhydrous Salts of Polyhedral Borates

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Introduction: The production of anions (*closo*-[1-$C_mB_nH_o$]$^{p-}$ where m = 0,1; n = 10-12; o = 10,12; p = 1,2), in the form of alkali metal salts (e.g. Li^+, Na^+) leads to the formation of many hygroscopic hydrates. The aim of the project was to achieve the lowest possible water content for these salts and to find suitable methods for the preparation of nearly anhydrous salts and for the accurate detection of very small amounts of water. In addition, it is very difficult to achieve almost complete removal of solvated water or other solvents from the above anions using vacuum technologies. ^{1}H NMR analysis can be used to determine the small amount of hydrated water. However, NMR does not appear to be an accurate method for determining water content and gives only an approximate indication of the water present in the samples measured.

Results: The degree of desolvation depends on many parameters, such as the amount, dipol moment and relative permittivity of the substance to be desolvated, the size and shape of the reaction vessel and, most importantly on the chemical or physical method used to remove the water content. The combined, chemical and physical method for desolvation of the studied salts has been developed. Methods for the determination of low water content in solid samples using coulometric Karl Fisher titration and quantitative ^{1}H NMR have also been used.

Summary: This project focuses on the development of a new technology for the production of nearly anhydrous sodium, lithium and magnesium salts of the anions *closo*-[1- $CB_{11}H_{12}]^-$, and *closo*-[1-$CB_9H_{10}]^-$, as well as the anions *closo*-$[B_{12}H_{12}]^{2-}$, *closo*-$[B_{10}H_{10}]^{2-}$ and *closo*-$[B_{12}X_{12}]^{2-}$, where X is Cl, Br and I. This work also focuses on the development and optimisation of the determination of water in selected samples using various analytical methods.

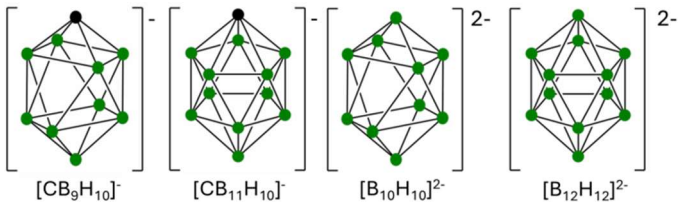

Figure 1: General structures of studied anions and dianions

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Direct Carbon-Functionalization of Cobalt Bis(dicarbollide) Anion with Azides and Amines and Cage-Controlled Acid-Base Properties

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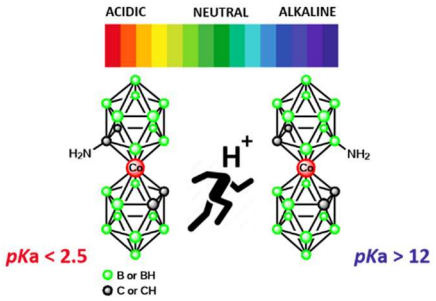
We report the first synthesis of primary amines directly bound to the carbon vertices of the cobalt bis(dicarbollide)ion—an advancement that significantly broadens the organometallic chemistry of this well-established 3D scaffold. Mono- and disubstituted carbon azides were prepared through lithiation followed by reaction with tosyl azide, and subsequently reduced to corresponding amines. An alternative Curtius rearrangement route was also developed for mono-amino derivatives, offering milder conditions and higher chemoselectivity. Compounds containing azido group attached *via* a linker were prepared from the respective mesyl esters and NaN_3 in DMF. Attempts to engage these azides in CuAAC "click" reactions revealed a sharp reactivity contrast: while azides bearing ethylene or propylene linkers underwent efficient cycloadditions with alkynes, those attached directly to cage carbon atoms were inert under standard conditions. We attribute this lack of reactivity to a combination of electronic withdrawal from the cage and steric strain near the azido group. Beyond synthesis, we explored the chemical behavior and structure-acidity relationships of these new C-bound amines. Protonation constants (pK_a) were determined by capillary electrophoresis and supported by quantum-chemical calculations. The results showed a marked difference in basicity depending on substitution site and the presence of alkyl linkers—underscoring the influence of the cage environment on electronic properties. The C-bound amines represent a structurally compact yet functionally rich class of cobaltacarborane derivatives, offering new potential for bioconjugation, inhibitor design, and supramolecular assembly.



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Carborane-thiazole conjugates as inhibitors of mushroom tyrosinase

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The most common of cancer skin malignancies is melanoma, usually found on the skin exposed to sunlight, but also on the skin of hands and feet, eyes, and mucous membranes of the gastrointestinal tract. The increased activity of tyrosinase in this type of cancer leads to the accumulation of melanin in the cells. Melanin belongs to a group of dyes that strongly absorb harmful UV radiation, which can protect melanoma cells during radiotherapy, and as the antioxidant may reduce the effectiveness of chemotherapy [1]. Melanin has also been found to have carcinogenic role in a pathway known as melanin chemiexcitation. As a result of activation of nitric oxide synthase (NOS) and NADPH oxidase by UV radiation, melanin is converted into a carbonyl form, which may form adducts with DNA or proteins, causing irreversible damage. Possible solution to this problem is the use of tyrosinase inhibitors, which inhibit the conversion of L-tyrosine to 3,4-dihydroxy-L phenylalanine (L-DOPA) and then to L-DOPA-quinone, which is one of the precursors of melanin. The search for new effective tyrosinase inhibitors that reduce the production of melanin in melanoma cells and thus increase its sensitivity to the therapies used is the subject of intensive research by our group.
The presented study depicted synthesis of new eleven carborane-thiazole conjugates with promising biological activity. The studies of inhibition activity towards the mushroom tyrosinase and enzyme inhibition kinetics were performed for all synthesized compounds. Analysis of mushroom tyrosinase inhibition showed compounds 4h and 4f as the most active. The measured IC_{50} values were 6 times lower than the IC_{50} values for the reference inhibitor of kojic acid, and 34 times lower than the values measured for ascorbic acid [2].

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Hirshfeld surface analysis and DFT calculations of boron- carbohydrate crystals

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The implementation of boron in diverse molecules along the past years have resulted in novel drugs that ameliorate different pathologies such as neurodegenerative and metabolic disorders.[1] Through computational studies it is possible to approximate the physicochemical properties and relative stability of crystals and correlate the predicted results with the experimental.[2,3] Obtaining crystalline structures is very useful in the field of medicine since the study of solid-state physics allows an approximation to the solubility and relative stability of different pharmacologically active compounds. The present work consisted of the synthesis of boron-containing compounds (BCCs) derived from arabinose and fructose which were crystallized and from the information obtained by single crystal X-ray diffraction these structures were analyzed using Hirshfeld surface (HS) and density functional theory calculations (DFT) under the B3LYP/6-31G (d,p) level of theory.

BCCs were synthetized as reported.[2] The products were crystalized and analyzed by X-ray diffraction. The crystallographic information files were submitted to DFT calculations to obtain different types of energy (polarization, dispersion and repulsion) and these structures were analyzed by Hirshfeld surfaces as in the reported protocol.[3] The HS's were mapped over d_{norm}, shape index and curvedness and each one represent the contribution of intermolecular interactions, convex and concave shape in the crystal and the planarity, respectively. Solubility test were performed to estimate the affinity of these compounds for polar and non-polar solvents and correlated with the HS's computed to confirm the stability of the compounds in solution. The total energy in of the crystal packing of the arabinose and fructose adducts were -38.9 kJ mol $^{-1}$ and -44.4 kJ mol $^{-1}$, respectively.

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Boron-containing compounds derived from L-amino acids as plant growth promoters

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Boron and phytohormones plays a key role in a diverse plant function including cell wall formation and stability, movement of sugar or energy into growing parts of plants, pollination and seed set. [1,2,3] The administration of exogenous melatonin improves the metabolism of plants as well in animals. [4,5] Plant growth is modified by different abiotic factors, mainly the concentration of micro and macro nutrients available in the soil. The implementation of exogenous substances that promote cell proliferation has been a critical point for the design of molecular structures capable of accelerating plant growth. The present work includes the design and evaluation of three boron-containing compounds (BCCs) derived from L-tryptophan as a potential plant growth promoters.

BCCs were simulated to obtain the free energy of binding of each compound in the phytomelatonin receptor 1 (PMT1), synthetized and administered in micro molar logarithmic concentrations ($10^{0.25}$ to $10^{2.75}$) in three groups (n=6) during three weeks to evaluate the growth of *Raphanus sativus.* After the three weeks, plant sections were analyzed to determine the elongation of stem and roots. Also, plasma chromatography was performed to quantify the metals present in soil an in the plants before and after the treatment with BCCs. The free energy of binding of the BCCs were from -8.3 to -8.6 kcal mol^{-1} in PMT1 and the percentage of elongations were: $10^{0.25}$ to $10^{0.75}$ mM 23.9% in root and 46.15% in stem, $10^{1.25}$ to $10^{1.75}$ mM 18.91% in root and 34.95% in stem, and $10^{2.25}$ to $10^{2.75}$ mM 32.14% in root and 30.32% in stem. The design, *in silico* evaluation, synthesis of BCCs and the administration of these compounds promotes the growth *of Raphanus sativus* in three weeks.

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Advances in Diclofenac Derivatives: Exploring Carborane-Substituted *N*-Methyl, Nitrile, Amidine and Lactam Analogs for Anti-Cancer Therapy

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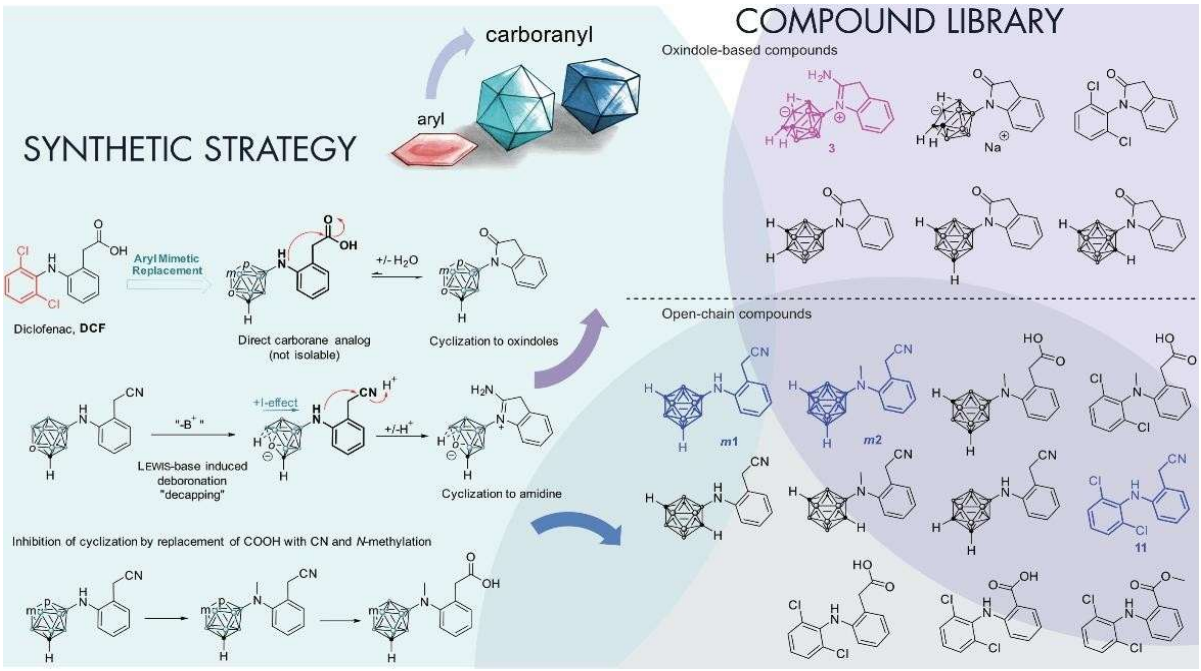

Figure 1. Overview of design concept, synthetic strategy and compound library of the phenyl- and carboranyl-based analogs of diclofenac.

We herein present our recent research efforts to design novel anti-cancer agents based on the well-established diclofenac framework fused with carborane clusters. Our studies focused on synthesizing and testing a range of carborane-substituted (pro)drug analogs of diclofenac featuring cyclic lactams and amidines as well as *N*-methylated open-ring derivatives. These compounds were evaluated for their anti-cancer potential against various colorectal cancer cell lines, including murine colon adenocarcinoma (MC38) and human colorectal carcinoma (HCT116, HT29). The redesigned molecules demonstrated a spectrum of anti-cancer activities, with one zwitterionic amidine species showing particularly strong cell division inhibition and selective cytotoxicity in MC38 cells, likely through both, COX-dependent and independent pathways. Our findings highlight the potential of carborane-based prodrugs as innovative cancer therapeutics, offering insights into their mechanisms and applications.

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POLYSACCHARIDE-BASED COLUMNS AS A TOOL FOR CHIRAL SEPARATIONS OF CARBORANES

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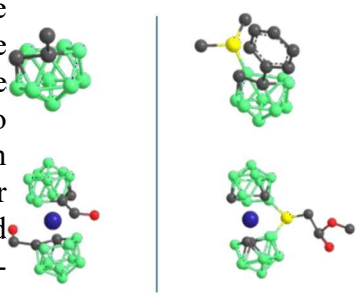
Cobalt bis(dicarbollide) and *nido*-7,8-dicarbaundecaborate derivates are highly stable, hydrophobic compounds, that have aroused interest in pharmaceutical research. [1] Some representatives of these substances are chiral, primarily due to asymmetric substitution. Considering the importance of chirality in pharmacy, it is crucial to establish reliable and rapid methods for separating enantiomers that are essential for further research and possible application of cobalt bis(dicarbollide) and *nido*-7,8-dicarbaundecaborate derivates. [2]



The aim of this work was to examine the behavior of chiral cobalt bis(dicarbollides) and *nido*-7,8-dicarbaundecaborates on polysaccharide-based columns in HPLC. Initial chiral screening was performed using the gradient conditions, which builds on the isocratic method previously developed by our research group [2]. In this work, the spectrum of chiral selectors and analytes was broadened. Subsequently, the method was converted to isocratic elution and optimized for each analyte.

It resulted in the baseline separation of 44 out of a total of 63 analytes. Zwitterionic compounds were generally better separated on the amylose-based column compared to anions. In contrast, the cobalt bis(dicarbollide) anions were better separated on cellulose-based columns. In general, the anions of *nido*-7,8-dicarbaundecaborates are known as challenging analytes for chiral separations. So far, only a few racemic mixtures of these species were resolved into enantiomers. [3,4] Herein, we achieved the baseline separation of one *nido*-7,8-dicarbaundecaborates for the first time on polysaccharide-based columns.

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Molecular dynamics of borocetamol: an acetaminophen analogue acting as a potential COX-2 inhibitor

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Boron-containing compounds are attractive as drugs for treating human maladies [1]. The main cause of physician consultation is pain, often related to an inflammatory process and fever. Acetaminophen (also known as paracetamol) is the most widely used over the counter antipyretic drug, nevertheless due to its overuse, it has become the main cause of acute liver failure. Boron compounds as a new alternative as pharmaceutical drugs is promising due to previous studies finding that they have higher affinity, potency and efficiency than their carbon counterparts [1]. Borocetamol (4-acetamidophenylboronic acid) has been recently described as a low hepatotoxicity agent limiting the pain of mice in a hot plate [2], but the effects limiting fever or in inflammatory processes is lacking. On the other hand, in silico studies help to reduce costs with screening potential new pharmaceutical drugs, and these studies helped to elucidate or support clear mechanisms of action for some drugs. With regards to its antipyretic effect, it has been shown that acetaminophen does interact with the inducible COX-2 enzyme and thus preventing the increase of prostaglandins, albeit locally.
In this study, borocetamol showed to interact with the same catalytic site of the peroxidase site of acetaminophen of the human COX-2 enzyme in a docking simulation, while molecular dynamics simulations were carried out to further observe the interactions between COX-2 and acetaminophen or borocetamol by using NAMD, and analyzed by CARMA software.

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Synthetic application of the electron-rich carboranes as catalysts with unique basic properties

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As a result of our recent research, a new class of polyhedral carboranes with unique basic properties was discovered. The heteroboranes are usually electronically deficient, however the coordination of suitable *N*-heterocyclic carbenes leads to an increase of the electron density in the cluster. Compounds with such a reversed polarity can subsequently act as relatively strong bases with a potential for synthetic application.[1]

Based on our findings we decided to deeply examine the reactivity of these carboranes and utilize them as catalysts in organic synthesis. After our initially obtained positive results with base-induced enolization, we decided to examine a catalytical Michel addition. As a model reaction for the optimization, we choose a reaction of *trans*-chalcone with acetylacetone catalysed by borane ***o*-2**. Later we broadened the scope using various types of Michael donors and the acceptor with higher reactivity – β-nitrostyrene.

We proved ***o*-2** to be an effective catalyst for many substrates within the Michael addition, moreover, it was successfully used in various aldol condensations or even in the conditions of Robinson annulation. Currently we are working on the preparation of a modified version of ***o*-2** containing chiral carbene ligands, with a potential of application in the stereoselective synthesis.

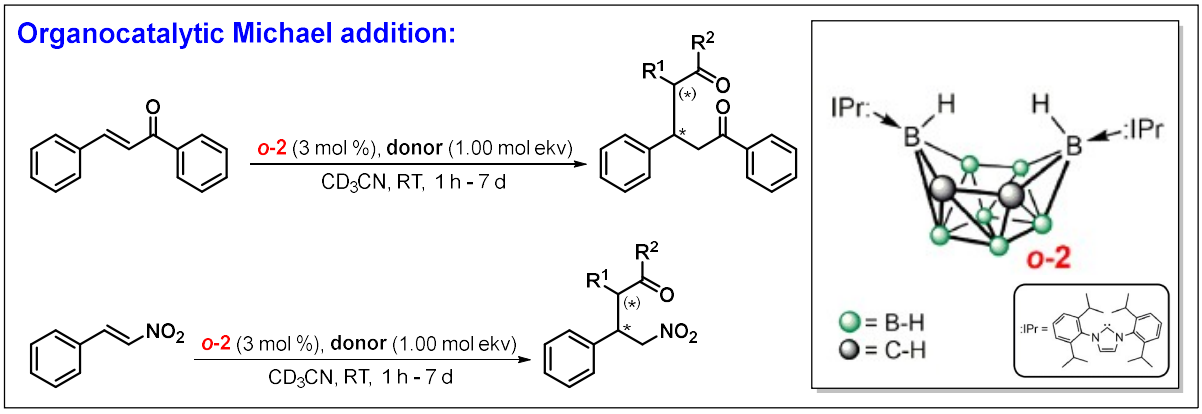

Figure 4. An overview of the developed conditions for the organocatalytic Michael addition and a structure of the tested catalyst – carborane ***o*-2**.

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Carborane-thiazole conjugates as 11β-hydroxysteroid dehydrogenase inhibitors

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Glucocorticoids belong to the group of steroid hormones produced by the adrenal cortex and they are necessary for the proper maintenance of metabolic (including lipid and carbohydrate metabolism) and homeostatic functions of the human body. Glucocorticoid secretion is regulated peripherally by the hypothalamic-pituitary-adrenal (HPA) axis in a double feedback fashion, but also at the tissue level by 11β-hydroxysteroid dehydrogenase type 1 (11β-HSD1) and type 2 (11β-HSD2). 11β-HSD1 is an enzyme that catalyzes the intracellular conversion of biologically inactive cortisone into biologically active cortisol, while 11β-HSD2 catalyzes the reverse reaction. Excess glucocorticoids disrupt the body's metabolic management, which leads to the development of metabolic disorders such as abdominal obesity, insulin resistance or dyslipidemia. The disorders in regulation of the activity of 11β-HSD1, especially that located in visceral adipose tissue, is the pathogenetic basis of diseases such as obesity or type 2 diabetes, which are related and constitute important components of the metabolic syndrome. Therefore, inhibition of 11β-HSD1 represents a promising therapeutic concept for the treatment of diseases associated with metabolic syndrome.

The 7 carborane-thiazole conjugates containing different aromatic substituents at C-4 of thiazole ring have been tested for inhibition of 11β-HSD1. All tested derivatives showed inhibitory activity in the range of 55.54 to 73.51% at a concentration of 10 μM. IC_{50} for all analysed compounds was lower than 10 μM (in the range 3.90 – 9.35 μM). These values are lower than those obtained for the known inhibitor - carbenoxolone. Furthermore, the analysed compounds are not selective. They also inhibit, although to a lesser extent (in the range from 19.34 to 32.55% at a concentration of 10 μM) the activity of 11β-HSD2. However, carborane derivatives are a group of compounds that has not been previously tested for 11β-HSD1 inhibition. Therefore, the fact that all analysed compounds show significant inhibitory activity in relation to this enzyme isoform, and less activity in relation to the isoform 2, gives the possibility to search for a selective 11β-HSD1 inhibitor in this group, e.g. by modifying the structure of the studied compounds.[1]

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Beyond Antibiotics: Designing Metallacarborane-Containing Peptides for the Treatment of Bacterial Infections

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Antimicrobial resistance (AMR) poses a significant global health threat, ranking among the top ten threats to humanity according to the World Health Organization [1]. The rise of multidrug-resistant (MDR), extensively drug-resistant (XDR), and pan-drug-resistant (PDR) pathogens is linked to their increasing insensitivity to traditional antibiotics [2].

Antimicrobial peptides (AMPs) offer a promising solution to combat drug-resistant infections [3]. These peptides, which possess cationic and hydrophobic regions, can disrupt bacterial cell membranes, leading to bacterial death [4]. However, challenges such as instability, high costs, and toxicity to normal cells must be addressed.

Metallacarboranes are stable compounds consisting of one or more boron hydride clusters coordinating a metal cation. They possess unique structures and properties that make them a promising platform for the development of new antimicrobial agents [5].

In our studies, we conjugated metallacarboranes with ultrashort cationic peptides to combine their advantages in the fight against bacterial infections. The synthesis of these conjugates and their physicochemical characteristics will be presented. Additionally, we will demonstrate their antibacterial efficacy and toxicity.

ACKNOWLEDGMENTS

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1,2-Dicarba-dodecaborane in direct electrocatalysis

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The 1,2-dicarba-*closo*-dodecaborane (*ortho*-carborane) holds a prominent position within the family of polyhedral boron clusters due to its stability and well-characterized bonding properties and reactivity. *Ortho*-carborane exhibits a reversible sequential two-electron redox couple, proceeding through a radical monoanion to a dianion.[1] The reductive potential of the dianion has been successfully employed in the reduction of divalent silicon and germanium to their rare zerovalent counterparts, which were stabilized by silylene-substituted *ortho*-carborane.[2] Furthermore, *ortho*-carborane has been utilized as an electrocatalyst in the reduction of 1,2-dibromoalkanes to alkenes, where its presence resulted in a 0.5 V decrease in the overpotential required for the reduction of the substrate.[3]

This contribution describes the immobilization of *ortho*-carborane onto the electrode surface via covalent bonding. The resulting materials were investigated for their stability during repeated redox cycles and subsequently evaluated in direct electrocatalytic reactions.

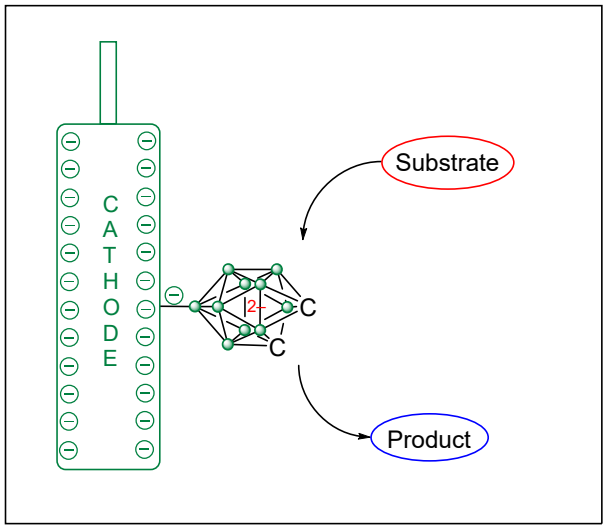

Figure 1: Schematic depiction of immobilized *ortho*-carborane on the electrode for direct electrocatalytical reduction.

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Determination of boron concentration in biological samples using the MARIA Research Reactor infrastructure: development of a code

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The development of a gamma spectrum analysis program for determining boron concentration in biological samples hinges on several critical methodological choices. First, selecting an effective deconvolution method is essential for accurately separating overlapping spectral features [1, 2]. Proper peak area counting is equally vital, necessitating algorithms that can precisely integrate the signal while mitigating errors due to noise. Equally, the subtraction of the background spectrum must be rigorously addressed to ensure that the contributions from ambient radiation are correctly removed[3].

Furthermore, potential interferences from nearby gamma emissions require careful consideration, often leading to the selection of the best mathematical model for peak shape description. Models such as Gaussian or Voigt functions are frequently employed these approaches can enhance the fidelity of peak characterization. Finally, the choice of fitting techniques, typically involving nonlinear least squares methods, is critical for minimizing residuals and obtaining reliable quantitative results[4, 5].

In sum, integrating these advanced spectral analysis components can pave the way for a robust program capable of delivering precise measurements of boron concentration in complex biological matrices.

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Selected Boron Clusters as Substrates for Coupling Reactions with Peptides: Properties and Biological Response

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Boron neutron capture therapy (BNCT) relies on boron-containing compounds that can accumulate in tumor tissues while maintaining favorable biological properties. Sodium mercaptododecaborate (BSH) has been extensively studied as a boron carrier, but its non-selective biodistribution and limited cell membrane permeability have prompted the search for alternative boron clusters with enhanced characteristics.[1, 2].

This study evaluates the properties of two boron clusters: trimethylammonium 1-mercapto-1-carbadodecarnorate (TMA) and triethylammonium decahydrodecaborate (TEA) in comparison to BSH(mercaptododecaborate dianion), focusing on their potential application in BNCT. The investigation encompasses serum stability, lipophilicity, biodistribution, cytotoxicity, and biological responses, including protease activity and apoptosis induction. The results indicate that TMA and TEA exhibit slightly higher lipophilicity than BSH, which may enhance their interaction with cell membranes. All three compounds undergo internalization into the membrane, suggesting their potential for effective cellular uptake.

TMA demonstrates superior serum stability and more favorable biodistribution, leading to increased tumor accumulation compared to TEA and BSH. Cytotoxicity assessments reveal that TMA is less toxic to healthy cells than TEA while maintaining efficacy against cancer cells. Additionally, TMA modulates protease activity and induces apoptosis in tumor cells, indicating supplementary therapeutic mechanisms.[1]

In conclusion, TMA not only exhibits improved biological and physicochemical properties over TEA and BSH but also shows enhanced reactivity in peptide conjugation reactions. This attribute renders TMA particularly promising for the development of boron carriers functionalized with peptides, thereby augmenting its potential application in BNCT and targeted drug delivery systems.

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Exploring the Stability and Properties of Zirconium and Hafnium MOFs with Carborane Ligands

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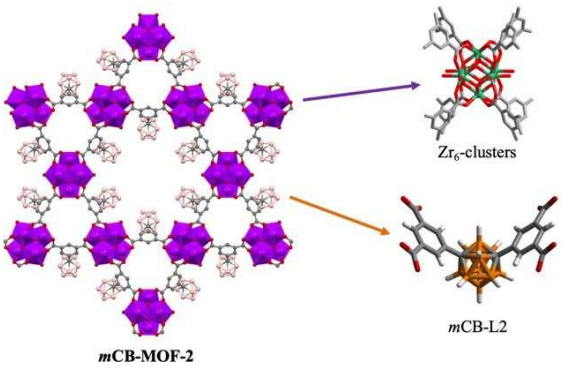
Porous coordination polymer materials, also known as metal-organic frameworks (MOFs), have gained significant research interest due to their high tunability, structural diversity, and wide range of potential applications. However, ensuring their stability is crucial for real-world applications. In recent years, we have demonstrated that incorporating hydrophobic carborane linkers into MOF structures enhances their hydrolytic stability.[1-3] In our studies, we reported the first Zirconium-based MOF featuring a meta-carborane carboxylate ligand, $[Zr_6(\mu_3\text{-}O)_4(\mu_3\text{-}OH)_4(OH)_4(H_2O)_4(m\text{CB-L2})_2]$ (***m*CB-MOF-2**). This highly porous and robust material was found to effectively capture pesticides from water and photodegrade glyphosate into exclusively non-toxic products.[1]

The present work aims to systematically investigate and compare the key factors affecting the stability of porous Zirconium (Zr) and hafnium (Hf) MOFs, a topic that remains relatively unexplored in the MOF literature.[4] Zr and Hf, both group IVB elements, share highly similar physicochemical properties, enabling the isostructural synthesis of Zr- and Hf-based MOFs. Given their chemical resemblance but distinct atomic weights, these MOFs provide an ideal system to explore how increased atomic weight influences thermal stability and how the different nature of these metals can affect the framework hydrophobicity and properties. We will describe the synthesis and structure of a new Hf-based MOF featuring a meta-carborane carboxylate ligand and its properties.



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Novel TADF emitters based on boracyclic groups with enhanced electron-accepting properties

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Emitters of thermally activated delayed fluorescence (TADF) have gained significant attention from both academia and industry since their introduction in third-generation organic light-emitting diodes (OLEDs). These emitters not only offer higher energy efficiency than those from the first generation, but are also cheaper, less toxic and more stable than metal-based phosphorescent compounds typically used in the second generation.

The goal of presented research is the design, synthesis and characterization of new TADF emitters containing strong boron-based acceptor: 10*H*-dibenzo[*b,e*][1,4]thiaborinine 5,5-dioxide (**SO2B**). To date, this is one of the strongest acceptors described in the literature in this context.[1] Current efforts also focus on enhancing electron-accepting properties of **SO2B** moiety by introducing substituents, such as fluorine atoms. These strong acceptors are paired with relatively weak donors, such as those derived from anisole or thiophene. The presence of delayed fluorescence for that kind of molecules has been already confirmed experimentally. Measurements with multichannel scaling (MCS) technique revealed that they exhibit emission characterized by lifetimes in excited state in the range of few microseconds.

The proposed design strategy enables the development of compounds that exhibit blue emission while maintaining delayed fluorescence. This approach addresses the challenge of balancing the contradictory requirements for blue TADF emitters – because the easiest way to achieve effective emission following TADF mechanism is pairing strong donor with strong acceptor, but also this leads to its bathochromic shift.

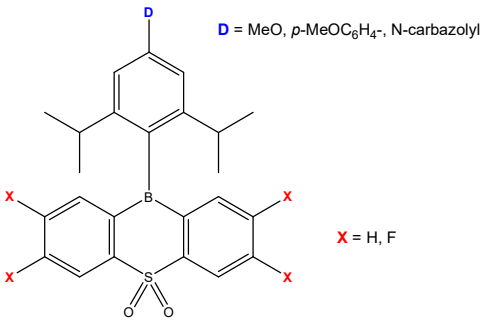

Figure 5 Structure of studied emitters

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