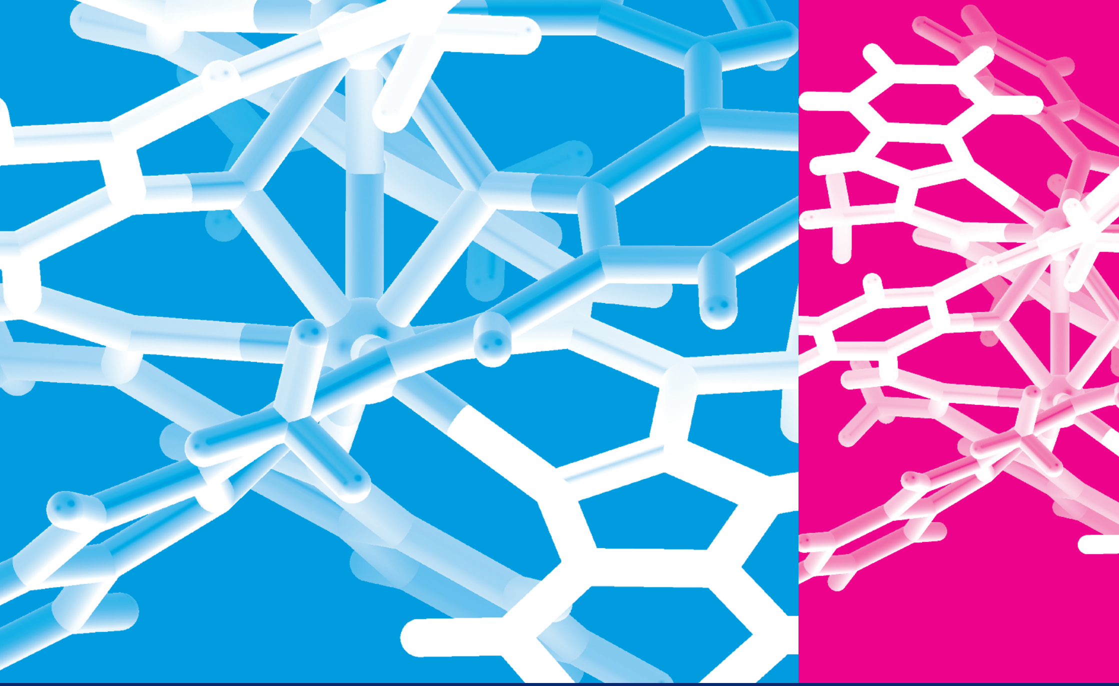

Montpellier, 28-31 August 2023

2ND FRENCH-POLISH CHEMISTRY CONGRESS

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Short history of French-Polish Chemistry Meetings

Ie Assises began with the evening gala – Soiree d'hommage à Jean-Marie Lehn – on July 23, 2015 at the Embassy of the Republic of Poland in Paris, dedicated to **Prof. Jean-Marie Lehn** from the University of Strasbourg, Nobel laureate in chemistry in 1987, the member of the College de France. Another important event was a popular science lecture given by Prof. Jean-Marie Lehn "De la Matière à la Vie: Chimie? Chimie" in French, his native language. The audience had no doubts that Prof. Jean-Marie Lehn is a virtuoso of chemis¬try. July 24, 2015 was the day of the scientific conference Assises Franco-Polonaises de Chimie, where 15 lectures were given. At the end of the conference, young scientists, PhD students at the Faculty of Chemistry, Adam Mickiewicz University, presented the results of their research to Prof. Jean-Marie Lehn.

On March 14-15, 2018 at the Scientific Station of the Polish Academy of Sciences in Paris second scientific symposium took place – IIe Assises Franco-Polonaises de Chimie. The festive evening on March 14, 2018 at the Embassy of the Republic of Poland in Paris was dedicated to **Prof. Jean-Pierre Sauvage**, University of Strasbourg, Nobel laureate in the field of chemistry in 2016 together with Sir J. Fraser Stoddart and Professor Ben L. Ferin¬ga, member of French Académie des Sciences, co-inventor of molecular machines, who gave a popular science lecture entitled "Molecular machines in biology and in chemistry". In addition, on March 15, 2018, 17 lecturers presented their achievements in various fields: from supramolecular chemistry through catalysis, hybrid materials, graphene to applica¬tions in sensors and power engineering.

The French-Polish Chemistry Congress in 4th-6th 2019 focused over 100 scientists! The program included lectures by the **Nobel Laureate in Chemistry – Prof. Jean-Marie Lehn** and other notable chemists: **Prof. Krzysztof Matyjaszewski, Prof. Bruno Ameduri, Prof. Karol Grela, Prof. Mir Wais Hosseini and Prof. Adam Proń**. Several plenary and invited lectures as well as oral communications and poster presentations were also held.

CONFERANCE PROGRAMME

MONDAY 28th

14:00 **REGISTRATION** & ROUND TABLE OVER A COFFEE & **POSTER SESSION**

15:00 **OPENING CEREMONY**

Chairman: Prof. Piotr Pawluć

15:15 **Prof. KAROL GRELA**, University of Warsaw/Institute of Organic Chemistry, Polish Academy of Sciences
RUTHENIUM CATALYZED FORMATION OF TETRASUBSTITUTED OR CROWDED C–C DOUBLE BONDS—A CHEMICAL STORY IN THREE ACTS

Chairman: Dr. Bruno Ameduri

15:45 **Prof. GUILLAUME MAURIN**, University of Montpellier (ICGM)
COMPUTATIONALLY ASSISTED ADVANCES IN MOF-BASED MIXED MATRIX MEMBRANES

Chairmen: Prof. Łukasz Albrecht, Prof. Michael Smietana

16:15 **Prof. Dariusz Matoga**, Jagiellonian University Kraków
PORE FUNCTIONALIZATION OF METAL-ORGANIC FRAMEWORKS FOR PROTON CONDUCTION

16:30 **Prof. Wojciech Bury**, University of Wrocław
PRE- AND POSTSYNTHETIC STRATEGIES APPLIED TO MOFS - TOWARDS SELECTED CATALYTIC APPLICATIONS

16:45 **Dr. Ingrid Suzana**, Sorbonne Université
SUPRAMOLECULAR MAGNETIC DENDRIMERS

17:00 **Dr. Grzegorz Markiewicz**, Adam Mickiewicz University Poznań
SELF-ASSEMBLY OF A FLUORESCENT HYDROGEN-BONDED CAPSULE BASED ON AN AMINO-ACID FUNCTIONALISED TETRAPHENYLETHYLENE

17:15 **Dr. Iwona Nierengarten**, University of Strasbourg CNRS
PILLAR[5] ARENE SCAFFOLDS: FROM MULTIFUNCTIONAL NANOMATERIALS TO MOLECULAR MACHINES AND ROTAXANES

17:30 **Prof. Janusz Dąbrowski**, Jagiellonian University Kraków
PHOTODYNAMIC IMMUNOTHERAPY: RECENT ADVANCES AND FUTURE CHALLENGES

17:45 **Prof. Katarzyna Matczyszyn**, Wroclaw University of Science and Technology
THE SYNTHESIS ANDUSE OF FOLIC ACID-DERIVED CARBON NANODOTS AS FLUORESCENT MARKERS FOR NON-INVASIVE IMAGING OF MORPHOLOGICAL CHANGES IN LIPIDIC MESOPHASES.

18:00 **Prof. Martin Jönsson-Niedziółka**, Institute of Physical Chemistry, Polish Academy of Sciences
POINT-OF-CARE TESTING FOR C-REACTIVE PROTEIN IN A SEQUENTIAL MICROFLUIDIC DEVICE

18:15 **POSTER SESSION**

TUESDAY 29th

9:00 MORNING COFFEE & **POSTER SESSION**

Chairman: Prof. Wojciech Macyk

9:45 **Prof. TEOFIL JESIONOWSKI**, Poznań University of Technology
FUNCTIONALIZED ADVANCED HYBRID MATERIALS FOR ENVIRONMENTAL AND BIOSENSING APPLICATIONS

Chairmen: Prof. Marcin Hoffmann, Prof. David Virieux

10:15 **Dr. Michele Salmain**, Sorbonne Université
INTRACELLULAR LOCALIZATION OF CYTOTOXIC HALF-SANDWICH IRIDIUM(III) COMPLEXES BY ADVANCED HIGH RESOLUTION IMAGING TECHNIQUES

10:30 **Prof. Robert Podgajny**, Jagiellonian University Kraków
SCO TRANSITIONS, SITE SELECTIVITY AND CORE-SHELL COMPOSITES IN [W(CN)8]-BRIDGED COORDINATIONCLUSTERS FAMILIES

10:45 **Prof. Elżbieta Wojaczyńska**, Wrocław University of Science and Technology
RING EXPANSION IN NITROGEN HETEROCYCLES

11:00 **Prof. Alberto Marra**, Institut des Biomolécules Max Mousseron (IBMM)
SYNTHESIS OF BIO-SOURCED ANTIOXIDANTS BY PHOTOINDUCED THIOL-ENE COUPLING UNDER CONTINUOUS-FLOW CONDITIONS

11:15 **Dr. Dorota Czajkowska-Szczykowska**, University of Białystok
MACROCYCLIC MOLECULAR ROTORS WITH STEROIDAL FRAMEWORKS – SYNTHESES AND SOME PROPERTIES

11:30 **Prof. Piotr Młynarz**, Wrocław University of Science and Technology
CELLULAR METABOLOME IN RESPONSE TO EXTERNAL CONDITIONS

11:45 **Prof. Beata Nowicka**, Jagiellonian University Kraków
SWITCHABLE COORDINATION POLYMERS IN BETTER SHAPE

12:00 **Dr. Jakub Brzeski**, University of Gdańsk
A THEORETICAL STUDY ON THE ALKYLIMINO SUBSTITUTED SULFONAMIDES

12:15 **Prof. Justyna Walkowiak-Kulikowska**, Adam Mickiewicz University Poznań
AMPHIPHILIC TELECHELIC POLYMERS FORMULATED USING A CLICK CHEMISTRY APPROACH

12:30 **Dr. Tadeusz Muzioł**, Nicolaus Copernicus University in Toruń
STRUCTURAL STUDIES OF COMPLEXES WITH [FE(OX)3]3- AND [FE(OX)2(H2O)2]- UNITS

12:45 **Dr. Karolina H. Markiewicz**, University of Białystok
MEMBRANE-ACTIVE POLYMERS FOR DRUG DELIVERY: RAFT SYNTHESIS, DRUG ENCAPSULATION, AND BIOLOGICAL EVALUATION

13:00 GROUP PHOTO

13:15 LUNCH BREAK

TUESDAY 29th

Chairman: Prof. Violetta Patroniak

15:00 **Prof. ARTUR CIESIELSKI**, University of Strasbourg/Adam Mickiewicz University Poznań
FUNCTIONAL 2D MATERIALS: FROM SMART DIAPERS TO CARDIOVASULAR HEALTH MONITORING

Chairmen: Dr. Michele Salmain, Prof. Łukasz John

15:30 **Prof. Elżbieta Regulska**, University of Białystok
MODIFIED TERNARY METAL OXIDES: EN ROUTE TO FUNCTIONAL MATERIALS

15:45 **Prof. Sławomir Boncel**, Silesian University of Technology
FROM FUNCTIONALIZATION TO FUNCTIONALITY – PHYSICOCHEMISTRY OF NANOCARBONS TOWARD APPLICATIONS

16:00 **Prof. Magdalena Rowińska-Żyrek**, University of Wrocław
METAL BINDING TO ANTIMICROBIAL PEPTIDES - A SMALL STEP FOR STRUCTURAL CHEMISTRY, A BIG LEAP FOR MEDICINAL APPLICATIONS

16:15 **Prof. Volodymyr Sashuk**, Institute of Physical Chemistry, Polish Academy of Sciences
FROM ENZYMES TO CUCURBITURILS: EXPANDING THE HORIZONS OF CATALYSIS

16:30 **Prof. Monika Wałęsa-Chorab**, Adam Mickiewicz University Poznań
STRUCTURE-PROPERTY RELATIONSHIP OF MATERIALS FOR ELECTROFLUOROCHROMIC APPLICATIONS

16:45 **Dr. Wojciech Smułek**, Poznan University of Technology
BIOAVAILABILITY OF ANTIBIOTICS MODIFIED WITH PLANT SURFACTANTS

17:00 **Prof. Joanna Niedziółka-Jönsson**, Institute of Physical Chemistry, Polish Academy of Sciences
SILVER NANOWIRES AS BUILDING BLOCKS FOR SENSORS

17:15 **Dr. Mateusz Kowalik**, University of Gdańsk
ANTICANCER STUDY ON IRIDIUM AND RHODIUM HALF-SANDWICH COMPLEXES WITH BIPYRIDYLSULFONAMIDE LIGAND

17:30 **Dr. Guillaume Vives**, Sorbonne Université
SWITCHABLE MOLECULAR TWEEZERS: A VERSATILE PLATFORM TO CONTROL MULTIPLE PROPETIES

17:45 **Dr. Suzanne Peyrottes**, CNRS Research Associate (IBMM)
UA2239: AN ACYCLIC NUCLEOSIDE PHOSPHONATE WITH POTENT ANTIMALARIAL ACTIVITY & UNEXPECTED MECHANISM OF ACTION

18:00 **POSTER SESSION**

WEDNESDAY 30th

9:30 MORNING COFFEE & **POSTER SESSION**

Chairman: Prof. Mariusz Makowski

10:00 **Prof. MIŁOSZ PAWLICKI**, Jagiellonian University Kraków
π-CONJUGATED SYSTEMS DOPED WITH BORON

Chairmen: Prof. Joanna Gościańska, Prof. Jerzy Zając

10:30 **Dr. Umut Ugur Ozkose**, University of Montpellier
DEVELOPMENT AND FUNCTIONALIZATION OF NOVEL POLYMERIC MATERIALS FROM POLY(OXAZOLINE)S FOR THEIR POTENTIAL BIOAPPLICATIONS

10:45 **Prof. Anna Kajetanowicz**, University of Warsaw
HIGH CONCENTRATION RING CLOSING METATHESIS FOR EFFICIENT SYNTHESIS OF MACROCYCLIC MUSK COMPOUNDS

11:00 **Dr. Marcin Lindner**, Institute of Organic Chemistry, Polish Academy of Sciences
AMBIPOLAR N-DOPED PAHS. A UNIQUE STRATEGY FOR THE EFFICIENT TADF OLED EMITTERS

11:15 **Prof. Till Bousquet**, University of Lille
PHOTOCATALYSIS IN HETEROCYCLIC CHEMISTRY

11:30 COFFEE BREAK & **POSTER SESSION**

Chairman: Dr. Mihail Dimitru Barboiu

12:00 **Prof. SEBASTIEN ULRICH,** CNRS Research Associate (IBMM)
DYNAMIC POLYMERS AS SMART FLUOROGENS

Chairmen: Dr. Renata Marcia de Figueiredo, Dr. Maciej Zaranek

12:30 **M.Sc. Zachary Pastorel**, University of Montpellier
DNA-BASED ASYMMETRIC PHOTOCATALYSIS

12:40 **M.Sc. Aleksandra Ciesielska**, University of Gdańsk
DETERMINATION OF LOW-MOLECULAR COMPOUNDS INTERACTIONS WITH DNA BIOMOLECULE USING SWITCHSENSE TECHNOLOGY

12:50 **M.Sc. Marion Gras**, University of Montpellier
CATALYTIC APPROACH FOR AMIDE COUPLING FOR THE DEVELOPMENT OF PEPTIDE-OLIGONUCLEOTIDE CONJUGATES

13:00 **M.Sc. Gracjan Kurpik**, Adam Mickiewicz University Poznań
STIMULI-RESPONSIVE SUPRAMOLECULAR TRANSFORMATIONS BETWEEN HOMOMETALLIC COMPLEXES AND HETEROMETALLIC POLYMERIC MATERIALS

13:10 **M.Sc. Laura Borrel**, University of Montpellier
INDOLIZINE BASED LIGANDS: SYNTHESIS OF BISOXAZOLINE AND PHOSPHINOOXAZOLINE ANALOGUES

WEDNESDAY 30th

13:20 **M.Sc. Paulina Nowicka**, University of Gdańsk
COMPLEXING PROPERTIES OF LIGANDS WITH THIAZOLYL-HYDRAZONE SYSTEM TOWARDS CADMIUM IONS

13:30 **M.Sc. Paras Wanjari**, University of Montpellier
SELF-ASSEMBLED PROTON AND WATER CHANNELS WITH PHOTO-TUNABLE TRANSPORT PROPERTY

13:40 **M.Sc. Anaïs Guillou**, University of Montpellier
SYNTHESIS OF NOVEL ANTIVIRAL NUCLEOSIDE ANALOGUES BEARING A PYRAZOLE MOIETY

13:50 **M.Sc. Agata Kowalska**, University of Gdańsk
SYNTHESIS AND CHARACTERIZATION OF CORE-SHELL NANOMATERIALS BASED ON GOLD NANOPARTICLES

14:00 **M.Sc. Pierre Plouard**, University of Montpellier
RU(II)-CATALYZED HIGHLY ENANTIOSELECTIVE TRANSFER HYDROGENATION OF α-KETO PHOSPHONATES

14:10 **END OF MEETING**

Amphithéâtre Godechot,
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FUNCTIONAL 2D MATERIALS: FROM SMART DIAPERS TO CARDIOVASULAR HEALTH MONITORING

Artur Ciesielski[1,2]

[1] *Université de Strasbourg, CNRS, ISIS, 8 allée Gaspard Monge, 67000 Strasbourg, France.*
ciesielski@unistra.fr
[2] *Center for Advanced Technologies, Adam Mickiewicz University, Uniwersytetu Poznańskiego 10, 61-614*
artur.ciesielski@amu.edu.pl

Two-dimensional materials (2DMs) exhibiting a high surface-to-volume ratio are unique scaffolds whose interactions with the environment drive their application as sensitive elements in chemical sensing. They allow prompt reconfiguration of the architectures of the sensor, whose response to the detection of chosen analyte becomes no longer limited by extrinsic factors such as the slow diffusion of target molecules through the active material or the presence of structural traps for small molecules/ions. The unique features of 2DMs determine the highest responsiveness, sensitivity, and reversibility combined with the lowest limit of detection in the sensing process.

Pristine 2DMs are being widely exploited as highly sensitive elements in chemical and physical sensors, although they suffer from the lack of intrinsic selectivity towards specific analytes. Here, we showcase the most recent strategies explored in our laboratories on the use of (supra)molecular interactions to harness selectivity of suitably functionalized 2D materials for chemical and physical sensing. We discuss how to achieve selectivity in (chemical) sensors along with other relevant characteristics, such as high sensitivity, response speed, and reversibility, by suitable functionalization and incorporation of low-dimensional materials into powerful transducers.

Among several examples, we will discuss piezoresistive pressure sensor based on a millefeuille-like architecture of reduced graphene oxide (rGO) intercalated by covalently tethered molecular pillars holding on-demand mechanical properties are fabricated. By applying a tiny pressure to the multilayer structure, the electron tunnelling ruling the charge transport between successive rGO sheets yields a colossal decrease in the material's electrical resistance. We will also discuss novel generation of humidity sensors based on a simple chemical modification of rGO with hydrophilic moieties, i.e., triethylene glycol chains. Such a hybrid material exhibits an outstandingly improved sensing performance compared to pristine rGO such as high sensitivity (31% increase in electrical resistance when humidity is shifted from 2 to 97%), an ultrafast response (25 ms) and recovery in the subsecond timescale, low hysteresis (1.1%), excellent repeatability and stability, as well as high selectivity toward moisture.

Acknowledgments: This work was supported by the National Science Centre (Grant No. 2015/18/E/ST5/00188, 2019/33/N/ST5/00052 & 2020/39/D/ST4/01182). The work was also supported by the European Commission through the Graphene Flagship Core 2 project (GA-785219).

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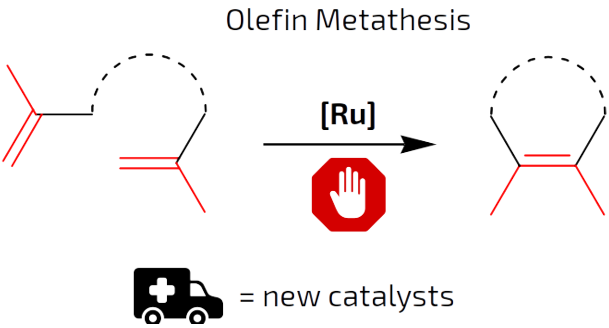
RUTHENIUM CATALYZED FORMATION OF TETRASUBSTITUTED OR CROWDED C–C DOUBLE BONDS—A CHEMICAL STORY IN THREE ACTS

Karol Grela

Biological and Chemical Research Centre, Faculty of Chemistry, University of Warsaw, Żwirki i Wigury Street 101, 02-089 Warsaw, Poland
prof.grela@gmail.com (www.karolgrela.eu, @GrelaGroup)

Ruthenium-catalyzed olefin metathesis reactions represent an attractive and powerful transformation for the formation of new carbon¬-carbon double bonds (1). This area is now quite familiar to most chemists as numerous air and moisture stable ruthenium (2) catalysts are available that enable a plethora of olefin metathesis reactions.

However, formation of substituted and crowded double bonds still remain a challenge, making applications of this methodology difficult (3). This limitation can be solved by designing new, more active and stable catalysts. During the lecture three different approaches to this problem will be presented.



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FUNCTIONALIZED ADVANCED HYBRID MATERIALS FOR ENVIRONMENTAL AND BIOSENSING APPLICATIONS

Teofil Jesionowski

Poznan University of Technology, Faculty of Chemical Technology, Institute of Chemical Technology and Engineering, Berdychowo 4, PL-69965 Poznan, Poland
teofil.jesionowski@put.poznan.pl

The lecture will focus on current trends in the fabrication and development of functionalized advanced hybrid materials. Additionally practical utilities of those materials will be also emphasized. Methods of their production, characteristics, how and above all the most important areas of their use will be indicated. An extremely important element of research is the work devoted to neutralization of contaminants with metals harmful to the environment or substances of organic origin.

Materials of natural origin, obtained from biomass or other sources, are of great interest among scientists. Lignin and its derivatives are becoming increasingly important in this respect. Hybrid materials produced with lignin and selected oxides can serve as advanced fillers, eco-friendly components of abrasives or biosensors as well as cement additives. On the other hand, an interesting field of research concerns the mineralization of chitin under extreme environmental conditions. Sea sponges or their derivatives (skeletons, including carbonized forms), due to their unique spatial structure and properties, are also the subject of numerous studies. They are used as adsorbents of harmful metals and carriers in the immobilization of enzymes. Together with dyes, both natural and synthetic, adsorbed on their surface, they form hybrid systems with antioxidant, antibacterial and catalytic properties. Recently, the use of deep eutectic solvents in the design of materials for tissue engineering has also become very important.

In turn, another direction of development of hybrid materials is their use as carriers in the immobilization of enzymes, followed by the production of enzymatic biosensors. For this purpose, nanomagnetite, lignin, polydopamine, poly(caffeic acid), etc. are used as components, as well as suitable enzymes dedicated to environmental or medical applications.

Acknowledgements
This work was supported by National Science Center Poland under the research grant no. 2021/43/B/ST8/01854. The author would like to thank all those who participate in the research in the area included in this paper.

COMPUTATIONALLY-ASSISTED ADVANCES IN MOF-BASED MIXED MATRIX MEMBRANES

Guillaume Maurin

ICGM, Univ. Montpellier, CNRS, ENSCM, Montpellier, France
guillaume.maurin1@umontpellier.fr

There is actually a need to develop optimized Mixed Matrix Membranes (MMMs) based on highly engineered MOFs and polymers to combine the best of both worlds. Our group developed an innovative computational toolbox to construct and characterize the MOF/polymer composites at the atomistic scale. This offers a unique opportunity to anticipate the most compatible components that drives the feasibility and stability of the MMMs without the need to experimentally scan the multiple combinations of possible pairs (MOFs/polymers) which is time consuming and impossible to be achieved in an equitable time. Monte Carlo/Molecular Dynamics simulations were further deployed to predict the thermodynamic adsorption/separation and permeability performances of the corresponding MMMs. Diverse avenues (functionalization of both polymers and MOFs, defective MOF surface, shape/size of the MOF/polymer interface) were systematically explored with the objective to gain insight into the main parameters that control the performance of the MMMs. This presentation will deliver a series of recent examples of highly compatible MOF/polymer pairs that led to MMMs with outstanding performance for energy-efficient separations (CO_2/CH_4, CO_2/N_2, N_2/CH_4….)

P-CONJUGATED SYSTEMS DOPED WITH BORON

Miłosz Pawlicki

Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Kraków, Poland
pawlicki@chemia.uj.edu.pl

Strongly conjugated carbon-based systems are extensively explored in several aspects focusing on optimisation of synthetic paths and followed by understanding the properties hidden within the skeletons of different size and shape. An extended conjugation based on *sp*2 hybridization of carbon allows tuning of the behaviour extracted from the number of available p-electrons eventually controlling optical and magnetic properties. An incorporation of a heteroatom into p-extended system is a separate possibility of modification that can be treated as a source of modulation of the optical properties. A boron involvement into those systems is a vibrant field deeply modifying the recorded properties [1] and based on the properties of boron itself and an electron deficiency of this element that deeply disturbs the electron distribution in defected p-conjugated systems,[2,3] but also stabilizes derivatives with a paratropic character typical for antiaromatic derivatives.[4,5]

The precisely planned strategy for formation of hybrid structures linking in one skeleton acene(s) or heteroacenes modulated by a presence of a specific defect predefined for binding small cation creates strictly designed systems. It results in, depending on the complexity of final molecule, observation of local effects of conjugation efficiently influencing properties of each subunit. A specific construction opens a possibility for observation of the reactivity characteristic for isolated unsaturated units[6] in addition creating an opportunity for switching on the global diatropic currents.[2-5] All those effects will be presented and discussed focusing on the influence of boron centre on the delocalization paths within precisely designed structural motifs introducing triangular defect(s) open for a post-synthetic modifications[7] either by entrapping of a central ion or redox switching, showing the synthetic approach followed by the spectroscopic behaviour extended by XRD analysis and theoretical support.

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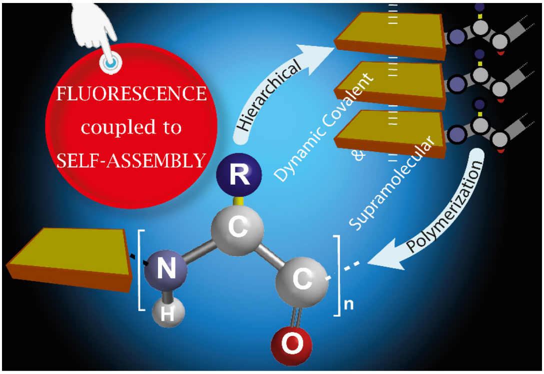
DYNAMIC POLYMERS AS SMART FLUOROGENS

Sébastien Ulrich

Institut des Biomolécules Max Mousseron (IBMM), CNRS, Université de Montpellier, ENSCM, Montpellier, France
sebastien.ulrich@cnrs.fr

The bottom-up self-assembly of responsive functional materials is an important quest that benefits from recent progresses in the area of supramolecular polymers. Looking beyond the archetypical Benzene TriscarboxAmide (BTA) system,[1] we have been attracted by the challenge and opportunities of inserting new functional aromatic cores with supramolecular polymers, and we selected TetraPhenylEthene (TPE) for its known property of Aggregation-Induced Emission (AIE).[2] Implementing a dynamic covalent self-assembly approach of TPE derivatives and modified peptides,[3] we reported the one-pot formation of (multi)-responsive fluorescent cages[4] and organo-gels.[5] In this talk, we will disclose new results showing that fluorescent supramolecular polymers can emerge, from a virtual library formed in aqueous media, by selection and auto-catalytic amplification.[6]



Dynamic self-assembly of fluorescent polymers from aromatic-peptide conjugate building blocks.

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2ND FRENCH-POLISH CHEMISTRY CONGRESS

FROM FUNCTIONALIZATION TO FUNCTIONALITY – PHYSICOCHEMISTRY OF NANOCARBONS TOWARD APPLICATIONS

Sławomir Boncel

Silesian University of Technology, Faculty of Chemistry, Department of Organic Chemistry, Bioorganic Chemistry & Biotechnology, NanoCarbon Group, Krzywoustego 4, 44-100 Gliwice, Poland
slawomir.boncel@polsl.pl

The most challenging problem of transfer of the extraordinary properties of nanocarbons (NCs) of various dimensionalities (carbon nanotubes, CNTs, graphene, quantum dots, etc.) from nano- to macroscale is control over their surface properties. Physicochemical modifications of NCs – enabling their full individualization as accompanied by non-compromised morphology – are essential for electrical, thermal, mechanical, and biological properties translatable to numerous applications (**Fig. 1**).

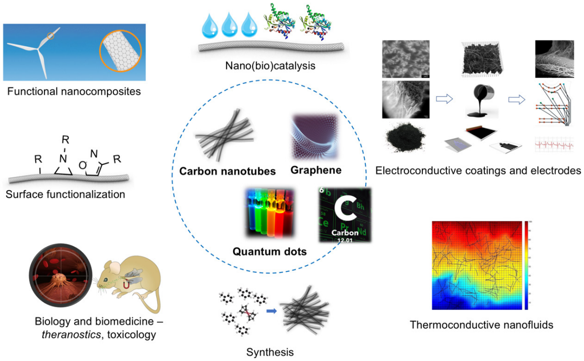

Fig. 1 Main application routes of physicochemically modified nanocarbons

The herein proposed transformations, encompassing covalent and non-covalent functionalization routes, can yield NCs of enhanced properties. Concerning the 'properties-by-design' approach, we have prepared, *inter alia*, textronics for Holter electrocardiography [1], conductive coatings [2], high-performance heat transfer fluids [3], phase change materials [4], and drug delivery systems [5] – all based on NCs of tunable hydrophilicity.

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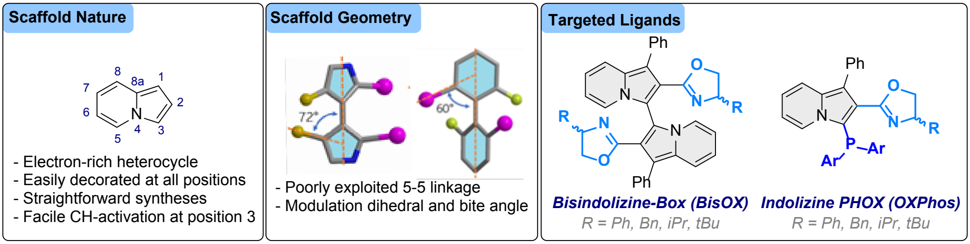
INDOLIZINE BASED LIGANDS: SYNTHESIS OF BISOXAZOLINE AND PHOSPHINOOXAZOLINE ANALOGUES

Laura BORREL, David VIRIEUX and Tahar AYAD

ICGM Univ Montpellier, CNRS, ENSCM, Montpellier, France.
laura.borrel@etu.umontpellier.fr

Chirality plays a fundamental role in the pharmaceutical industry as it strongly influences the biological properties of small molecules. Over the past decades, there has been a growing trend towards developing single enantiomers. In 2021, out of the 50 drugs approved by the FDA, 75% were enantiopure, and no racemic mixture reached the market. This trend highlights the significance of studying methods to selectively obtain one enantiomer. Asymmetric catalysis has emerged as a preferred approach for this purpose, employing enantiopure ligands in combination with transition metals being widely used as catalysts. Notably, significant progress has been made in developing such ligands. However, the quest for a "universal" ligand that is effective across a wide range of transformations remains ongoing.

Biheteroaromatic atropochiral ligands have demonstrate remarkable efficiency in various enantioselective transformations, despite being lest extensively studied compared to their carbocyclic analogues. For example, tetraMe-BITIANP has exhibited more promising than the landmark BINAP ligand in the reduction of α- and β-oxoesters (1). Building upon this pioneering work, a limited number of *C*2-symmetric atropisomeric diphosphines characterized by two interconnected 5- or 6-membered heteroaromatic rings have been developed and successfully used as efficient chiral inducers in asymmetric catalysis. To further expand this family of ligands, we aim to develop a new toolbox of chiral ligands and organocatalysts with diverse stereoelectronic properties for challenging asymmetric transformations, from a common indolizine precursor and using an efficient, scalable and cost-effective process. (2). The synthesis and stereoelectronic properties of a wide range of phosphinooxazoline (PHOX) analogues as well as a new bisoxazoline ligands (BOX) will be discussed (3).



Scheme 1: Scaffold nature, geometry of targeted indolizine ligands.

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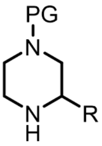
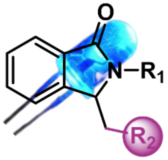
PHOTOCATALYSIS IN HETEROCYCLIC CHEMISTRY

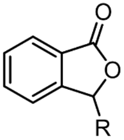
Nathan Martin, Lucas Fortier, Aurélien Moncomble, Eric Deniau, Lydie Pélinski, Till Bousquet

University of Lille, CNRS, UMR 8181, Unité de Catalyse et Chimie du Solide, F-59000 Lille, France
till.bousquet@univ-lille.fr
nwak@edu.pl

This presentation showcases the emerging field of visible light photocatalysis in organic chemistry, with a focus on its green and sustainable nature. The utilization of visible light as a powerful tool for activating chemical reactions has gained significant attention in recent years. This talk will delve into three specific transformations: the synthesis of piperazines, phthalides, and the arylation of 3-methyleneisoindolinones. These reactions offer high yields and demonstrate the effectiveness of blue LED irradiation as a light source. Visible light photocatalysis provides a promising alternative to traditional activation methods, enabling sustainable and selective transformations in organic synthesis. The results presented contribute to the understanding and advancement of this rapidly growing field.







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A THEORETICAL STUDY ON THE ALKYLIMINO SUBSTITUTED SULFONAMIDES

Jakub Brzeski, Aleksandra Ciesielska, Mariusz Makowski

University of Gdańsk, Jana Bażyńskiego 8, 80-309 Gdańsk, Poland
jakub.brzeski@ug.edu.pl

Antibiotics play an essential role in combating bacterial diseases. Unfortunately, bacteria rapidly develop strategies to minimize the impact of antimicrobials and increase their resistance [1]in part due to widespread resistance. The target of sulfonamides, and the basis for their selectivity, is the enzyme dihydropteroate synthase (DHPS. As a consequence, the battle against bacterial infections becomes more and more demanding. During the search for new antibiotics, it is essential to assess fundamental characteristics of potential antimicrobials, such as pK_a (acid dissociation constant), possible formation of non-covalent interactions, and hydrophobicity. Bearing this in mind, five sulfonamide derivatives varying in the length of the alkylamine chain were studied with the use of quantum chemical methods. Based on the findings, three-potential acid-base equilibria together with corresponding pK_a values for each of the compounds under investigation were proposed. It was found that the application of Muckerman's approach [2] for the pK_a determination leads to results that are in great agreement with experimental results. It was also found that the formation of intramolecular hydrogen bonds by studied sulfonamides significantly affects the corresponding pK_a values. Said interactions are formed between the alkylamine group (donor) and sulfonamide group (acceptor) of the studied sulfonamides. Moreover, it was determined that the calculated partition coefficients (measured as *logP* values) correlate with the number of carbon atoms in the alkylamine chain. The results found within the project provide valuable insights into the structural, physicochemical, and thermodynamic aspects, facilitating a better comprehension of the potential activity of studied sulfonamides.

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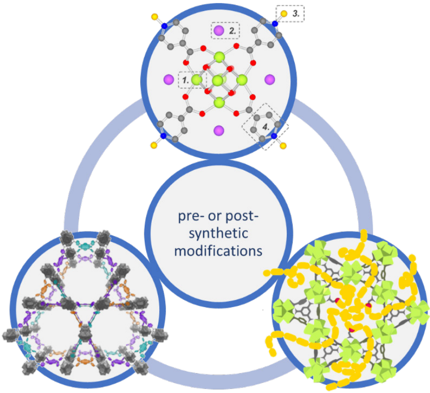
PRE- AND POSTSYNTHETIC STRATEGIES APPLIED TO MOFS - TOWARDS SELECTED CATALYTIC APPLICATIONS

Wojciech Bury, Marzena Pander, Rodrigo Gil-San-Millan

Faculty of Chemistry, University of Wrocław, F. Joliot-Curie 14, 50-383 Wrocław, Poland
wojciech.bury@uwr.edu.pl

The observed rapid growth of interests in metal-organic frameworks (MOFs) has been the result of their numerous intriguing properties, which lead to many potential applications of MOFs, including gas storage, separations, heterogenous catalysis, biomedical applications, and others. Proper selection of building blocks allows to design MOF structure and often its desired physicochemical properties [1]. Post-synthetic modifications of MOFs allow for their further functionalization, expanding their possible applications [2]. Nevertheless, presynthetic design of MOFs is of great importance for the construction of multivariate systems. In this presentation our approach to the application of MOFs as platforms and precursors for further transformations into functional systems will be presented.



The aim of our studies was to evaluate pre- and postsynthetic functionalization strategies in model zirconium-based MOFs to test the possibility of incorporating new functions into MOFs with special focus on three research topics: (1) catalytic synthesis of cyclic carbonates under mild reaction conditions [3], (2) synthesis of polymer@MOF hybrids based on radical polymerization of acrylic monomers [4], and (3) imprinting desired compositions into MTV-MOFs to obtain heterogenous catalysts for decomposition of liquid hydrogen sources [5].

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DETERMINATION OF LOW-MOLECULAR COMPOUNDS INTERACTIONS WITH DNA BIOMOLECULE USING

Aleksandra Ciesielska*, **Sandra Brzeska, Mariusz Makowski**

University of Gdańsk, Faculty of Chemistry, Wita Stwosza 63, 80-308 Gdańsk
*aleksandra.ciesielska@phdstud.ug.edu.pl

The growing problems of drug resistance and cancer diseases are a major obstacle for modern medicine. Therefore, it is necessary to search for new drugs with a broader spectrum of biological activity. One approach to finding new drugs is target-based drug discovery. Molecular targets may include proteins, enzymes, receptors, and other cellular components involved in disease pathways or physiological processes. DNA can be a molecular target for drugs in certain contexts. These drugs may work by directly binding to DNA and disrupting its structure, or by inhibiting enzymes involved in DNA replication or repair. Other drugs may target specific DNA sequences or genes to modulate gene expression or correct genetic defects.

Determining the strength of binding to DNA, and thus understanding the mode of action of a given compound, is therefore crucial. The most commonly used approaches to this type of research are spectroscopic and electrochemical methods. They can be used to determine the constant value (K) of the interaction equilibrium between a potentially active molecule and the DNA helix in solution [1]. However, these techniques have some limitations. The study of the binding equilibrium of the DNA molecule in solution gives limited insight into the kinetics of the processes taking place. In the standard approach, these methods do not allow for determining the rate of the binding reaction, nor do they provide direct information about the dissociation process of the resulting adduct. An interesting alternative to the above methods may be the switchSENSE technology, which uses chips with a gold surface covered with fragments of nucleic acid strands. The essence of this technique lies in the possibility of studying the interaction between the ligand and the analyte in real time, in the flow of the buffer. In turn, its simplicity results from the use of a signaling system attached to the DNA strand, which, based on changes in fluorescence intensity, provides information about the ongoing interactions, without the need to label the tested systems [2]. This technique can be extremely useful in the study of compounds with potential biological activity, e.g. new pharmaceuticals.

The conducted research consisted in determining the type of binding and the strength of interaction of low-molecular compounds with the DNA helix using the switchSENSE technique. The analyzed compounds include the intercalator - ethidium bromide described in the literature [3] and pyrazine-2-thiocarboxamide (PTCA), which is a pyrazine derivative with proven antifungal properties, and studies of its interaction with DNA have already been carried out using, among others, spectrophotometric and voltammetric methods [4]. In addition, the interactions of sulfonamide derivatives of different aminoalkyl chain lengths [5] with the DNA biomolecule were investigated. Due to the resulting limitations of some methods, it was impossible to determine the association constant for these compounds. Therefore, the switchSENSE technique was used for this purpose, which allows to determine the influence of the length of the alkylamino chain on interactions with DNA.

Acknowledgments: This work was supported by the National Science Centre (NCN) under Grant No. UMO-2019/33/B/ST4/00031

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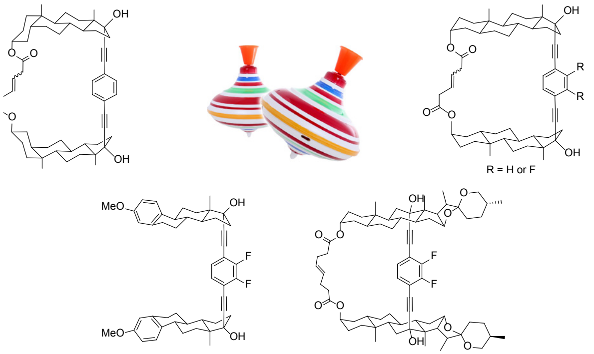
MACROCYCLIC MOLECULAR ROTORS WITH STEROIDAL FRAMEWORKS – SYNTHESES AND SOME PROPERTIES

Dorota Czajkowska-Szczykowska[1], Marek J. Potrzebowski[2], Miguel A. Garcia-Garibay[3], Rosa Santillan[4], Jacek W. Morzycki[1]

[1] *Faculty of Chemistry, University of Bialystok, K. Ciołkowskiego 1K, 15-245 Białystok, Poland*
[2] *Centre of Molecular and Macromolecular Studies, Polish Academy of Sciences, Sienkiewicza 112, 90-363 Lodz, Poland*
[3]*Department of Chemistry and Biochemistry, University of California, Los Angeles, California 90095, United States*
[4]*Departamento de Química, Centro de Investigación y de Estudios Avanzados del IPN, Ciudad de México Apdo. Postal 14-740, 07000, México*
dorotac@uwb.edu.pl



The careful design of applicable artificial molecular machines is based on structural and dynamic analogies between macroscopic objects and small molecules. Scientists are trying to integrate them into organized assemblies to achieve a level of exquisite control over molecular motion and function. These are intended to perform valuable work on their immediate environment. Such inspirations was taken from Nature, which has evolved a large group of molecular machinery, such as ATP synthase or skeletal muscle [1].

The synthesis of compounds with a wheel-and-axis molecular architecture, possessing sufficient free volume for the rotational motion, was considered [2]. Relatively small group, termed *rotator*, linked to some voluminous groups (called *stators*) with large moment of inertia is the most desired. In this purpose, the preparation of molecular rotors based on steroidal molecules performing dynamic processes in the crystalline state will be presented [3].

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PHOTODYNAMIC IMMUNOTHERAPY: RECENT ADVANCES AND FUTURE CHALLENGES

Janusz M. Dąbrowski

Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Krakow, Poland
janusz.dabrowski@uj.edu.pl

Innovative approaches for combating resistant cancers through the stimulation of the immune system show great potential. One notable example of such therapeutic strategies is photodynamic therapy (PDT), which operates on the principles of photochemistry. PDT not only exerts direct effects on cancer cells but also disrupts tumor vasculature and activates the host immune system. However, to achieve successful therapeutic outcomes, including the eradication of primary tumors and distant metastases, the design of appropriate photosensitizers (PSs) with desired optical and photophysical properties is imperative. These properties enable efficient generation of reactive oxygen species (ROS) under tumor microenvironmental (TME) conditions, particularly hypoxia. [1-2]

Consequently, this work places particular emphasis on the photochemical characteristics of bacteriochlorin-based photosensitizers, with a focus on their intense NIR absorption and sufficiently long-lived triplet states that enable ROS generation. ROS not only initiate an inflammatory reaction but also induce the expression of heat-shock proteins, promote immune cell infiltration, and establish long-term immune memory. The distinctive features of PDT open up new possibilities for combining PDT with agents that stimulate the immune response, as well as with immunotherapy, specifically those based on PD-1/PD-L1 blockade. Furthermore, this work provides an overview of our recent findings regarding the synthesis of TEM-targeted conjugates possessing desired spectroscopic and photochemical properties, as well as enhanced selectivity and biological activity. [3-5]

Lastly, some limitations of PDT are discussed, and a future scenario is outlined for the development of PDT as a standalone therapy and in combination with immunotherapy to overcome these challenges.

ACKNOWLEDGEMENTS
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ACTIVITY PROFILING OF VIRAL PROTEASES FROM SARS-COV-2

Marcin Drąg[1], Wioletta Rut[1], Katarzyna Groborz[1,9], Linlin Zhang[2,3,4,9], Xinyuanyuan Sun[2,3,4], Mikolaj Zmudzinski[1], Bartlomiej Pawlik [5,6], Xinyu Wang[7], Dirk Jochmans[7], Johan Neyts[7], Wojciech Młynarski[5], Rolf Hilgenfeld[2,4,8], Zongyang LV[9], Stephanie Patchett[11], Digant Nayak[9, 10], Scott J. Snipas[12], Farid El Oualid[13], Tony T. Huang[11], Miklos Bekes[14], Shaun K. Olsen[9, 10]

[1.] Department of Chemical Biology and Bioimaging, Wroclaw University of Science and Technology, Wroclaw, Poland. [2.] Institute of Molecular Medicine, University of Lübeck, Lübeck, Germany. [3.] Institute of Biochemistry, Center for Structural and Cell Biology in Medicine, University of Lübeck, Lübeck, Germany. [4.] German Center for Infection Research (DZIF), Hamburg-Lübeck-Borstel-Riems Site, University of Lübeck, Lübeck, Germany. [5.] Medical University of Lodz, Lodz, Poland. [6]. Postgraduate School of Molecular Medicine, Medical University of Warsaw, Warsaw, Poland. [7.] Laboratory of Virology and Chemotherapy, Department of Microbiology, Immunology and Transplantation, Rega Institute, KU Leuven, Leuven, Belgium. [8.] Center for Brain, Behavior, and Metabolism, University of Lübeck, Lübeck, Germany. [9.] Medical University of South Carolina, Charleston, SC 29425, USA. [10.] Department of Biochemistry and Structural Biology University of Texas Health Science Center at San Antonio, San Antonio, TX 78229, USA. [11.] Department of Biochemistry and Molecular Pharmacology, New York University School of Medicine, New York, NY 10016, USA. [12.] Sanford Burnham Prebys Medical Discovery Institute, La Jolla, CA 92037, USA. [13.] UbiQ Bio B.V., 1098 XH, Amsterdam, Netherlands, [14.] Independent Consultant.
marcin.drag@pwr.edu.pl

Proteases are key players in the development of viral diseases. Recent studies show that proteases operate in a network that involves the activity of many different proteolytic enzymes at the same time. Given the fact that more and more proteases are actively involved in viral diseases, there is an urgent need to develop new chemical tools that, thanks to the activity of enzymes, can be used for their precise monitoring or the search for drug candidates.

Our group has recently developed technology to obtain new types of ultrasensitive chemical tools (substrates, inhibitors, activity-based probes) for major families of medically important proteases. Using this novel, unique and very efficient technology called Hybrid Combinatorial Substrate Library (HyCoSuL) we have demonstrated that protease substrate specificity can be significantly enlarged by the use of unnatural amino acids in peptide sequence.

In December 2019, the first cases of infection with a novel coronavirus, SARS-CoV-2, were diagnosed. To address this emerging problem, we focused on the SARS-CoV-2-Plpro and SARS-CoV-2-Mpro that constitutes one of the most attractive antiviral drug targets. We used a combinatorial substrate library and performed comprehensive activity profiling of both proteases. The lecture will present modern techniques of creating tools for the study of SARS-CoV-2-Plpro and SARS-CoV-2-Mpro focusing on biochemical characterization, bioimaging, crystal structures and antiviral properties as well as provide a structural framework for the design of inhibitors as antiviral agents and/or diagnostic tests.

Kasperkiewicz et al. Proc. Natl. Acad. Sci. U S A. 2014; Poreba et al., Nature Protocols, 2017; Rut et al, Nature Chemical Biology, 2021; Rut et al. Chemical Science, 2020; Rut et al., Science Advances, 2020

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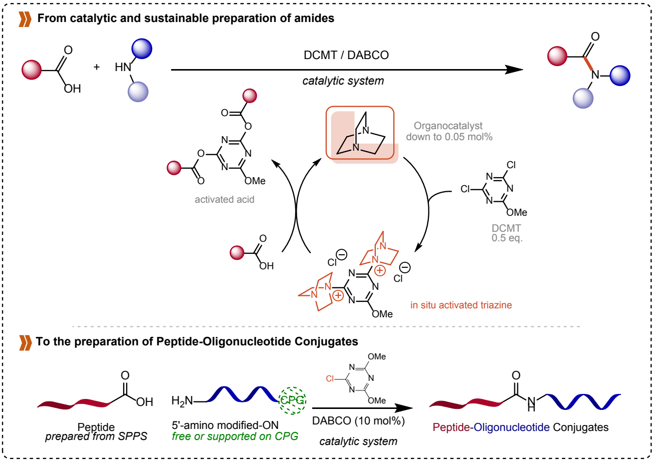
CATALYTIC APPROACH FOR AMIDE COUPLING FOR THE DEVELOPMENT OF PEPTIDE-OLIGONUCLEOTIDE CONJUGATES

Marion Gras, Pauline Adler, Michael Smietana

ChemBioNAC, IBMM, Université de Montpellier, CNRS, ENSCM, 1919 Route de Mende, 34293 Montpellier, Cedex 5, France ; www.chembionac.com
marion.gras@etu.umontpellier.fr

Amides are one of the most important functional groups in organic chemistry, with significant importance in the pharmaceutical industry and life sciences. Numerous efficient coupling reagents have been described, but most of them are not atom-economic and generate non-recoverable by-products.[1] The development of sustainable approaches for amide bond formation is therefore still needed. We have thus developed a novel catalytic method for the direct synthesis of amides from carboxylic acids and amines. This approach demonstrates excellent efficiency across a wide range of substrates, without causing epimerization of chiral stereocenters, and is applicable to solid-phase peptide synthesis (SPPS).[2]



Subsequently, this new approach was extended to the synthesis of peptide-oligonucleotide conjugates (POC). POC are widely used as biologically relevant compounds: the oligonucleotide serves as the therapeutic agent (anti-sense, siRNA etc.) while the peptide helps for cell penetration (amongst other applications).[3] In this context, we will present the results of our study dedicated to the synthesis of POC both in aqueous solution and on CPG solid support, using our catalytic approach.

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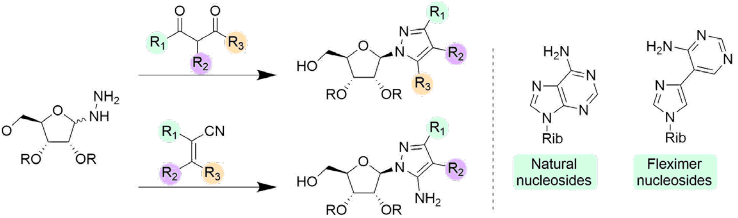
SYNTHESIS OF NOVEL ANTIVIRAL NUCLEOSIDE ANALOGUES BEARING A PYRAZOLE MOIETY

Anaïs Guillou, Suzanne Peyrottes, Jean-Jacques Vasseur, Michael Smietana, Christophe Mathé

Institut des Biomolécules Max Mousseron, Université de Montpellier, CNRS, ENSCM, 1919 Route de Mende, Montpellier, France
anais.guillou@etu.umontpellier.fr

Nucleoside analogues play a significant role in antiviral therapies, as they can interact and inhibit multiple essential enzymes such as viral polymerases.[1] While several chemical modifications have already been described,[2] the emergence of new viruses and re-emergence of known RNA viruses reactivated the search for broad-spectrum antivirals and new biologically active scaffolds. The present work focuses on nucleobase modifications.

Base-modified nucleosides are usually synthetized by reaction of protected pentofuranosides with a modified nucleobase thus forming the glycosidic bond. Here, we described a linear approach starting from an osidic precursor having a pre-formed C-N bond, thus avoiding regioselectivity and stereoselectivity issues usually encountered during *N*-glycosylation reactions. While a handful pyrazole nucleosidic analogues have been synthetized in the 70s starting from D-ribosylhydrazine these compounds have not been evaluated on polymerases.[3,4] We report here the synthesis of 25 new nucleoside analogues synthetized by reacting D-ribosylhydrazine with 1,3-dicarbonyl compounds and acrylonitrile derivatives



This work was further extended to the synthesis of fleximer nucleoside analogues. This term defines nucleosides in which the purine base has been cleaved into two heterocycles linked by a bond that allows rotation.(5,6containing two or more planar moieties in the heterocyclic base, connected by a bond that permits rotation. Such analogs have been proposed as molecular probes for detecting enzyme–substrate interactions and studying the transcription and translation of nucleic acids, but subsequently have attracted the interest of researchers by their antiviral and antitumor activity. The methods used in the synthesis of such compounds, along with their structural features and also biological activity are considered in this review.","container-title":"Chemistry of Heterocyclic Compounds","DOI":"10.1007/s10593-020-02713-5","ISSN":"0009-3122","issue":"6","journalAbbreviation":"Chem Heterocycl Compd (N Y) These compounds were initially designed in order to study enzyme-substrate interactions, but they have shown interesting antiviral and antitumor activities. In our case, the synthesis of the fleximers was achieved using Suzuki-Myaura cross-coupling of various boronic acid derivatives with a bromopyrazole nucleoside synthetized by the method described above.

Acknowledgement: The GAVO consortium is gratefully acknowledged for supporting this project.

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POINT-OF-CARE TESTING FOR C-REACTIVE PROTEIN IN A SEQUENTIAL MICROFLUIDIC DEVICE

Suchanat Boonkaew, Katarzyna Szot-Karpińska, Joanna Niedziółka-Jönsson,
Martin Jönsson-Niedziółka

Institute of Physical Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, Warsaw 01-224, Poland
martinj@ichf.edu.pl

Point-of-care testing (POCT) devices have revolutionized the detection of biomarkers and diseases, including SAR-CoV-2, cancer, diabetes, and cardiovascular diseases (CVDs) [1]. These devices offer easy-to-use, portable, rapid, and cost-effective features. However, the complex reagent manipulation process hinders their performance. In this study, we present a microfluidic sensor device that simplifies reagent handling using C-reactive protein (CRP) as a model biomarker.

To enable sequential reagent delivery, we employed capillary-driven microfluidics that combines a fast- flow and delayed-flow channel. The device was assembled using transparency PET film and double-sided adhesive tape with a passive pump paper serving as a waste reservoir and fluid flow controller and a screen-printed electrode, using chronocoulometry (CC) to quantify CRP concentration. Once the running buffer is loaded, the device performs automated washing of unbound antigens and sequential transport of the redox reagent, completing the analysis within 15 minutes. In contrast, quantitative CRP measurements usually relies on antibodies and enzyme-linked immunosorbent assay (ELISA), which requires measurements in a specialized laboratory. Additionally, as an alternative to antibodies, a P3- CRP peptide was developed and utilized as a new bioreceptor for CRP detection, prepared through phase display technology. The device's performance using both antibody and P3-CRP peptide was examined, demonstrating a detection limit as low as 47 pg mL-1 with a wide linear range spanning 5 orders of magnitude.

To validate its applicability, the device was tested with serum and whole blood samples, yielding satisfactory results. This microfluidic device holds great potential for low-cost, easy-to-use, and point- of-need diagnostics. Its impact extends beyond CRP detection, since the general concept can be extended to other biomarkers.

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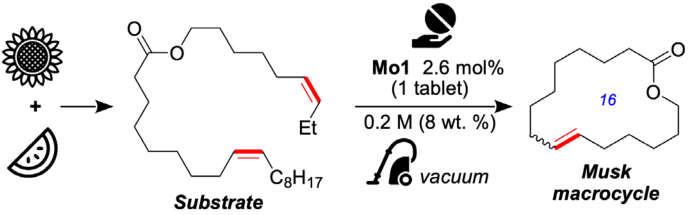
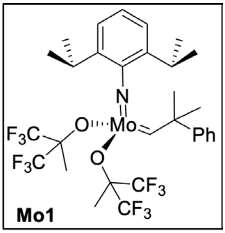
HIGH CONCENTRATION RING CLOSING METATHESIS FOR EFFICIENT SYNTHESIS OF MACROCYCLIC MUSK COMPOUNDS

Anna Kajetanowicz

Biological and Chemical Research Centre, Faculty of Chemistry, University of Warsaw, Żwirki i Wigury 101, 02-089 Warsaw, Poland
a.kajetanowicz@uw.edu.pl

Macrocyclic musk compounds are valuable raw materials for the flavor and fragrance industry, and olefin metathesis reaction, since Fürstner's pioneering research [1], has been a convenient method for their synthesis [2]. For many years, macroRCM was carried out at high dilutions to avoid the formation of undesired side products, but recently there has been increasing attention to designing catalysts that allow to increase the reaction concentration to 0.02-0.1 M [3]. The employment of reactive distillation, which allows the preparation of musk-scented compounds in the presence of both ruthenium and molybdenum catalysts at concentration of 0.2 M or higher, makes us prominent participants in this general trend [4]. During the presentation I will highlight our key findings.





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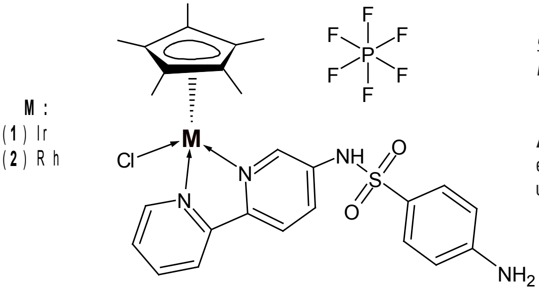
ANTICANCER STUDY ON IRIDIUM AND RHODIUM HALF-SANDWICH COMPLEXES WITH BIPYRIDYLSULFONAMIDE LIGAND

Mateusz Kowalik[1], Joanna Masternak[2], Mateusz Olszewski[3], Natalia Maciejewska[3], Katarzyna Kazimierczuk[3], Jerzy Sitkowski[4,5], Mariusz Makowski[1]

[1] *Faculty of Chemistry, University of Gdańsk, Wita Stwosza 63, 80-308 Gdańsk, Poland*
[2] *Institute of Chemistry, Jan Kochanowski University in Kielce, Uniwersytecka 7, 25-406 Kielce, Poland*
[3] *Faculty of Chemistry, Gdańsk University of Technology, Gabriela Narutowicza 11/12, 80-233 Gdańsk, Poland*
[4] *Institute of Organic Chemistry, Polish Academy of Science, Marcina Kasprzaka 44/52, 01-224 Warszawa, Poland*
[5] *National Medicines Institute, Chełmska 30/34, 00-725 Warszawa, Poland*
mateusz.kowalik@ug.edu.pl

Among many types of non-platinum compounds, half-sandwich organometallic complexes have attracted great interest in chemotherapeutic studies [1]. Their biological activity is mainly modulated by the choice of appropriate chelating ligand. Sulfonamides were used for the treatment of various bacterial, fungal, and protozoal infections. However, they have been also recently investigated in cases of cancer chemotherapy [2].

Herein, two half-sandwich complexes $[(\eta^5\text{-Cp})\text{IrCl(L)}]\text{PF}_6$ (**1**) and $[(\eta^5\text{-Cp})\text{RhCl(L)}]\text{PF}_6$ (**2**) were prepared by treating pentamethylcyclopentadienyl chloride dimers of Ir(III) or Rh(III) with the obtained 4-amino-*N*-(2,2'-bipyridin-5-yl)benzenesulfonamide ligand (**L**) and NH_4PF_6 (Scheme 1). The crystal structures of **L** and complexes **1** and **2** were obtained and then analyzed. Coordination reactions of the bipyridylsufonamide ligand to the central ions were confirmed by MS, UV-Vis, FT-IR, NMR (^{1}H, ^{13}C, and ^{15}N) spectroscopies, and stability study. Moreover, the interactions of compounds **L**, **1,** and **2** with HSA and also CT-DNA binding studies have been investigated. Additionally, the reactivity of complexes toward GSH and NADH has been spectrophotometrically tested. The compounds were then evaluated for their antiproliferative activity against four cancer cell lines: A549, HCT-116, MCF7, Nalm-6, and nonmalignant HEK293. It has been observed that the Ir(III) complex **1** was found to exhibit a lack of antiproliferative properties against the tested cancer cell lines. The sulfonamide ligand (**L**) and the Rh(III) complex (**2**) were studied in detail for the colon cancer HCT-116 cell line, and a detailed biological analysis was performed.



Scheme 1. The structure of half-sandwich Ir(III) and Rh(III) complexes with sulfaligand.

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SYNTHESIS AND CHARACTERIZATION OF CORE-SHELL NANOMATERIALS BASED ON GOLD NANOPARTICLES

Agata Kowalska, Elżbieta Adamska, Beata Grobelna

Faculty of Chemistry, University of Gdansk, Wita Stwosza 63, 80-308 Gdansk, Poland
agata.kowalska@phdstud.ug.edu.pl

Currently, nanotechnology is the dominant field of science, which creates many opportunities. In addition, it is a research direction that is undergoing intensive development. Interest in nanomaterials is applied in many industries, one of the most important aspects is nanomedicine [1]. Gold nanoparticles have been known for a long time, among others, thanks to their applications in the medical industry. For example in cancer therapy, they are used as carriers of anticancer drugs or in photothermal therapy [2].

Synthesizing and reproducibility of results is one of the more difficult steps and often debatable of technology at the nanometer scale. Our research group worked on the procedure for obtaining core-shell nanostructures consisting of a gold core and a silica shell, which is a fundamental element for further research. We have successfully obtained spherical gold nanoparticles coated with silica, which is intended to improve the stability of the obtained nanomaterials and reduce potential toxicity. In addition, we also performed a basic characterization of the material, determined the size, shape, and stability, and confirmed the presence of gold in the sample.

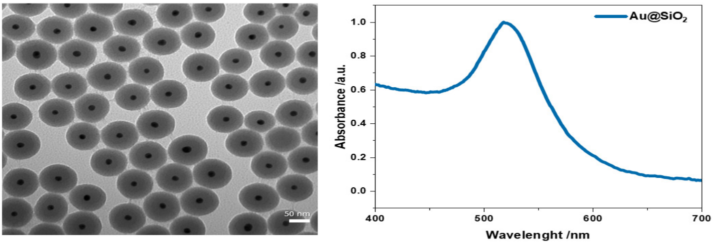

Figure 1. Transmission Electron Microscopy image and absorption spectra for Au@SiO2

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STIMULI-RESPONSIVE SUPRAMOLECULAR TRANSFORMATIONS BETWEEN HOMOMETALLIC COMPLEXES AND HETEROMETALLIC POLYMERIC MATERIALS

Gracjan Kurpik,[1,2] Anna Walczak,[1,2] Grzegorz Markiewicz,[1,2] Jack Harrowfield,[3]
Artur R. Stefankiewicz[1,2]

[1] *Center for Advanced Technology, Uniwersytetu Poznańskiego 10, 61-614 Poznań, Poland*
[2] *Faculty of Chemistry, Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland*
[3] *ISIS, Université de Strasbourg, 8 allée Gaspard Monge, 67083 Strasbourg, France*
gracjan.kurpik@amu.edu.pl, ars@amu.edu.pl

Metal-ligand interactions are the primary driving force in the generation of simple coordination compounds, as well of metallosupramolecular architectures with a high degree of complexity and a precisely defined structure (1). Taking into account the character of a coordinate bond, *i.e.* its high strength but commonly dynamic nature, coordination-driven self-assembly processes are characterized by high controllability at the molecular level with respect to directionality, reversibility and post-synthetic switchability (2). In the presented research, a bifunctional ligand 4,4-dimethyl-1-(pyridin-4-yl)pentane-1,3-dione (H**L**) able to provide two distinct coordination sites, *i.e.* anionic β-diketonate (after deprotonation) and neutral pyridine, has been used in the synthesis of Ag(I), Pd(II) and Pt(II) complexes that then have been applied as metalloligands for the construction of new heterometallic polymeric materials (3). The ambidentate nature of **L**$^-$ enables switching between different modes of coordination within mononuclear complexes or their conversion into polymeric species in a fully controllable way. The coordination-driven processes can be triggered by various stimuli, *i.e.* a metal salt addition or acid-base equilibria, and presents an efficient strategy for the generation of metallosupramolecular materials. As a consequence of self-assembly, new multimetallic coordination aggregates have been synthesized and characterized in depth in solution as well as in the solid state. Furthermore, the Pd-based assemblies have been found to be efficient catalyst precursors in the Heck cross-coupling reaction, demonstrating a direct impact of compositional and morphological differences on their catalytic activity.

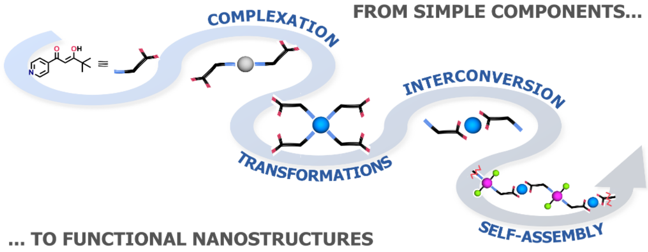

*Figure 1. Supramolecular transformations within coordination-driven assemblies based on H**L**.*

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AMBIPOLAR N-DOPED PAHS. A UNIQUE STRATEGY FOR THE EFFICIENT TADF OLED EMITTERS.

[a]Jakub Wagner, [c]Dharemendra Kumar, [c]Michał Andrzej. Kochman, [b]Adam Kubas, [c]Przemysław Data, [d]Eli. Zysman-Colman, M. Lindner

[a] Institute of Organic Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, 01-224 Warsaw, Poland;
[b] Institute of Physical Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, 01-224 Warsaw, Poland;
[c] Łódź University of Technology, Department of Chemistry, Stefana Żeromskiego 114, Łódź 90-543, Poland
[d] University of St-Andrews, Purdie Building, North Haugh, KY16 9ST St Andrews, United Kingdom
marcin.lindner@icho.edu.pl

Although bowl-shaped N-pyrrolic polycyclic aromatic hydrocarbons (PAHs) can achieve excellent electron--donating ability, their application for optoelectronics is hampered by typically low photoluminescence quantum yields (PLQYs). [1] To address this issue, we report a efficient synthetic strategy towards nonplanar N-PAHs with intrinsic D-A electronic structures [2] which are, for the first time, applied as yellow to orange TADF/RTP OLED emitters (Fig. 1, 1). The entirely fused, and curved system leads remarkable PLQY (up to 86%) OLEDs fabricated with the developed N-PAHs as TADF/RTP emitters were unprecedented for this class of compounds showing EQE as high as 12% along with satisfactory operational stability. We next performed a facile post-functionalization of our core structure introducing a set of auxiliary donors (Fig. 1, 2), at the meta position of protruding phenyl ring of quinoxaline.[3] This modification let us to obtain a set of highly emissive dyes (PLQY up to 96%) and successfully fabricate a series of TADF OLEDs devices with a yellow to orange-red electroluminescent emission color. Their analyses revealed significant EQE up to 21.9% and pronounced luminance (up to 31 000 cd/m2) which is the highest recognized for N-doped PAHs investigated in OLED domain. We furthermore challenged the synthesis of pyridine-based dyes (Fig. 1, 3) to change the dipole orientation of the acceptor structure. [4] This resulted in significant batochromic shift of the emission to the desired NIR region. The photophysical properties together with NIR OLED device characteristics are being studied and will be soon reported.

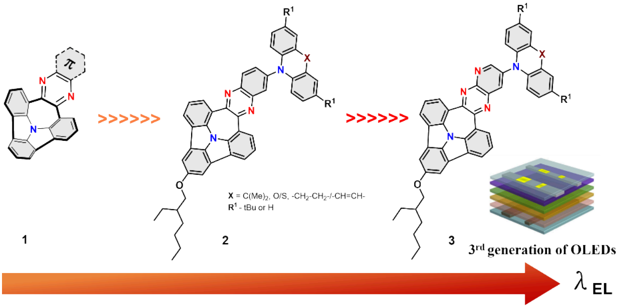

Figure 1. Evolution of ambipolar N-doped PAHs as TADF OLED emitters.

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SELF-ASSEMBLY OF A FLUORESCENT HYDROGEN-BONDED CAPSULE BASED ON AN AMINO-ACID FUNCTIONALISED TETRAPHENYLETHYLENE

Anna Brzechwa-Chodzyńska,[‡ab] Grzegorz Markiewicz,[‡ab] Piotr Cecot,[ab] Jack Harrowfield,[c] Artur R. Stefankiewicz[ab]

a) Faculty of Chemistry, Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, Poznań 61-614, Poland
b) Center for Advanced Technology, Adam Mickiewicz University, Uniwersytetu Poznańskiego 10, Poznań 61-614, Poland
c) Université de Strasbourg, ISIS, 8 allée Gaspard Monge, Strasbourg 67083, France
grzegorz.markiewicz@amu.edu.pl

A newly designed TPE derivative is presented,[1] which due to its functionalization with amino-acid side arms, can self-assemble into a chiral, non-covalent dimeric capsule in solvents of low polarity. The capsule is held together by four pairs of hydrogen bonds formed between amino acid COOH units, leaving amide linkers unoccupied. Surprisingly, the dimerization in the ground state does not affect the fluorescent properties of TPE core, as those are governed by the excited state equilibrium involving excimer species. However, due to the strong AIE tendency of the TPE, photoluminescence quantum yields up to 24% can be attained in the aggregated state.

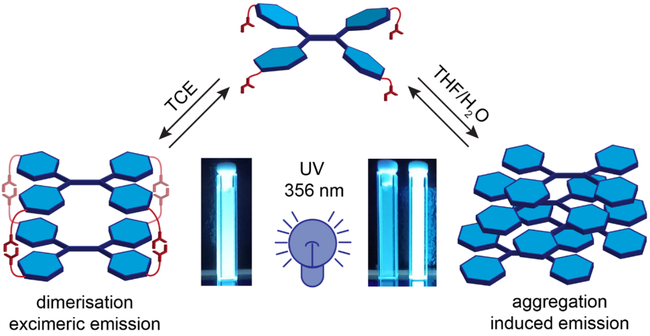

Figure 1. Schematic representation of the self-assembly and photoluminescent properties of an amino-acid functionalised tetraphenylethylene.

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MEMBRANE-ACTIVE POLYMERS FOR DRUG DELIVERY: RAFT SYNTHESIS, DRUG ENCAPSULATION, AND BIOLOGICAL EVALUATION

Karolina H. Markiewicz

Faculty of Chemistry, University of Bialystok, Ciolkowskiego 1K, 15-245 Bialystok, Poland
k.markiewicz@uwb.edu.pl

Drug delivery is a complex process involving drug administration, absorption, and transport through tissues until the bioactive molecules bind to the target site and achieve a therapeutic effect. The pharmaceutical substance may encounter many natural barriers, mainly cell membranes, during this path. The efficiency of the drug-membrane interaction is one of the most essential pharmacological features determining the biological activity of a drug.[1,2] In this view, the synthesis of new drugs or drug delivery systems containing membrane-active mediators, which exert their pharmacological effects by modulating the environment of cell membranes, might be a valuable strategy to improve drug efficacy.

The presented study concerns lipid-polymer conjugates as drug carriers. Reversible addition-fragmentation chain transfer (RAFT) polymerization was used to obtain amphiphilic (co)polymers containing derivatives of lipids such as cholesterol or diacylglycerols in the main chain or side chains. The (co)polymers were formed into polymeric nanoparticles (PNPs) with and without encapsulated drug molecules and characterized in terms of their physicochemical and biological properties. The biological evaluation indicated compatibility with the representatives of host cells and cytotoxicity toward selected cancer cell lines.[3-5]

The research is supported by the National Science Centre, Poland, grant no. NCN/2019/35/B/ST5/03391.

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SYNTHESIS OF BIO-SOURCED ANTIOXIDANTS BY PHOTOINDUCED THIOL-ENE COUPLING UNDER CONTINUOUS-FLOW CONDITIONS

Alberto Marra[1] and Marie-Christine Scherrmann[2]

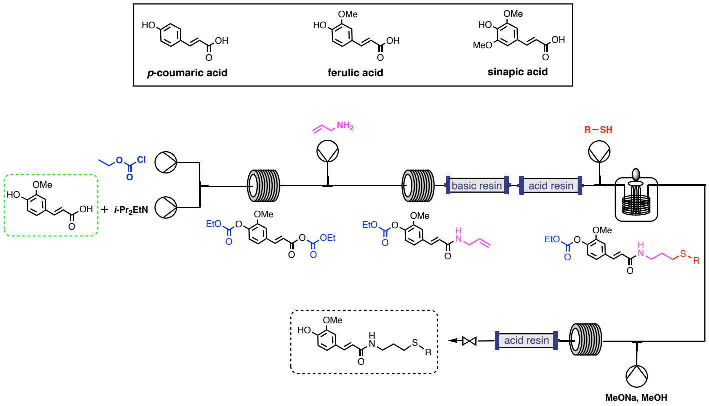
[1] *Institut des Biomolécules Max Mousseron (IBMM), Pôle Chimie Balard, Montpellier, France*
[2] *Institut de Chimie Moléculaire et des Matériaux d'Orsay (ICMMO), Université Paris-Saclay, Orsay, France*
Alberto.Marra@umontpellier.fr

The use of antioxidants as additives to maintain quality and durability of products is indispensable in a considerable range of industries (from fuels to food), thus, there is a true potential for the development of processes for the large-scale synthesis of new antioxidants from bio-sourced molecules. Technical lignins are by-products recovered from the industrial fractionation of lignocellulosic biomass, either from the paper industry or from biorefinery processes developed for the production of bioethanol. These by-products contain phenolic compounds, which can be extracted by organic solvents, mainly constituted of *p*-coumaric, ferulic, and sinapic acids, well-known antioxidants.

Since polar antioxidants are more efficient in an apolar medium, and conversely, apolar antioxidants are more efficient in a polar medium (the so-called "polar paradox"), the tuning of the antioxidant activity of these acids can be achieved by introducing polar or apolar residues. To preserve the functions involved in the antioxidant activity (phenolic OH and conjugated double bond), we functionalized these compounds taking advantage of their carboxylic group.

The reaction of the latter with 2 equiv. of ethyl chloroformate gave the mixed anhydride, *O*-protected as ethyl carbonate, that was coupled with allylamine to give the allyl amide. The totally chemo- and regio-selective photoinduced (UV-A, 365 nm) radical addition of a thiol to the terminal alkene (Thiol-Ene Coupling, TEC), in the presence of a photoinitiator, produced the stable sulfide that was then *O*-deprotected by transesterification (see Figure below). Bio-sourced hydrophilic (e.g. sugar thiols) and hydrophobic (e.g. fatty acid thiols) thiols have been employed in the thiol-ene coupling.

The new molecules will be exploited for skin care applications (sunscreen and anti-aging formulations).



This work aims at developing a safe and efficient process easy to scale up to an industrial scale by using parallel reactor systems (numbering up). They represent a valid alternative to conventional reaction vessels because the reduced diameter of coil reactors allows improved control of mass and heat transfer as well as light penetration.

THE SYNTHESIS ANDUSE OF FOLIC ACID-DERIVED CARBON NANODOTS AS FLUORESCENT MARKERS FOR NON-INVASIVE IMAGING OF MORPHOLOGICAL CHANGES IN LIPIDIC MESOPHASES.

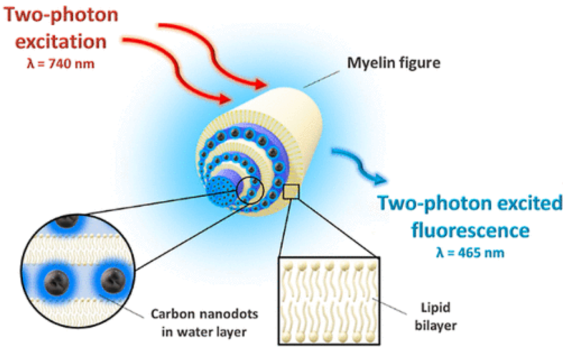
Dominika Benkowska-Biernacka, Sebastian G. Mucha, Katarzyna Matczyszyn

Institute of Advacned Materials, Faculty of Chemistry, Wroclaw University of Science and Technology, Wyb. Wyspianskiego 27, 50-370 Wroclaw, Poland
Katarzyna.matczyszyn@pwr.edu.pl

Presented studies are focused on designing new fluorescent probes that are bright, biocompatible, and derived from folic acid. Folic acid-derived carbon nanodots (FA CNDs) were developed and characterized for their structural and optical properties. These CNDs showed significant fluorescence performance under both linear and non-linear (two-photon) excitation, making them suitable for imaging applications (1,2).

The goal of the research is to understand membrane-mediated processes by imaging morphological changes in lipidic mesophases. Non-invasive imaging is crucial for this purpose. We used confocal fluorescence microscopy and two-photon excited fluorescence microscopy to investigate the distribution of FA CNDs within the bioinspired myelin figures in a three-dimensional manner.[3]

The research demonstrated that FA CNDs can effectively serve as fluorescent markers for imaging different forms and components of multilamellar microstructures within the phospholipid-based myelin figures.



In summary, the study successfully introduced and characterized folic acid-derived carbon nanodots as excellent fluorescent markers for non-invasive imaging of bioinspired myelin figures, enabling the visualization and study of structural changes in lipidic mesophases. The research findings have potential applications in the understanding of membrane-related processes and could further the development of imaging techniques in the biological and medical fields.

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PORE FUNCTIONALIZATION OF METAL-ORGANIC FRAMEWORKS FOR PROTON CONDUCTION

Dariusz Matoga

Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Kraków, Poland
dariusz.matoga@uj.edu.pl

Coordination polymers based on organic linkers, or so-called metal-organic frameworks (MOFs) are a large group of materials characterized by modularity, crystallinity and porosity [1]. These features create unique opportunities to design and explore them in a variety of applications, such as catalysis, sensorics or energy storage and conversion. For example, MOFs capable of proton conduction (PC-MOFs) are drawing the attention of researchers as potential solid electrolytes in fuel cells. Several general strategies have been established for the synthesis of PC-MOFs, the most effective of which are installing Brønsted acid groups on linkers and filling voids with acidic ions or molecules [2]. In this presentation, three original synthetic approaches for obtaining PC-MOF materials will be presented.

The first strategy is based on chlorosulfonation of selected organic building blocks, which leads to the installation of terminal sulfonic groups in the targeted MOF backbones. Its implementation has yielded a few new PC-MOFs including sulfonated zirconium-based frameworks, selected for discussion [3].

The second strategy allows inducing and tuning of proton conductivity in MOF with open metal sites using a solvent-free mechanochemistry and thiocyanate salts with protic cations. Contrasting examples for discussion will include the flexible JUK-1 framework, undergoing remarkable reversible MOF-MOF or MOF-HOF transformations, and the rigid CPO-27 platform, whose modification leads to highly conductive materials even under anhydrous conditions (4).

The third strategy utilizes inverse electron-demand Diels-Alder reaction as a covalent post-synthetic modification of MOFs containing a tetrazine entity, carried out under mild conditions with functionalized dienophiles. This approach is being developed with new MOFs and known platforms [5].

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CELLULAR METABOLOME IN RESPONSE TO EXTERNAL CONDITIONS

Badr Qasem, Wojciech Wojtowicz, Piotr Młynarz

Department of Biochemistry, Molecular Biology and Biotechnology, Faculty of Chemistry, Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław
piotr.mlynarz@pwr.edu.pl

Metabolomic studies of cell cultures allow for advanced qualitative and quantitative analysis of low molecular weight compounds – metabolites, which are changed under different stimuli. The hypoxia, hyperoxia, and reoxygenation conditions with different cell culturing times are still metabolically unexplored. The oxygen and nutrients bioavailability in time determine very distinctly cell intra and extracellular metabolome. For this reason, different flux metabolites changes reflect the characteristic pattern of each studied condition. Therefore, any studies which are used for the cell culture assessment under the influence of the potential drug, nanotechnological structures, and physical stimulation should be considered with particular care.

STRUCTURAL STUDIES OF COMPLEXES WITH [FE(OX)$_3$]$^{3-}$ AND [FE(OX)$_2$(H$_2$O)$_2$]$^{-}$ UNITS.

Tadeusz M. Muzioł[1], Natalia Tereba[1], Robert Podgajny[2], Julia Reszkowska[1], Grzegorz Wrzeszcz[1]

[1]*Faculty of Chemistry, Nicolaus Copernicus University in Toruń, Gagarina 7, 87-100 Toruń, Poland*
[2]*Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Kraków, Poland*
tmuziol@chem.umk.pl

In multifinctional materials several properties are shared, e.g. magnetic, porous, luminescence, chirality [1]. Oxalate anions are widely studied mainly due to (i) a variety of coordination modes and (ii) chirality of trisoxalatometallate unit resulting in a variety of topologies which can be tuned by proper selection of auxiliary ligands/molecules.

We prepared $\{[Co(bpy)_2(ox)][Cu_2(bpy)_2(ox)Fe(ox)_3]\cdot 8.5H_2O\}_n$ (**1**) and $(Hacr)[Fe(ox)_2(H_2O)_2]\cdot H_2O$ (**2**) complexes (acr = acridine). They were characterised by spectroscopic, thermal and magnetic methods. For single crystals X-ray diffraction experiments were performed. The porosity (**1**) or luminescent (**2**) measurements were carried out. For both compounds XAS experiments were performed at PEEM/XAS beamline of National Synchrotron Radiation Centre SOLARIS (Kraków) for $L_{2,3}$ edges of iron, copper and cobalt.

In (**1**) four different coordination modes of oxalate anion was observed [2]. The compound shows complicated topology with chains composed of alternately arranged $[Cu_2(bpy)_2(ox)]^{2+}$ $[Fe(ox)_3]^{3-}$ moieties. They are connected *via* non-covalent forces and along *a* axis they are separated by $[Co(bpy)_2(ox)]^+$ block balancing the charge providing the porous material (Fig.1). The channels accounting for 16.9% of the cell volume are filled with tightly bound water molecules. Water adsorption experiments are described by a D'arcy andWatt model being the sum of Langmuir and Dubinin–Serpinski isotherms. We developed our own approach to describe the topology of the complex based on the semiclassical model (SC) and molecular field (MF) model. In (**2**) being a hybrid compound compartmentalization occurs with columns of (Hacr)+ cations separated by $[Fe(ox)_2(H_2O)_2]^-$ anions and water molecules.

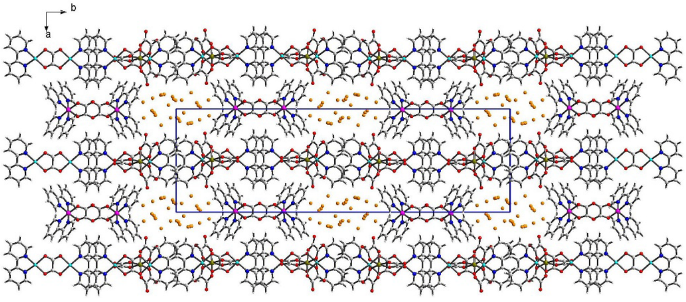

Fig. 1 Packing of $[Co(bpy)_2(ox)][Cu_2(bpy)_2(ox)Fe(ox)_3]\cdot 8.5H_2O$ shows voids filled with water molecules.

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SILVER NANOWIRES AS BUILDING BLOCKS FOR SENSORS

Joanna Niedziółka-Jönsson

Institute of Physical Chemistry Polish Academy of Sciences, Kasprzaka 44/52, 01-224 Warsaw, Poland
jniedziolka@ichf.edu.pl

The unique physical and chemical properties of silver nanowires (AgNWs) make them ideal candidates for designing advanced structures with on-demand properties required for building different sensors. Much of this flexibility comes down to the unique characteristic of having one dimension in the macroscopic range, whereas the other two are firmly in the nanoscale. Light, in the visible or near-infrared part of the spectrum, can excite collective oscillations of free electrons in the transverse directions of silver nanowires, and such oscillations can result in propagating surface plasmon polaritons travelling down the length of the metal nanowire. Since the length of the wires can exceed tens of micrometres, they are visible under standard optical microscopes and can relatively easily be manipulated with microprobes.

Here, we will discuss the tuning of silver nanowires synthesised using wet-chemistry, followed by various strategies of surface functionalisation. Using wide-field fluorescence microscopy we studied antibody-antigen interaction and real-time bioconjugation of photosynthetic proteins to modified silver nanowires pushing our sensitivity towards the single molecule level. The latter is possible due to plasmonic enhancement of protein fluorescence by the silver nanowire. This approach can be universally applied in studying molecule-nanostructure interactions for real-time fluorescence-based sensing.

Proper surface functionalisation is also a key point in studying plasmon propagation in silver nanowires. AgNWs are perfect structures for remote excitation of fluorophores in close vicinity to the nanowire. One such example is long nanowires connected to a drop of quantum dot emitters at one end of the wire that be excited by illuminating the other end of the nanowire. The QD drops can also be used to transfer energy from one nanowire to the next, forming the beginning of an optical network of plasmonic wires. The waveguiding properties of nanowires can also be used for remotely controlled photocatalysis.

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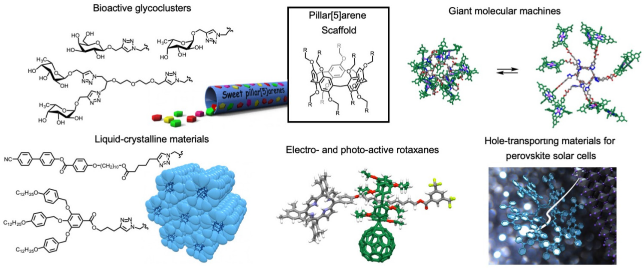
PILLAR[5]ARENE SCAFFOLDS: FROM MULTIFUNCTIONAL NANOMATERIALS TO MOLECULAR MACHINES AND ROTAXANES

Iwona Nierengarten, Jean-François Nierengarten

Laboratoire de Chimie des Matériaux Moléculaires, Université de Strasbourg et CNRS,
(LIMA – UMR 7042), Ecole Européenne de Chimie, Polymères et Matériaux (ECPM),
25 rue Becquerel, 67087 Strasbourg Cedex 2 (France).
iosinska@unistra.fr

With their ten peripheral substituents, pillar[5]arene[1] derivatives are attractive compact nanoscaffolds for the construction of multifunctional compounds with specific properties. The copper catalysed alkyne-azide cycloaddition (CuAAC) reaction has been particularly useful for the ten-fold post-functionalization of pillar[5]arene building blocks bearing ten peripheral azide or terminal alkyne functions. A wide range of advanced materials and bioactive compounds build on a pillar[5]arene scaffold have been thus prepared in recent years. Examples include efficient hole transporting materials for perovskite solar cells,[2] redox-driven molecular machines,[3] and multivalent glycoclusters targeting bacterial lectines.[4] On the other hand, the pillar[5]arene moiety is also a supramolecular receptor offering additional features to the multifunctional materials. This has been for example used to modulate the liquid crystalline properties of pillar[5]arene columnar assemblies[5] and to develop photo- and electro-active rotaxanes.[6] Our latest advances in this particular field will be presented.



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SWITCHABLE COORDINATION POLYMERS IN BETTER SHAPE

Beata Nowicka,[1] Magdalena Fitta,[2] Aleksandra Pacanowska[2]

[1] Jagiellonian University, Faculty of Chemistry, Gronostajowa 2, 30-387 Krakow, Poland
[2] Institute of Nuclear Physics, Polish Academy of Sciences, Radzikowskiego 152, 31-342 Kraków, Poland
beata.nowicka@uj.edu.pl

Coordination networks constitute an important and versatile group of molecular magnetic materials. Their modular structure enables merging at the molecular level various desirable properties, like magnetic order, optical transparency bistability and sensitivity to externals stimuli. However, in the crystalline form coordination networks are usually characterised by unfavourable surface and mechanical properties, which hinder their practical applications. Embedding them in an organic polymer matrix is a promising pathway to prevent their degradation and create materials with desired mechanical properties originating from the choice of the polymer and the fabrication method (Figure 1).

The 1D $\{(NH_4)[Ni(cyclam)][Fe(CN)_6]\ 5H_2O\}_n$ (NiFe) coordination network shows multistability at ambient temperature and humidity conditions: it can coexists in three phases differing in colour and magnetic susceptibility. Moreover, the phase transitions, which are connected with metal to metal charge transfer between $Ni^{II/III}$ and $Fe^{II/III}$ ions, are fully reversible and can be induced by different stimuli, including temperature, pressure and humidity changes [1]. These unusual properties make the NiFe network a perfect candidate for the construction of humidity, pressure and temperature sensors. However, the compound in the crystalline form is brittle and in contact with water it recrystalizes to a different network and loses its switchable properties. Therefore, in order to improve its stability and mechanical properties we prepared composites based on polycaprolactone (PCL) or poly(2-vinylpyridine-*co*-styrene) (P2VP-PS) with embedded nano to micro-sized crystallites of NiFe. The composites were obtained in the form of films or electrospun mats. The materials were characterised by SEM imaging with detection of backscattered electrons to visualise morphology, as well as the size and distribution of the NiFe particles. Magnetic and water vapour sorption measurements show that the switchability between the three forms of the original compound is retained in the composites, with slightly modified conditions of phase transitions.

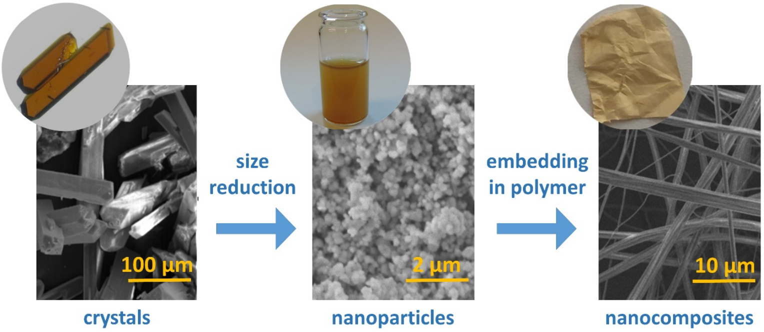

Figure 1. Ideogram showing the change of the form of a coordination polymer from crystals to an electrospun nanocomposite mat.

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COMPLEXING PROPERTIES OF LIGANDS WITH THIAZOLYL-HYDRAZONE SYSTEM TOWARDS CADMIUM IONS

Paulina Nowicka,* Sandra Brzeska, Mariusz Makowski

University of Gdańsk, Faculty of Chemistry, ul. Wita Stwosza 63, 80-308 Gdańsk, Poland
paulina.nowicka@phdstud.ug.edu.pl

According to the report of the World Health Organization (WHO) cancer is currently the biggest global health problem. Based on data from the Globocan 2020 Report it is estimated that in 2040 there will be an increase in the incidence of cancer worldwide by 47% compared to 2020, which will translate into 28.4 million new cases of cancer [1]. The greatest success in the case of compounds used in anticancer therapy so far is the discovery of cisplatin. However, its serious side effects and increasing drug resistance are the main problems in treatment, especially in the advanced stage of the disease. Therefore, the search for new compounds for the treatment of cancer focuses mainly on the search for coordination compounds that would contain a metal ion other than platinum as the central atom. The biological activity of hydrazone ligands containing a thiazole system in its structure and the coordination bonds formed by them with some d-block metal ions is already known in the literature [2,3]. Numerous research studies have proven that metal ions that are generally considered harmful when coordinated with various ligands can modify or stimulate the biological activity of such systems [4]. The research results showed that combinations of cadmium with appropriate ligands, as a result, showed greater cytotoxic activity against some cancer cells than either the ligand or cisplatin alone [5].

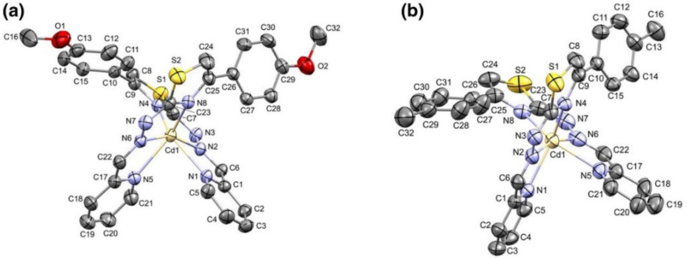

Fig. 1. Molecular structures of the tested complexes [3].

The study aimed to determine the complex-forming properties of hydrazone ligands containing a thiazole system. The research included checking the influence of the substituent (at the aromatic ring) on the spectroscopic properties and the complexing ability concerning cadmium ions. As part of the research, it was necessary to perform a spectral analysis of the tested compounds. Based on changes in the absorbance of the tested systems interacting with Cd^{2+} ions, the values of the gradual and cumulative stability constants of the resulting coordination connections were also determined. In addition, by changing the traditionally used salt as a source of cadmium(II) ions, it was also possible to determine the effect of metal salt hydrolysis on the coordination process.

Acknowledgments

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DEVELOPMENT AND FUNCTIONALIZATION OF NOVEL POLYMERIC MATERIALS FROM POLY(OXAZOLINE)S FOR THEIR POTENTIAL BIOAPPLICATIONS

Umut Ugur OZKOSE[1,2]

[a]*ICGM, University of Montpellier, CNRS, ENSCM, 34095 Montpellier, France*
[b]*Department of Chemistry, Faculty of Science and Letters, Piri Reis University, Tuzla, Istanbul, Turkey*
umut-ugur.ozkose@umontpellier.fr

The polyoxazoline polymers (POx) were discovered as poly(N-acylethylenimine) in 1966, and have caught researchers' attention only in recent years. This is because they stand out in many ways as they exhibit non-cytotoxicity, structural adaptability, susceptibility, high biocompatibility, narrow molecular weight distribution, responsiveness to pH and temperature, high functionalization and copolymerization, versatility, and stealth behavior to attachment of biological moieties such as labeling and targeting groups. To this respect, they became spotlighted as multi-pronged polymer-based biomaterials and a popular choice to replace polyethylene glycol (PEG), which infamously suffer from oxidation under in vivo conditions.

POx are cut out in the diversified amount of biomedical fields such as scaffolds for 3D cell culture, polymer therapeutics, tissue adhesives, surface modification, antimicrobial agents, and matrix excipient for solid dispersions. Here, the methodology described will provide flexibility to obtain the amphiphilic block copolymers to self-assemble into various morphologies, comprising ellipsoids, tubular structures, toroids, vesicles, micellar structures by using functional poly(oxazoline)s (POx), poly(ethyleneimine)s (PEI), poly(ε-caprolactone)s (PCL), and poly(L-lactide)s (PLA). The obtained amphiphilic block copolymers will be distinguished applicants in biomedical studies such as pharmaceutics, drug or gen delivery systems, stabilizing agents, cosmetics and processing aids.

On the other hand, the use of functionalized clay in living cationic ring opening polymerization (CROP) of 2-ethyl-2-oxazoline (EtOx) will ease the growing polymer chains with living nature of the polymerization in the silicate interlayers and fabricate well-defined poly(2-ethyl-2-oxazoline) (PEtOx) polymers with controlled molecular weight and narrow molecular weight distribution. It is expected that PEtOx/clay nanocomposites will be used in the production of novel biomaterials for significant applications such as drug delivery, protein adsorption and antibacterial material.

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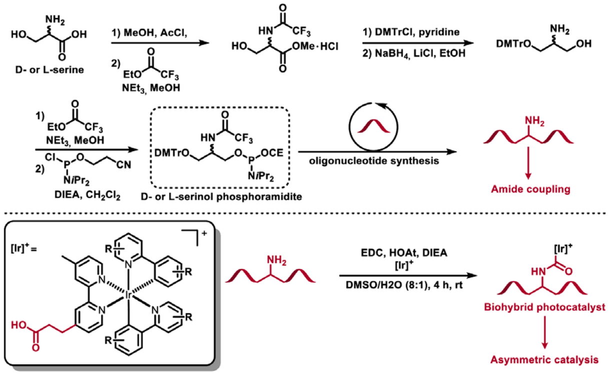
DNA-BASED ASYMMETRIC PHOTOCATALYSIS

Zachary PASTOREL[a], **Juliette ZANZI**[b], **Yves CANAC**[b], **Olivier BASLE**[b], **and Michael SMIETANA**[a]

[a] *Institut des Biomolécules Max Mousseron, équipe ChemBioNAC, Université de Montpellier, Montpellier, France*
[b] *Laboratoire de Chimie de Coordination, Université Paul Sabatier, Toulouse, France*
zachary.pastorel@etu.umontpellier.fr

Chirality is a crucial factor in molecular recognition processes observed in biological systems. While chemists have developed a large variety of chiral ligands able to generate enantiopure compounds, asymmetric biocatalysis, relying on stereoselective, energy-efficient, and environmentally friendly processes, has witnessed significant advancements in recent years.[1] In this context, our group has been dedicated to developing a series of highly enantioselective transformations that rely on the transfer of chirality of the DNA double helix.[2] This approach is based on the covalent or non-covalent anchoring of an achiral Cu(II) bipyridine ligand into natural or modified DNA.[3] More recently, the ligand was introduced inside an oligonucleotide through the synthesis of a serinol phosphoramidite synthon which, after being incorporate, was coupled via an amide link to bipyridines (Figure).



Similarly, drawing inspiration from natural photosynthesis, photocatalyzed reactions have experienced rapid growth and have found application in various chemical transformations.[4] In continuation of our work, we decided to embark in the synthesis of modified DNA functionnalized with a Ir(III) photocatalyst. This was achieved by reacting our serinol-modified oligonucleotide with acid-modified photocatalysts. We will present the synthesis of this new hybrid photocatalyst and its applications in enantioselective photocatalysis (Figure).

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UA2239: AN ACYCLIC NUCLEOSIDE PHOSPHONATE WITH POTENT ANTIMALARIAL ACTIVITY & UNEXPECTED MECHANISM OF ACTION

Thomas CHEVIET,[1] Marie ALI,[2] Sharon WEIN,[2] Rachel CERDAN,[2] and Suzanne PEYROTTES[1*]

[1] *Institut des Biomolécules Max Mousseron (IBMM), UMR 5247 UM-CNRS-ENSCM, Equipe Nucléosides & Effecteurs Phosphorylés, Montpellier*
[2] *Laboratory of Pathogens Host Interactions* (LPHI)*, UMR 5235 UM-CNRS, Montpellier*
suzanne.peyrottes@umontpellier.fr

Plasmodium parasites cause malaria, one of the most devastating infectious diseases. The treatment of malaria essentially relies on antimalarial drugs. However, the emergence of resistance to all existing antimalarial drugs, including artemisinin derivatives (ACTs), strengthens the urgency to find new ones and with new mode of action. To this end, we synthesized and screened a new family of Acyclic Nucleoside Phosphonates (ANPs), that are documented to target DNA synthesis. ANPs are well-known antiviral drugs, and have also been described as inhibitors of *Pf*HGXPRT (hypoxanthine-guanine-xanthine phosphoribosyl transferase), one of the main enzyme involved in the *Pf* purine metabolism.[1]

Herein, we report syntheses and in vitro biological activities of a novel series of ANPs, highlighting among them a very promising lead (UA2239) which was selected for further *in vitro* & *in vivo* investigations.

UA2239, showed antimalarial activity on asexual stages in vitro (*P. falciparum*, IC_{50}=76.6 ± 9 nM) and in vivo (*P. berghei*, ED_{50}=0.5mg/kg/day).[2] This compound is also active against the sexual stage inhibiting male gametocyte exflagellation (P. berghei). Unexpectedly, DNA synthesis is not affected by UA2239. In order to identify the main target and understand the mode of action of UA2239, we generated resistant strains and sequenced their whole genome.

In conclusion, our results unraveled a promising antimalarial compound UA2239, which acts through a novel molecular mode of action, that is different from previously known ANPs acting as *Pf*HGXPRT inhibitors. Deciphering its full mechanism of action at the molecular levels will pave the way for the development of an original antimalarial compound.

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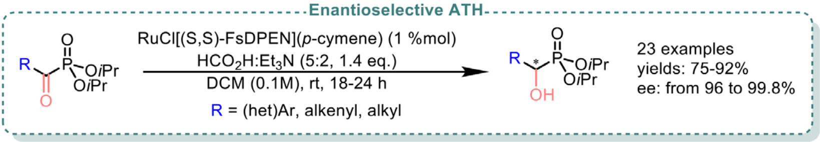
RU(II)-CATALYZED HIGHLY ENANTIOSELECTIVE TRANSFER HYDROGENATION OF Α-KETO PHOSPHONATES

Ulysse Elmerich,[a] Ludovic Clarion,[b] Pierre Plouard,[a,b] Séverine LOISEAU,[b] Jean Luc Pirat,[a] Pierre-Georges Echevarria,[c] Tahar Ayada,* and David Virieux,*

[a] *ICGM Univ Montpellier, CNRS, ENSCM, 1919 route de Mende, Montpellier, France*
[b] *Phost'In Therapeutics, 104 Rue de La Galera, 34090 Montpellier, France*
[c]*Minakem Recherche, 145 Chemin des Lilas, Beuvry-La-Forêt 59310, France*
pierre.plouard@phostin.com

Optically active α-hydroxyphosphonic acids and phosphonates constitute an important class of biologically active compounds that have a wide-range of activities.[1] They have been also considered as convenient precursors for a variety of biologically significant chiral phosphonate derivatives, including chiral α-amino phosphonates. Because their biological activities usually depend on the absolute configuration, catalytic enantioselective synthesis of these compounds has been explored. Among the numerous methods developed such as asymmetric Pudovik[2] or Abramov reaction,[3] asymmetric reduction of easily available α-ketophosphonates is an efficient and convenient pathway. However, most of these methods suffer from several drawbacks such as relatively high catalyst loading, expensive metal catalyst, high H_2 pressure and/or result in low enantioselectivity.

Consequently, there is considerable space for improvement. Asymmetric Transfer Hydrogenation (ATH) has proven to be one of the most versatile, safe and powerful approach for the synthesis of enantiopure hydroxyl compounds. However, despite tremendous advances in this field, its application in the selective reduction of α-ketophosphonates, which are privileged motifs in pharmaceutical and agrochemical industries, remains largely unexplored[4],[5]. Herein, we report an efficient Ru-catalyzed asymmetric transfer hydrogenation across a broad range of substrates, including aryl, alkenyl and alkyl α-substituted ketophosphonates, providing a rapid access to enantiomerically enriched α-hydroxy phosphonates. Compared with existing methods, our approach offers several advantages, such as mild reaction conditions, operational simplicity, limited waste generation, broad substrate scope (23 diversified examples), high to excellent yields (up to 92%) and excellent to nearly perfect levels of stereoinduction (up to 99.8% ee).



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SCO TRANSITIONS, SITE SELECTIVITY AND CORE-SHELL COMPOSITES IN [$W(CN)_8$]-BRIDGED COORDINATION CLUSTERS FAMILIES

Le Shi,[1,2] Jedrzej Kobylarczyk,[1,3] Barbara Sieklucka,[1] Katarzyna Dziedzic-Kocurek,[4] Jan J. Stanek,[4] Sylvie Ferlay,[5] Robert Podgajny[1]

[1]*Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Krakow, Poland.*
[2]*Stoddart Institute of Molecular Science, Department of Chemistry, Zhejiang University, Hangzhou 310027, P. R. China.*
[3]*Institute of Nuclear Physics PAN, Radzikowskiego 152, 31-342 Kraków, Poland.*
[4]*Marian Smoluchowski Institute of Physics, Jagiellonian University, 30-348 Krakow, Poland.*
[5]*University of Strasburg, CNRS, CMC UMR 7140, F-67000 Strasbourg, France.*
robert.podgajny@uj.edu.pl

An attractive strategy for new potential platforms with switchable functions is construction of polynuclear spin-crossover (SCO) coordination complexes with speciation of coordination sites hosting active d-metal ions. In this contribution, we present unique examples of binary $\mathbf{M_9W_6@M'_9W_6}$ and $\mathbf{Fe_6Co_3W_6@Mn_9W_6}$, as well as ternary $\mathbf{M_9W_6@M'_9W_6@M''_9W_6}$ (M, M' M" – divalent 3d metal ions; W – [$W(CN)_8$]$^{n-}$) milimetr-sized molecular core-shell crystals.[1] We discuss their heteroepitaxial growth, interface size and possibility of enveloping the SCO active core with various types of shells, based on the previously elaborated series of primary crystals (Figure 1).[2,3] Further on, we reveal a new series of topologically identical 11-nuclear heteropolymetallic 3d-5d $\mathbf{M_7L_xW_4}$ or 3p-3d-5d $\mathbf{Na_1M_6LW_4}$ clusters (M = Fe^{II}, Co^{II} or Ni^{II}; L organic ligands, $x = 1$ or 2).[4] $\mathbf{Fe_7L^1W_4}$ exhibits decently resolved double-step SCO, whereas $\mathbf{NaCo_6L^1W_4}$ and $\mathbf{Co_7L^2_2W_4}$ approach the first examples of Co(II)-centered SCO in {Co[$W(CN)_8$]$^{n-}$} systems. We tend to discuss the impact of coordination M site speciation, single-crystal to single-crystal (SCSC) transformation and intermolecular contacts on the quality of SCO processes. *Acknowledgements*: NCN (Poland), Opus 18, No. 2019/35/B/ST5/01481.

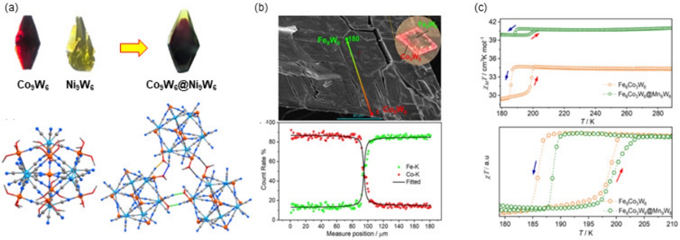

Figure 1. *Construction and properties of core-shell crystals based on the 15-nuclear octacyanidotungstate-bridged* $\mathbf{M_9W_6}$ *clusters:*[1] *(a) crystals appearance and crystal structure, (b) interface image and SEM/EDX characterization, and (c) magnetic* $\chi_M T(T)$ *data for seed* $\mathbf{Fe_6Co_3W_6}$ *phase and core-shell* $\mathbf{Fe_6Co_3W_6@Mn_9W_6}$ *composites (*H_{dc} *= 1000 Oe, the sweep rate of 1 K/min).*

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MODIFIED TERNARY METAL OXIDES: EN ROUTE TO FUNCTIONAL MATERIALS

Elzbieta Regulska

University of Bialystok, Ciolkowskiego 1K, 15-245 Bialystok, Poland;
e.regulska@uwb.edu.pl

Water pollution and ongoing shortage of energy are matters of global concern. The scarcity of pure water, growing amounts of disposed pharmaceuticals and unsustainable energy use occur all over the world. Those issues evoke a need for functional materials. As such, modified ternary metal oxides (MTMOs) appear as promising platforms for catalysis and energy applications. These materials present superior physicochemical features beyond the sum of their individual components. The MTMOs show outstanding performance in air and water purification, self-cleaning surfaces, antimicrobial deactivation, and energy related processes. Inorganic semiconductors (ISs) can harvest the light in the broad spectral range. Their excitation generates electron-hole pairs with the attractive lifetimes. The ternary metal oxides offer faster charge-carrier generation and higher charge mobility with respect to the organic semiconductors. The latter together with the defined energy band edges of TMOs translate to the particular applications, i.a. oxygen/hydrogen evolution, carbon dioxide reduction, methane conversion, photocatalytic water remediation, etc. The presented herein series of studies refers to the synthesis and characterization of functional materials that exhibit photo- and electrocatalytic properties, are capable of energy storage, or conversion. To this end, the mixed metal oxides modified with carbon nanostructures (GQDs, rGO), or doped with rare-earth metals were synthesized. The obtained materials were further examined towards their application as photocatalysts, electrocatalysts and energy storage materials.

METAL BINDING TO ANTIMICROBIAL PEPTIDES - A SMALL STEP FOR STRUCTURAL CHEMISTRY, A BIG LEAP FOR MEDICINAL APPLICATIONS

Adriana Miller[a], Dorota Dudek[a], Aleksandra Hecel[a], Joanna Olesiak-Bańska[b], Aleksandra Mikołajczyk[c], Agnieszka Matera-Witkiewicz[c], Magdalena Rowińska-Żyrek[a]

[a] *Faculty of Chemistry, University of Wrocław, 50-383, Wroclaw, Poland*
[b] *Faculty of Chemistry, Wrocław University of Science and Technology, 50-370, Wrocław, Poland*
[c] *Screening Laboratory of Biological Activity Tests and Collection of Biological Material, Faculty of Pharmacy, Wroclaw Medical University, 50-556 Wroclaw, Poland*
magdalena.rowinska-zyrek@uwr.edu.pl

Antimicrobial peptides are considered as potential treasure troves for new antimicrobial therapeutics; although they have existed for millions of years, pathogenic resistance against them is rarely described. Their activity can, in numerous cases, be enhanced by the presence of metal ions – metal coordination can change the charge and structure of the peptide, thus affecting the AMPs mode of action via membrane disruption, production of reactive oxygen species, inhibition of cell wall or nucleic acid and protein synthesis [1].

We focus on several families of metal binding AMPs, showing relationships between the coordination chemistry, structure, stability, mode of action and biological activity of their Cu(II) and Zn(II) complexes, explaining the effect of the preorganisation of the Zn(II) binding site of marine clavanins on their antifungal activity [2], the needle-like mode of action of the Zn(II)-pramlintide (amylin analogue) complex [3], the effect of charge on semenogelin complexes [4] and the impact of the local change of structure of calcitermin (human airways AMP) complexes on their antibacterial activity [5].

Acknowledgments:
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INTRACELLULAR LOCALIZATION OF CYTOTOXIC HALF-SANDWICH IRIDIUM(III) COMPLEXES BY ADVANCED HIGH RESOLUTION IMAGING TECHNIQUES

Robin Ramos,[a] Alfonso Annunziata,[b] Sadek Amhaz,[a] Joëlle Sobczak-Thépot,[a] Michèle Salmain[b]

a INSERM, Sorbonne Université, Centre de recherche Saint Antoine, CRSA, F-75012 Paris, France
b Sorbonne Université, CNRS, Institut Parisien de Chimie Moléculaire, IPCM, F-75005 Paris, France
michele.salmain@sorbonne-universite.fr

Bioorthogonal chemistry is currently an essential tool in chemical biology and is especially useful to visualize (bio)molecules in the cellular context and even in whole animals (1). By definition, bioorthogonal reactions involve chemical functions that exclusively react with one another without interference from nucleophiles present in abundance in biological media. On the other hand, information on the distribution of biologically active molecules at the subcellular level is extremely useful in the comprehension of their mechanism of action.

In the context of metal-based anticancer agents development, we recently introduced a family of half-sandwich iridium(III) complexes with promising antiproliferative properties on cultures of cancer cells, inducing regulated cell death by apoptosis. To get insight into their cell uptake and localization, we slightly modified their structure to introduce a chemical handle for in-cell bioorthogonal fluorescence labeling (Figure 1a).

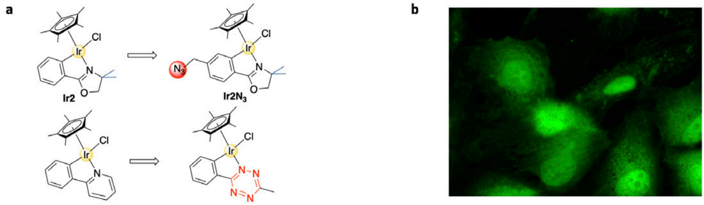

Figure 1. (a) “Clickable” iridium complexes for in cell fluorescent labeling; (b) Huh-7 cells treated with 1 µM azido complex for 1 h, then fixed and incubated with FITC-alkyne under CuAAC conditions

Azide and tetrazine functions were selected for the purpose and the corresponding neutral [(Cp*)iridium(C^N)Cl] complexes were synthesized accordingly. In-cell reactions with fluorescein derivatives carrying a partner terminal alkyne or bicyclononyne (BCN) group were achieved, allowing the complexes distribution to be precisely determined in fixed or even live cells (Figure 1b). Further staining of organelles with specific dyes enabled to determine that the iridium complex preferentially accumulates in the cytoskeleton network and the nucleus. In addition, chemical mapping of iridium in cells exposed to **Ir2** was also achieved by Synchrotron Radiation X-ray fluorescence (SR-XRF) microscopy. This localization gives useful clues to understand the mechanism by which these iridium complexes exert their cytotoxicity on cancer cells.

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FROM ENZYMES TO CUCURBITURILS: EXPANDING THE HORIZONS OF CATALYSIS

Volodymyr Sashuk

Institute of Physical Chemistry, Polish Academy of Science, Kasprzaka 44/52, 01-224 Warsaw, Poland
vsashuk@ichf.edu.pl

Enzymes have long been recognized as natural catalysts that enable fast, selective, and controllable chemical reactions. However, their inherent limitations, such as low stability, narrow reaction scope, and high cost, have motivated researchers to explore alternative catalytic systems. In this presentation, I will discuss a family of macrocyclic compounds known as cucurbiturils, which exhibit similarities to enzymes in terms of structure and catalytic capabilities, while overcoming the limitations associated with traditional enzyme systems. In particular, I will show the acceleration of hydrolysis (1) and condensation (2, 3) reactions, selective product formation (2, 3), uncompetitive inhibition (4), and remotely controlled catalysis (3).

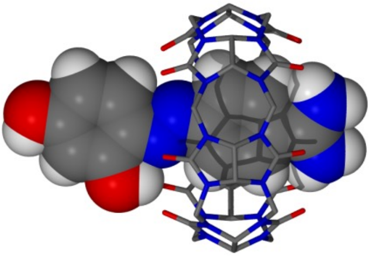

Figure 1. X-ray structure of the product of the hydrolysis reaction trapped within the cucurbit(6)uril cavity.

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BIOAVAILABILITY OF ANTIBIOTICS MODIFIED WITH PLANT SURFACTANTS

Wojciech Smułek*, Natalia Burlaga, Adam Grzywaczyk, Aleksandra Makiej, Amanda Pacholak, Agata Zdarta, Ewa Kaczorek*

Institute of Chemical Technology and Engineering, Poznan University of Technology, Berdychowo 4, 61-131 Poznań, Poland
wojciech.smulek@put.poznan.pl, ewa.kaczorek@put.poznan.pl

The increase in antibiotic use is one of the most important challenges of the 21st century. The increasing number of strains of pathogenic microorganisms that are resistant to antibiotics is prompting the use of antibiotics in ever-increasing doses, which translates into increasing emissions of these compounds into the environment. The presence of these compounds in the environment negatively affects the organisms living there, but also stimulates the spread of antibiotic resistance among microorganisms. Thus, the aim of our research is to stimulate the biodegradation of antibiotics in the environment, as well as to increase their toxic effect against pathogenic microorganisms. In both of these strategies, surfactants of natural origin are used as a tool to increase the bioavailability of antibiotics to the cells of microorganisms.

Natural surfactants used in this study will be plant saponins from e.g. *Saponaria officinalis* (soapwort), or *Sapindus mukorossi* (soapnuts). The tested antibiotics will belong to different groups, including: aminoglycosides, nitrofurans or polypeptides. In the research, the interaction of plant surfactants with tested antibiotics to obtain higher bioavailability. The main stage of the project is determination of the influence of plant surfactants on the transport of antibiotics through the membrane of bacterial cells as well as modifications of cell membrane permeability and adhesion properties of bacterial cells (including atomic force microscopy tests – see Fig. 1).

The measurable effect of the project will be significant extensions of the current state of knowledge and the development of environmental microbiology and sciences, biological safety, the environment and human health protection.

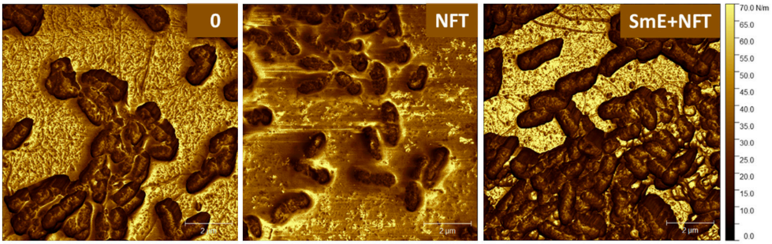

Figure 1. Atomic force microscopic images of Pseudomonas aeruginosa NFT3, color axis represents stiffness values (forward approach); 0 – untreated cells, NFT – cells exposed to nitrofurantoin, SmE+NFT – cells exposed to both S. mukorossi L. extract and nitrofurantoin.

Acknowledgements

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SUPRAMOLECULAR MAGNETIC DENDRIMERS

Ingrid Suzana,[1] Moritz Malischewski[2] and Valérie Marvaud[1]

[1]IPCM-CNRS, UMR 8232, Sorbonne Université, Paris, France,
[2]Fachbereich Chemie, Freie Universität, Berlin, Deutschland.
Ingrid.suzana@sorbonne-universite.fr

Design of molecular materials has attracted a great deal of attention in recent years. Owing to their molecular nature, they are associated with soft chemistry routes, light density, optical transparency or tuneable physical properties. More specifically, our interest is focused upon supramolecular architectures that have the potential of featuring luminescent, magnetic and photo-switching properties.

Hetero-poly-metallic complexes combining up to four different metallic ions, are obtained according to a smart supramolecular approach that consists in using “complexes as ligands”. In other words, coordination complexes, either mononuclear or polynuclear, are employed as functional precursors for multifunctional assemblies such as hetero-tetra-metallic complexes or coordination dendrimers. This method is advantageous as it affords many variations in synthetic parameters, and the properties of the precursors are well established.

Our synthetic strategy essentially relies on oxalate-, anilate- and cyanide-based coordination chemistry.[1] The key building blocks are original trinuclear complexes that feature high-spin molecule, single-molecule magnet or luminescent properties. And second, para- and dia-magnetic magnetic oxalates/anilates as well as photo-switching cyanido complexes act as structure-directing entities for supramolecular and dendritic assemblies.

To date, we have developed the first multifunctional hetero-tetra-metallic complexes having both magnetic and photo-switching properties. The versatility of the synthetic approach was demonstrated by getting several families of hetero-tetra-metallic complexes, with no less than 18 different compounds.[2] In this presentation, we report the first instance of metallodendrimers with singlemolecule magnet properties, a fascinating tuneable decanuclear architecture.[3]

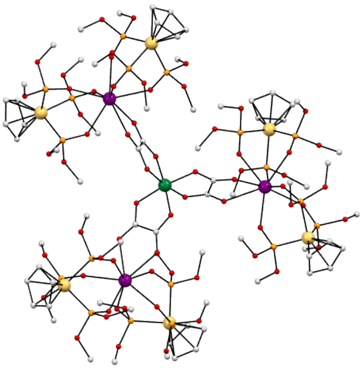

Figure. X-ray structure of the hetero-tri-metallic dendrimer CrLn3Co6 with Ln = Gd, Tb, Dy. Solvent molecules and hydrogen atoms have been omitted.

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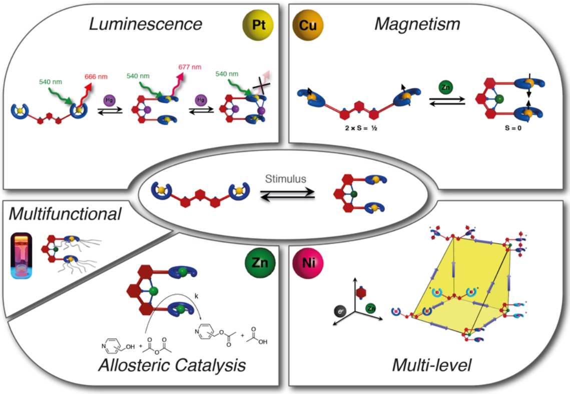
SWITCHABLE MOLECULAR TWEEZERS: A VERSATILE PLATFORM TO CONTROL MULTIPLE PROPERTIES

Guillaume Vives

Institut Parisien de Chimie Moléculaire, Sorbonne Université, 4 Place Jussieu, 75005, Paris, France.
guillaume.vives@sorbonne-universite.fr

In recent years, molecular machines[1] have attracted increasing interest for their ability to control motion at the molecular level. However, artificial systems are far from achieving the complexity of natural systems and harnessing their inherent properties to perform useful functions remains a major challenge. We are interested in an innovative approach to control physical or chemical properties at the molecular level by exploiting the mechanical motion of molecular switches capable of dynamic interconversion between different states.



We have developed a family of switchable molecular tweezers based on a terpyridine ligand functionalized in 6 and 6" positions by Metal-salen complexes. The open tweezers adopt a 'W' shaped conformation that can be switched to a 'U' shaped one by a coordination stimulus bringing into proximity the two functional salen complexes. By using Pt(II) or Cu(II)-salen complexes a drastic modulation of luminescence[2] or magnetic[3] properties was respectively achieved. We also exploited the modularity of our platform to combine ion triggered mechanical motion with the redox activity of Ni(II)-salen complexes. A remarkable six level switch was obtained by combining three orthogonal stimuli.[4] A notable substrate-dependent allosteric regulation of the catalytic activity of Zn(II) tweezers was obtained in the acetylation of pyridine-methanol substrates.[5] More recently, we wished to exploit the large structural reorganization of the tweezers to develop switchable organogels.[6] The reversible sol-gel transition induced by the mechanical motion will be highlighted.

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AMPHIPHILIC TELECHELIC POLYMERS FORMULATED USING A CLICK CHEMISTRY APPROACH

Justyna Walkowiak-Kulikowska, Katarzyna Żymańczyk, Anna Szwajca, Joanna Wolska

Faculty of Chemistry, Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
justyna.a.walkowiak@amu.edu.pl

Polymers containing perfluoroalkyl groups are classified as PerFluoroAlkyl Substances PFASs, that are currently attracting much attention and care. Unlike non-polymeric PFAS representatives, fluorinated polymers are considered to be of low environmental, human and biota hazard as they have negligible monomer and oligomer content and low or no leachability, no bioavailability or bioaccumulation, no chronic toxicity or carcinogenicity, and no reproductive, developmental or endocrine toxicity. [1]. Since non-polymeric amphiphilic PFASs have found application, for example, in manufacturing protective coatings for packaging, as they prevent the absorption of water, grease, or dirt, the aim is to replace long-chain PFASs with short-chain and alternative fluorinated and non-fluorinated compounds. Fluorinated amphiphilic polymers can provide an affordable alternative to non-polymeric substances, as the desired properties can be achieved by introducing the relevant modification, avoiding the risk of bioaccumulation and toxicity [2].

The objective of the presented work was to synthesize amphiphilic aromatic polymers using "click" reactions of suitable building blocks in the form of azido-functionalized derivatives of fluorinated aromatic polymers and propargyl derivatives of monosaccharides (Figure 1). Telechelic α,ω-diazido-functionalized fluorinated polymers were obtained by azidation reaction of α,ω-diiodo-functionalized macromolecules that were previously obtained by iodine transfer copolymerization (ITcoP), while propargyl derivatives of the monosaccharides glucose and glucosamine were obtained by literature-known, two-step syntheses [3,4]. Equally important was to fully characterize structural, thermal, and surface properties.

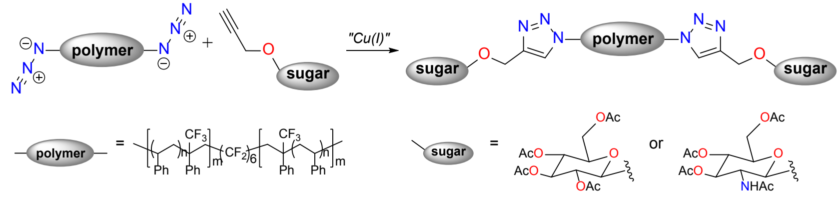

Figure 1: Click chemistry as an efficient tool toward telechelic amphiphilic polymers.

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STRUCTURE-PROPERTY RELATIONSHIP OF MATERIALS FOR ELECTROFLUOROCHROMIC APPLICATIONS

Kacper Muras, Monika Wałęsa-Chorab

Faculty of Chemistry, Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
mchorab@edu.pl

Electrochromic and electrofluorochromic materials can switch between two different states of emission or coloration in a reversible manner and due to this they represent one of the most extensively studied materials in recent years.[1–4] Dual functioning electrochromic and electrofluorochromic materials, which show a reversible electrochromism combined with the changes in the emission properties, can be used for the construction of dual-mode displays that can work in both emissive and reflective modes (Figure 1).

In order to investigate the influence of the structure of organic compound on its electrochromic, electrofluorochromic and luminescent properties, compounds of different structure were designed and synthesized. The electrochemical properties of the obtained compounds were examined in order to assess their suitability for use as materials in electronic devices. It was found that the tested compounds show the ability to change the redox state reversibly. Subsequently, the electrochromic, solvatochromic, and electrofluorochromic properties of the obtained compounds were studied. It was confirmed that the investigated compounds exhibit the expected properties, and the impact of structural differences on these properties was assessed.

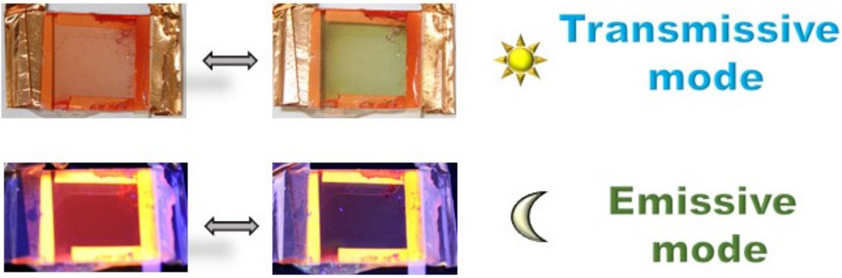

Figure 1. The example of dual-functioning device based on donor-acceptor compound.

The research were financially supported by the National Science Center (Poland) within project SONATA BIS No. 2019/34/E/ST5/00103.

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SELF-ASSEMBLED PROTON AND WATER CHANNELS WITH PHOTO-TUNABLE TRANSPORT PROPERTY

Paras Wanjari, Mihail Barboiu

Institute Des Membranes, University of Montpellier, 300 Av. du Professeur Emile Jeanbrau, 34090 Montpellier.
Mihail-Dumitru.Barboiu@umontpellier.fr

Artificial Ion transporters have been reported in the literature owing to their application as potential therapeutics in channelopathies such as cystic fibrosis, muscular dystrophies, etc. In recent times, these systems have also been explored for their application in treating cancer by creating ionic imbalance across the cell membrane and triggering apoptosis. Although these systems had the ability of transporting ions across the artificial bilayer membranes, their application in biological system is limited due to the absence of the ability to control the ion transport. Moreover, one of the very important properties of the natural transmembrane proteins is their ability to regulate the transport of ions which was lacking in these artificial systems. Therefore, chemists came up with the idea of developing stimuli responsive systems which can activate only with the help of external trigger such as pH, voltage, light(1) or in the presence of certain enzyme(2). Among these stimuli, light has been useful because of its biocompatible and inert nature. Various photoresponsive ion transporters have been reported in literature but none of them have extended specifically to proton and water transporters. Herein, we have attempted to introduce the photoresponsive nature of transport in self-assembling proton and water channels by introducing molecular photoswitches such as acylhydrazones and azobenzene.

One of the strategies involves designing an acyl hydrazone linked imidazole-based channel that can adjust the interlayer distance using light and redox stimuli. In the trans configuration, hydrogen bonding between layers enhances stacking. However, when switched to the cis conformer using specific wavelengths of light, intramolecular hydrogen bonding disrupts and in turn disrupts the stacking. Another approach uses azobenzene based water channels, which can control water transport by manipulating I- quartet formation through external electromagnetic irradiation. Integration of tetra-o-fluoro azobenzene with histamine promotes I- quartet formation in the cis form, while hindering it in the trans-form. Stacking across the membrane can be facilitated by hydrogen bonding between the four amide bonds (figure 1).

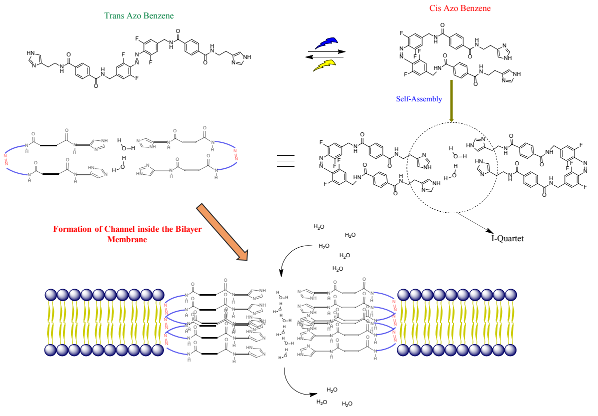

Figure 1: Representation of Azobenzene based photo-responsive Water or Proton Channel.

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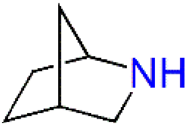
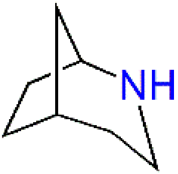
RING EXPANSION IN NITROGEN HETEROCYCLES

Elżbieta Wojaczyńska

Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland
elzbieta.wojaczynska@pwr.edu.pl

2-Azanorbornane (2-azabicyclo[2.2.1]heptane), which can be prepared in a stereoselective manner using the aza-Diels-Alder reaction between cyclopentadiene and an enantiopure imine, serves as a versatile chiral platform for the preparation of a variety of ligands and catalysts for asymmetric synthesis and compounds exhibiting biological activity [1]. Among the possible modifications of the bicyclic system, an interesting possibility of expansion of the six-membered ring under the conditions of Mitsunobu reaction was observed [2], which opens the route to 2-azabicyclo[3.2.1]octane derivatives. In the presentation, various transformations of this type will be presented, as well as a comparison of the properties of isomeric compounds bearing an expanded and unaltered skeleton.





Acknowledgement
Harmonia project, funded by the National Science Centre, Poland (grant number: 2018/30/M/ST5/00401) is gratefully acknowledged.

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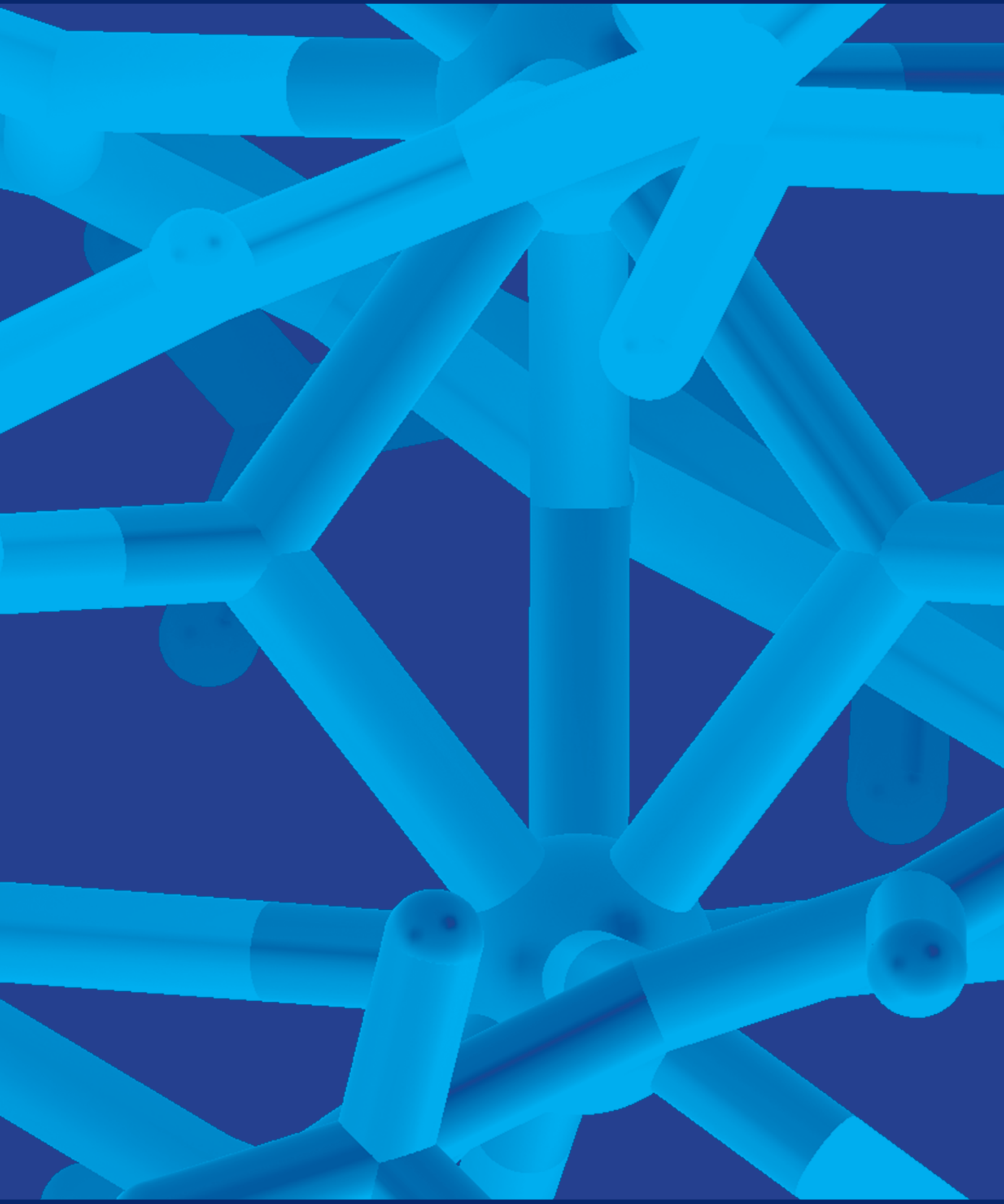


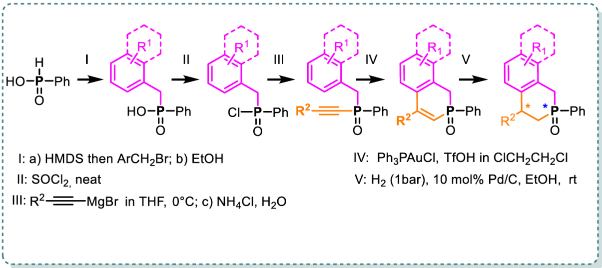
HYDROPHOSPHONYLATION OF COUMARINS AND ISOPHOSPHINOLINE 2-OXIDES

K-P. Mengue Me Ndong*,[a,b], A. R. Issaka Ibrahim*,[a,c] M. Hariri,[a] G. Mwande-Maguene,[b] J. Lebibi,[b] A. T. Ilagouma,[c] T. Ayad,a J-L. Pirat,[a] D. Virieux[a]

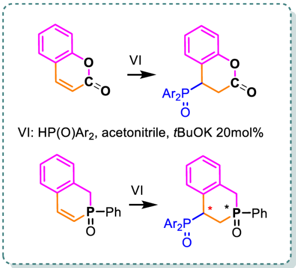
[a] *Institut Charles Gerhardt/UMR 5253/AM2N, ENSC, Montpellier, France*
[b] *Université des Sciences et Techniques de Masuku, Franceville, Gabon*
[c] *Faculté des Sciences, Université Abdou Moumouni, Niamey, Niger*
karen-pacelye.mengue-me-ndong@enscm.fr
abdrachid2i@gmail.com

We developed an efficient synthesis of a new family of compounds, namely isophosphinoline 2-oxides, a six-membered phosphorus heterocycle specifically designed for the discovery of new pharmacophores or building blocks for medicinal chemistry. They were obtained in five steps from cheap Hphenylphosphinic acid using a gold-catalyzed hydroarylation reaction as a key step [1].

In a second time, we explored the reactivity of coumarins and their phosphorus analogues, the isophosphinoline 2-oxides, through Michael additions. These modifications were successful, allowing to modulate the structural features of these heterocycles [2].



I: a) HMDS then ArCH$_2$Br; b) EtOH
II: SOCl$_2$, neat
III: R^2—≡—MgBr in THF, 0°C; c) NH$_4$Cl, H$_2$O
IV: Ph$_3$PAuCl, TfOH in ClCH$_2$CH$_2$Cl
V: H$_2$ (1bar), 10 mol% Pd/C, EtOH, rt



VI: HP(O)Ar$_2$, acetonitrile, *t*BuOK 20mol%

Preliminary biological results showed moderate to good activities on different bacterial strains [2].

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MULTIRESPONSIVE SWITCHING BETWEEN DIFFERENT SUPRAMOLECULAR AGGREGATES SELF-ASSEMBLED FROM A SINGLE AMINO ACID-DERIVED NAPHTHALENEDIIMIDE

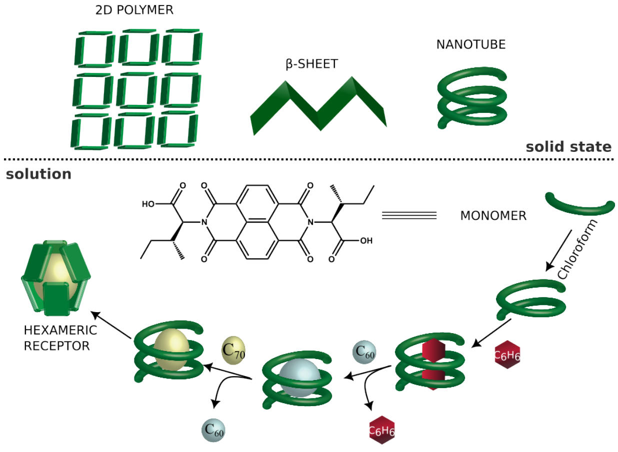
Wiktoria Adamska[1], Grzegorz Markiewicz[1], Jack Harrowfield[2], Artur Stefankiewicz[1]

[1]Faculty of Chemistry, Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland, Center for Advanced Technology, Adam Mickiewicz University, Uniwersytetu Poznańskiego 10, 61-614 Poznań, Poland
[2]Institut de Science et d'Ingénierie Supramoléculaires, Université de Strasbourg, 8 Allée Gaspard Monge, 67083 Strasbourg, France
wikada2@amu.edu.pl

Over the last decade, amino acid derived naphthalenediimides (NDIs) were proved to be a versatile components for the non-covalent self-assembly of distinct chiral supramolecular polymers with tunable structures and complexity. The most widely studied product are the helical nanotubes held together by the cooperation of COOH-HOOC and CH-O hydrogen bonding.[1]

Many noncovalent supramolecular structures may be formed from amino acid-derived NDIs, each of which differs not only in terms of global morphology but also in terms of the thermodynamics and kinetics of its formation. The significance and strength of the intermolecular interactions as well as the influence of guest molecules (e.g. C_{60} and C_{70}) differ, which in turn causes a controllable variation in the self-assembly products.[2]

In this report, we show that a single NDI component may yield up to six different supramolecular assemblies depending on the conditions applied. While in the solid the polymerization yields either nanotube, β-sheet, or 2D cage-like polymer, switching to the solution has shown that the self-assembly is highly sensitive to the influence of solvent polarity, concentration as well as the guest molecules. Namely, in chlorinated solvents the NDI-Ile form the metastable helical nanotubes, while in aromatic solvents of lower polarity, longer and more stable polymers can be observed due to templating effects.



Furthermore, in the presence of guest molecules such as C_{60}/C_{70} fullerenes, NDI-Ile forms either a guest-filled supramolecular nanotube or hexameric receptor, depending on the sample' concentration and temperature.

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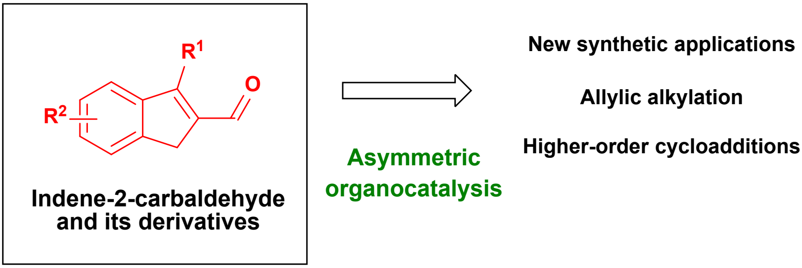
NEW SYNTHETIC APPLICATIONS OF INDENE-2-CARBALDEHYDE AND ITS DERIVATIVES – HIGER-ORDER CYCLOADDITIONS AND BEYOND

Łukasz Albrecht

Lodz University of Technology,Faculty of Chemistry, Zeromskiego 116, 90-924, Łódź, Poland
lukasz.albrecht@p.lodz.pl

Cycloaddition reactions constitute one of the most usable synthetic methodologies, giving access to various, interesting building blocks. The most popular [4+2] Diels-Alder and 1,3-dipolar cycloadditions are well-recognized, as different variants of these reactions already appeared in literature, including catalytic and asymmetric methodologies. Different approach in the field of cycloaddition reaction focuses on the reactions in which more than 6π take part. These processes are called higher-order cycloadditions, discovered in 70' and being currently an objective of intensive studies [1].

Indene-2-carbaldehyde and its derivatives constitute an interesting group of substrates capable of participating in higher order cycloadditions [1]. The aim of our research was to develop new synthetic applications of this interesting group of reactants. We have demonstrated that indene-2-carbaldehyde and its derivatives readily participate in enantioselective allylic alkylation of Morita-Baylis-Hillman carbonates [2] and cascade reaction initiated by higher-order cycloaddition. Reactions were carried out under organocatalytic conditions and proceeded with complete regio- and stereoselectivities.



Indene-2-carbaldehyde and its derivatives

Asymmetric organocatalysis

New synthetic applications

Allylic alkylation

Higher-order cycloadditions

This project was realized within the Opus programme (grant number: UMO-2021/41/B/ST4/03385) from the National Science Centre, Poland.

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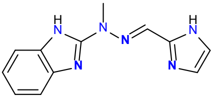
APPLICATION OF COBALT COMPLEXES WITH SHIFF BASE LIGANDS AS PRECATALYSTS FOR HIGHLY SELECTIVE HYDROBORATION OF ALKYNES

Piotr Andruszak, Maciej Zaranek, Piotr Pawluć

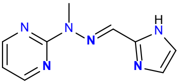
Adam Mickiewicz University, Faculty of Chemistry, Department of Organometallic Chemistry, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
pioand3@amu.edu.pl

Organoboronic compounds are known as one of the simple fundamental reagents in modern organic chemistry. Their main advantage is that they can be used in reactions with a broad spectrum of reagents such as halides, amides or metalorganics compounds [1]. They are usually obtained by hydroboration of unsaturated compounds, such as alkenes or alkynes. This reaction is usually carried out with addition of catalyst, mainly complexes of PGMs (platinum group metals), such as rhodium or iridium [2]. Depleting deposits of these metals, and their increasing cost, are prompting the search for equally efficient, but still more sustainable alternatives, such as cobalt, iron, or nickel complexes [3-4].

Our recent research showed that using cobalt(II) complex with 3N-donor ligand **L I** as a catalyst in hydrosilylation of alkenes leads to highly selective generation of α products [5]. Switching the benzimidazole fragment with pyrimidine one, as shown in the **L II** scheme, allowed for the development of conditions for equally selective preparation of β products, this time in the hydroboration of alkynes. The main advantages of this reaction system are mild conditions and the tolerance to a wide spectrum of functionalized terminal alkynes.



L I



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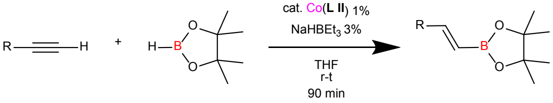

Scheme of hydroboration in the presence of cobalt catalyst

The poster will present the results and difference in activity of cobalt (II) complexes with Schiff base ligands in the alkyne hydroboration.

Acknowledgement
Research funded by the National Science Center under the grant nr UMO-2019/35/B/ST4/00329

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INVESTIGATION OF THE LINEAR VIOLOGENS AS PROMISING MATERIALS FOR ELECTROCHROMIC APPLICATIONS

Radosław Banasz, Monika Wałęsa-Chorab

Faculty of Chemistry, Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
radban@amu.edu.pl

Viologens can occur in several stable redox states and their color changes are the result of reduction of a dication form to a radical cation and then to neutral form. The change of substituent on the nitrogen atoms or insertion of different units between pyridine rings can leads to the modification of electrochromic properties of the viologens [1].

In our group we obtained benzothiadiazole- and benzoselenadiazole-based linear viologens containing styrene groups [2]. The prepared compounds were characterized by NMR spectroscopy and HR-ESI-MS method. The electrochemical characterization of viologens **1** and **2** and their respective polymers **poly-1** and **poly-2** were examined by cyclic voltammetry. The spectroelectrochemical properties of the polymers were further investigated in terms of their usefulness as active materials in electrochromic devices (Figure 1). The thin films of the polymers were easily obtained by the photopolymerization of the appropriate monomer. Electrochromic behaviour of patternable polymers coated onto ITO glass have been investigated after applying the appropriate negative potentials. The conducted research makes up the first example of using styrene derivatives in the photopolymerization of electrochromic compounds. The usefulness of the styrene derivatives in the formation of patterns of active materials has been shown and it provided an alternative way for the formation of patterns for large-area electrochromic segmented displays.

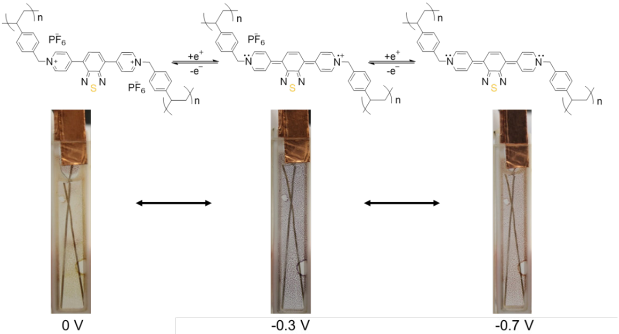

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Figure 1. Photographs of polyviologen in dication form (left), radical cation (middle) after applying the appropriate potential for poly-1.

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Acknowledgments

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G4 RNA FOLDING REPRESENTS ANOTHER LAYER OF NON-GENETIC, NON-EPIGENETIC, BUT STRUCTURAL REGULATION OF GENE EXPRESSION

Agnieszka Belter

Institute of Bioorganic Chemistry, Polish Academy of Sciences, Noskowskiego 12/14, 61-704 Poznań, Poland
abelter@ibch.poznan.pl

G-quadruplexes are secondary structures that typically form from guanine-rich sequences, both in RNA and DNA. In a G-quadruplex, four guanine bases come together to form a planar square-shaped structure, where each guanine base interacts with two neighbouring guanines through hydrogen bonds and are stabilized by stacking interactions and monovalent cations, such as potassium. The sine qua non of G-quadruplex structure are only two things: a putative G-quadruplex-forming sequence (four or more runs of consecutive G bases), and monovalent cations. So, taking into account the ubiquity of G4 motifs in the human genome and transcriptome (>700 000 and >13 000 quadruples forming sequences, respectively in DNA and RNA) and a high concentration of potassium ions in cells, one can expect huge number of G4s in the cells. Moreover, it is not difficult to imagine that this 'knot' stable structures, when appear in RNA or DNA may exert regulation on a variety of biological processes.

The breakthrough in understanding G-quadruplexes RNA in cellular context was the observation that there is a huge gap between the number of 4G-motifs and G-quadruplex structure in eukaryotic cells, which suggests that eukaryotic cells have innate strategy to regulate G4 formation, somehow avoid this knoty structures.

The aim of my research is to identify the components of cellular molecular machinery responsible for unfolding RG4 regions and maintains them in an unfolded state. To gain this, I chose a model G4 RNAs (Mango and Broccoli RNA) and prepared the cell lines with stable expression of these RNAs. Then, I chose a sensitive method to monitor the dynamic (folded and unfolded stages) of these model G-quadruplexes RNA in the cells. To sum up, I prepared a cellular model, which could be used in a high throughput screen to identify the components of cellular molecular machinery responsible for unfolding RG4 regions. The model could be a step forward to understand the mechanism of RNA quadruplex structure regulation in cellular context and the precise role of G4s RNA in cellular processes.

The research is supported by National Science Centre, Poland [grant UMO2018/28/C/NZ1/00497].

DEVELOPMENT OF CHEMICAL TOOLS FOR IN VITRO AND IN VIVO STUDIES OF GHRELIN /DOPAMINE RECEPTOR HETERODIMERS

Célia Bouacha, Jean-Alain Fehrentz, Sonia Cantel & Séverine Denoyelle

Institute of Biomolecules Max Mousseron (IBMM, Team F9, Montpellier University
sonia.cantel@umontpellier.fr
severine.denoyelle@umontpellier.fr

G protein-coupled receptors (GPCRs) represent a large family of transmembrane proteins and are involved in the regulation of numerous physiological functions. Recent studies indicate that GPCRs heterodimerization may induce the activation of alternative pathways. Its impact on molecular processes has not yet been elucidated, hence the need to design chemical tools to study the GPCR's heteromers. [1] Considered to be powerful tools for studying receptor dimerization, bivalent ligands can be used to link the orthosteric sites of a dimer. Because of their selective recognition properties, they can be used to specifically target cells expressing heterodimers receptors.

The growth hormone secretagogue receptor (GHSR), a GPCR known for regulating numerous central and peripheral physiological processes, has been studied for many years in the laboratory.[2], [3] Recent studies indicate that the GHSR forms heteromers with other GPCR like the dopamine D2 receptor (D2R). GHSR heterodimerization with D2R has been demonstrated to induce a modulation of feeding behavior. To study these heterodimeric complexes, the development of bivalent ligands has been considered. These original ligands consist of peptide or non-peptide pharmacophores of the GHSR and well established small molecule pharmacophores of the D2R linked by a spacer. The advantages of the generated bivalent ligands may include higher affinity and selectivity compared to respective monovalent ligands along with an improved or modified physiological response. [4]

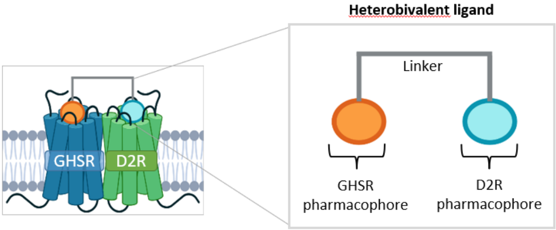

Figure 1: Structure of heterobivalent ligands

Generating such bivalent ligands and working on the nature of the GHSR ligands (agonist, antagonist, and inverse agonist), like the length, functionalization, hydrophobicity, and rigidity of the spacer, may provide a better understanding of biological processes involving GHSR-D2R heteromers. (Figure 1) These ligands may offer significant therapeutic tools for the treatment of specific GPCR heteromers involved in pathologies such as obesity. [5]

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ACCESS TO VALUABLE ORGANOGERMANES VIA EARTH-ABUNDANT CATALYSIS

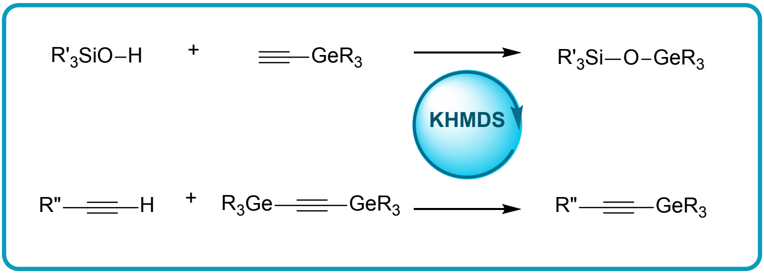
Konstancja Broniarz, Grzegorz Hreczycho

Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
konstancja.broniarz@amu.edu.pl

Organogermanium compounds have gained interest in recent years due to their unique properties. They can be considered as useful building blocks for more complex organic molecules, because of their low toxicity and high stability. Germasiloxanes attracted attention due to their high refractive index, low dielectric constant and biocompatibility.[1] They can be formed via classical stoichiometric methods of condensation of chlorogermanes with silanols or metal silanolates and in reaction between germoxanes and silyl azides.[2–4] Because of the inconvenient nature of the process (including production of corrosive or explosive by-products, sensitive nature of substrates) scientists searched for more efficient ways to synthesize germasiloxanes, which led to the development of coupling reactions of organosilicons with various germylation agents.[5–6]

High cost and environmental load of transition metal catalysts have caused a huge spike of interest in more sustainable and eco-friendly approaches utilizing main group species as catalysts.[7–9]

In this poster communication, we present an efficient protocol for catalytic O- and sp C-germylation using potassium bis(trimethylsilylamide) as the catalyst leading to functional germasiloxanes and alkynylgermanes in good yields.



Scheme 1: Scheme of synthesis of germasiloxanes and alkynylgermanes.

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DIASTEREOSELECTIVE SYNTHESIS AND BIOLOGICAL ACTIVITY OF NEW FLUORINATED α-AMINOPHOSPHONATES

Karolina Ciesielska[1], Donata Pluskota-Karwatka[1], Maciej Kubicki[1], Grzegorz Dutkiewicz[1], Dariusz Wawrzyniak[2]

[1]*Faculty of Chemistry, Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland*
[2]*Institute of Bioorganic Chemistry, Polish Academy of Sciences, Noskowskiego 12/14, 61-704 Poznań, Poland*
karcie5@amu.edu.pl

α-Aminophosphonates are an important group of chemical compounds which, due to their structural similarity to natural α-amino acids, exhibit a number of biological activities, such as for example antiviral, antibacterial and anticancer [1-3]. Among the already known α-aminophosphonates, compounds containing fluorine constitute especially important group. The presence of this element in the structure of chemical compounds can significantly change their chemical, physical and biological properties [4].

The title α-aminophosphonates were synthesized using the Pudovik method by subjecting the previously obtained imines [5] to hydrophosphonylation. Fluorinated benzaldehyde derivatives and enantiomerically pure amines were used for the synthesis of imines. Therefore, the imine hydrophosphonylation resulted in the formation of diastereomeric mixtures of the expected products. The products were obtained with good yields and satisfactory or very good diastereomeric ratios (Figure 1), and subjected to structural and biological studies. The preliminary results obtained are very promising.

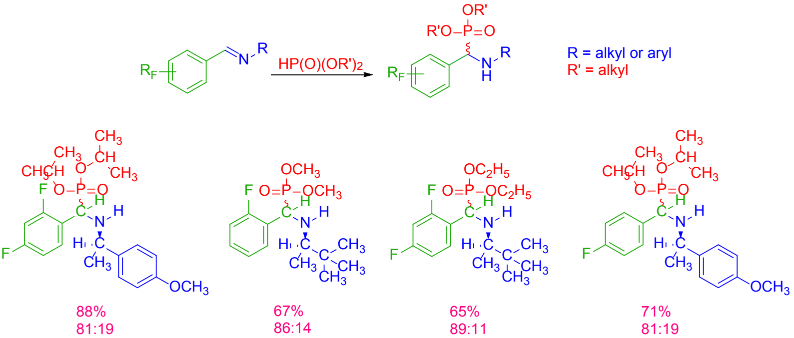

Figure 1: Scheme of imine hydrophosphonylation and exemplary structures, yields and diastereomeric ratios of the α-aminophosphonates obtained.

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TUNING THE POROSITY AND PARTICLE MORPHOLOGY OF ZIF-BASED CARBONS FOR IMPROVED ADSORPTION OF DYES

Aleksander Ejsmont, Agata Jankowska, Joanna Goscianska

Adam Mickiewicz University, Faculty of Chemistry, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
aleksander.ejsmont@amu.edu.pl

Carbon nanomaterials are widely applied in adsorption processes, catalysis, or energy storage. Their performance is influenced by specific surface area development, morphology, and particle size. Metal-organic frameworks (MOFs) represent a new type of carbon precursors, which at the same time act as a structure-directing agent that allows governing carbon porosity.

In the present study, we developed the preparation of carbon materials with different particle shapes and pore sizes, by using zinc-based zeolite imidazole structures (ZIFs), i.e. ZIF-8 and ZIF-CO_3-1. The 2-methylimidazole in the ZIFs, acting as an organic linker, was the main source of carbon and additionally enriched the carbon samples with nitrogen. ZIFs were synthesized by a solvothermal method employing dimethylformamide for ZIF-8 and a mixture of dimethylformamide and distilled water for ZIF-CO_3-1. In their syntheses, zinc acetate and zinc oxides with spherical and flower-like morphologies were applied as metal sources. Subsequently, all metal-organic frameworks were carbonized at 1000 °C and the resulting carbons were subjected to detailed physicochemical characterization.

Analyses revealed that the obtained materials have morphologies similar to ZIFs while they differ significantly in porosity. Carbons prepared from ZIF-8 are microporous, while a double system of pores (micro- and mesopores) was noted for ZIF-CO_3-1-derived carbons. An increase in the pore size of samples provided greater adsorption of auramine O and brilliant green dyes. Moreover, a unique morphology of windmill-shaped carbon particles was achieved (Figure 1), characterized by highly developed specific surface area, contrary to the non-porous ZIF-CO_3-1 precursor.

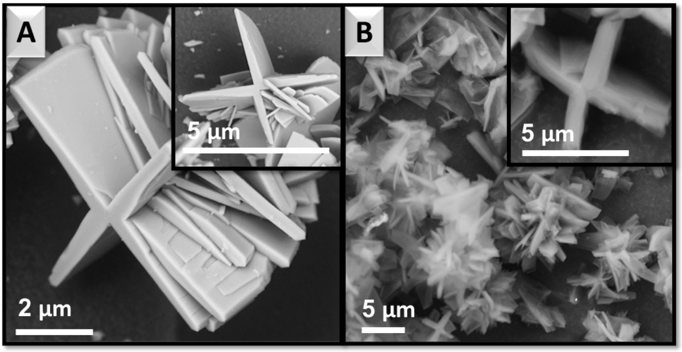

Figure 1. The windmill-shaped ZIF-CO_3-1 precursor (A) and ZIF-derived carbon material (B).

MIL-88A-BASED DRUG DELIVERY SYSTEM FOR ANTI-MIGRAINE THERAPY

Aleksandra Galarda, Joanna Goscianska

Adam Mickiewicz University, Faculty of Chemistry, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
alegal2@amu.edu.pl

In recent years, a new class of crystalline materials, metal–organic frameworks (MOFs) have been of great interest in biomedical applications. They are characterized by unique properties, i.e. large surface area and pore volume, biocompatibility, high drug-loading capacity, and sustainable drug release [1]. Drug delivery systems based on metal-organic frameworks could be applied to treat many diseases, including migraine, cancer, and inflammation. One of the most commonly used medications for migraine attacks is diclofenac with analgesic and antipyretic properties. However, it has low bioavailability reached by oral administration and very short half-time, which requires repeated dosing [2]. Hence, there is a need to develop a porous carrier delivering diclofenac in a controlled manner at the target site of the body.
The aim of the study was the synthesis optimization, characterization, and applicationof MIL-88A materials as diclofenac delivery systems. Metal-organic frameworks were prepared via the solvothermal method with the use of iron(III) chloride as a metal precursor and fumaric acid as a linker. The synthesis of samples was performed in distilled water or N,N-dimethylformamide (DMF) at different temperatures. In order to evaluate the properties and potential of synthesized materials as drug carriers, diclofenac adsorption and release were carried out.

The results have shown, that the highest specific surface area (326 m2/g) and pore volume (0.47 cm3/g) were obtained for material synthesized in DMF at 70 ºC. Scanning electron microscopy images indicated the hexagonal rod- or spindle-like morphology of samples depending on the solvent used during preparation. The materials are promising adsorbents of diclofenac with sorption capacities ranging from 833 mg/g to 2021 mg/g. Drug adsorption onto the surface of MIL-88A samples is mainly based on the hydrogen bond formation, electrostatic, and metal cation–π interactions. It was found that selecting the appropriate carriers allows for precise control of the kinetics of the diclofenac release from their surface.

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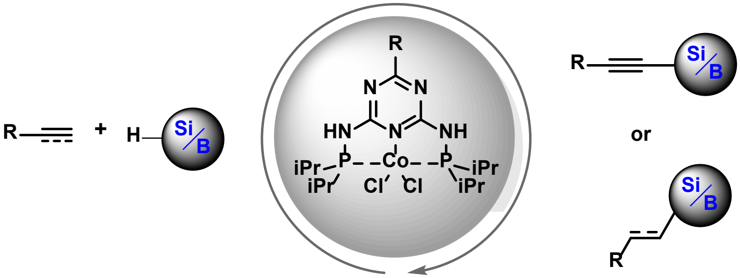
COBALT PINCER-TYPE COMPLEXES DEMONSTRATE UNIQUE SELECTIVITY IN THE REACTIONS WITH UNSATURATED SILICON AND BORON

Grzegorz Hreczycho, Krzysztof Kuciński, Hanna Stachowiak-Dłużyńska, Dariusz Lewandowski, Ewelina Szafoni

Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
g.h@amu.edu.pl

Modern chemical synthesis highly focuses on the sustainability of the carried-out reactions mainly by minimizing the amount of used and generated hazardous substances. This is mostly achieved by using catalysts that permit the activation of new reaction pathways which enable increased process selectivity and the utilization of less reactive substrates.[1]

An interesting example of recently intensively studied homogeneous catalysts is pincer cobalt complexes. They are known for their relatively simple synthesis, exhibiting high stability, activity, and selectivity in hydrogenation, hydroboration, hydrosilylation, or bond-forming reactions.[2] Their important feature is the possibility of affecting their selectivity by simply changing the reaction conditions or the structure of the ligand.



In this communication, I will present a synthesis of organoboron and organosilicon compounds, which have been catalyzed by cobalt pincer complexes. These complexes were synthesized using inexpensive and commercially available reagents in a gentle and straightforward manner. The presented methodology enables ligand-controlled synthesis regarding the principles of sustainable chemistry leading to a valuable group of compounds.[3-5]

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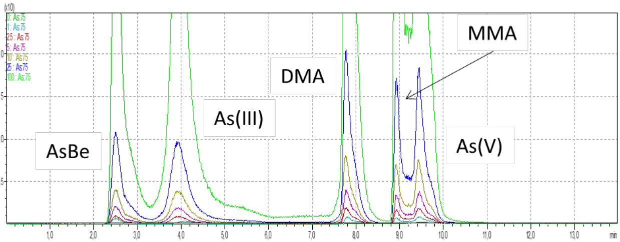
SPECIATION ANALYSIS OF WATER- AND FAT-SOLUBLE ARSENIC SPECIES IN VARIOUS SAMPLES USING HPLC-ICP-MS – LITERATURE STUDY AND RESEARCH RESULTS

Dorota Jakkielska, Anetta Zioła-Frankowska

Department of Analytical Chemistry, Faculty of Chemistry, Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
dorjak@amu.edu.pl

Arsenic (As) is one of the most toxic elements and it can cause chronic health effects such as cancer, cardiovascular disease and diabetes. It is present in both organic and inorganic forms and compounds. The interest in arsenic toxicity has been mainly focused on inorganic forms, while the organic ones were considered non-toxic. However, in recent years it has been shown that organic forms can also show toxicity and in the case of arsenolipids comparable or even higher than inorganic forms [1, 2]. Arsenic occurs in the form of both water- and fat-soluble forms (arsenolipids) in foods. Marine products are one of the largest sources of arsenic in the human diet and may contain compounds, such as arsenites – salts containing arsenic(III), arsenates – salts containing arsenic(V), methylarsonic acid (MMA), dimethylarsinic acid (DMA), arsenobetaine, arsenocholine, arsenosugars and arsenolipids. Marine organisms, such as fish, shellfish and seaweed, are high in total arsenic, but more than 90% of it occurs in organic forms [3]. The total arsenic content is not sufficient to determine toxicity and accurately determining various forms in which arsenic occurs in food is a major challenge for food safety authorities and institutions. The current regulations and restrictions regarding the exposure to arsenic mainly focus on its inorganic forms. Therefore, the aim of the study is to develop effective methods of speciation analysis of water- and fat-soluble arsenic forms (arsenolipids), using high performance liquid chromatography with inductively coupled plasma mass spectrometry (HPLC-ICP-MS). Arsenolipids are not commercially available, hence synthesis of selected arsenolipids is planned. Certified reference materials and honey samples have been analyzed for water-soluble arsenic species.



Overlaid chromatograms for the standard solutions, concentrations 0 – 100 μg/L, of arsenobetaine (AsBe), As(III), dimethylarsinic acid (DMA), monomethylarsonic acid (MMA) and As(V).

The research is funded by ID-UB (Initiative of Excellence - Research University) Proposal No.: 054/13/SNŚ/0037.

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REMOVAL OF SUNSET YELLOW FCF AND TARTRAZINE FROM WATER WITH THE USE OF MODIFIED FLY ASH-BASED MCM-41

Agata Jankowska[1], Rafał Panek[2], Wojciech Franus[2], Joanna Goscianska[1]

[1]Adam Mickiewicz University, Faculty of Chemistry, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
[2]Lublin University of Technology, Faculty of Civil Engineering and Architecture, Nadbystrzycka 40, 20-618 Lublin, Poland
agache1@amu.edu.pl

The growth of the human population and world development have contributed to the generation of vast amounts of toxic pollutants and in consequence environmental degradation. Organic dyes, including sunset yellow FCF and tartrazine, are among the most common water contaminants that endanger wildlife and people, therefore, their effective elimination is of great importance [1].

The research aimed to analyze the potential of pure and functionalized MCM-41 in the removal of selected azo dyes from water solutions. Silica material of MCM-41 type was subjected to modifications with different amounts of (3-aminopropyl)trimethoxysilane (APTMS). The physicochemical characterization of the samples (MCM-41, MCM-41$_{\text{APTMS-0.4}}$, MCM-41$_{\text{APTMS-1}}$) was carried out and the impact of adsorbate solution pH and initial concentration, as well as temperature of the adsorption process, on the sorption capacities of materials toward dyes was determined (Figure 1).

The modification of MCM-41 led to a decline in the intensities of XRD reflexes which indicates a partial disruption of the structure ordering caused by the closing pore entrances with $-NH_2$ groups. The generation of basic oxygen functional groups on the surface of MCM-41$_{\text{APTMS-0.4}}$ (2.74 mmol g^{-1}) and MCM-41$_{\text{APTMS-1}}$ (3.49 mmol g^{-1}) and disappearance of acidic groups present on pure MCM-41 was also observed. Sorption capacities of silica materials were the highest at pH 2 and, depending on the adsorbent, at room temperature or 45 °C. It is the result of electrostatic attraction between the negatively charged molecules of azo dyes and the positively charged surface of the samples. The modification with aminosilanes led to an increase in the sorption capacities of materials. Research proved that modified fly ash-based silica adsorbents can effectively eliminate azo dyes from aqueous solutions.

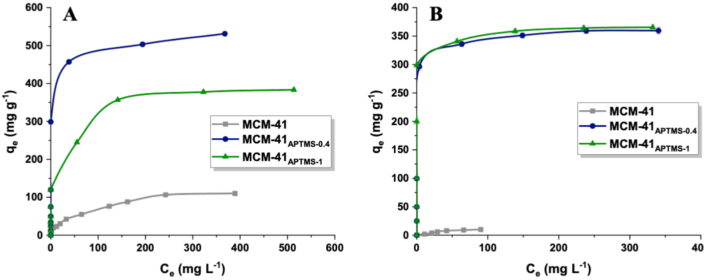

Figure 1. Isotherms of sunset yellow FCF (A) and tartrazine (B) adsorption on the synthesized samples.

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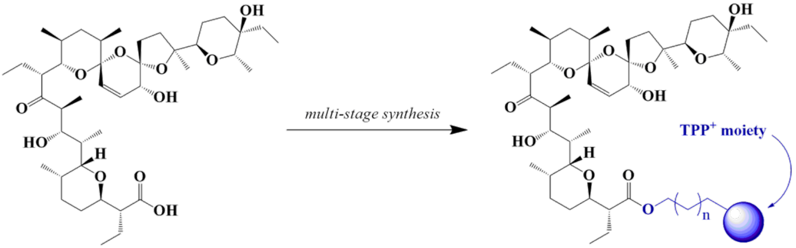
SYNTHESIS, CYTOTOXICITY, AND ANTIMICROBIAL ACTIVITY OF TRIPHENYLPHOSPHONIUM SALTS OF SALINOMYCIN

Marta Jędrzejczyk[1], Magdalena Mielczarek-Puta[2], Małgorzata Podsiad[2], Marta Struga[2], Adam Huczyński[1]

[1]Department of Medical Chemistry, Faculty of Chemistry, Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
[2]Chair and Department of Biochemistry, Medical University of Warsaw, Banacha 1, 02-097, Warszawa, Poland
marta.jedrzejczyk@amu.edu.pl

Salinomycin (**SAL**) belongs to the group of ionophore antibiotics, which are compounds of natural origin and exhibit a very wide spectrum of biological properties. **SAL** for the first time was isolated from *Streptomyces albus* in 1974, during screening tests devoted to seeking new antibiotics. Nowadays, **SAL** is commonly used in veterinary medicine as a coccidiostatic agent for poultry and cattle [1]. It has been proven that **SAL** is one of the most active among natural polyether ionophores and exhibits biological activity such as antibacterial, antiparasitic, antiviral, and antiproliferative. A vast spectrum of biological properties of **SAL** is related to its ability to coordinate cations and transport them through bilayer lipid membranes, which leads to the disruption of a concentration gradient in the intracellular environment and then to programmed cell death called apoptosis [2].

Triphenylophosphonium cation (TPP$^+$) is widely known as a mitochondrial targeting moiety and literature data suggest that conjugation natural compounds with TPP$^+$ is an interesting research direction [3]. Therefore in our work we conducted the synthesis of **SAL** bioconjugates with triphenylphosphonium cation by modification at C-1 position. We investigated their antiproliferative activity using human cancer cell lines. Additionally, we tested their antibacterial properties against Gram-positive and Gram-negative bacteria. The synthesis of **SAL** derivatives and biological research were funded by the project OPUS (grant 2021/41/B/ST4/00088) funded by the National Science Centre, Poland (NCN) to A. Huczyński.



SAL

n = 2 or 4

Figure 1. Structure of SAL and its analogues.

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RESEARCH ON HETEROGENOUS PERACETIC ACID-BASED ADVANCED OXIDATION PROCESSES

Dariusz Kiejza[a*], Joanna Karpińska[b], Urszula Kotowska[b], Elżbieta Regulska[b]

[a]University of Bialystok, Doctoral School of Exact and Natural Sciences, Ciolkowskiego 1K Str., 15-245 Białystok
[b]University of Bialystok, Faculty of Chemistry, Department of Analytical and Inorganic Chemistry, Ciolkowskiego 1K Str., 15-245 Białystok
*d.kiejza@uwb.edu.pl

The use of an Advanced Oxidation Process (AOP) provides a viable and effective option for removing organic contaminants by oxidizing a wide range of chemicals. According to the definition AOPs are based on *in situ* generation of strong oxidants for the oxidation of organic compounds. This includes processes based on action of variety reactive species, mainly oxygen reactive forms such as ·OH, $O_2^{\cdot -}$, $^1O_2$, $HO_2^{-\cdot}$, which constitute the majority of available AOPs, but also other processes applied the other oxidizing species especially sulfate or chlorine radicals. Recently, the attention of scientists is focused on organic peracids, among many, acetic peracid. Acetic peracid is known and applied for years as a very efficient sterilizing and disinfecting agent. In recent years, there has been observed an increase in interest in the use of PAA as an oxidant for the degradation of organic pollutants due to its high oxidizing potential E^0=1,960V [1]. The PAA molecule contains a peroxide (-O-O-) moiety which is thermodynamically unstable. Its dissocciation starts a chain of reactions which lead to the generation hydroxyl radical, acetic and to the lesser extend the methyl radicals. Despite the fact that PAA is thermodynamically unstable, the dissociation kinetics of the -O-O- bond is too small to obtain a sufficiently high concentration of reactive species in solution. Various activation methods are used to accelerate this process [2]. One of them is the use of heterogeneous activators [3]. The presented work concerns the search for new durable and effective activators of peracetic acid peracid. In the study, the usefulness of nickel cobaltite ($NiCo_2O_4$) as an activator of PAA in the degradation process of 10 organic compounds from the bisphenol group was checked. Nickel cobaltite, belonging to the group of mixed transition metal oxides, is characterized by photocatalytic properties, low toxicity, and easiness of production, but also the ability to create various nanostructures [4]. The compound was obtained by sol-gel method by precipitation with ammonia. Then, the bisphenol removal process was optimized by selecting appropriate process conditions. The optimal amount of catalyst (115 mg/l), PAA concentration (7 mM) and pH (7) in the system were selected by analysis of the response surface in the experimental design method (DoE, central composition plan). The possibility of reusing cobaltite in subsequent oxidation cycles was checked. The obtained results indicate that in the next 4 cycles, there is a slight decrease in the activity of the activator. However, already in the fifth cycle, a significant decrease in $NiCo_2O_4$ activity was observed, manifested by a decrease in bisphenol degradation efficiency.

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ZINC OXIDE-BASED MATERIALS AS FUNCTIONAL ADMIXTURES FOR CEMENT COMPOSITES

Izabela Klapiszewska [1,*], Teofil Jesionowski [2], Łukasz Klapiszewski [2], Agnieszka Ślosarczyk [1]

[1]*Poznań University of Technology, Faculty of Civil and Transport Engineering, Institute of Building Engineering, Piotrowo 5, PL-60965 Poznan, Poland*
[2]*Poznań University of Technology, Faculty Chemical Technology, Institute of Chemical Technology and Engineering, Berdychowo 4, PL-60965 Poznan, Poland*
izabela.klapiszewska@put.poznan.pl

The use of nanoparticles creates the possibility of new solutions, including the improvement of materials used in the construction sector, because the introduction of such systems into the matrix causes the densification of the structure, increasing its packing. Nanoparticles are also often characterized by a developed specific surface area, which affects the cement hydration process by increasing the pozzolanic reaction. This leads to an improvement in the strength of composite. There are also literature reports about the beneficial effect of nanoparticles on the transition zone between the aggregate and the paste [1]. The introduction of zinc oxide to the cement composite allows for the reduction of empty spaces in the cement matrix, which leads to the effectiveness of inhibiting the corrosion process and the effect of sodium nitrite in concrete mixes containing ZnO. The durability tests carried out showed that the addition of a superplasticizer is a very important element to ensure adequate workability [2]. It is also worth noting that zinc oxide is one of the most attractive materials with antimicrobial activity [3,4]. Additional advantages it has are its relatively low price, high chemical activity and light sensitivity [5].

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CONSTRUCTION MATERIALS MODIFIED WITH FUNCTIONAL NANO- AND MICROMATERIALS WITH PHOTOCATALYTIC AND ANTIMICROBIAL PROPERTIES

Łukasz Klapiszewski [1,*], Patryk Jędrzejczak [1], Izabela Klapiszewska [2], Agnieszka Ślosarczyk [2], Teofil Jesionowski [1], Jaroslav Riha [3]

[1] Poznan University of Technology, Faculty of Chemical Technology, Institute of Chemical Technology and Engineering, Berdychowo 4, PL-60965 Poznan, Poland
[2] Poznan University of Technology, Faculty of Civil and Transport Engineering, Institute of Building Engineering, Piotrowo 5, PL-60965 Poznan, Poland
[3] Zentiva, k.s, U Kabelovny 130/22, Prague 102 00, Czech Republic
lukasz.klapiszewski@put.poznan.pl

Biodeterioration is one of the causes of degradation of building materials and can significantly affect erected buildings, especially public buildings, such as hospitals, pharmaceutical laboratories, offices, schools, historic buildings. This topic has gained particular attention in recent years, when the COVID-19 pandemic made it necessary to separate special clean and polluted zones in buildings, which turned out to be a great challenge. This situation drew additional attention to research activities undertaken by numerous research centers for over 20 years, but still not implemented, and related to the use of metal nanoparticles and metal oxides in preventing the multiplication and development of microorganisms in building materials.

Nanoparticles of selected metals and metal oxides can effectively act on both gram-positive and gram-negative bacteria, fungi, molds and algae, limiting their growth and thus extending the life of building materials and newly constructed structures. In addition, they can also have a positive effect when used as bioactive coatings on existing buildings, very often of historical significance. Among such materials, the most important are: nanoparticles of silver, copper, titanium dioxide, zinc oxide or copper oxide. Their effectiveness in inhibiting microorganisms significantly depends both on the physicochemical properties of the nanoparticles themselves, such as: size, shape, surface area and their concentration, as well as on the properties of the building material substrate, in particular on porosity, water absorption and pH.

Acknowledgment: This work was supported by the National Science Center Poland under research project no. 2019/35/B/ST8/02535. Furthermore, part of the research was funded by the European Union's Horizon 2020 Research and Innovation program under the Marie Skłodowska-Curie grant agreement No 778051, and the Ministry of Science and Higher Education of Poland 5014/H2020 – MSCA-RISE/2019/2.

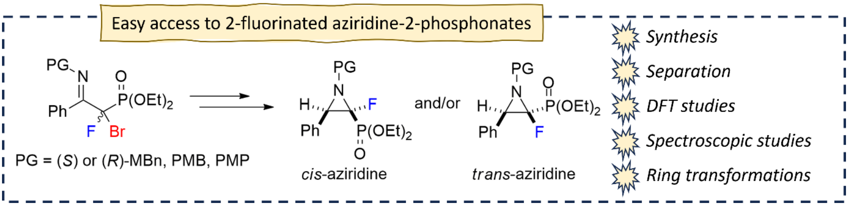
ACCESS TO 2-FLUORINATED AZIRIDINE-2-PHOSPHONATES FROM α,α-HALOFLUORINATED β-IMINOPHOSPHONATES

Mateusz Klarek[a], **Tomasz Siodła**[a], **Tahar Ayad**[b], **David Virieux**[b], **Magdalena Rapp**[a]

[a] *Adam Mickiewicz University, Uniwersytetu Poznanskiego 8, 61-614 Poznan, Poland*
[b] *ICGM Univ. Montpellier, CNRS, ENSCM, Montpellier, France*
matkla@amu.edu.pl

The aziridine motif frequently appears in biologically active compounds [1,2]. Therefore, this heterocyclic three-membered ring motif also serves as an attractive building block for organic transformations owing to the strained ring system and its ability to undergo highly regio- and stereospecific ring-opening reactions [3]. A particular group of azaheterocyclic compounds are aziridine-2-phosphonates, which could be used as starting material in the synthesis of aminophosphonates.

Herein, we disclose the first example of the synthesis of *N*-inactivated aziridines substituted by a fluorine and phosphonate moiety at the same carbon atom [4]. We propose a convenient strategy starting from the condensation of the β-ketophosphonate with primary amines, followed by a one-pot halofluorination reaction yielding titled α,α-halofluorinated β-iminophosphonates. Reduction of the imine bond allows form amines suitable for intramolecular cyclization and the construction of three-membered fluorinated aziridines (Scheme 1). The synthesized products are air-stable and don't undergo spontaneous degradation. Based on the spectroscopic and theoretical studies as well as literature reports, we determined the *cis*/*trans* geometry of the obtained heterocycles. We also present the impact influence of fluorine atom on the reactivity of aziridine-2-phosphonates *via* an acid- catalyzed ring opening reaction or selective transformation to non-fluorinated aziridine.



Scheme 1. Synthesis of 2-fluoro aziridine-2-phosphonates through α,α-halofluorinated β-iminophosphonates transformations.

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THE USE OF WOLFFIA ARRHIZA (L.) HORKEL EX WIMM. TO REMOVE TEN BISFENOLS FROM WATER

Urszula Kotowska, Weronika Polińska, Joanna Karpińska

Faculty of Chemistry, University of Białystok, Ciołkowskiego 1K Str., 15-245 Białystok, Poland
ukrajew@uwb.edu.pl

The industrial development and growing human interference with nature cause an increasing number of hazardous substances in the environment, including aquatic ecosystems. One of the pollutants most often detected in the environment is bisphenol A (BPA). Due to the endocrine effect of BPA and the introduced legal restrictions, were developed structural analogs of BPA, which can be even more harmful. The main source of bisphenols entering the environment is municipal and industrial wastewater, due to the fact that the applied wastewater treatment processes are not sufficiently effective. The aim of this study was to investigate the effectiveness, kinetics and mechanism of removal of ten bisphenols: F, E, A, C, B, G, Cl_2, Z, AP, M from aqueous solution during contact with smallest vascular plant *W. arrhiza*.

Experiments were carried out in sterilized vessels, where 1 g of *W. arrhiza* and 100 mL of an aqueous solution with Hutner's medium and bisphenols (100 µg/L) were placed. Changes in the content of bisphenols were examined by GC-MS technique on the day of starting the culture and after 1, 2, 3, 5, 7 and 14 days. The removal of bisphenols proceeded according to pseudo-first order kinetics. The efficiency of removing bisphenols within 14 days of culture ranged from 95% to 99.5%. The optimal conditions for the bisphenols removal was as follows: pH 7, amount of plant 25 g per liter of polluted water and dailyexposure time 16 h. The decrease in bisphenol concentration occurred at a different rate each day of cultivation, reaching values of process rate constants, ranging from 0.22/day to 0.38/day. Bisphenol Cl_2 was the most intensively removed by the plant, while bisphenol M was the slowest to be removed from solution.

Phytoremediation processes do not use energy inputs, reagents or complicated equipment. What's more, thanks to their high efficiency, they have a chance to be combined with processes in conventional wastewater treatment plants.

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STABILITY STUDIES OF COLLOIDAL SYSTEMS CONTAINING FUNCTIONALIZED ORGANOSILICON COMPOUNDS

Klaudia Krysiak, Julia Leśniewska, Miłosz Frydrych, Bogna Sztorch, Robert Przekop, Anna Olejnik

Centre for Advanced Technology, Adam Mickiewicz University, Uniwersytetu Poznańskiego 10, 61-614 Poznań, Poland
Faculty of Chemistry, Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
klaudia.krysiak.uam@gmail.com

A colloid is a two-phase system in which one substance is dispersed in another. Emulsions are examples of colloids that consist of two immiscible liquids that are stabilized by emulsifier [1]. Recently modified polyhedral oligomeric silsesquioxanes (POSS) have been applied as emulsifying agent in colloidal systems [2].

The aim of the present research was to check the emulsifying properties of three different octaspherosilicates functionalized with 4-allyloxy-2-hydroxybenzophenone and polyethylene glycol (PEG). In this study it was evaluated if the length and amount of polyethylene glycol groups attached to core of POSS have influence on the stability of emulsions. Three POSS with different ratio of olefins such as 4-allyloxy-2-hydroxybenzophenone and PEG were synthesized by hydrosilylation reaction using Karstedt catalyst. Each of them was analyzed by Fourier Transform Infrared Spectroscopy and contact angle measurement to determine their hydrophilic-lipophilic balance. By knowing the nature of each compound obtained different types of emulsions were prepared. The stability of colloidal systems was analyzed by centrifugation test, optical microscope, multiple light scattering, and laser diffraction methods.

The results have shown that the length of PEG chain had no influence on the wetting angle and the hydrophilic-lipophilic balance. It was also proved that the more PEGs attached to the octaspherosilicate core, the greater hydrophilicity, and the better emulsifying properties of organosilicon compounds and thus the more stable emulsion can be obtained

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CURCUMIN DERIVATIVES AND THEIR NANOFORMULATIONS USING MICELLES WITH POTENTIALACTIVITY AGAINST BLADDER CANCER

Kuźmińska Joanna[1], Kobyłka Paulina[2], Kucińska Małgorzata[2], Stawny Maciej[1], Jelińska Anna[1], Goslinski Tomasz[3]

[1] Chair and Department of Pharmaceutical Chemistry, Poznan University of Medical Sciences, 6 Grunwaldzka St., Poznan, Poland;
[2] Chair and Department of Toxicology, Poznan University of Medical Sciences, Dojazd 30 St., Poznan, Poland;
[3] Chair and Department of Chemical Technology of Drugs, Poznan University of Medical Sciences, 6 Grunwaldzka St., Poznan, Poland;
jkuzminska@ump.edu.pl

Bladder cancer is responsible for approximately 200,000 deaths annually worldwide, accounting for 2.1% of all cancer deaths. The epidemiology of this disease is a growing problem, despite the development of new anti-cancer therapies (1). Curcumin is a phytochemical with proven anticancer activity. However, its clinical use is limited due to unfavorable physicochemical and pharmacokinetic parameters. To improve bioactivity of curcumin new curcumin fluoro derivatives were synthesized, but they have lower solubility (2). The way to modify the bioavailability is a strategy based on the use of carriers, such as liposomes or micelles, which can contribute to improving pharmacokinetic and pharmacodynamic parameters. The assumptions of the presented project concern: (I) synthesis of curcumin derivatives with higher stability and biological activity, (II) encapsulation of the most active curcuminoid in micelles, (III) evaluation of the effect of curcuminoid encapsulation on the survival of normal and cancerous bladder cells in an *in vitro* model.

The research used classical chemical synthesis methods. The presented curcuminoids were characterized by the following techniques: NMR, HRMS (ESI), HPLC, and UV-Vis. The micelles were prepared using a solubilizer, a crystallization inhibitor, and a matrix-forming polymer reagent called Soluplus®. Characterization of the size of the resulting micelles was performed using the Dynamic Light Scattering (DLS) technique, while encapsulation efficiency (EE) was evaluated using HPLC. The in vitro model test was performed for a human bladder cancer line and a human fibroblast cell line. Cell survival after incubation with the tested compounds was assessed using the MTT assay. The results provided new information on the use of micelles as an effective carrier for phytochemicals, including the possibility of modulating the biological activity and improving the selectivity of curcumin derivatives.

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COBALT PNP TYPE COMPLEXES AS A UNIVERSAL TOOL FOR THE SYNTHESIS OF ORGANOMETALLIC COMPOUNDS

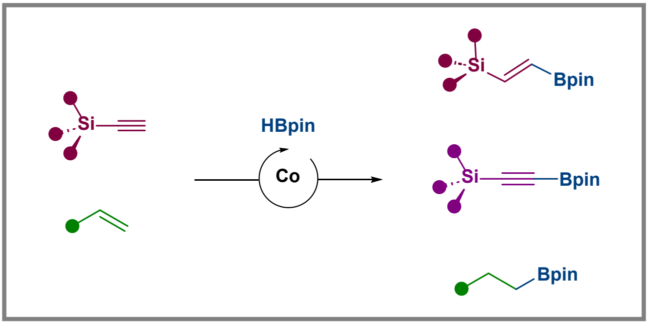
Dariusz Lewandowski, **Grzegorz Hreczycho**

Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
darlew1@amu.edu.pl

The unique properties of organometallic compounds make them interesting synthons used to construct complex molecules. They find applications in the production of advanced intelligent materials, bioactive molecules, or catalysts.[1] Moreover, the organometallic moiety allows further functionalization by the easy introduction of new functional groups into the molecule, leading to highly complex molecules.[2]

Recently, a high emphasis has been placed on conducting syntheses in a sustainable and environmentally friendly manner. Consequently, most of the methods currently being developed for the production of organometallic compounds are based on catalytic reactions proceeding under mild conditions and avoiding the formation of by-products.[3] In this context, pincer cobalt complexes seem to be of particular interest, which has found application in many catalytic processes due to their high thermal and chemical stability, as well as the possibility of fine-tuning their properties.[4]

In this communication, we will present methods for the synthesis of organoboron and organosilicon compounds by hydroboration reaction. The presented procedures are conducted considering the principles of green chemistry and utilize PNP-type cobalt pincer complexes built on a triazine backbone to synthesize highly valuable synthons.



Scheme 1: Syntheses of organometallic compounds catalyzed by pincer cobalt complexes.

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MCPA HERBICIDE RAPID AND SELECTIVE REMOVAL USING 2-BUT-3-ENYL-2-OXAZOLINE-BASED MOLECULARLY IMPRINTED POLYMERS

Aleksandra Lusina, Michał Cegłowski

Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
aleksandra.lusina@amu.edu.pl

Molecularly imprinted polymers (MIPs) are polymeric systems possessing tailor-made sites selective toward specified analytes. The recognition property is a result of remembering shape, size, and the presence of functional groups from analyte molecules, thus the milestone is the thoughtful designing of integrations that can be formed. Physical stability, selectivity, relatively low-cost synthesis, and reusability caused high interest in MIPs' application in various fields [1]. Poly-2-but-3-enyl-2-oxazoline (P(BuOx)) is a polymer that comes from the poly-2-oxazolines (POx) class of compounds. Their beneficial properties like biocompatibility, stealth behavior, dispersity, stability, nonionic character, and solubility in water and organic solvents, caused POx to have broad applications [2]. 2-Methyl-4-chlorophenoxyacetic acid (MCPA), one of the widely used herbicides in Europe, shows high toxicity and low biodegradability [3]. The use of the herbicides over years has resulted in considerably increased pollution problems of surface and groundwater [4]. To prevent the environmental hazard and human risks of MCPA it is necessary to develop new methods allowing its effective removal. The aim of the work was the synthesis of P(BuOx)-based MIPs for selective removal of MCPA from the environmental water samples (Fig.1). Prepared materials, differentiated by the amount of 3-mercaptopropionic acid (3MPA) at the side chain, were then subjected to the adsorption examinations that prove the unique recognition property toward MCPA. The obtained results from the adsorption isotherm investigations showed that the increased amount of donor groups caused more efficient recognition systems. Moreover, the adsorption results were approximately 5 times better than for non-imprinted materials.

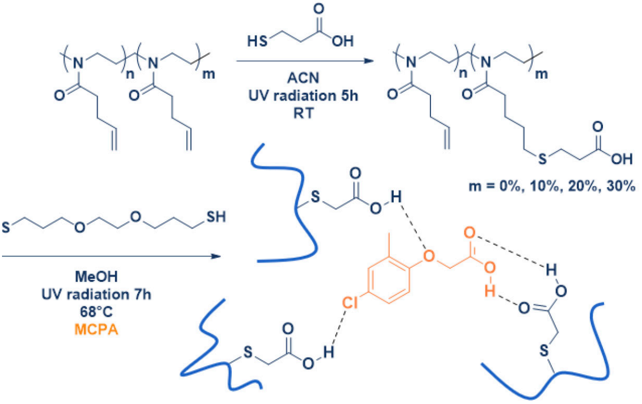

Figure 1. The overview of the proposed MIPs' synthesis methodology.

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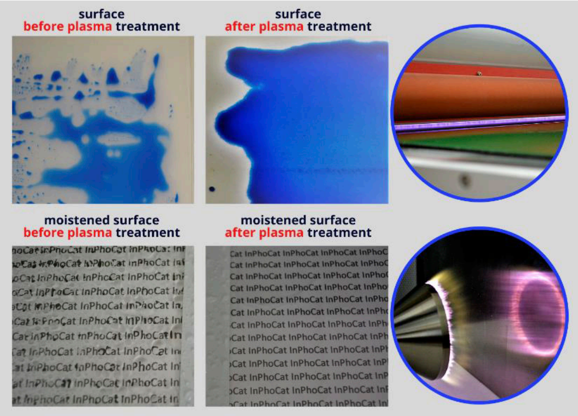
PLASMA SURFACE TREATMENT – IMPROVEMENT OF ADHESION AND DURABILITY

Karolina Zając[1,2], Joanna Macyk[2], Paweł Wyżga[2], Wojciech Macyk[1,2], Andrzej Kotarba[1]

[1] *Faculty of Chemistry, Jagiellonian University, Kraków*
[2] *InPhoCat – Innovative Photocatalytic Solutions Sp. z o.o., Kraków*
jmacyk@inphocat.pl



Surfaces of many materials, such as polymers, glass, ceramics, metals require extremely careful pre-treatment using chemical and/or physical methods to enable uniform and durable application of various coatings. One of the techniques used for this purpose is plasma pre-treatment, known as plasma cleaning, plasma etching, plasma modification or surface activation. The application of plasma makes it possible to obtain functional coatings with anti-corrosion, antibacterial or controlled wettability properties. Our studies are focused on understanding the surface chemistry of various substrates activated with atmospheric plasma and therefore a possibility of bonding of functional coatings to them. Such knowledge enables the design and rational selection of components of coatings, as well as optimal preparation of substrates both on a laboratory and production scale.

Selected materials: polymer foils, polypropylene nets, and conductive glass were exposed to atmospheric plasma. Surface wettability, expressed as the contact angle, was monitored at different exposures to plasma. Adhesion, homogeneity and morphology (smoothness) of the coatings were evaluated using SEM and AFM. The synthesized and characterized coatings were applied in various tests, including photoelectrochemical activity (photocurrent tests), antibacterial effectiveness (microbiological tests), and photocatalytic activity.

Acknowledgements

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INVESTIGATIONS OF LIGAND-MACROMOLECULES INTERACTIONS BY USING DSC, ITC AND FLUORESCENCE SPECTROSCOPY TECHNICS

Krzysztof Żamojć, Dariusz Wyrzykowski, Joanna Makowska

Faculty of Chemistry, University of Gdańsk, Wita Stwosza 63, 80-308 Gdańsk, Poland
joanna.makowska@ug.edu.pl

The ITC (isothermal titration calorimetry) method is a useful tool for investigating metal-ligand interactions in solution (1). However, sometimes the experiment is not feasible, e.g. due to the poor solubility of the tested compounds or because of the requirements connected with a high concentration of samples. Therefore, it has been proved that fluorescence spectroscopy is an alternative method for studying the interaction of macromolecules with metal ions (2). The fluorescence quenching corresponds to any process that decreases or eliminates the fluorescence intensity, lifetime or quantum yield of luminescent species as a result of the interactions with other chemical compounds. The high sensitivity, non-destructivity and simplicity of fluorescence spectroscopic techniques make them the most widely used for the analysis of the interactions between fluorescent peptides and metal ions that cause quenching. Generally, the fluorescence quenching can reveal the accessibility of quenchers to the fluorophore groups of proteins, help to understand protein binding mechanisms and provide important information on the nature of the binding phenomenon. The DSC (differential scanning calorimetry) method is a method complementing the above-mentioned methods used in studies of interactions of macromolecules with other systems (3). Thanks to it, we are able to determine the thermal stability of the samples before and after the possible reaction of complexation, which could be useful in the design of new compounds.

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SYNTHESIS AND SPECTROSCOPIC INVESTIGATIONS OF SCHIFF BASE LIGAND AND ITS AG(I) COMPLEXES AS DNA AND BSA BINDERS

Martyna Mańka[1,2], Martyna Szymańska[1], Izabela Pospieszna-Markiewicz[1], Ariel Adamski[1], Zbigniew Hnatejko[1], Maciej Kubicki[1], Agata Campisi[3], Giuseppe Consiglio[4], Marta Fik-Jaskółka[1], Violetta Patroniak[1]

[1] Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
[2] Institut de science et d'ingénierie supramoléculaires (ISIS), University of Strasbourg, 8 All. Gaspard Monge, 67000 Strasbourg, France
[3] Department of Drug Sciences and Health, University of Catania, 95125 Catania, Italy
[4] Dipartimento di Scienze Chimiche, Università degli studi di Catania, viale A. Doria 6, I-95125 Catania, Italy
martyna.manka@amu.edu.pl

Schiff base-type compounds and their Ag(I) complexes exhibit a broad spectrum of properties, including, among others, biological activity. [1] Due to the photosensitivity of Ag(I) compounds, research is being carried out on their use as photoactive drugs. This would allow activation of the chemotherapeutic only after irradiation at the target site, ensuring control of the drug and thus reducing the side effects that occur with standard chemotherapy. [2] The action of Ag(I) complexes involves the slow release of silver ions, which can then interact with DNA and proteins or lead to the production of reactive oxygen species, resulting in cell death. [3]

The aim of the project was the synthesis of Schiff base-type ligand and its coordination compounds with silver ions, and then, using spectroscopic techniques: UV-vis and fluorescence, study of their interaction with model biomolecules: CT-DNA (*Calf thymus*-DNA) and BSA (*Bovine Serum Albumin*). The obtained results may contribute to the design of modern anti-inflammatory or anticancer drugs that will be able to cause apoptosis when delivered with a protein to inflammatory cells.

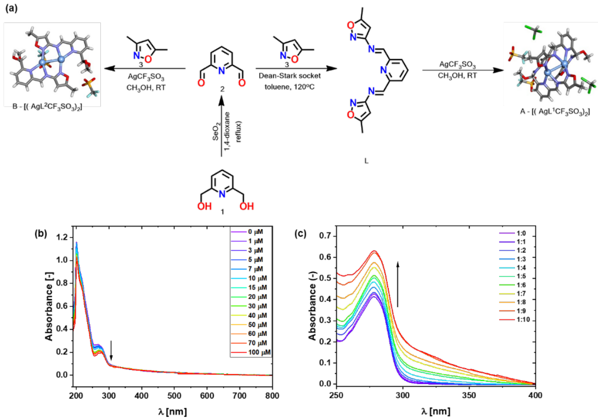

Figure 1. (a) The schematic presentation of the synthetic pathways of ligand L and silver(I) complexes of A and B. Absorption spectra of complex A in the presence of increasing concentrations of (b) CT-DNA (0-100 μM) and (c) BSA (0-100 μM).

This work was supported by IDUB-UAM "PhD Minigrants"

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EXPANDING THE FRONTIERS OF MULTIFUNCTIONALITY: LANTHANIDE(III) ION COMPLEXES EXHIBITING MAGNETIC AND LUMINESCENT PROPERTIES

Dawid Marcinkowski[1], Maciej Kubicki[1], Violetta Patroniak[1], Przemysław Woźny[1], Marcin Runowski[1], Robert Podgajny[2], Adam Gorczyński[1]

[1] *Faculty of Chemistry, Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland*
[2] *Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Kraków Poland*
dawid.marcinkowski@amu.edu.pl

The rational design and appropriate modification of molecular architectures are primary steps in the generation of tailor-made advanced multifunctional materials. Materials based on supramolecular approach are readily tunable at the molecular level, and in principle, information programmed into the molecular-scale building blocks can be translated through the nano- and micro-scales up to the macroscopic level [1].

Herein we demonstrate the synthesis and characterization of lanthanide(III) complexes with Schiff base and macrocyclic ligands exhibiting magnetic and high-pressure luminescence properties. In the first part of the study we will demonstrate the extent to which the trityl group can influence the formation of Single Molecule Magnets (SMMs) based on lanthanides and hydrazone ligands that differ with the number of coordination binding pockets [2]. I the second part, we will show two Nd(III) macrocyclic complexes as a multifunctional platform. Detailed magnetic and luminescence studies allow us to obtain first high-pressure barometer based on macrocyclic Nd(III) complex and new field induced Nd(III) Single Ion Magnet, where energy barrier of spin reversal is quite competitive among compounds based on Nd(III), sharing the 20-30 K range with just a few literature examples [3].

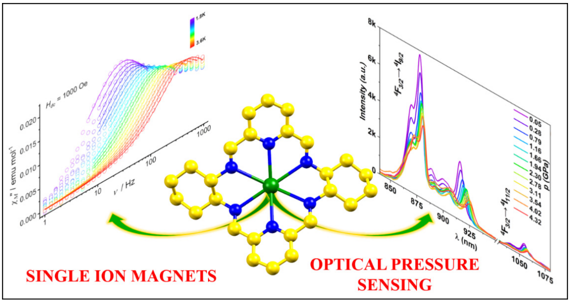

Figure 1. Schematic representation of presented studies.

This work was supported by: PRELUDIUM grant UMO-2022/45/N/ST4/00344 from National Science Centre, Poland and the project "The University of Tomorrow II".

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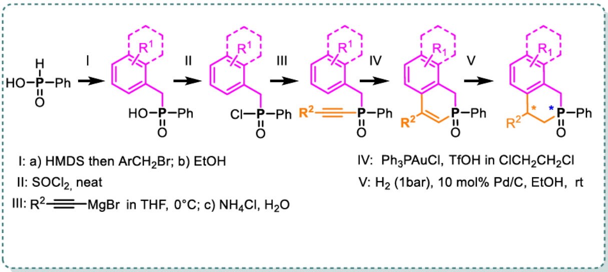
HYDROPHOSPHONYLATION OF COUMARINS AND ISOPHOSPHINOLINE 2-OXIDES

K-P. Mengue Me Ndong*,[a,b], A. R. Issaka Ibrahim*,[a,c] M. Hariri,[a] G. Mwande-Maguene,[b] J. Lebibi,[b] A. T. Ilagouma,[c] T. Ayad,[a] J-L. Pirat,[a] D. Virieuxa

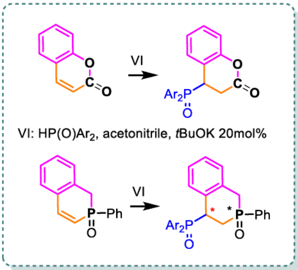
[a] *Institut Charles Gerhardt/UMR 5253/AM2N, ENSC, Montpellier, France*
[b] *Université des Sciences et Techniques de Masuku, Franceville, Gabon*
[c] *Faculté des Sciences, Université Abdou Moumouni, Niamey, Niger*
karen-pacelye.mengue-me-ndong@enscm.fr
abdrachid2i@gmail.com

We developed an efficient synthesis of a new family of compounds, namely isophosphinoline 2-oxides, a six-membered phosphorus heterocycle specifically designed for the discovery of new pharmacophores or building blocks for medicinal chemistry. They were obtained in five steps from cheap Hphenylphosphinic acid using a gold-catalyzed hydroarylation reaction as a key step [1].

In a second time, we explored the reactivity of coumarins and their phosphorus analogues, the isophosphinoline 2-oxides, through Michael additions. These modifications were successful, allowing to modulate the structural features of these heterocycles [2].



I: a) HMDS then $ArCH_2Br$; b) EtOH
II: $SOCl_2$, neat
III: R^2–≡–MgBr in THF, 0°C; c) NH_4Cl, H_2O
IV: Ph_3PAuCl, TfOH in $ClCH_2CH_2Cl$
V: H_2 (1bar), 10 mol% Pd/C, EtOH, rt



VI: $HP(O)Ar_2$, acetonitrile, *t*BuOK 20mol%

Preliminary biological results showed moderate to good activities on different bacterial strains [2].

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POLYAZOMETHINES BASED ON COMPLEXES OF TRANSITION-METAL IONS

Sergiusz Napierała, Maciej Kubicki, Monika Wałęsa-Chorab

Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
sergiusz.napierala@amu.edu.pl

Electrochromic materials have emerged as a promising class of compounds that change their color in response to an electrical stimulus, holding immense potential in various technological application[1]. Among these materials, transition metal complexes have garnered significant attention due to their unique electronic properties and undergoing a reversible redox processes concomitant with the color change[2].

Polycondensation is one of the polymeric complexes obtaining method[3]. To obtain complexes of transition-metals with ability to undergo a polycondensation reaction, ligand **L** was synthesized[4]. The ligand **L** contains unbound amine groups capable to reaction with the appropriate dialdehydes. The transition-metal complexes of ligand **L** and Fe(II) as well as Cu(II) exhibit a reversible redox process and color changes, and were used to synthesize polyazomethines in polycondensation reaction with dialdehydes (fig. 1.). Subsequently, the electrochemical properties of the synthesized complexes were investigated using cyclic voltammetry and other relevant techniques. During research, polymeric complexes containing Fe(II) and Cu(II) were prepared and their electrochromic and electrochemical properties have been investigated.

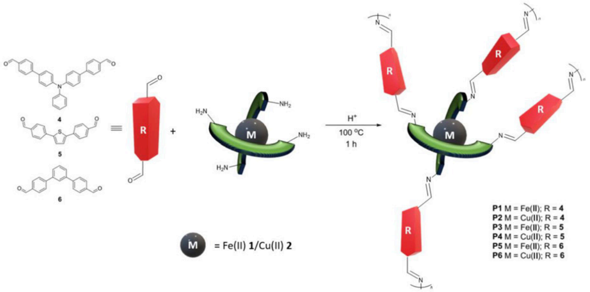

Figure 1. Scheme showing the preparation of transition-metal-complex-based polyazomethines **P1–P6**.

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QUANTIFICATION OF 2,4-DICHLOROPHENOXYACETIC ACID USING IMPRINTED POLYETHYLENEIMINE AS A SELECTIVE ADSORBENT

Tomasz Nazim, Michał Cegłowski

Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
tomnaz@amu.edu.pl

The technique of molecular imprinting has many advantages for adsorption purposes. Molecularly imprinted polymers (MIPs) are promising materials for applications, that rely on adsorption mechanism. The key advantage of MIPs lies in their selectivity, as they can be tailored to adsorb specific target molecules or groups of molecules. This selectivity is achieved through the imprinting process, which creates binding sites in the polymer that are compatible with the target molecule. Additionally, MIPs exhibit remarkable stability, enabling them to withstand harsh chemical and physical conditions, thus expanding their applicability across various domains. Moreover, MIPs are highly reusable, as they can be regenerated and reused multiple times without a significant decline in performance [1-3].

This research work describes the synthesis and adsorption properties of molecularly imprinted polymers based on linear polyethyleneimine. The polymer was functionalized with glycidol to study the effect of the introduced hydroxyl groups on the properties of the molecularly imprinted polymer. The new analytical method was employed to perform quantification of 2,4-dichlorophenoxyacetic acid (2,4-D). The method involves adsorption of 2,4-D from solution and the subsequent analysis of solid materials using ambient plasma mass spectroscopy. Molecular imprinting was conducted using two bisepoxide cross-linkers: 1,4-butanediol diglycidyl ether (BDE) and neopentyl glycol diglycidyl ether (NGDE). The analytical setup proposed demonstrated a significant enhancement in detection limits by 200 times compared to pure solution analysis. Furthermore, excellent recoveries were obtained when quantifying 2,4-D in river water samples. These results serve as strong evidence that the suggested analytical configuration is highly effective for detecting 2,4-D in real water samples.

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THE ROLE OF ACETAZOLAMIDE ACTIVE COMPLEXES WITH IN(III) IONS RELATED TO KINETICS AND MECHANISM OF THE ELECTRODE PROCESS IN THE SURFACTANT PRESENCE; THE „CAP-PAIR" EFFECT

A. Nosal-Wiercińska, M. Martyna, A. Pawlak

Maria Curie-Skłodowska University in Lublin, Pl. Marii Skłodowskiej-Curie 2,20-031 Lublin,
agnieszka.nosal-wiercinska@mail.umcs.pl

Acetazolamide is a drug used in the treatment of glaucoma and epilepsy [1]. Knowledge of the electrochemical properties of drugs is very important for a deeper understanding of their metabolic pathways or 'in vivo' redox processes. There is therefore a need to study the mechanisms of action of drugs and to search for new systems for controlled drug release, which can be used to monitor a patient's condition.

The process of In(III) ions electroreduction in the presence of acetazolamide, hexadecyltrimethylammonium bromide (CTAB) and sodium dodecyl sulphate (SDS) was investigated in terms of the 'cap - pair' effect [2] using an innovative electrode made from a cyclic renewable film of liquid silver amalgam (R-AgLAFE) [2].

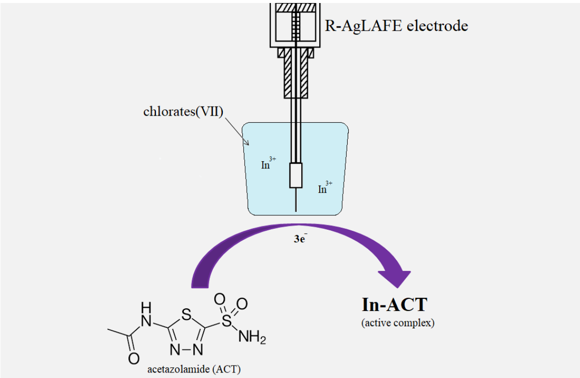

Fig. 1. Scheme of In(III) ions electroreduction in chlorates(VII) including the mediating role of active complexes in the charge (electron) transfer.

The control of the multi-step electroreduction process of In(III) ions was demonstrated through the chemical reaction of the formation of In - ACT active complexes on the electrode surface, which mediate electron transfer. The active complexes are the substrate in the electroreduction process and their different structures and properties are the reason for the varied catalytic activity of acetazolamide. In contrast, the formation of mixed adsorption layers of ACT - CTAB or ACT - SDS changes the dynamics of this process towards inhibition.

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THE APPLICATION OF MACHINE LEARNING METHODS TO THE PREDICTION OF NOVEL LIGANDS FOR RORΓ/RORΓT RECEPTORS

Damian Nowak[1,2], **Rafał Bachorz**[2], **Marcin Ratajewski**[2], **Joanna Pastwinska**[2], **Kaja Karas**[2], **Iwona Karwaciak**[2], **Marcin Hoffmann**[1]

[1]*Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland*
[2]*Institute of Medical Biology of Polish Academy of Sciences, Lodowa 106, 93-232 Lodz, Poland*
damian.nowak@amu.edu.pl

In this work, we have developed and applied a computational procedure for creating and validating predictive models capable of estimating the biological activity of ligands (Fig. 1). The combination of modern machine learning methods, experimental data, and the proper setup of molecular descriptors led to a set of well-performing models. We have thoroughly inspected both the methodological space and various possibilities for creating a chemical feature space.

The resulting models were applied to the virtual screening of the ZINC20 database [1] to identify new, biologically active ligands of RORγ receptors [2, 3], which is a subfamily of nuclear receptors. Based on the known ligands [4] of RORγ, we have selected candidates for which we have calculated the predicted activities with the best-performing models. We have chosen two candidates that were experimentally verified. One of these candidates indeed triggers the biological activity of the RORγ receptors, which we consider proof of the efficiency of the proposed methodology.

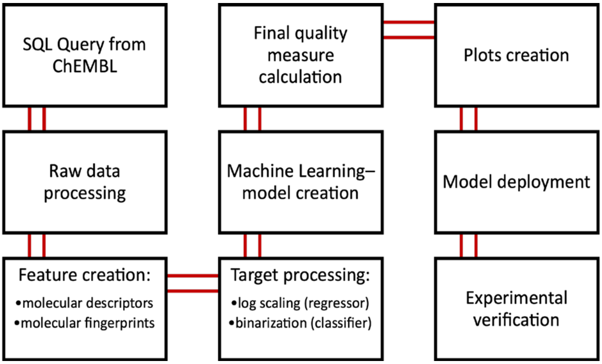

Figure 1. The workflow procedure enables the generation and storage of the best-performing models for regression and classification.

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SYNTHESIS, CHARACTERIZATION, AND CATALYTIC APPLICATION OF HIERARCHICAL ZEOLITES CONTAINING VANADIUM OR TANTALUM IONS

Agnieszka Feliczak-Guzik, Paulina Szczyglewska, Izabela Nowak

Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
nowakiza@edu.pl

Transition metals play a significant role as catalysts in inorganic synthesis. In addition, they are increasingly used in organic catalytic reactions due to their undoubted advantages. Many chemical compounds used in everyday life are produced using them because they are relatively biocompatible. Vanadium and tantalum are attracting increasing scientific attention. This is because vanadium is a relatively non-toxic and inexpensive element, so it plays an important role in biochemistry and medicinal chemistry, and its diversity in coordination chemistry has also led to applications in synthesis and catalysis [1]. Tantalum, on the other hand, is an element very similar to niobium in terms of its physicochemical properties. According to literature reports, tantalum is increasingly used in catalysis. Hence, the aim of our research was the synthesis, characterization, and application of hierarchical materials modified with tantalum and vanadium ions in the epoxidation reaction of cyclohexene.

Hierarchical zeolites are materials characterized by possessing so-called secondary porosity (an additional pore system, usually in the mesopore range, i.e. from 2 to 50 nm), thus allowing reactant molecules to access the active sites of the material while maintaining the acidity and crystallinity of the zeolites. All synthesized materials were characterized by using various techniques, including XRD, TEM, SEM, and low-temperature nitrogen adsorption/desorption isotherms, and applied to the cyclohexene epoxidation reaction. Based on the results, the systems were found to have high activity and selectivity in the aforementioned reaction, which was carried out by two methods: conventional and microwave-assisted. The microwave method did not affect the acceleration of the cyclohexene epoxidation process - the cyclohexene conversion results obtained were comparable. The vanadium-containing catalysts showed slightly higher catalytic activity compared to the tantalum catalysts. In turn, the tantalum-modified catalyst was more selective toward the production of cis-1,2-cyclohexanediol. These results confirm that hierarchical FAU zeolite materials containing vanadium or tantalum ions are potentially interesting catalysts for epoxide rearrangement reactions.

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ANGELICA L. COUMARINS POTENTIAL TO MODULATE GLUCOSE-INDUCED INSULIN SECRETION AND THEIR MECHANISM OF ACTION

Andrzej Patyra [1,2,3], Soufiyan Omhmmed[1], Justine Vaillé[1], Sylvie Péraldi-Roux[1] , Jean-François Quignard JF [4] , Anna Kiss[2] , Jérémie Neasta[1] , Catherine Oiry[1]

[1] *Institut des Biomolécules Max Mousseron, Université de Montpellier, CNRS, ENSCM, Montpellier, France*
[2] *Department of Pharmaceutical Biology, Medical University of Warsaw, Warsaw, Poland*
[3] *Doctoral School, Medical University of Warsaw, Warsaw, Poland*
[4] *Université de Bordeaux, Centre de Recherche Cardio-Thoracique de Bordeaux, INSERM U1045, Pessac, France*
catherine.oiry-cuq@umontpellier.fr

Pancreatic β-cell function and notably glucose-induced insulin secretion play a pivotal role in glucose homeostasis. We have previously shown that natural molecules like flavonoids or ellagitannin metabolites potentiate glucose-induced insulin secretion through a mechanism implicating the activation of L-type Ca^{2+} (CaV) channels and ERK 1/2 [1-3]. According to some studies, extracts from Angelica L. species shown similar effects on insulin secretion [4-5]. Thus, this study aimed at isolating and studying active constituents of three pharmacopeial Angelica roots.

Twenty-two coumarins were isolated from the roots of Angelica archangelica L., Angelica dahurica (Hoffm.) Benth. & Hook.f. ex Franch. & Sav., and Angelica pubescens Maxim through Soxhlet extraction in n-hexane, and column and preparative chromatography methods. The structure of the compounds was analyzed and confirmed using UHPLC-DAD-MS and NMR methods. Pharmacological experiments were performed on the INS-1 β-cell line. Insulin release was quantified by the homogeneous time-resolved fluorescence method. The mechanism of action was studied using patch clamp and fluorescence microscopy techniques.

Some of the studied compounds were able to modulate glucose-induced insulin secretion acting on the membrane potential, as well as by activating voltage-gated calcium channels and increasing intracellular calcium concentrations. Overall, the results demonstrate a new pharmacological activity of coumarins present in traditionally used Angelica roots.

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AMINO ACIDS WITH TRIFLUOROMETHYLATED OLEFINIC MOTIF

Karolina Paszek, Katarzyna Koroniak-Szejn, Henryk Koroniak

Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
karolina.paszek@amu.edu.pl

Chemical modifications of peptides to improve their biological activity, *in vivo* stability or bioavailability have been studied extensively [1]. Recently, a lot of attention has been focused on the synthesis of fluorinated pharmaceuticals, which have a variety of biological activity depending on the amount and type of fluorinated substituent in the molecule. The incorporation of fluorine into amino acids and peptides established a completely new class of compounds and their applications in design of new peptidomimetics [2].

Herein, we present the synthesis of modified amino acid with a trifluoromethyl group based on a typical modification of *L*,α-amino acids performed by a nucleophilic trifluoromethylation reaction using the Ruppert-Prakash reagent ($TMSCF_3$). Our main focus is the synthesis of analogues of amino acids bearing trifluorometylated olefinic moiety. One of the most important structural properties of trifluoromethylalkene isosteres is the reproduction of β - turn structure of the original peptide [3]. Replacement of peptide bonds with non-hydrolyzable mimetic is one of the most promising approaches toward overcoming the major drawbacks of peptides by displaying higher metabolic stability, good bioavailability and enhanced receptor affinity and selectivity [4].

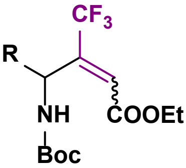

Figure 1. Fluorinated amino acids derivatives with olefinic moiety.

We thank National Science Centre Poland (NCN, grant HARMONIA 2017/26/M/ST5/00437), The Excellence Initiative – Research University (IDUB UAM, Minigrant doktorancki 054/13/SNŚ/0042) and Project "The University of Tomorrow II" POWR.03.05.00-00-Z303/18 for financial support.

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CHITIN-BASED POROUS BIOCARBONS FOR EFFICIENT ADSORPTION OF LIQUID CONTAMINANTS

Aleksandra Bazan-Wozniak, Robert Pietrzak

Adam Mickiewicz University Poznań, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
pietrob@amu.edu.pl

The main aim of the study presented was to obtain biocarbons by chemical and physical activation of empty shells (casings) of pupae of *Hermetia illucens* fly. The obtained biocarbons were characterized by determination of their physicochemical and sorption capacities towards methylene blue. The impact of a number of experimental parameters, including: mass of biocarbon sample, speed of shaking of adsorbent/adsorbate system, time of adsorbent/adsorbate contact, dye concentration and pH of the dye solution, on the effectiveness of the dye removal, was checked. Thermodynamics of the process of sorption was analyzed to assess the practical suitability of the obtained adsorbents for adsorption of dye from wastewater. The possibility of reuse of the biocarbon adsorbents was checked by characterization of the dye desorption.

The adsorbents were found competent for removal of methylene blue from its water solution, economically favorable and characterized by high sorption capacity, in particular the sample activated with potassium carbonate. The most effective adsorbent, obtained by activation with potassium carbonate, was characterized by the specific surface area of 1167 m^2/g and its sorption capacity towards methylene blue was 641 mg/g. The model best describing the process of adsorption on the adsorbents studied was that of Langmuir isotherm. The process of dye removal was described by the pseudo- second order model, which indicates that chemisorption took place between the adsorbent and adsorbate. The methylene blue adsorption on the biocarbons studied was endothermic and spontaneous. An increase in pH of the initial dye solution above pH_{pzc} of carbon, led to an increase in the sorption capacity. The highest efficiency of desorption was obtained for 0.5 mol/L of HCl, while the lowest for NaCl solution and distilled water. Higher efficiency of desorption in HCl is mainly a consequence of better solubility of methylene blue in this eluent and its polarity higher than that of the other ones. In future the stability of the studied adsorbents and the possibility of their reuse should be tested in actual wastewater.

THE UNEXPLORED POTENTIAL OF FRESHWATER ALGAE. STEPWISE EXTRACTION WITH SEPARATION OF SEVERAL GROUPS OF CHEMICAL COMPOUNDS AND THEIR ANALYSIS

Zuzanna Piotrowicz, Łukasz Tabisz, Bogusława Łęska, Radosław Pankiewicz

Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
zuzanna.piotrowicz@amu.edu.pl

Algae are a well-known and widely used source of active and nutritional compounds, as well as raw stock for biofuels. However, when we talk about algae as a raw material, we usually mean marine algae. Meanwhile in many European countries freshwater algae occupy inland reservoirs, and this significant biomass can also potentially be used in similar applications. As we found out, our domestic freshwater algae are an equally good source of active ingredients as some marine species. A stepwise extraction process developed by us allowed for the separation of individual fractions of active compounds for further analysis. The use of solvents of different polarity (hexane, ethanol and water) enabled the isolation of several different groups of active compounds contained in algae, such as lipids and carotenoids, polyphenols and polar dyes, and sulphated polysaccharides. Lipids for example can be used as a raw material for the production of biodiesel. Particular emphasis was placed on the analysis of phenolic fractions, which have not only antioxidant properties, but also may yield important information about conditions in the habitat. As polyphenols are secreted by algae as a result of various types of environmental stress, their concentration both in the thallus itself and in the waters surrounding the mats can be used for ecological monitoring.

The use of complementary, semi-quantitative colorimetric methods enables the creation of a simplified profile of antioxidant compounds, including phenolic compounds. In addition, the analysis of the lipid fraction allows to supplement the profile with the content of carotenoids and to estimate what part of the non-polar fraction are fat-soluble vitamins. Sulphated polysaccharides, isolated for the first time from freshwater species by our team, can be used in the pharmaceutical, food and cosmetic industries.

Research was carried out thanks to the financial support of the National Science Center grant number 2018/31/B/NZ8/00280.

LIGNOSULFONATE-ASSISTED IN SITU DEPOSITION OF PALLADIUM NANOPARTICLES ON CARBON NANOTUBES FOR THE ELECTROCATALYTIC SENSING OF HYDRAZINE

Patrycja Płócienniczak, Tomasz Rębiś, Amanda Leda, Grzegorz Milczarek

Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
patrycja.plocienniczak@amu.edu.pl

Hydrazine (N_2H_4) is a significant chemical compound with high reactivity and strong reducing properties. It finds extensive use in fuel cells, antioxidant production, as well as in the synthesis of pesticides, herbicides and pharmaceutical products. It is also used in the photographic industry [1-3]. Due to its widespread and commercial use, hydrazine and its derivatives are frequently detected in the environment, which can pose a significant threat to living organisms. Hydrazine has been found to be highly neurotoxic, carcinogenic, and mutagenic. Due to the rising consumption of hydrazine, it is essential to implement effective procedures for the detection of hydrazine in the environment using simple and sensitive analytical techniques.

To overcome this problem, electrodes modified with various noble metal nanoparticles (NMNPs) should be considered. NMNP-electrodes exhibit distinctive characteristics, including enlarged surface area and enhanced mass transport, resulting in significant electrocatalytic activity [4,5]. The detection of N_2H_4 through electrochemistry seems to show promising results when using palladium-based electrodes. Palladium nanoparticles (NPd) diminish the oxidation potential of hydrazine and facilitate dinitrogen formation [6].

This study proposes a straightforward and eco-friendly technique to prepare a N_2H_4 sensor based on the in situ NPds electro-reduction on the surface of lignosulfonate-coated multi-walled carbon nanotubes. This hybrid material demonstrates potent electrocatalytic properties for hydrazine oxidation, i.e. excellent activity and high sensitivity of 0.166 $\mu A\ \mu M^{-1}\ cm^{-2}$.

The findings of this study and the knowledge gained on coordination chemistry and transition metal complexes will be applied in a NCN research project Sonata 16 UMO-2020/39/D/ST4/01182 "*Multifunctional character of copper(II) macrocyclic complexes – utilization in atom transfer radical polymerization (ATRP) and molecular nanomagnetism (MNM)*", led by Adam Gorczyński, PhD.

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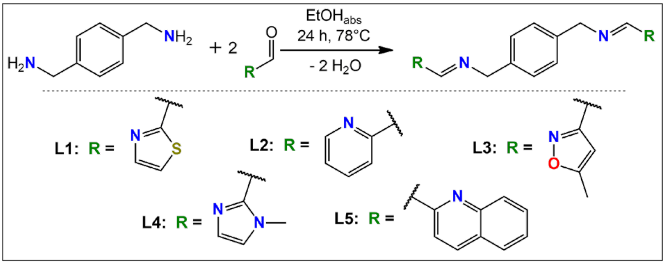
NEW N4-DONOR LIGANDS AS SUPRAMOLECULAR GUESTS FOR DNA AND RNA

Izabela Pospieszna-Markiewicz, Marta Fik-Jaskółka, Ernest Ewert, Violetta Patroniak

Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
izap@edu.pl

Coordination polymers are a particular type of coordination compound, which includes a class of materials consisting of metal ions and organic linkers (Schiff base ligands) connected together with coordination bonds. Schiff base chemistry is shown to be useful in the synthesis of covalent organic frameworks and other nano- and microstructures. Due to their many advantages, e.g., vast diversity and facility of synthesis, they have found numerous applications, especially in the currently developing areas of research, such as catalysis, gas storage and separation, magnetism, nonlinear optics, desalination, etc. If designed appropriately, i.e., using ions of metals endowed with low toxicity, coordination polymers can be used for biomedical purposes, including drug delivery, bioimaging, or biosensing. Some of these materials may exert antimicrobial activities, and their mechanisms of action may vary. For instance, they can be based on ions that have antibacterial properties, such as Ag(I) or Cu(II), whose release follows slow polymer degradation. Another way of eradicating microorganisms is to generate reactive oxygen species or hydrogen peroxide via photocatalysis, which occurs with some metal-organic frameworks based on Zn(II) ions and 2-methylimidazole ligands [1].

We reports the synthesis of different Schiff base N4-donor compounds carrying p-xylyl spacers in their structure. In more detail we obtained Schiff base ligands (Scheme 1) (**L1-L5**). Ligand **L1** was used as an organic linker in coordination polymers containing Cu(I) (**Polymer1**) and Ag(I) (**Polymer2**) ions.



Scheme 1. *Synthesis of ligands L1–L5 with molecular representations of all derivatives including the respective R moieties.*

Subsequently evaluated for their ability to interact with two models of nucleic acids: calf-thymus DNA (CT-DNA) and the RNA from yeast Saccharomyces cerevisiae (simply indicated as RNA). In order to determine whether ligands interact with the DNA helix, a spectrophotometric titration was performed in our study. The method consists of measuring the UV absorbance of the ligands after each of the subsequent portions of CT-DNA (calf thymus DNA) is added . The mechanisms of action of many bioactive compounds depend on their binding with DNA; hence, determining the interaction between the molecules and DNA is crucial for understanding, at a molecular level, the origin of their possible therapeutic effects. Chemical compounds may interact with DNA variously—via covalent bonding, intercalation between base pairs, electrostatic, interactions with the phosphate-rich backbone, or binding to either minor or major grooves [2].

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DESIGN OF MULTIFUNCTIONAL LANTHANIDE BASED SUPRAMOLECULAR SYSTEMS

Dominika Prętka, Dawid Marcinkowski, Maciej Kubicki, Violetta Patroniak, Adam Gorczyński

Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
dominika.pretka@amu.edu.pl

The facility to control the nature and crystal structures of molecular architectures still remains one of the most important aspects in the search for new supramolecular systems with specific properties, especially when it comes to design multifunctional systems, which can be applied to many areas of science. Important factors influencing creation of finals assemblies involve external variables used during synthesis such as reaction conditions, temperature, concentration, solvent, stoichiometry, pH, etc, as well as choice of specific building blocks and metal ions to the forming compounds having regard to size and shape, steric effect, coordination sphere [1], the presence of different intermolecular forces like hydrogen bonds, metal-ligand interactions or other weak non-covalent interactions e.g. electrostatic, van der Waals electrostatic and π-interactions [2-5], that have a direct impact of their related multifunctional properties resulting from their possibilities to present rich structural diversity.

In the present project we synthesized a series of lanthanide(III) complexes, which were structurally characterized and examined by a variety of coordination modes around the Ln(III) centres as the result of utilization of the appropriate counterions, lanthanide ions, ligands molecules or reaction conditions with the aim of better understanding how slight structural changes influence tuning of desired properties.

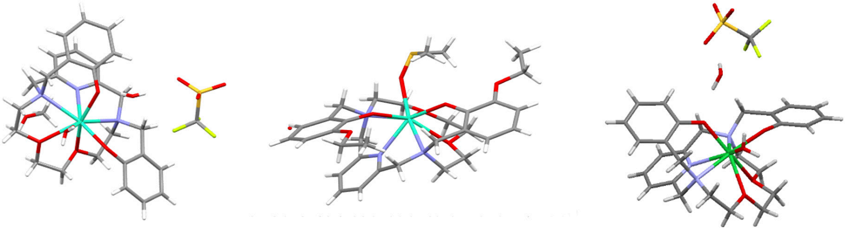

Figure 1. Crystal structures of obtained lanthanide(III) metal complexes.

This work was supported by (PI: AG): SONATA grant UMO-2020/39/D/ST4/01182 from National Science Centre, Poland

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NEGISHI CROSS-COUPLING REACTION CATALYZED BY SIMPLE COBALT-CONTAINING CATALYTIC SYSTEM

Jakub Robaszkiewicz[1], **Maciej Zaranek**[1, 2], **Piotr Pawluć**[1, 2]

[1]*Faculty of Chemistry, Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland*
[2]*Center of Advanced Technologies, Adam Mickiewicz University, Uniwersytetu Poznańskiego 10, 61-614 Poznań, Poland*
jrobaszkiewicz@amu.edu.pl

Transition metal-catalyzed cross-coupling is widely applied method for the synthesis of pharmaceuticals, agrochemicals, and fine chemicals[1]. In the Suzuki cross-coupling reaction, boronic compounds are used, which takes advantage of stability of organoboron molecules compared to eg. organolithium or organotin species used in Murahashi and Stille cross-coupling. Furthermore, organotin compounds are associated with high toxicity, mutagenic and cancerogenic effects. The great advantage of organozinc reagents used in Negishi cross-coupling is that they have the ability to provide fast transmetalation. The most common catalytic systems of these transformations are based on precatalysts that contain platinum-group metals (PGM) and often require the addition of ligands. However, they do not comply with the principles of Green Chemistry because of their high price and possible leaching into the reaction causing impurities in the product. The huge impact in modern organometallic chemistry of 3-d metal complexes such as of iron, nickel, and cobalt is observed. First-row transition metals, in comparison to PGMs, are considerably cheaper and they are less toxic, which is important for medical purposes. There are numerous articles containing palladium and nickel catalysts in Negishi reactions but only a few with cobalt species [2][3].

This poster is going to show our work on the Negishi cross-coupling of benzylzinc bromide with aryl iodides catalyzed by a simple cobalt salt. Aryl iodides and benzylzinc bromide were used as the substrates without any additives to give 15 products with good yields and selectivity of 95%.

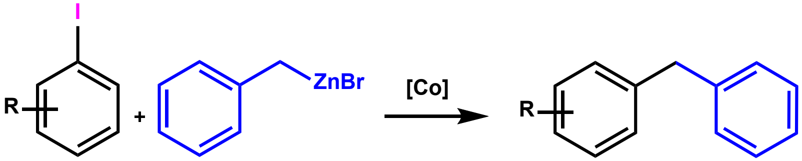

Figure 1. Model reaction system of Negishi cross-coupling.

Acknowledgments
This work was supported by National Science Centre (Poland), Grant no. UMO-2019/35/B/ST4/00329.

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PIANO-STOOL FE(II)/RU(II) CARBONYL COMPLEXES BEARING MALEIMIDATO, PHOSPHINE OR PHOSPHITE LIGANDS: SYNTHESIS, CHARACTERIZATION, AND CYTOTOXICITY WITHIN LIVING CELLS

Bogna Rudolf[a], Sujoy Das,[a] Aneta Kosińska,[a] Kinga Wzgarda-Raj,[b] Agnieszka Rybarczyk-Pirek,[b] Michał Juszczak,[c] Magdalena Kluska,[c] Katarzyna Woźniak,[c]

[a]*Department of Organic Chemistry, Faculty of Chemistry, University of Lodz, 91-403 Lodz, Poland.*
[b]*Department of Physical Chemistry, Faculty of Chemistry, University of Lodz, Pomorska 163/165, 90-236, Lodz, Poland.*
[c]*Department of Molecular Genetics, Faculty of Biology and Environmental Protection, University of Lodz, Pomorska 141/143, 90-236, Lodz, Poland.*
bogna.rudolf@chemia.uni.lodz.pl

In recent times, organometallic complexes containing transition metals like Fe, Ru etc. are being massively investigated for their versatile physico-chemical applications.[1-4] As an example, (η^1-*N*-maleimidato) metallocarbonyl compounds have been found to be efficient biomarkers due to their specific absorption bands in the mid-IR spectral range resulting from the stretching vibrations of carbonyl ligands. Maleimide derivatives are commonly used in bioconjugation processes due to their reactivity towards bio-thiols.[5] The search for an appropriate ligand that effectively controls the stability and reactivity of metal complexes plays an essential role in organometallic chemistry.[6]

Herein, we report a series of (η^5-cyclopentadienyl) $M^{II}(CO)(\eta^1$-maleimidato) complexes (M= Fe, Ru) with alkyl/aryl phosphine or phosphite ligands, their synthesis, characterization, X-ray diffraction analysis followed by their influences in peripheral blood mononuclear (PBM) cells as normal cells and different cancer cell lines like human leukemic, HL-60 and non-small-cell lung cancer cells, A549. Each of reported complexes were synthesized by photolysis, using visible or UV light with a satisfactory yield and purity. NMR (^{1}H, ^{31}P, ^{13}C), FT-IR and ESI-MS spectral study were utilized for their characterization. X-ray diffraction analysis further confirmed the structures of many of them.

To study the genotoxic potential of complexes in cancer cells, we selected those complexes that were the most cytotoxic for these cells and were less cytotoxic for normal PBM cells, comparing IC_{50} doses. We also used the plasmid relaxation assay to determine the potential of these complexes to directly damage DNA.

In the search for new anticancer drugs, selective activity of these complexes towards cancer cells and lack of effect on normal cells are of key importance. For this reason, iron(II) and ruthenium(II) complexes described here are expected to open new ways for anticancer research.

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HIGHLY SELECTIVE SYNTHESIS OF SILOXANES CATALYZED BY COBALT COMPLEXES

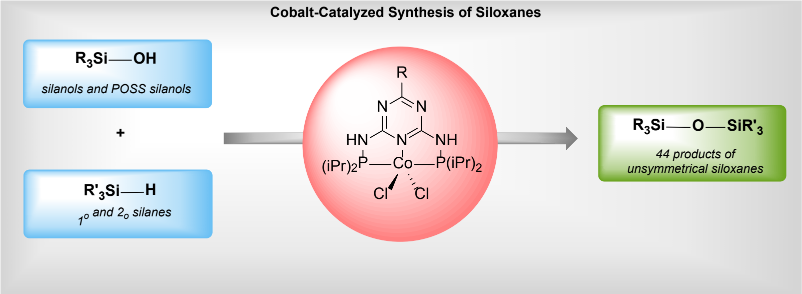
Ewelina Szafoni, Grzegorz Hreczycho

Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
ewesza1@amu.edu.pl

Siloxane motifs -Si-O-Si- are ubiquitous building blocks in chemical synthesis and industry. They are highly valued for their unique properties, being used in a myriad of different fields including medicine, cosmetology, the textile industry, etc.

Siloxanes can be accessed via well-developed stoichiometric methods, mainly by the use of chlorosilanes. Therefore, in recent years, there have been extensive investigations on other methods proceeding via catalytic cross-coupling reactions between silanols with different silylating agents. Silylation processes based on transition metal catalysts are well known, but due to the high costs of catalysts used in these reactions, this method is not economical. Other routes of siloxane synthesis have many disadvantages that reduce the attractiveness of these methods. Currently, due to green and sustainable chemistry, catalytic processes are based on cheap, naturally abundant metal catalysts. They show high selectivity and very low toxicity, which means that they are used in homogeneous catalysis. Catalytic systems based on pincer ligands are very popular among researchers. Cobalt catalysts based on a triazine ring skeleton show high activity even under mild conditions and at low concentrations.(1,2)

In this communication, we report dehydrogenative coupling reactions between hydrosilanes and silanols using the PN5P cobalt pincer complex. It is a very efficient method because it does not require harsh conditions and the use of additional pre-catalyst activators, which makes it a sustainable alternative to other catalytic and traditional methods.(3)



Scheme 1: Reaction of silanes with silanols using a cobalt complex.

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THE IMPACT OF NITROGEN HETEROATOMS ON PORE DEVELOPMENT AND CO2 SORPTION CAPACITY OF ACTIVATED CARBONS DERIVED FROM FURFURYL ALCOHOL

Agnieszka Kałamaga, Rafał J. Wróbel

West Pomeranian University of Technology in Szczecin, Faculty of Chemical Technology and Engineering, Department of Catalytic and Sorbent Materials Engineering, Piastów Ave. 42, 71-065 Szczecin, Poland
rafal.wrobel@zut.edu.pl

The purpose of this research is to study the impact of nitrogen heteroatoms on the pore development of activated carbons applied in CO2 adsorption.

The typical cheap carbonaceous material precursors exhibit drawbacks such as mineral matter and inhomogeneous porosity. In order to avoid the impact of the mineral matter and natural origin pores on the porosity development, ultra-pure activated carbons were prepared from furfuryl alcohol via 3 step synthesis. Firstly, furfuryl alcohol was polymerized to polyfurfuryl alcohol. Subsequently, the polymer was subjected to the carbonization at 600oC for 4 h under the following atmospheres: N2, NH3 and NH3/air (ratio 3:2). Afterwards, obtained carbons were activated under CO2 atmosphere at 1000oC from 1 h to 3 h.

The high purity of obtained carbons was confirmed by X-ray photoelectron spectroscopy (XPS). Deconvolution of N 1s, O 1s and C 1s signals allowed to determine the functional groups on the surface of activated carbons. The highest concentration of nitrogen achieved material after carbonization under NH3/air atmosphere amounting 25 at. %.

Sorption capacities of CO2 were determined at 30oC and at atmospheric pressure using the thermobalance (TGA) in temperature swing adsorption (TSA). The highest CO2 uptake (2.3 mmol/g at 30oC) reached activated carbon after carbonization under N2 carbonization and activated for 2 h. On the other hand, the lowest CO2 adsorption achieved material after carbonization under NH3/air atmosphere and activated for 3 h (0.3 mmol/g at 30oC).

Based on the N2 adsorption/desorption isotherms (BET) it can be observed that the porosity of activated carbons decreases with the increase of the nitrogen concentration. The adsorption of CO2 at 0oC confirms that the volume of pores lower that 1 nm (crucial for high CO2 uptake) also decreases, which negatively affects the CO2 adsorption.

Presented results are useful in activated carbons preparation, especially for CO2 adsorption.

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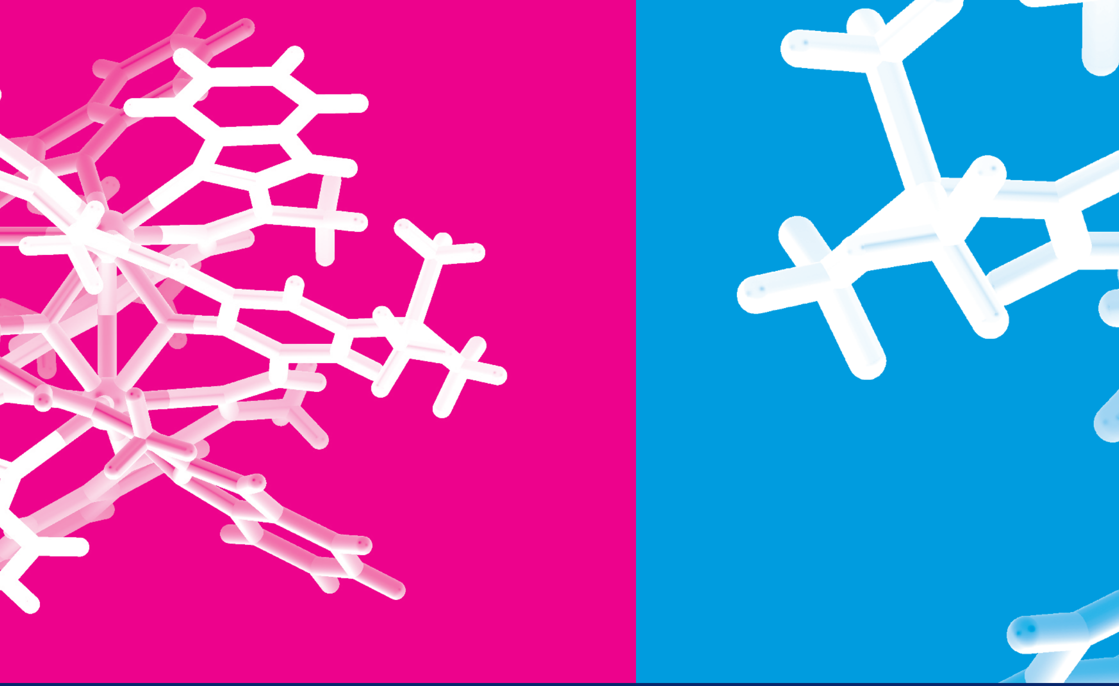

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National Superior School of Chemistry Montpellier
École nationale supérieure de chimie de Montpellier
240 Av. du Professeur Emile Jeanbrau, 34090 Montpellier, France