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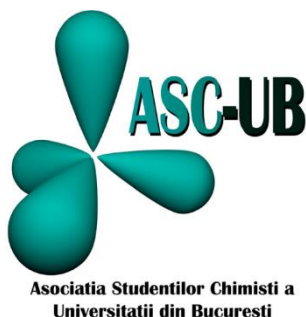
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Content

Section 1 - Bachelor Level	6
Alexandra Georgiana Bălan & Andreea Soc, Mădălina Elena Moisă - <i>Site-specific immobilization of phenylalanine ammonia-lyase from Arabidopsis thaliana</i>	7
Maria Alexandra Bălan, Adina Răducan- <i>Enzymatic Degradation of Epirubicin</i>	8
Claudiu Andrei Crîmpîță, Petruța Oancea - <i>Photochemical degradation of Safranin</i>	9
Stefan Dimitriu, Marius Andruh - <i>Functionalization of 5-bromosalicylaldehyde as Mannich, Schiff-base, and imino-nitroxide ligands. New Ni(II), Mn(II), and Cu(II) complexes</i>	10
Rareș George Dornea, Ciprian Ionuț Raț - <i>Assessment of the Lewis acidity of organoantimony compounds by theoretical and experimental methods</i>	11
Andrada-Irina Eremia, Nicoleta Sandu, Adela Dobre, Anamaria Hanganu, Codruța Popescu, Mihaela Matache, Anca Păun - <i>Synthesis of 1,3,4-oxadiazole-based thiols for metal ion detection purposes</i>	12
Andrei-Gabriel Grecu, George Costache, Nicoleta Sandu, Marius Lucian Matache, Mihaela Matache - <i>Study of the Influence of Interfering Substances on Glucose Readings of Commercial Glucometers</i>	13
Ana-Maria Luntraru, Marilena Ferbinteanu Cimpoesu - <i>Synthesis and Structural Analysis in a New Series of Mn(III) complexes</i>	14
Adriana-Flavia Lupea, Catalin Salagean, Hani El-Naggar, Monica Baia, Lucian Baia, Cosmin Coteț - <i>Thermally Reduced 3D Graphene Oxide Membranes: Preparation and Characterization</i>	15
Diana Troana, Cristina Matache, Marilena Ferbinteanu Cimpoesu - <i>Syntheses and Crystal Structures of the Metal Complexes Based on Pyrazole-carboxylic Acid Ligands</i>	16
Stefania-Minodora Rujoiu, David Iulia Gabriela - <i>Voltammetric determination of vitamin B6</i>	17
Maria-Mihaela Serban, Cătălin C. Anghel, Niculina Hădade - <i>N-Heterocyclic Carbene-Based [2]Rotaxanes: design and synthesis of the building blocks</i>	18
Daniel Vasile Toderel, Niculina D. Hădade, Alexia M. Frîncu, Ana Maria Cosmeniu - <i>Toward a New Activity-Based Probe: Synthesis and Characterization of an Epoxysuccinyl-based Peptide</i>	19
Maria-Alexandra Cernica, Ana-Maria Brezoiu - <i>Studies on the production of fermented soy products</i>	20
Teodora-Christina Purice, Nicoleta Sandu, George Costache, Anamaria Hanganu, Codruța Popescu, Mihaela Matache - <i>Synthesis of TEMPO-Functionalised Hydrazide Precursor for N-Acylhydrazones</i>	21
Cătălin Turcu, Simona Nica, Marius Andruh - <i>Unleashing the Power of Photoswitchable Ligands: New Cu(II) Complexes with Azo Derivatives of ortho-Vanillin</i>	22
Valentin L. Virgil, Augustin M. Mădălan - <i>Luminescent molecular materials based on chalcones</i>	23
Andreea-Diana Zamfirescu, Marilena Ferbinteanu Cimpoesu - <i>Synthesis and Structural Particularities of d-f Ionic Complexes</i>	24

Section 2- Master Level	25
Cosmina Bohan , Alexandra Pop - <i>Synthesis, structural characterization and reactivity of organoselenium ligands</i>	26
Robert I. Botea , Augustin M. Mădălan - <i>Mono- and binuclear complexes with polydentate imino and amino ligands</i>	27
Marian-Gabriel Gâsnac , Dana-Elena Popa - <i>Voltammetric study of atropine</i>	28
Vlad Penciu , Adrian-Alexandru Someșan - <i>Organotin(IV) compounds with Sn-O-E bonds (E= C, Si)</i>	29
Section 3 - PhD Level	30
Cătălina-Diana Cristea , Toboc A, Stan C, David V - <i>Development of a detection method for some oligopeptides forbidden in doping control</i>	31
Giuseppe Stoian , Elena Toma, Bogdan Cojocaru, Madalina Tudorache, Joanna Gościańska, Simona Coman - <i>CQD@ZnO heterostructures with enhanced photocatalytic properties</i>	32

Section 1- Bachelor Level

Site-specific immobilization of phenylalanine ammonia-lyase from *Arabidopsis thaliana*

Alexandra Georgiana Bălan & Andreea Soc, Mădălina Elena Moisă

Babeş-Bolyai University, Faculty of Chemistry and Chemical Engineering, 11 Arany Janos, 400028, Cluj-Napoca, Romania

The development of synthetic processes based on biotransformation has advanced significantly in recent years. Rather than using hazardous chemicals, enzymatic processes offer exceptional chemo-, regio- and enantioselectivity and efficiency. Enzymes can replace traditional catalysts in a biocompatible, biodegradable, cost-effective beneficial way, making a substantial contribution to the development of environmentally benign and sustainable chemical/biotechnological production processes.

One of the main challenges in using enzymes in synthesis is their rather low operational stability, which nonetheless can be considerably increased through enzyme immobilization. By doing so, the catalyst can be easily removed from the reaction mixture, thus facilitating its reuse in additional reaction cycles. To achieve high stability while maintaining the biocatalytic activity, high efficiency has been shown through site-specific enzyme immobilization, generally requiring protein engineering.

Maleimide/thiol coupling of engineered enzymes with cysteine residues introduced at specific positions on the enzyme surface to maleimide-functionalized supports is a straightforward, adaptable, and effective method for site-specific enzyme immobilization. This method produces highly stable and functional biocatalysts.

It is already well known that phenylalanine ammonia-lyases (PALs), which naturally catalyse the non-oxidative deamination of L-phenylalanine to *trans*-cinnamic acid, are effective biocatalysts for the synthesis of both D- and L-phenylalanine derivatives [2], important building blocks in both medicinal and synthetic chemistry. In the recent biotransformation of various substituted phenylalanine and *trans*-cinnamic acid analogues, PAL from *Arabidopsis thaliana* (*At*PAL) outperformed the well-researched PAL from *Petroselinum crispum* [3].

Motivated by the prior successful site-specific immobilization of *Pc*PAL [4] and considering the high similarity between *Pc*PAL and *At*PAL, we concentrated our research on developing the site-specific immobilization of *At*PAL through maleimide/thiol coupling, having the ultimate goal to create effective procedures for the synthesis of optically pure phenylalanine derivatives.

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Enzymatic Degradation of Epirubicin

Maria Alexandra Bălan, Adina Răducan

*University of Bucharest, Faculty of Chemistry, Bulevardul Regina
Elisabeta 4-12, Bucharest, 030018, Romania*

Epirubicin is an anthracycline drug used in combination with other medications to treat breast cancer in patients who have had tumor removal surgery. As a consequence of increasing cases of breast cancer worldwide, a significant amount of anthracyclines are present in aquatic environment, where they can have negative effects on any living organism, including cytotoxicity, genotoxicity, mutagenicity, teratogenicity, and endocrine disruption. Therefore, it is essential to find effective methods for their degradation in order to keep them out of the environment. The employment of specific enzymes is one of the advanced oxidation methods (AOPs) being investigated to remove pharmaceuticals from wastewaters. In the presence of hydrogen peroxide as cosubstrate, horseradish peroxidase (HRP) is utilized to remove a large number of phenolic compounds. The degradation of epirubicin in the presence of HRP and hydrogen peroxide was studied in an unbuffered medium, using a spectrophotometric method (monitoring absorbance at $\lambda_{\max}=480$ nm in time) at different initial concentrations of all components. The kinetic parameters according to a simple Michaelis-Menten model were estimated, showing that HRP has a high affinity for epirubicin. Moreover, the operational inactivation constant of HRP is smaller than the values obtained for other substrates, emphasizing that the method could be applied for removal of anthracyclines from wastewaters.

Photochemical degradation of Safranin

Claudiu Andrei Crîmpitã, Petruța Oancea

*University of Bucharest, Faculty of Chemistry, Bulevardul Regina
Elisabeta 4-12, Bucharest, 030018, Romania*

Azine-type dye, Safranin, is commonly used in various fields of applications like microbiology, histology, and food industry. However, its wide use also raises concerns about environmental pollution and potential health risks. One of the ways to address these issues is to develop efficient and sustainable methods for the degradation of safranin.

In this study, we investigated its photochemical degradation by homogeneous advanced oxidation processes in the presence of hydrogen peroxide (H_2O_2), persulfate ($\text{S}_2\text{O}_8^{2-}$) and non-iron Fenton process. The photodegradation experiments were carried out in a laboratory scale UV reactor using a low-pressure mercury lamp which emits at $\lambda = 254$ nm. For Visible range was used medium-pressure mercury lamp with power 250 W. The reaction was followed spectrophotometrically, by monitoring the variation of Safranin absorbance in time at 518 nm and 276 nm, respectively. The absorption spectra showed the formation of an intermediate and the presence of isosbestic points. By comparing the rate constants of each set of measurements, we were able to reach a conclusion regarding the method that proved to be the most efficient in terms of photodegradation. Using a first-order kinetics approach, we evaluated the degradation rate of Safranin. In order to establish the optimal operating conditions, was also studied the influence of different parameters (the pH of the medium, the initial concentration of copper salt, ferrous ion, persulfate, hydrogen peroxide) on the rate constants and the best results were obtained by the UV/ $\text{S}_2\text{O}_8^{2-}$ system.

These degradation systems tend to be clean, cost-effective, and efficient processes for the removal of several types of dyes from wastewater.

Functionalization of 5-bromosalicylaldehyde as Mannich, Schiff-base, and imino-nitroxide ligands. New Ni(II), Mn(II), and Cu(II) complexes

Stefan Dimitriu,^{a,b} Marius Andruh^{a,b,c}

^a *University of Bucharest, Faculty of Chemistry, Regina Elisabeta Blvd. 4-12, Bucharest, Romania*

^b *"C. D. Nenitzescu" Institute of Organic and Supramolecular Chemistry, of the Romanian academy, Splaiul Independenței nr. 202B, Bucharest, Romania*

^c *Scientific supervisor*

5-bromosalicylaldehyde is known to form a wide range of ligands, using Mannich and Schiff reactions [1]. In this work, several coordination compounds were synthesized, based on two successive functionalizations of 5-bromosalicylaldehyde. At first, Mannich reactions were performed, using N-methylpiperazine, piperazine and tris[2-(methylamino)ethyl] amine. The new ligands and the intermediates have been characterized by NMR spectroscopy and mass spectrometry. For one ligand the crystal structure has been solved. Further, the formyl groups were converted into either imino-nitroxide free stable radical moieties or Schiff bases. Complexes of both simple and functionalized Mannich products were obtained, using Ni(II), Mn(II), and Cu(II) metal ions. Their structures were determined using single-crystal X-ray diffraction measurements.

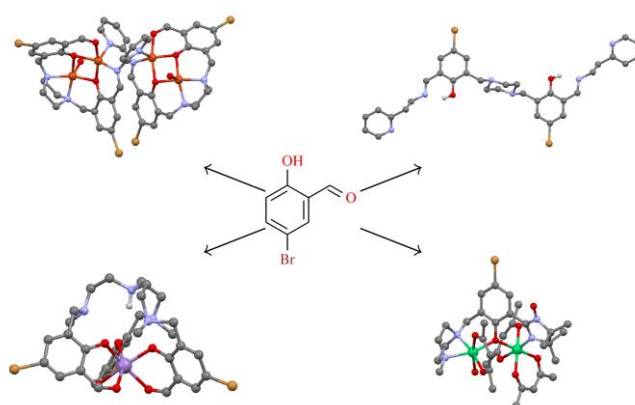


Figure 1: Crystal structure of a Schiff base and three coordination compounds containing 3d metal ions, obtained starting from 5-bromosalicylaldehyde (hydrogen atoms bonded to carbon and fluorine atoms were omitted for clarity)

Acknowledgements: S. D. is grateful to Dr. Constantin Drăghici, and Ph.D. students Andrei Pătrașcu, Cristian Spînu, and Mihai Răducă for their help.

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Assessment of the Lewis acidity of organoantimony compounds by theoretical and experimental methods

Rareș George Dornea, Ciprian Ionuț Raț

Babeș-Bolyai University, Faculty of Chemistry and Chemical Engineering, Center of Supramolecular Organic and Organometallic Chemistry, 11 Arany Janos, 400028, Cluj-Napoca, Romania

We report the molecular structure determined by X-ray diffraction of the adduct of $\text{PhSbCl}_2(o\text{-O}_2\text{C}_6\text{Cl}_4)$ (**1**) with THF. The synthesis (Figure 1) and spectroscopic characterization of $\mathbf{1}\cdot\text{THF}$ have been previously reported.^[1]

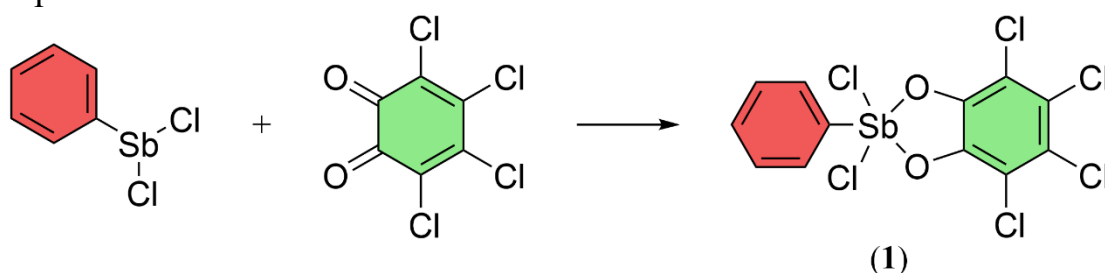


Figure 1. Synthesis of compound **1**.

The Lewis acidity of compound **1** and of the series of organoantimony(V) compounds $\text{R}_n\text{SbCl}_{3-n}(o\text{-O}_2\text{C}_6\text{Cl}_4)$ [$\text{R} = 2\text{-(Me}_2\text{NCH}_2\text{)C}_6\text{H}_4$; $n = 1\text{-}3$] has been evaluated by theoretical methods.^[2] The results have been compared with experimental data of Gutmann-Beckett^[3] and Childs^[4] methods (Figure 2).

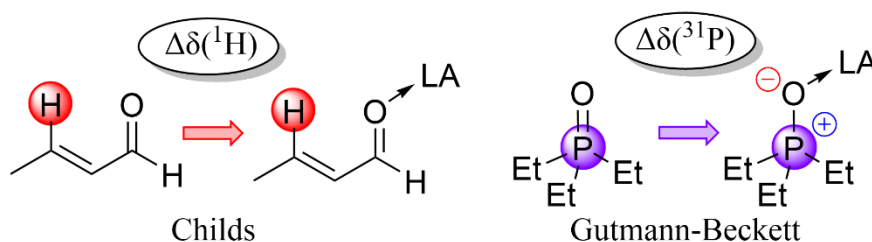


Figure 2. The working principle of the experimental methods (LA = Lewis acid).

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Synthesis of 1,3,4-oxadiazole-based thiols for metal ion detection purposes

Andrada-Irina Eremia,¹ Nicoleta Sandu,¹ Adela Dobre,¹ Anamaria Hanganu,^{1,2} Codruța Popescu,¹ Mihaela Matache,¹ Anca Păun¹

¹*University of Bucharest, Faculty of Chemistry, Department of Inorganic, Organic Chemistry, Biochemistry and Catalysis, 90 Panduri Street, 050657 Bucharest, Romania*

²*Institute of Organic and Supramolecular Chemistry "C. D. Nenitzescu" of the Romanian Academy, 202B Spl. Independenței, 060023 Bucharest, Romania.*

Thiorganic compounds are adaptable ligands capable to coordinate transition metals in a wide range of oxidation state[1]. Compounds bearing the 1,3,4-oxadiazole core, mainly the 2,5-disubstituted ones, have been continuously developed due to their emissive properties, but also due to their ability to act as ligands for various metal ions[2], making them very good candidates to act as sensors for various analytes using luminescent techniques.

Herein, we describe synthesis of a tris-1,3,4-oxadiazolethiol. Preparation of the target compound (Figure 1) started with the esterification of benzene-1,3,5-tricarboxylic acid. The resulted ester was treated with hydrazine hydrate to synthesize the hydrazide and finally, the heterocyclic ring was closed with carbon disulfide to obtain the tris-thiol/thione. All compounds were purified and characterized by physical and spectral analysis (NMR).

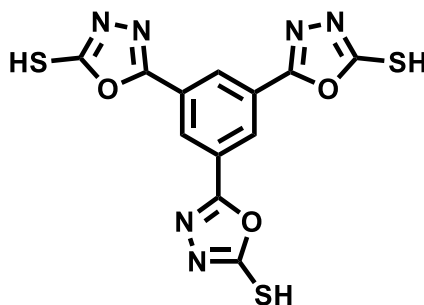


Figure 1. Structure of the tris-thiol, the target compound

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Study of the Influence of Interfering Substances on Glucose Readings of Commercial Glucometers

Andrei-Gabriel Grecu¹, George Costache¹, Nicoleta Sandu¹, Marius Lucian Matache², Mihaela Matache¹

1. Department of Inorganic Chemistry, Organic Chemistry, Biochemistry and Catalysis, Faculty of Chemistry, University of Bucharest, Bucharest, 90 Panduri Street, 050663, Romania

2. Research Centre for Environmental Research and Impact Studies, Faculty of Geography, University of Bucharest, 1 Nicolae Balcescu Blv. Bucharest, 030167, Romania

Herein, we report results obtained during a research training program [1] in which the authors participated. The study aimed to investigate the influence of three interfering substances, namely ascorbic acid, oxalic acid, and mannose on three commercially available glucometers in Romania. The tests were conducted on aqueous buffer glucose solutions along with different interfering substances at physiologically relevant concentrations to establish the influence of these interferents on the final glucometer readings. We found that ascorbic acid displayed a significant interference – up to an approximately 7-fold increase from the reference value, on all tested devices and both oxalic acid and mannose exhibited interference on the devices tested at different concentration ranges.

[1] ReachSci Training Program, www.reachsci.org

Synthesis and Structural Analysis in a New Series of Mn(III) complexes

Ana-Maria Luntraru , Marilena Ferbinteanu Cimpoesu

University of Bucharest, Faculty of Chemistry, Department of Inorganic, Organic Chemistry, Biochemistry and Catalysis, 90-92 Road Panduri, Bucharest 050657, Romania

New Mn(III) complexes are analysed in the frame of the spin-crossover phenomenon (SCO). SCO is a good candidate for new technologies of information processing and storage, being a firm example of bistability, implying a tunable electronic structure transformations change, along with the molecular ground state and all of the displayed optical and magnetic properties. [1]

In this work we report the synthesis, and structural analysis of manganese (III) complex based on pentadentate Schiff Bases. The compounds were synthesised via template condensation reaction between different amine and salicylaldehyde derivatives. From the obtained series complexes, the compound 1D-[Mn(salen)(N₃)] (**1**) and [Mn(sal-N-1,4,7)(N₃)] (**2**) were characterised by single crystal X-ray diffraction. For all compounds spectral and magnetically studies are ongoing.

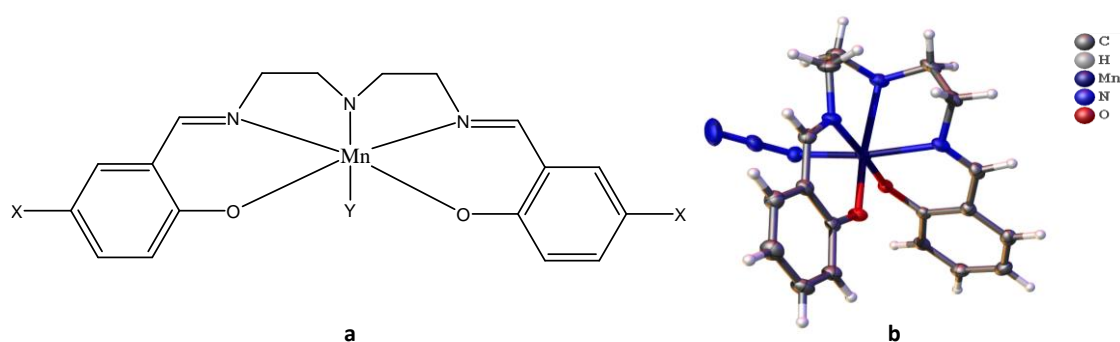


Figure 2. (a) The formula of Mn(III) complexes with pentadentate Schiff Base, X=H, Br and Y=N₃⁻, NCO⁻, NCS⁻, CH₃COO⁻. (b) Asymmetric units for (**2**)

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Thermally Reduced 3D Graphene Oxide Membranes: Preparation and Characterization

Adriana-Flavia Lupea¹, Catalin Salagean², Hani El-Naggar², Monica Baia^{2,3}, Lucian Baia^{2,3}, Cosmin Cotet^{1,3}

¹Babeş-Bolyai University, Faculty of Chemistry and Chemical Engineering, Cluj-Napoca, Romania

²Babeş-Bolyai University, Faculty of Physics, Cluj-Napoca, Romania

³Babeş-Bolyai University, Institute for Research, Development and Innovation in Applied Natural Sciences, Cluj-Napoca, Romania
adriana.lupea@stud.ubbcluj.ro

New materials with improved morpho-structural and technical properties is a demand for supporting the high technological development. In this context, carbon nanomaterials represented by 2D graphene materials [1] including graphene, graphene oxide (GO), reduced graphene oxide (rGO), etc., have been found to present a great potential for use in the construction of cheaper miniaturized devices with a higher degree of technical performance.

In this study, monolithic 3D free-standing GO membranes are obtained using a suspension of 2D GO nanoseets prepared via an innovative sono-chemical oxidation pathway [2]. Subsequently, using an original method carried out in ambient conditions (i.e. not performed by using an inert gas) [3], these electrical insulator materials were thermally reduced (100, 200, and 300°C) to produce rGO membranes. In this way, a reduction in electrical resistivity at about 600Ω/cm was achieved for rGO membrane thermally treated at 300 °C for 10 min. X-ray diffraction (XRD), optical microscopy (OM), and scanning electron microscopy (SEM) were used to characterize the produced monolith GO and rGO membranes. The obtained data confirms that by increasing the thermo-reduction temperature (performed in open ambient atmosphere) a switch of the material from the electrical insulator field to electrical conductor one can be achieve without to have the burning of the GO material.

Acknowledgements

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Syntheses and Crystal Structures of the Metal Complexes Based on Pyrazole-carboxylic Acid Ligands

Diana Troana, Cristina Matache, Marilena Ferbinteanu Cimpoesu

University of Bucharest, Faculty of Chemistry, Department of Inorganic Chemistry, Organic Chemistry, Biochemistry and Catalysis, 90 Panduri Street, 050657 Bucharest, Romania

The design of crystalline materials is an important research area including interesting structural features and potential application. We targeted functional materials with d or f metal ions and heterocyclic carboxylic acids ligands. The pyrazole-carboxylic acids are versatile ligands due to their multi-coordination mode by the N and O donor atoms on the heterocyclic rings and the carboxyl groups (Fig.1). As protons donors and acceptors, the pyrazole nitrogen atoms and carboxylic oxygen atoms in pyrazole-carboxylic acids can not only coordinate metals to form M–N and/or M–O bonds, but also provide intermolecular hydrogen bonds for assembling the complex into high-dimensional networks. We synthesized and structurally characterized pyrazole-carboxylic acids, as well their complexes with Fe(II), Eu(III) and Ho(III) ions. We analyzed Fe(II) complexes in the frame of the spin transition processes and the lanthanide-based compounds as luminescent and magnetic materials.

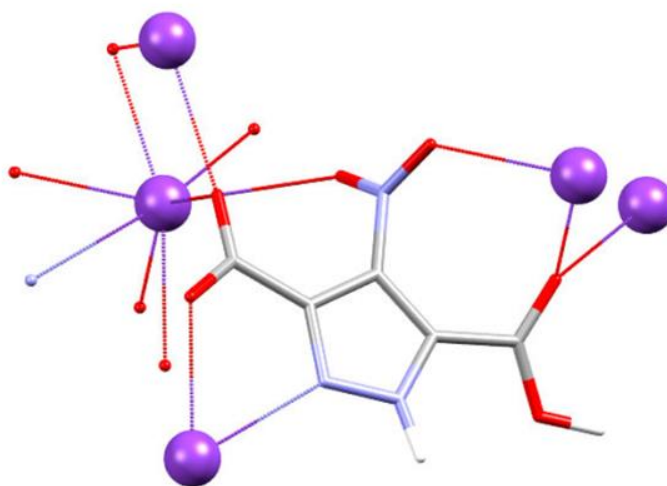


Figure 1. Asymmetric unit for K^+ salt of 4-nitro-1H-pyrazole-3,5-dicarboxylic acid determined by single crystal X-ray diffraction.

Voltammetric determination of vitamin B6

Rujoiu Stefania-Minodora, David Iulia Gabriela

University of Bucharest, Faculty of Chemistry, Department of Analytical Chemistry and Physical Chemistry, 90-92 Panduri Av., District 5, Bucharest, Romania.

Vitamin B6 (VB6) is a water-soluble vitamin with three major forms: Pyridoxin (predominantly used in clinical treatment), pyridoxal, and pyridoxamine, as well as their phosphorylated derivatives. VB6 plays a major role as a coenzyme in different reactions within the metabolisms of lipids, hemes, nucleic acids, proteins, or carbohydrates [1].

This work presents the voltammetric determination of vitamin B6 at a glassy carbon electrode (GCE). The influence of the supporting electrolyte pH was investigated in the range 1.81-12.48 by cyclic voltammetry (CV) and differential pulse voltammetry (DPV) in Britton Robinson Buffer (BRB) and NaOH solutions. The peak potential shifted linearly towards more positive potentials with increasing pH values. The $E_p=f(\text{pH})$ dependence suggested that the electrode process involved an equal number of electrons and protons. The highest peak currents were recorded in BRB pH 1.81 and 0.1 M NaOH solution, these electrolytes being used for further studies.

CV recorded at various scan rates emphasized that VB6 oxidation was diffusion controlled in both media.

DPV was employed for VB6 quantitative determination. The peak current varied linearly with the analyte concentration in the ranges $1 \times 10^{-5} - 3 \times 10^{-4}$ M and $1 \times 10^{-5} - 1 \times 10^{-4}$ M VB6 in NaOH and BRB pH 1.81, respectively. The limits of detection and quantification were 3.72×10^{-6} M and 1.24×10^{-5} M VB6 in NaOH and 4.71×10^{-6} M VB6 and 1.57×10^{-5} M VB6 in BRB pH 1.81. The DPV at GCE was applied to VB6 determination from a pharmaceutical solution. The recoveries obtained by the calibration curve method and by the standard addition method were 98.63% and 94.97%, respectively.

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***N*-Heterocyclic Carbene-Based [2]Rotaxanes: design and synthesis of the building blocks**

Maria M. Șerban, Cătălin C. Anghel, Niculina Hădade

Babeș-Bolyai University, Faculty of Chemistry and Chemical Engineering, Supramolecular Organic and Organometallic Chemistry, 11 Arany Janos, 400028 Cluj-Napoca, Romania;
maria.mihaela.serban@stud.ubbcluj.ro

Rotaxanes are mechanically interlocked molecules (MIMs) that have important applications as molecular devices for information storage and processing^[1]. We consider of interest to design a [2]rotaxane embedding a NHC moiety in the axle part (Fig. 1), in order to boost the catalytic activity of the Cu(I) metallic center. Our proposed strategy involved the synthesis of two key intermediates: an azide, alkyne functionalized macrocycle precursor and a dumbbell (axle + stoppers) segment. Herein, we present the auto-*click* synthesis of the dumbbell unit. All compounds have been characterized by NMR spectroscopy and high-resolution mass-spectrometry. With the dumbbell molecule in hand, we are now focused on interlocking it with the macrocycle precursor to obtain the proposed NHC-based [2]rotaxanes.

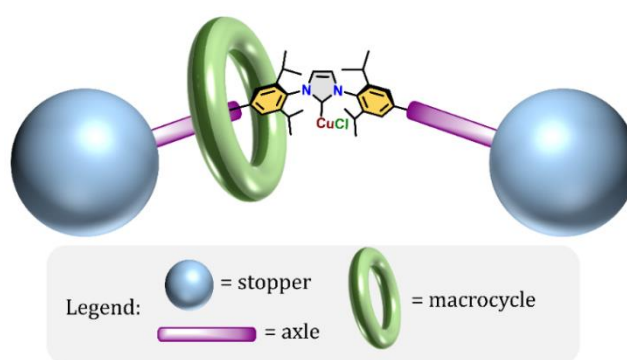


Fig. 1: Schematic representation of the target [2]rotaxane

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Toward a New Activity-Based Probe: Synthesis and Characterization of an Epoxysuccinyl-based Peptide

Daniel Vasile TODEREL
**Niculina D. HĂDADE, Alexia M. FRÎNCU, Ana Maria
COSMENIUC**

*Babeş-Bolyai University, Faculty of Chemistry and Chemical
Engineering, Supramolecular Organic and Organometallic Chemistry
Center, 11 Arany Janos, 400028 Cluj-Napoca, Romania,
daniel.toderel@stud.ubbcluj.ro*

Activity based probes (ABPs) are powerful chemical tools for investigation of biological processes.[1,2] ABPs act by irreversibly modifying the active site of an enzyme. These molecules possess three main structural components: a reactive group (also known as „warhead”) for reaction with the target enzyme, an affinity region, required to direct reactivity to the active site, a linker to modulate solubility and avoid steric hindrance and an analytical handle (detection tag), for the visualization and purification of the modified enzyme. [1] In this context we focused on developing a new ABP that has an epoxysuccinate-based “warhead”. This moiety is known to be a common inhibitor for the papain family. [2] To get access to the target compound, the linker, affinity region and warhead structural moieties were synthesized by classic solution chemistry and eventually assembled by Solid-Phase Peptide Synthesis method, using the Fmoc strategy, into the final ABP. The detection tag was designed to be attached using the copper (I) catalyzed alkyne-azide cycloaddition (CuAAC), *click* reaction. [3] The obtained precursors were characterized by NMR spectroscopy and MS, while the modified peptide was analysed by RP-HPLC and MS. Our future work will be directed toward the use of this ABP in order to assess Cathepsin B activity, a member of papain family.

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Studies on the production of fermented soy products

Maria-Alexandra Cernica, Ana-Maria Brezoiu

University Politehnica of Bucharest, Faculty of Chemical Engineering and Biotechnologies, Department of Chemical and Biochemical Engineering, 1-7 Gh. Polizu Street, District 1, Bucharest, Romania.

Milk-based yogurt contains important levels of lactose, which could be a problem for more than 68% of consumers with lactose malabsorption. For them, soy-based fermented products, as they are named accordingly to recent laws in vegetal products labelling [1], are considered a good alternative having low levels of both cholesterol and unsaturated fatty acids, compounds that are unhealthy and associated with various diseases [2].

However, due to the lack of lactose, it is considered a hurdle for microorganisms to produce lactic acid from oligosaccharides [3], which gives consistency (gel-like structure) and the acidity of yogurt. To overcome this disadvantage, the addition of xanthan gum in samples is proposed, a food additive acting as both a thickening agent and emulsifier and being used widely in the food industry.

Two sets of experiments were conducted, in which soy-based drink obtained in the laboratory and store-bought were used and xanthan gum and inoculum were added. Furthermore, in some samples, blueberry dried or frozen puree were added to enhance organoleptic properties and achieve functional food products [4]. Before and after the fermentation, a set of analyses were conducted: total acidity, pH, total soluble solids, rheological behavior as well as water binding capacity of samples [5]. Results support the obtaining of fermented soy products with improved features and nutritional values.

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Synthesis of TEMPO-Functionalised Hydrazone Precursor for *N*-Acylhydrazones

Teodora–Christina PURICE¹, Nicoleta SANDU¹, George COSTACHE¹, Anamaria HANGANU^{1,2}, Codruța POPESCU¹, Mihaela MATACHE¹

¹University of Bucharest, Faculty of Chemistry, Department of Organic Chemistry, Biochemistry and Catalysis, Research Centre of Applied Organic Chemistry, 90-92 Panduri Street, RO-050663 Bucharest, Romania; ²Institute of Organic Chemistry “C.D. Nenitescu” of the Romanian Academy, 202B Spl. Independenței, RO060023 Bucharest, Romania.

N-acylhydrazones are versatile building blocks in organic synthesis and have significant interdisciplinary applications (e.g., therapeutic activity, self-healing hydrogels, drug carriers [1-3]). Their most convenient synthetic procedure is by reaction between *N*-acylhydrides (hydrazides) and aldehydes. Free stable radicals are thermodynamically and kinetically stable paramagnetic species. Among these, TEMPO is one of the most widely known due to its enhanced stability [4], and TEMPO-functionalised derivatives enable study of redox-active materials. Therefore, combining properties of stable free radicals to behaviour of *N*-acylhydrazones could be of high interest [5].

Herein we describe synthesis and characterisation of a stable free radical (TEMPO) decorated dihydrazone as a precursor for *N*-acylhydrazones, as well as the intermediates, using ¹H-NMR, ¹³C-NMR, ESR and Mass Spectroscopy. We obtained pure compounds in good yields, and we investigated their physical properties, including melting point, solubility, and retention factor.

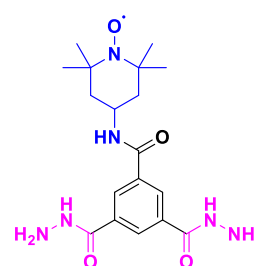


Fig. 1. Target compound

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Unleashing the Power of Photoswitchable Ligands: New Cu(II) Complexes with Azo Derivatives of *ortho*-Vanillin

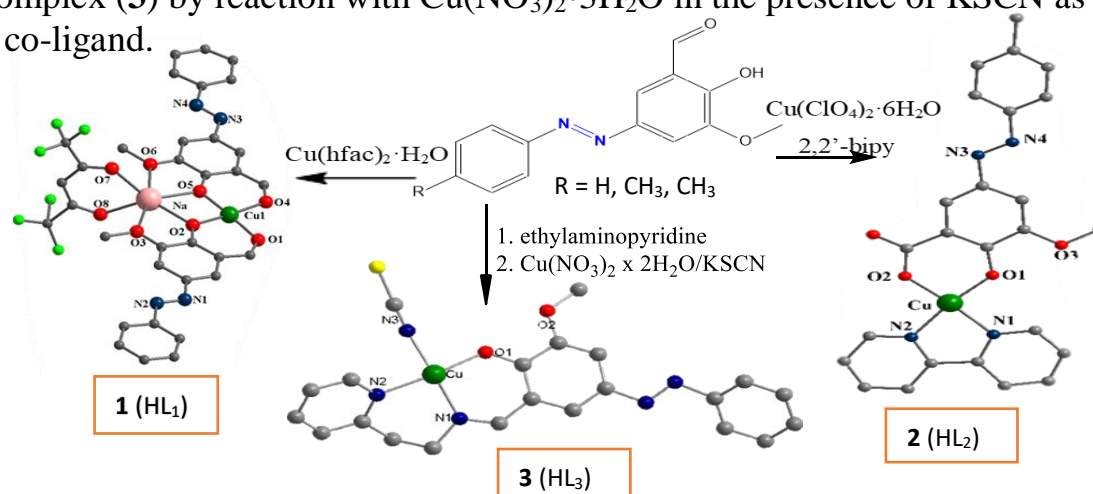
Cătălin Turcu^{a,b}, Simona Nica^{b,c} and Marius Andruh^{a,b,c}

^aUniversity of Bucharest, Faculty of Chemistry, Bdul Regina Elisabeta 4-12, București

^b“C. D. Nenitzescu” Institute of Organic and Supramolecular Chemistry, Splaiul Independenței 202B, București

^cScientific supervisor

Ortho-vanillin has a versatile coordination chemistry owing to its ability to readily form Schiff base compounds.¹ This property has made Schiff base derivatives popular as building blocks for assembling homometallic and heterometallic complexes featuring asymmetric bicompartimental pockets.² To further advance our research, we pursued the development of photoactive organic and coordination compounds by functionalizing *o*-vanillin with azobenzene moiety (**HL**₁, **HL**₂ and **HL**₃). By reacting these organic ligands with various copper salts, two types of mononuclear complexes were obtained. For instance, treating **HL**₁ with [Cu(hfac)₂] \cdot H₂O yielded [Cu(**L**₁)₂Na(hfac)], **1** complex. On the other hand, with Cu(ClO₄)₂ \cdot 6H₂O and 2,2'-bipyridine as a co-ligand, complex of type **2** was isolated. In this case, copper(II) displayed its oxidative character, leading to *in situ* oxidation of the aldehyde to the corresponding carboxylic acid. Lastly, the Schiff base ligands of the azo-tailored *o*-vanillin afforded complex (**3**) by reaction with Cu(NO₃)₂ \cdot 3H₂O in the presence of KSCN as a co-ligand.



Acknowledgement: The authors are thankful to Cătălin Maxim and Teodora Mocanu for their contribution to these results.

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Luminescent molecular materials based on chalcones

Valentin L. Virgil, Augustin M. Mădălan

Inorganic Chemistry Department, Faculty of Chemistry, University of Bucharest, Regina Elisabeta Blvd. 4-12, Bucharest – 030018, Romania

Chalcones are organic species that belong to the class of α,β -unsaturated ketones. Chalcone compounds have a common chemical scaffold of 1,3-diaryl-2-propen-1-one, also known as chalconoid, that can exist as *trans* and *cis* isomers, with the *trans* isomer being thermodynamically more stable. Chalcones present numerous applications such as bioactive substances, fluorescent materials, and chemical intermediates. Because of their conjugated systems, chalcones with proper electron-pulling and electron-pushing functional groups on the benzene ring(s) can be fluorescent making them potential chemical probes for mechanistic investigations and imaging/diagnosis.¹

Our perspective is to obtain luminescent complex combinations based on chalcones synthesized from 2-acetylpyridine and different aldehydes (9 - anthracenecarboxaldehyde, 2-naphthaldehyde, fluorene-2-carboxaldehyde and 1-pyrenecarboxaldehyde). Further, we want to investigate their behavior in photochemical processes in complex combinations using 3d (Figure 1) or 4f metal ions.

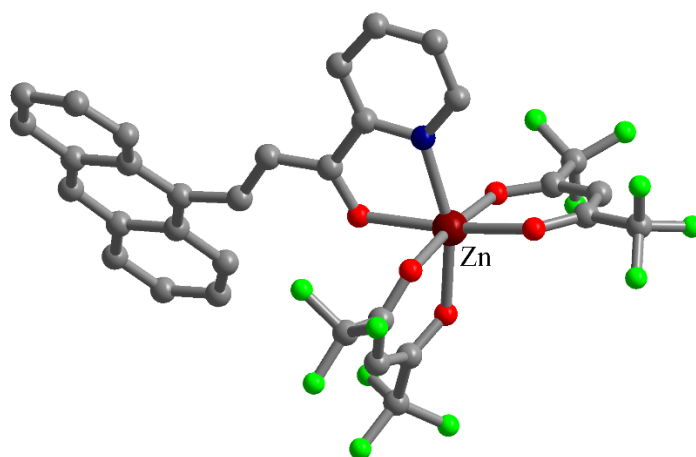


Figure 3. Perspective view of the crystal structure of the complex $[\text{ZnL}_1(\text{hfac})_2]$. The hydrogen atoms were omitted for clarity

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Synthesis and Structural Particularities of d-f Ionic Complexes

Andreea-Diana Zamfirescu, Marilena Ferbinteanu Cimpoesu

University of Bucharest, Faculty of Chemistry, Department of Inorganic Chemistry, Organic Chemistry, Biochemistry and Catalysis, 90 Panduri Street, 050657 Bucharest, Romania

Lanthanide based Metal-Organic Frameworks (Ln-MOF) are a class of porous materials capable of adsorbing and interacting with small molecules, with various applications like small molecule sensing, catalysis, gas capture, separation, luminescence, and even drug delivery.[1]

Targeting Ln-MOF with a particular interest in their luminescence capacity, we study new Zn-Ln ionic complexes series, as soluble building blocks and structure-driven topologies of phenanthroline based Zn(II) cation complexes (Fig.1.). The structural particularities of the obtained complexes are investigated by single crystal X-Ray diffraction and spectral measurements.

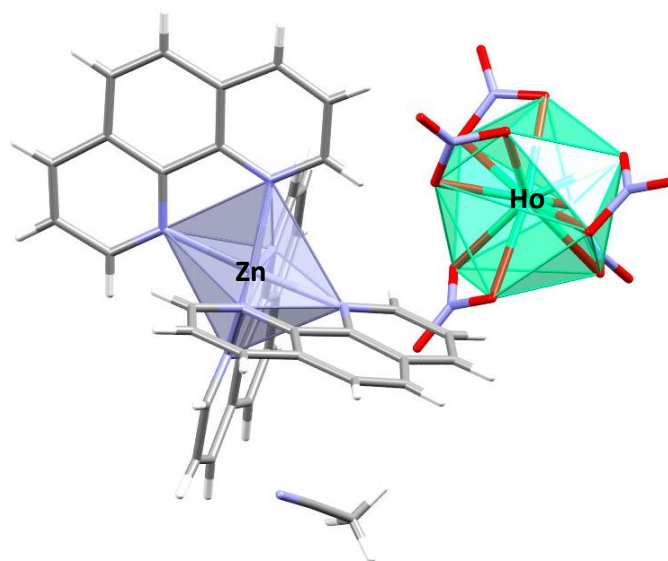


Figure 1. Molecular structure of synthesized Zn-Ho ionic complex. All Zn-Ln complexes from the analysed series are isostructural.

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Section 2 - MASTER Level

Synthesis, structural characterization and reactivity of organoselenium ligands

Cosmina Bohan and Alexandra Pop

*Supramolecular Organic and Organometallic Chemistry Centre,
Chemistry Department, Faculty of Chemistry and Chemical Engineering,
Babeş-Bolyai University, 11 Arany Janos, 400028 Cluj-Napoca, România;*

cosmina.bohan@stud.ubbcluj.ro

Multidentate ligands, which contain both *soft* (chalcogen) and *hard* (nitrogen, oxygen) donors atoms incorporated into the skeleton have shown a wide coordination pattern toward transition metals, being able to stabilize the metal complexes with promising biological, optical or catalytic activity.^{1,2}

We report here the synthesis and structural characterization of new heteroleptic diorganoselenium(II) of RSeBu type (R = [2-(CH₂O)₂CH]C₆H₄; 2-(OCH₂)C₆H₄) and diorganodiselenium(I) of R₂Se₂ type (R = [2-(CH₂O)₂CH]C₆H₄; 2-(OCH₂)C₆H₄; 2-{2-C₆H₄-(4*H*)-oxazol-5-one}C₆H₄). The reactivity of [2-{2-C₆H₄-(4*H*)-oxazol-5-one}C₆H₄]₂Se₂ was studied towards silver(I) and zinc(II) salts.

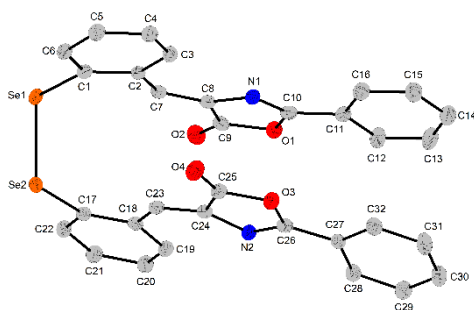


Figure 1. Molecular structure of [2-{2-C₆H₄-(4*H*)-oxazol-5-one}C₆H₄]₂Se₂

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Mono- and binuclear complexes with polydentate imino and amino ligands

Robert I. Botea, Augustin M. Mădălan

Inorganic Chemistry Laboratory, Faculty of Chemistry, University of Bucharest, Regina Elisabeta Blvd. 4-12, Bucharest – 030018, Romania

Polydentate imino and amino ligands play a significant role in the design of homo- and heteropolynuclear complexes containing 3d, 4d and/or 4f metal ions. Typically, the synthesis of such complexes involves a stepwise process in which the 3d ion is introduced first, followed by the use of the resulting complex as a ligand towards the 4f ion.

In this study, a series of novel polydentate Schiff base ligands were synthesized using N-(1-naphthyl)ethylenediamine and various phenol aldehydes. These imino ligands and, subsequently, the amino derivatives obtained by reduction of the imines were employed either alone or in combination with other chelatic ligands to produce mono- and binuclear complexes. X-ray diffraction on single crystal was utilized to structurally characterize the ligands and complexes. The investigation revealed the versatility of these types of imino and amino derivatives functioning as bidentate, tridentate, or tetradentate ligands. Figure 1 shows the sequential synthesis of a heterobinuclear Zn(II)-Tb(III) complex.

Additionally, the optical properties (IR, UV-Vis, luminescence) of the ligands and complexes were analysed in the solid state.

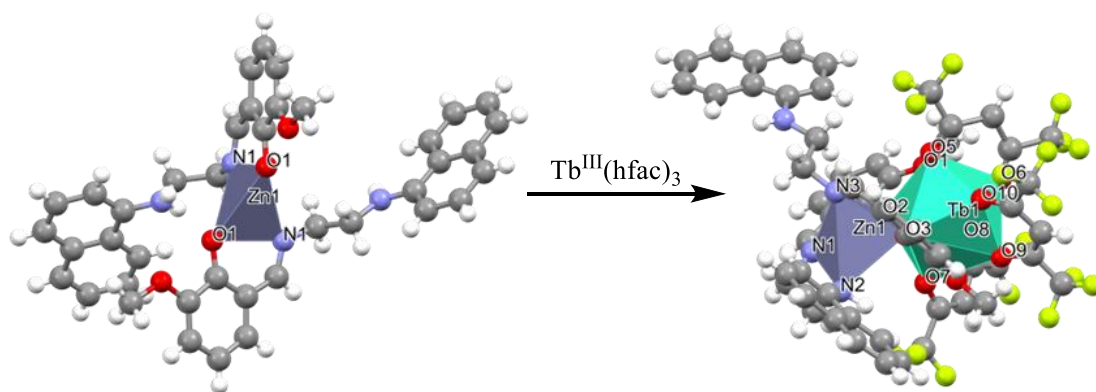


Figure 1. Stepwise synthesis of a heterobinuclear Zn(II)-Tb(III) complex

Voltammetric study of atropine

Marian-Gabriel Gâsnac, Dana-Elena Popa

*University of Bucharest, Faculty of Chemistry, Department of Analytical
Chemistry and Physical Chemistry,
90-92 Panduri Road, Bucharest-5, Romania*

Atropine (ATR) is a tropane alkaloid found in plants and belongs to the *Solanaceae* family. It is used to dilate the pupils before eye exams, in the treatment of amblyopia and other ophthalmological conditions, septic shock, heart and gastrointestinal diseases, as an antidote against opium, muscarine and phosphorus-based pesticides poisoning [1]. Voltammetric techniques are fast, simple, cost-efficient, versatile and non-destructive, being extensively used in pharmaceutical analysis for determination of different active ingredients. Thus, cyclic voltammetry (CV) and square wave voltammetry (SWV) were availed to study the electrochemical behaviour and for the quantification of ATR from pharmaceutical formulations. As a working electrode a cheap, disposable and eco-friendly bare pencil graphite electrode (PGE) was used [2].

By studying the influence of the nature and the pH value of the supporting electrolyte it was assessed that Na₂B₄O₇/NaOH buffer (pH = 10.4) is the best suited. Moreover, it was demonstrated that in the electrode process protons are also involved, the number of protons being equal to that of the electrons. Applying CV and varying the scan rate it was proved that ATR oxidation is diffusion controlled and it was established that two electrons are transferred in the electrode process. Employing SWV two linearity ranges were obtained: 7.5·10⁻⁶ M - 5.0·10⁻⁴ M and 5.0·10⁻⁴ M - 1.0·10⁻³ M. The detection and the quantification limits were calculated as 1.78·10⁻⁶ M and 5.39·10⁻⁶ M, respectively. The accuracy and the precision of the results were evaluated. The possible interference of different compounds present in the analysed matrix on the quantification of ATR was studied.

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Organotin(IV) compounds with Sn-O-E bonds (E= C, Si)

Vlad Penciu, Adrian-Alexandru Someșan

*Supramolecular Organic and Organometallic Chemistry Centre, Faculty of Chemistry and Chemical Engineering, Babeș-Bolyai University
11 Arany Janos, 400028 Cluj-Napoca, Romania*

Organotin(IV) compounds containing Sn-OR bonds (alkoxides) or Sn-OSiR₃ bonds (siloxides) have mostly been studied in the last 20 to 40 years. Compared to the organotin(II) derivatives, these compounds are less common, and their reactivity was less investigated.

We report the synthesis of new triorganotin(IV) alkoxides and siloxides bearing one phenyl group and two *ortho*-substituted phenyl-1,3-dioxolane fragments as ligands. The halide [2-((CH₂O)₂CH)C₆H₄]₂SnPhI (**1**) was used as the starting material in all syntheses. The organotin(IV) methoxide [2-((CH₂O)₂CH)C₆H₄]₂SnPhOMe (**2**) and siloxide [2-((CH₂O)₂CH)C₆H₄]₂SnPhOSiPh₃ (**3**) were obtained in good yields and characterized by multinuclear (¹H, ¹³C, ¹¹⁹Sn) NMR spectroscopy. The attempt to synthesize the organotin(IV) derivative with the *tert*-butoxy group led to the formation of the more stable oxide [2-((CH₂O)₂CH)C₆H₄]₂SnPh]₂O (**4**), bearing the Sn-O-Sn fragment. Compound **4** was characterized by multinuclear NMR spectroscopy and its identity was confirmed by elemental analysis and mass spectrometry. The molecular structure of compound **3** was determined by single crystal X-ray diffraction, and its supramolecular associations were investigated. The organotin(IV) methoxide **2** is air- and moisture-sensitive and it decomposes with the formation of the oxide **4**.

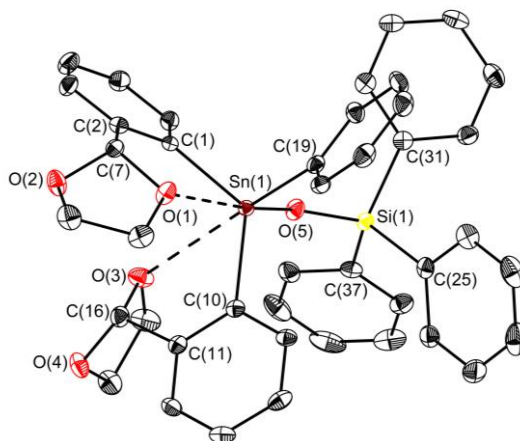


Figure 1: Molecular structure of compound **3**.

Section 3 - PhD level

Development of a detection method for some oligopeptides forbidden in doping control

Cristea CD^{1,2}, Toboc A², Stan C², David V¹

¹University of Bucharest, Faculty of Chemistry, Department of Analytical Chemistry, Sos. Panduri, no. 90, sect 5, Bucharest, 050663, Romania

²Romanian Doping Control Laboratory, Blvd Basarabia 37-39, sect 2, Bucharest, 022103, Romania

Doping control testing is one tool that Anti-Doping Organizations use to level the playing field and protect clean sports. The use of growth hormone-releasing hormones (GHRHs) is prohibited in sports according to the regulations of the World Anti-Doping Agency (WADA). The Minimum Required Performance Level (MRPL) for GHRH class is 1 ng/mL from urine, which shall imply for the initial testing procedure a limit of detection less than or equal to 50% of the corresponding MRPL (≤ 0.5 ng/mL). Considering the complexity of urine samples and the low concentrations at which these analytes should be detected, the analysis of GHRHs is a challenging task and for this purpose we developed a validated analytical method based on weak cation exchange solid phase extraction followed by LC-MS/MS analysis, which can detect a concentration of 0.5 ng/mL.

CQD@ZnO heterostructures with enhanced photocatalytic properties

Giuseppe Stoian¹, Elena Toma¹, Bogdan Cojocar¹, Madalina Tudorache¹, Joanna Gościańska², Simona Coman¹

¹*Department of Organic Chemistry, Biochemistry and Catalysis, Faculty of Chemistry, University of Bucharest, Regina Elisabeta Blvd., no. 4-12, Bucharest 030016, Romania*

²*Adam Mickiewicz University, in Poznań, Uniwersytetu Poznańskiego 8, Poznań, Faculty of Chemistry, Department of Chemical Technology, 61-614, Poland*

Corresponding author: giuseppe.stoian@drd.unibuc.ro

Zinc oxide is a commonly used material for wastewater treatment, but still there are different practical barriers for its extensive applicability [1]. Therefore, research has been intensified to improve its performance. In this respect, novel CQD@ZnO heterostructures were recently developed with improved photocatalytic activity in selective oxidation and degradation processes [2].

In this work, we report a cheap and simple attempt for preparing CQDs, and then using CQDs to fabricate CQD@ZnO heterostructure.

The photocatalytic properties of these heterostructures were investigated in the degradation of methylene blue (MB), a representative of a class of dyestuff resistant to biodegradation. CQDs were produced from humins waste usually formed in the biomass dehydration while CQD@ZnO heterostructures were synthesized via two methods: hydrothermal deposition and one-pot hydrothermal synthesis. The materials were characterized using various techniques such as XRD, DRIFT and UV-VIS spectroscopy. For the photocatalytic degradation tests blue LED lamps emitting at 445-465 nm were used and the dye concentration was determined by using a UV-visible spectrophotometer adjusted at 664 nm.

The obtained results will be discussed and correlated with the main physico-chemical characteristics of CQD@ZnO materials.

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