

# ***Abstracts***

**for**

## **Faculty of Chemistry Conference**

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## CP1. Metal ion sorption on cross-linked chelating architectures

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The regulations concerning the release of heavy metal ions into the environment and the recycling of wastewaters contributed to the improvement of metal ions recovery processes. A multitude of techniques, such as solvent extraction, precipitation, ion exchange and membrane separation, were involved in metal ion removal, but they often fail due to several technical limitations, economical constraints or environmental issues. Fortunately, adsorption proved to be an advantageous process showing high efficiency for removal and recovery of metal ions from dilute effluents.<sup>1</sup> In this work, an overview on cross-linked chelating architectures involved in metal ion sorption, starting from organic ion exchangers towards polymer composites, will be presented.<sup>2-6</sup> The sorption efficiency of every system will be discussed taking into consideration the solution properties, the polymer nature (synthetic or natural), as well as the accessibility and availability of reactive groups. The possible mechanisms involved in the sorption process constitute another aspect that will be depicted. Additionally, the benefits of combining chitosan with natural zeolites will be detailed, the chitosan/zeolite composites revealing, besides the enhanced sorption capacity, a simpler and more accessible pathway for sorbent recycling.

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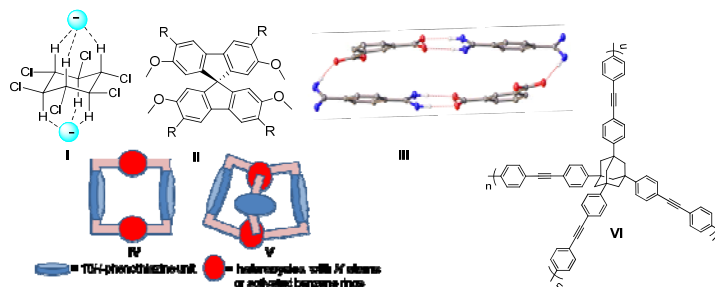
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## CP2. Self assembled architectures, innovative host-guest systems and COFs based on tetrahedric tectons

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Exciting self-assembled architectures generated by  $C(sp^3)\text{-H} \cdots X^-$  contacts using  $\beta\text{-HCH}$  as host and different anions as guests (I),<sup>1</sup> along with the solid state single crystal X-ray diffraction structures (built by hydrophobic interactions) of different octa-substituted 9,9'-spirobifluorene derivatives (II)<sup>2</sup> are presented in details. The role of CAHB (Charge-Assisted Hydrogen Bonding) in the combinations of diamidines with diacids (carboxylic or sulfonic) is investigated on a large series of compounds which show unexpected supramolecular constructions.<sup>3</sup> The aromatic nucleophilic substitution based synthesis of some cyclophanes (IV) and cryptands (V) exhibiting two or more phenothiazine units in the bridges is described and some applications (*e. g.* as logical gates) of these compounds are revealed. The synthesis by Sonogashira or Suzuki cross-coupling reactions of some COFs starting from tetrahedric classic building blocks (derivatives of tetraphenyladamantane or 9,9'-spirobifluorene) and some relevant absorption and catalysis properties of these macromolecular compounds are discussed.<sup>4</sup>



**Figure 1.** Representations (general formula or examples) of the main targets: anion- $\beta\text{-HCH}$  complexes (I), 9,9'-spirobifluorene derivatives (II) diamididine-dicarboxylic acid complex (III), phenothiazine based cyclophanes (IV) and cryptands (V), adamantane based COF (VI).

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### CP3. Functional pi-Conjugated Systems: from molecular design to applications

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The control of the electronic properties of pi-conjugated systems represents a key issue for the development of their multiple technological applications in:

- Electrode materials for energy storage, electro-catalysis or sensors
- Molecular architectures for molecular electronics.
- Active materials for organic light-emitting devices (OLEDs), field-effect transistors (OFETs) and organic photovoltaics (OPV).

Since each of these fields of application resorts to specific physical, chemical and electronic properties of the functional molecule and/or material, progress in these various areas requires the definition of appropriate guidelines for the design and synthesis of functional pi-conjugated systems. This objective involves both the tuning of the electronics properties at the molecular level and the control of intermolecular interactions that *in fine* determine the ultimate collective properties of the material.

These various aspects of the molecular and supramolecular engineering of functional pi-conjugated systems will be discussed on the basis of selected examples of molecules and materials designed for applications in electrode materials, molecular electronics and OPV.

## CO1. Vertical transport of continental air masses and their influence on the distribution of size resolved aerosols from Iasi, Romania

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Research on the mineral dust is of great interest for the atmospheric chemistry scientific community due to the impact of such particles on air quality, health and climate. The world's major source of mineral dust is the Sahara desert but continental air masses convectional lifting might have also very important contributions. In the present work the impact of long range transport phenomena, on the distribution of size resolved atmospheric aerosols from Iasi, north-eastern Romania, was studied. Over November 2015 till September 2016, size distribution of the interest species in the 0.0276-9.94  $\mu\text{m}$  size range was appropriately investigated by using 13 specific fractions collected with a cascade Dekati Low-Pressure Impactor (DLPI). Ionic chemical constituents of the collected particles have been determined by ion chromatography. Data analysis revealed that at the investigated site the distribution of size resolved aerosols can be highly influenced by the air masses origins and characteristics. April 2016 was remarked as the month with predominant air masses undertaking faster vertical transport, most probably taking place due to the locally/continentally driven buoyancy. Over the investigated period,  $\text{Ca}^{2+}$  and  $\text{Mg}^{2+}$  species, assigned usually as tracers of mineral dust, have been found to reside mainly in the coarse mode (with maxima close to 2.5  $\mu\text{m}$ ). Bimodal distributions with maxima in the 260-380 nm range and close to 2.5  $\mu\text{m}$  have been observed for  $\text{NO}_3^-$  ion, while  $\text{SO}_4^{2-}$  and  $\text{NH}_4^+$  ions were mainly present in the submicron size range.

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## CO2. Amphiphilic polysaccharide-based diblock copolymers prepared by click chemistry

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Biocompatible amphiphilic block copolymers were obtained by copper-catalyzed azide-alkyne cycloaddition (CuAAC) of propargyl ester of different deoxycholic acid polyesters with azide-functionalized dextrans (Dex6000, Dex11000, Dex25000). Alkyne-end-functionalized polyesters were prepared by polycondensation reaction of 3-succinoyloxy-bile acid with different oligo(ethylene glycol)s (OEG100, OEG200) followed by the coupling of the polyesters with propargyl alcohol. Azide-functionalized dextrans were obtained by reductive amination of the polysaccharide end group with a large excess of 1-azido-3-aminopropane.

The chemical composition of the copolymers was determined by <sup>1</sup>H-NMR and high pressure liquid chromatography (HPLC). Self-assembling in aqueous media of diblock copolymers was studied by dynamic light scattering (DLS) and transmission electron microscopy (TEM). DLS measurements revealed a monomodal size distribution of the aggregates with an average size in the range of 60-600 nm. TEM studies demonstrated that block copolymers could self-assemble into micelles or vesicles depending on the polymer composition and micellization procedure. Applicability of the synthesized self-assembling particles as drug carriers was evaluated by encapsulation/release experiments performed with biologically active substances (Curcumin, Nystatin, Rifampicin).

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### **CO3. The effects of *Origanummajorana* L. essential oil on an amyloid beta (1-42) rat model of Alzheimer's disease: cognitive and molecular approaches**

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Alzheimer's disease (AD) is a neurodegenerative progressive disorder characterized by elevated levels of amyloid beta (A $\beta$ ) peptides in the brain and progressive cognitive impairments. In the present study, the effects of *Origanummajorana* L. (1% and 3%) essential oil were assessed on spatial memory performance in an amyloid beta (1-42) rat model of Alzheimer's disease.

In traditional medicine, *Origanummajorana* L., also known as sweet marjoram, is recommended for the treatment of anxiety, and also as anti-inflammatory, antispasmodic and antidepressant agent. Y-maze and radial arm-maze tasks were used to assess the spatial memory on animal models. The A $\beta$ (1-42)-treated rats exhibited decreases of spontaneous alternations percentage within Y-maze task and increases of working memory and reference memory errors within radial arm maze task, and the inhalation of this essential oil significantly improved short term memory in Y-maze test, but did not exhibit impressive improvement in long term memory in radial arm maze test. The collected brain tissue samples were used for protein extraction in order to evaluate the changes induced in protein expression by the administration of sweet marjoram essential oil. Using mass spectrometric methods, it was observed that the essential oil influenced the expression of a large number of proteins with possible implications in the pathogenesis of AD.

These findings suggest that the *Origanummajorana* L.(1% and 3%) essential oil may be a potential candidate for the development of therapeutic agents to manage memory impairment associated with Alzheimer's disease.

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## CO4. Authentication of old heritage violins

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The violins of the famous Italian luthiers of Cremona of the period 1538 to 1740 became the most searched stringed instruments that were also real masterpieces. In chronological order the most famous luthiers are the following family members: **Amati** (Andrea Amati, 1505 – 1578; Antonio and Girolamo Amati; Nicolò Amati, 1596-1684 and Girolamo Amati/Hieronymus II, 1649-1740), **Stradivari** (Antonio Stradivari, 1644-1737; Francesco Stradivari, 1671-1743 and Omobono Stradivari 1679-1742), Bergonzi (Carlo Bergonzi, 1683-1747; Michele Angelo Bergonzi 1722–1758 and Zosimo Bergonzi 1725–1777) and **Guarneri** (Andrea Guarneri 1626 – 1698; Pietro Giovanni Guarneri/Pietro da Mantova, 1655 – 1720; Giuseppe Giovanni Battista Guarneri, 1666 – 1740; Pietro Guarneri/Pietro da Venezia, 1695 – 1762 and Bartolomeo Giuseppe Guarneri/del Gesù, 1698 - 1744). Of the more than 6,000 stringed instruments made by Stradivari family (the most popular tools, both during those ages and after) currently are 601 identified, a small part being sung, the majority being in museums or particular collections. The paper presents the main structural-functional, dendrochronological and chemometric features with archaeometric value, concerning the wood composition and vernishes, which were used in the authentication of old violins, analyzed in our team.

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## CO5. Alginate/clinoptilolite composite microspheres with enhanced sorption properties for Methylene Blue

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Over last years, water pollution became a huge environmental issue due to the large variety of residues originating from different human activities. Amongst all pollutants, dyes are considered as the most problematic ones due to their high toxicity, non-biodegradability, and carcinogenic potential.<sup>1</sup> The considerable amount of colored effluents resulting from numerous industrial domains such as textile, plastic, paper, food or cosmetic industry cannot be disposed without an adequate treatment. Various techniques, such as chemical oxidation, flocculation, biological treatment or adsorption were explored for the removal of cationic dyes. Among them, chemical or physical adsorption is generally recognized as an efficient and economic approach.<sup>2,3</sup> In our study, composites based on sodium alginate and clinoptilolite (Alg/CPL) were designed as microspheres for the removal of Methylene Blue (MB) from model aqueous solutions. FTIR spectroscopy, SEM, energy dispersive X-ray spectroscopy and water uptake measurements were considered for the characterization of Alg/CPL composites. Subsequently, the effect of sorbent dosage, CPL content, contact time and initial MB concentration on their sorption capacity was investigated. In the end, the mechanism controlling the sorption process was evaluated based on the kinetic parameters and sorption isotherms.

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## CO6. Extraction, isolation and characterization of inulin-type fructans from *Cichorium intybus* and *Taraxacum officinale*

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Inulin is a fructan-type polysaccharide, discovered in more than 30000 vegetable products, such as: *Helianthus tuberosus* (Jerusalem artichoke), *Cichorium intybus* (chicory), *Dahliapinnata* (dahlia) and *Polymnia sonchifolia* (yacon).<sup>1</sup> Due to therapeutic potential, inulin and its hydrolyzed form oligofructose are used in various sectors, such as food industry and pharmaceutical area.<sup>2</sup> Furthermore, inulin extracted from tubers cold-stored during 4 months can be used as a prebiotic food ingredient, representing a potential alternative to the available commercial inulin obtained from various vegetable roots.<sup>3</sup>

In the present work, the inulin-type fructans from *Cichorium intybus* and *Taraxacum officinale* roots was extracted, isolated and characterized to evaluate its therapeutic potential. The inulin content of these vegetable extracts was quantified using spectrophotometric methods and HPTLC technique. The highest content of inulin was found in *Cichorium intybus* roots. The prebiotic activity of inulin from these vegetable extracts was investigated in the presence of *Lactobacillus plantarum* strains, which showed a significant growth dynamics. In conclusion, *Cichorium intybus* and *Taraxacum officinale* roots are essential vegetable sources to extract the inulin, which has a significant nutritious, functional and bioactive role in foods and can be used as a protein stabilizer, respectively.

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## CO7. Synthesis, structure and properties of Cu(II) coordination compounds with water soluble thiosemicarbazone

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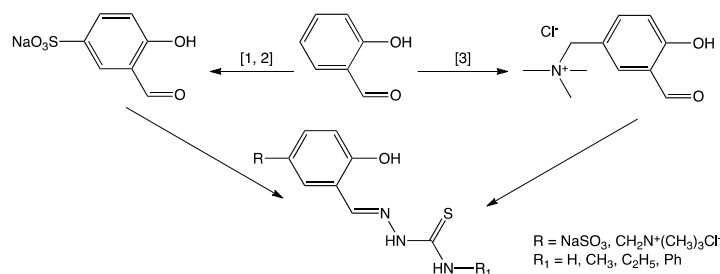
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The coordination chemistry of the transition metal complexes with thiosemicarbazide derivatives has been widely investigated due to their attractive chemical, physical and biological properties. Employing various thiosemicarbazide derivatives and different metal ions with different oxidation states allows the preparation of a wide number of coordination compounds with original structures and properties.

In this work we present a new way of activation of the thiosemicarbazide fragment and his condensation product with salicylaldehyde - thiosemicarbazone by coordination to the transition metals. An interesting point is to functionalize the salicylaldehyde thiosemicarbazone with strong ionic group to increase the solubility in water of products.

For this, we functionalize the five positions of the salicylic fragment by cationic groups like  $N^+(CH_3)_3$  and anionic groups like  $NaSO_3$ . First, was synthesized the corresponding salicylic aldehyde, and after his condensation products with N4 - substituted thiosemicarbazide was performed.



The obtained ligands were used for the synthesis of new coordination compounds with 3D transition metals.

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## CO8. Proteomic approach to characterize prolamins from corn

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Zeins are proteins called prolamins soluble in alcohols which can be extracted from corn. They can be used in biomedicine as drug delivery in the body, in production of bio-plastics or in food industry in the production of chewing gum. Proteomics is a modern "science" which studies peptides and proteins using various modern techniques. Among them, unidimensional electrophoresis and mass spectrometry have become more popular behind researchers in the last ten years.<sup>1</sup> However, in literature, there are a few articles that characterize zeins by mass spectrometry (MALDI-ToF- Matrix assisted laser desorbition ionization- Time of Flight) because they are numerous and each genotip, each sort of corn meal have a particular amino acid sequence and thus a particular zein primary sequence.<sup>2</sup> Mass spectrometry was used to analyze the composition of corn meal. Zeins were extracted using different methods and different "eco-friendly" solvents (alcohol solutions) followed by a detailed characterization using a proteomic approach. The obtained spectra were compared with those obtained from literature and they matched very well.<sup>3</sup>

**Acknowledgments:** This work was supported by the *PN-II-RU-TE-2014-4-092* project.

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## SC1. Impact of chain conformation on rheological behavior and biocompatibility of some semi-aliphatic polyimides

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Polymers with imidic structure are recognized as high performance plastics. They are utilized in multiple industry sectors owing to their outstanding chemical and physical features, including high oxidative stability, good resistance at raised temperatures, high mechanical strength, and elevated electrical insulation. Most polyimidic materials are obtained by solution processing method so rheological investigations are mandatory for ensuring quality products. This work aims to study the influence of polymer backbone conformation of some semi-aliphatic polyimides on their rheological behavior. Rheological data reveal that in the appropriate solvent, the polyimide solutions exhibit Newtonian behavior at low shear rates, which facilitate their processing into films with good uniformity. Shear oscillatory tests show that the polymer solutions exhibit a transition from the viscous flow to the elastic fluid flow, enabling their easy processing. Biocompatibility of the samples was assessed in regard with some basic blood components.

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## SC2. Contributions regarding the synthesis and characterization of compounds from the series $\text{ZnAl}_{2-x}\text{Cr}_x\text{O}_4$

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Compounds with a spinel structure and the general formula  $\text{ZnAl}_{2-x}\text{Cr}_x\text{O}_4$  ( $x = 0-2$ ) using fructose as complexing/fuel agent were obtained. Soluble salts of the reagents were dissolved in an aqueous solution alongside the complexing/fuel agent. The obtained solution was concentrated to form a gel. The gel was then heated until autocombustion was observed. After that, the heat treatment applied to the samples was between 500-900 °C. IR absorption spectroscopy was used as a method for the investigation the chemical reaction in the solid phase. The heating behavior of complexing/fuel agent was determined by thermal analysis. The samples obtained were characterized by X-ray diffraction to determine their structure and purity. The ends of the series  $\text{ZnAl}_2\text{O}_4$  and  $\text{ZnCr}_2\text{O}_4$  have many applications.

$\text{ZnAl}_2\text{O}_4$ , having a large specific surface area and a porous structure, is used as a catalyst and a catalyst support in various reactions such as: the photodegradation of dyes, alkylation of heterocycles, transesterification of vegetable oil, acetylation of amines, alcohols and phenols.<sup>1</sup>  $\text{ZnCr}_2\text{O}_4$  is used in: catalysis, toxic gas sensor and as a semiconductor.<sup>2</sup>

The physical and catalytic properties of the samples obtained by substituting chrome with aluminum in a zinc chromite ( $\text{ZnCr}_2\text{O}_4$ ) have been investigated.

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### SC3. Selectivity of transport capacity of the compounds based on 15-crown-5 and 18-crown-6 ethers

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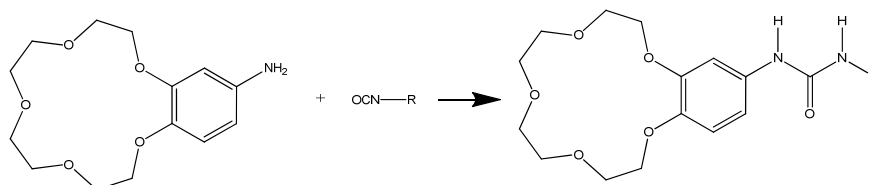
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Ionic exchange through double-layer lipid membranes is a key process in the basic activity of a living cell. KcsA (prokaryotic potassium channel from the soil bacteria *Streptomyces lividans*) is especially known for its high selectivity for potassium against sodium and other cations, but its lack of stability makes it an unsuitable candidate for use in artificial systems. This aroused the need for synthesis of a new molecule which would behave similarly to KcsA in a controlled environment.

This work's main focus is the synthesis and characterization of some compounds capable of forming supra-molecular structures within the double – layer membranes, thus creating pores with specificity for K<sup>+</sup> and Na<sup>+</sup>.

We synthesized compounds based on benzo-15-crown-5 ether and benzo-18-crown-6 ether, on which we attached urea to position 4' in order to promote self-assembly. On the other end of urea, we attached a linear or optic active branched alkyl group, like shown in figure 1:



where R is butyl, hexyl, octyl, dodecyl, (s)-(+)-2-hexyl, (r)-(-)-2-hexyl, (s)-(+)-2-octyl, (r)-(-)-2-octyl.

The reactions were performed in acetonitrile at reflux for 12 hours and the resulted compound precipitated at -20°C. The products were verified by NMR and MS:

The capacity of transport was analysed by fluorescence, using large unilamellar vesicles (LUVs).

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## P1. Dynamics of tebuconazole and other combination fungicide formulations in *Jonathan* and *Golden Delicious* apple leaves

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Tebuconazole (TEB), a systemic triazole fungicide, is nowadays widely used to control many diseases in fruits, nuts, cereal and vegetable crops.<sup>1</sup> As part of a more complex study, dissipation behavior of tebuconazole and clearly stated combinational fungicide formulations, on *Jonathan* and *Golden Delicious* apple leaves, from a local orchard (Miroslava) in Iasi, has been investigated in the present work. The interest products have been sequential sprayed (4 times) in full agreement with the producer's recommendation (Bayer) and the samples have been collected by following an own developed strategy such as to fulfill the requirements of the single first order (SFO) linear kinetic model (with at least six points after the product application). Levels of TEB in apple leaves, after appropriate extraction (ultrasound assisted) and cleanup procedure, were determined by using a gas chromatograph, Agilent 7890A, in tandem with a mass spectrometer, Agilent 5975C, Agilent Technologies, USA. The goodness of fit on the implied variables was assessed using statistical approaches as well as visual introspection on the residuals distribution. The data on the persistence of TEB in the investigated apple leaves showed that this parameter is highly controlled by a relatively fast dissipation process. The results obtained in the present study show that the dissipation parameters (constant rate and half-life times) are sensitive to the applied dose and also to the formulation of the fungicide combination.

**Acknowledgements:** CERNESIM is gratefully acknowledged for the infrastructure used to achieve the experimental tasks.

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## P2. Lanthanide Isopolyoxometalates: synthesis, structure and photocatalytic activity

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Photocatalysis is an attractive property for POMs because of potential applications in decomposition of water contaminants. Methyl Blue, Methylene Blue and Rhodamine 6G, which are typically difficult to decompose in waste water were employed to study the photocatalytic activities of synthesized POM.

Polyoxotungstate was obtained hydrothermally from Na<sub>2</sub>WO<sub>4</sub>·2H<sub>2</sub>O, Sm(NO<sub>3</sub>)<sub>3</sub> in an aqueous solution at a pH value of 7.4-7.55 adjusted by acetic acid solution. The characterization of the systems Sm<sup>3+</sup>- POM was accomplished by means of DRX, FTIR, UV-Vis spectroscopy and thermal analysis.

For the evaluation of catalytic activity, the catalyst was suspended in an aqueous solution of dyes in a Pyrex reactor. Photodegradation reactions of colorants upon 6W lamp irradiation employing POM as the photocatalyst have been examined by UV-Vis spectroscopy. The efficiency of catalyst was calculated by the following formula:

$$\text{Efficiency(\%)} = \frac{(A_0 - A)}{A_0} \cdot 100$$

where A<sub>0</sub> and A referred to the absorbance of the colorant before and after reaction, respectively.

The obtained results demonstrate that the catalytic activity of the compound depends on the reaction time, the catalyst amount, solvent polarity and volume of hydrogen peroxide.

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### **P3. Ecological footprint of recycled paper**

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Paper and paperboards are commonly used in corrugated boxes, milk cartons, folding cartons, bags and sacks, and wrapping paper, tissue paper, paper plates and cups. The types of paper used in food packaging are: Kraft paper, Sulfite paper, Greaseproof paper, Glassine, Parchment paper. Paper industry is considered a major user of natural resources, energy and a significant polluter. Recycling of paper supports sustainable development and by incorporating this method in waste management plans local governments can reduce the amount of waste landfilled, the environmental impacts associated, costs and others and can preserve forest, water and energy resources. The goal of this study is to establish the ecological footprint of recovered paper and compared with the footprint of paper obtained by virgin materials (wood). The functional unit chosen was 1 tonne of paper. All the inputs and outputs of the product system are calculated reported at functional unit. The data collected in the inventory phase were used further in the impact assessment stage. The software used for this evaluation was SimaPro. The results showed that 1 tonne of paper obtained by using virgin materials (wood) has the most significantly value for carbon dioxide indicator which means that processing of wood for obtaining the paper have a major influence on CO<sub>2</sub> emissions, followed by land occupation. Sorting of waste paper also have significant influence on CO<sub>2</sub> emissions and less influence on nuclear and land occupation. For recycled paper it was observed that for all impact categories are registered negative values which mean positive impacts on the environment. It can be concluded, after comparison of environmental impacts, that recycling of paper is the most suitable alternative in order to avoid the emissions of carbon dioxide and not only in the environment (pollution prevention) but also by saving virgin materials. The present study intended to highlight the importance of paper packaging recycling.

#### P4. Biosynthesis of silver nanoparticles from *Paeonia officinalis* aqueous extract

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Silver nanoparticles (AgNPs) exhibit particular physical-chemical properties which contribute to a continuous development of the researches in this field especially in the past decade. There are used different methods to obtain AgNPs, from the conventional (i.e.: chemical and electrochemical methods,  $\gamma$  radiations, etc.) to the unconventional ones (“green chemistry” methods).<sup>1</sup> Among the unconventional methods, the most used and studied are the ones based on plant extracts (aqueous or alcoholic) in the presence of silver nitrate (AgNO<sub>3</sub>), under heat or at room temperature, in the dark.<sup>2</sup>

Peony (*Paeonia officinalis*) has multiple therapeutic effects: fights acne, dermatitis or various skin inflammations as well as diminishes stomach aches. This plant contains tannins, alkaloids, oligoelements (calcium, magnesium, iron), vitamin C and flavonoids - phytocomponents that provide the aqueous extract obtained from *Paeonia officinalis* excellent properties to obtain AgNPs.<sup>3</sup>

This paper presents the synthesis of AgNPs from aqueous peony extract, in the synthesis both petals and leaves being used. In order to prove that AgNPs are obtained the UV-Vis, FTIR and DLS spectra were recorded. The results are presented in comparison with the chemical obtaining of AgNPs via sodium citrate method.

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## P5. DNA assisted functionalization of gold nanoparticles with cyclodextrin moiety

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In order to find new ways for the preparation of cyclodextrin functionalized gold nanoparticles, we employed synthetic DNA sequences and a mono functional  $\beta$ -cyclodextrin derivative to prepare final cyclodextrin coated gold nanoparticles. The design pathways included the synthesis, purification and characterization of isothiocyanate-modified  $\beta$ -cyclodextrin<sup>1</sup> (mono-6-isothiocyanate-6-deoxy- $\beta$ -cyclodextrin). In parallel, phosphine-coated gold nanoparticles were reacted together with synthetic DNA<sup>2</sup> containing two modifications: a thiol moiety (3' end) for attachment to the gold nanoparticle surface and an amine moiety (5' end) for the attachment of cyclodextrin through the formation of a thiourea bond. Thus, the DNA amino-modified gold nanoparticles were reacted together with the mono-6-isothiocyanate-6-deoxy- $\beta$ -cyclodextrin to yield the final gold nanoparticle with  $\beta$ -cyclodextrin shell. The starting, intermediate and the final product were characterized by nuclear magnetic resonance spectroscopy <sup>1</sup>H, <sup>13</sup>C NMR (organic derivatives), Transmission Electron Microscopy (TEM) and zeta potential measurements. The obtained functionalized nanoparticles are suitable for the preparation of supramolecular assemblies and afford the possibility to form inclusion complexes with the desired molecules for subsequent biomedical applications.

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## P6. Chain flexibility influence on optical and dielectric properties of some polyimides

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Polyimides represent a class of macromolecular materials widely used in advanced technologies particularly due their dielectric and optical properties. In this work, the group contribution theory was utilized to calculate molar volume and molar refraction. These are the essential parameters for estimation of the refractive index. The latter was further employed in determining the dielectric constant of the samples using Maxwell approximation. The different flexibility of the proposed polyimide structures was visualized through molecular modelling by applying molecular mechanics method. The results were discussed by highlighting the influence of chain flexibility on optical properties of studied structures. The resulted data are of great importance in pre-determining basic optical and dielectric characteristics of the imidic polymers (before starting the synthesis reactions) that are influencing the applicability of these materials on electronic domain.

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## P7. Binding of redox-active metals to peptides

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The interaction of redox-active metals with proteins is linked to production of reactive oxygen species (ROS), which have been associated with progression of several diseases, including neurodegenerative pathologies. Iron and copper ions can form highly toxic hydroxyl radicals, which oxidize biomolecules and subsequently lead to neuronal cell death.<sup>1,2</sup> Previous experiments based on NMR, MS, IR and microscopic techniques revealed significant changes in the structure of peptides associated with metal binding. The reduction of metals can involve either internal A $\beta$  amino acid side chains or an external reductant.<sup>3</sup> The spectroscopic studies indicated the involvement of histidine residues in metal binding, and of tyrosine, which is sensitive to free radical attack due to its conjugated aromatic ring.<sup>4</sup>

In the current study we have used MS and FT-IR spectroscopy to reveal the structural modifications of binding iron and copper active metals to peptides. Several truncated sequences and mutant forms of amyloid and neuroprotective peptides have been used in experiments. We observed that not only the histidine residues are involved in the binding process, but others like Tyr or Ser, carboxyl and amino groups.

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## P8. Phytochemical Screening of *Hexalobus monopetalus* (A. Rich.) Engl. & Diels, Plant Used in the Treatment of Gout in Chad

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In developing countries, illiteracy, poverty, social and cultural constraints and difficult access to modern medicine are that the population first made use of traditional medicine for treatment. According to the World Health Organization, more than 80% of the African population use of this medicine to meet their health needs.<sup>1</sup> One health problems in Chad, breeding country is gout where modern medicine offers very few solutions.

After an ethnobotanical survey of practitioners of traditional medicine, a phytochemical screening is performed on the bark of the root of *Hexalobus monopetalus* (A. Rich.) Engl. & Diels (*Annonacées*). It is variously used.<sup>2,3</sup> The pleasantly scented fruits are often eaten by monkeys and men.<sup>4</sup>

A brief analysis on the plant allowed to identify alkaloids, flavonoids, saponins, tannins and terpenes/steroids. The thin layer chromatography of the crude extract in dichloromethane was used for confirmation of the presence of alkaloids, flavonoids and terpenes. After extraction with solvents of increasing polarity, the GC-MS analysis of the cyclohexane extract revealed the presence of volatile compounds. The dichloromethane extract was fractionated and two fractions (HM F3 and HM F6) with a good profile was analyzed by standard chromatographic and spectroscopic techniques (TLC, HPLC, UV-VIS and FTIR).

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## **P9. Phytoremediation study of petroleum polluted soils using *Pleurotus Pulmonarius* mushrooms**

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After the evaluation of ICPA Institute of Bucharest in 2010, it was established that more than 50 000 ha of Romanian land are polluted with oil and oil products. The largest polluted areas are in Teleorman, Braila, Bihor, Dolj, Dambovita, Giurgiu and Gorj counties.<sup>1</sup> In addition, in areas of oil exploitation, most crop production is ceased because of siting the land surface of pipelines, wells being out of operation, storage of materials and waste, plus roads and paths built legally and unequally, power and telephone lines etc.<sup>1</sup> Technologies regarding soil remediation consist mainly of chemical and physical treatments on the soil profile in order to foster and accelerate the biodegradation process of spilled waste oil. There are also biological treatments, such as biodegradation, bioaccumulation or bioleach, which are implemented outside the site of polluted soil, directly at the site of polluted land or "in situ".

Since characteristics of oil-polluted soils vary according to the intensity of contamination, the time elapsed from the occurrence of pollution and also the depth reached by oil components, herein is presented a preliminary study concerning a bioremediation technology, using *Pleurotus Pulmonaris* mushrooms, like those implemented outside the site of polluted soil.<sup>2</sup> Infrared spectrometry was used to establish the preliminary content in petroleum compounds of analyzed soil, samples having been taken from two drills located in different places, at different depths and different distances from the center of the drill. Half of each sample of polluted soil was used as such and the other half was mixed in equal proportions with compost and they were subjected to phytoremediation with *Pleurotus Pulmonaris* myceliums. We have re-analyzed soil samples and the results showed a decrease of the petroleum compounds content in the samples that were subjected to phytoremediation with mushrooms, compared to the other samples.

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## P10. New bis-pyridine-imidazolium/benzimidazolium salts with acetophenone skeleton: synthesis and NMR characterization

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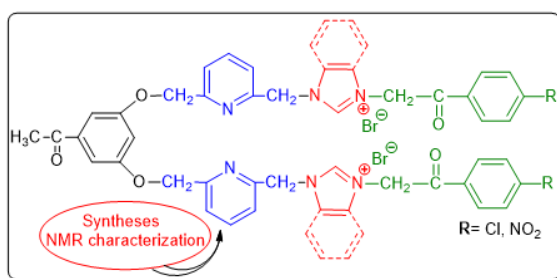
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An elaborate literature study of the derivatives with acetophenone skeleton, emphasize that are one of the most used classes of building blocks in supramolecular chemistry.<sup>1,2</sup> Also, quaternary salts with imidazole/benzimidazole moiety are described in the literature like compounds with biological properties: antibacterial, anti-inflammatory, anticancer.<sup>3,4</sup>

In this respect our goal was to synthesize and characterize new bis-pyridine-imidazolium/benzimidazolium salts with acetophenone skeleton. The syntheses were done in three



steps: **(I)** *O*-alkylation of 3,5-dihydroxyacetophenone with bis-chloromethyl pyridine, giving a halogenated derivative with increased reactivity; **(II)** *N*-alkylation of imidazole/benzimidazole with the compound obtained in first step; **(III)** quaternization

reactions of bis-pyridin-imidazole/benzimidazole derivatives with different *p*-substituted phenacyl bromides. The structures of new salts were proved using NMR experiments: <sup>1</sup>H NMR, <sup>13</sup>C NMR, 2D-correlations. The NMR spectra have been recorded on a Bruker Avance III 500 spectrometer operating at 500 MHz for <sup>1</sup>H and 125 MHz for <sup>13</sup>C.

**Acknowledgements:** This work was supported by PN-II-DE-PCE-2011-3-0038, no.268/05.10.2011. We also thanks to the POSCCE-O 2.2.1, SMIS-CSNR 13984-901, No. 257/28.09.2010 Project, CERNESIM, for NMR measurements.

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## P11. Synthesis and NMR characterization of novel anthracene-imidazolium/benzimidazolium salts

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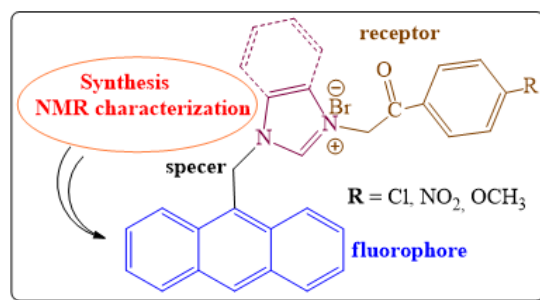
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The design and synthesis of receptors containing imidazole, benzimidazole or pyridine units, attached to a fluorophore, which is the anthracene moiety, have been extensively exploited, due to their biological and environmental importance.<sup>1,2</sup> Also, imidazolium/benzimidazolium salts are well known in the literature with biological properties: antibacterial, anti-inflammatory, anticancer.<sup>3,4</sup>

Having in view this considerations, our main objective was to synthesize and characterize novel anthracene-imidazolium/benzimidazolium salts with *p*-substituted-phenacyl moiety. The syntheses were conducted in only two steps: (I) *N*-alkylation of anthracene with imidazole/benzimidazole,

(II) quaternization reactions of anthracene-imidazole/ benzimidazole derivatives, in the first step, with different *p*-substituted phenacyl bromides. Thus, it obtained the desired **PETs**



obtained  
were

(photoinduced electron transfer), these being a typical fluorophore-spacer-receptor system. The structures of new salts were proved using NMR experiments (<sup>1</sup>H, <sup>13</sup>C, 2D-correlations), recorded on a Bruker Avance III 500 spectrometer, operating at 500 MHz for <sup>1</sup>H and 125 MHz for <sup>13</sup>C.

**Acknowledgements:** This work was supported by *PN-II-DE-PCE-2011-3-0038, no.268/05.10.2011*. We also thanks to the *POSCCE-O 2.2.1, SMIS-CSNR 13984-901, No. 257/28.09.2010* Project, *CERNESIM*, for NMR measurements

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## **P12. New composite materials based on hydroxyapatite (HAP) and novel functionalized poly(trimethylene carbonate) (PTMC) intended for biomedical applications**

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The autologous bone grafts are, despite their limitations, a high standard in bone reconstruction. To limit their disadvantages, non-resorbable implants made of titanium, PTFE, PE, silicone rubbers were considered. Given the high risk of infection inherent in permanent grafts, the research focused on biodegradable and resorbable scaffolds, Therefore, new bone tissue grown at the implant site is the best result to be aimed at.

A synthetic material must have osteoinductive (such as calcium phosphate ceramics with specific surface microstructures)<sup>1</sup> or osteoconductive (e.g., nanocomposites made of synthetic polymer matrices and calcium phosphates or biphasic calcium phosphate which is an intimate mixture of tricalcium phosphate and hydroxyapatite, HAP) properties in order to be successfully employed as bone-proliferating implant.

Thus, new composites based on novel functionalized poly(trimethylene carbonate) (PTMC) matrices and HAP were prepared and characterized, and they seem to be a promising solution. Given that PTMC have no negative effects on bone tissue, such as osteolysis at the implant site,<sup>2</sup> and considering the HAP will grow exposed during the gradual biodegradation of the novel PTMC matrix, creating a new scaffold for osteocytes migration and proliferation, these new composites may have satisfactory osteoinductive properties.

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### **P13. Polysaccharides as renewable polymer matrices for obtainment of multi-component polymer systems**

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*Dedicated to the memory of our dear friend and colleague,*

*Dr. Ruxanda Bodirlau, who recently passed away*

Polysaccharide based polymer units are suitable candidates for use as renewable fillers, in composite materials considering their partially crystalline structure which confers interesting properties. These properties are strongly influenced by the polymer components, their distribution, processing conditions and the interactions between them.

Multi-component polymer systems based on corn starch as thermoplastic polymer matrix and polysaccharide-based polymer matrices from renewable sources (softwood industrial pulp, straw from crop plant) were obtained and characterized. FTIR spectroscopy was performed for structural investigation, while surface and optical properties were investigated through water absorption and transparency measurements, respectively.

FTIR spectroscopy evidenced the changes in the structure of composite films, when hydrogen-bonding interactions between starch polymer matrix and fillers occurred. These interactions involved the hydroxyl, carbonyl and ether groups from the thermoplastic starch matrix and biopolymers components in composite formulations. The water sensitivity was slightly improved due to the addition of fillers in composite formulations, mainly in the first 5h of water sorption testing. Transparency of the starch based films is related to a large extent by the type of incorporated filler. Film samples comprising wheat straw were less transparent compared to those comprising softwood pulp.

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## P14. Study of the optical transparency of novel thermoplastic ternary copolyamide-clay hybrid materials

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The optical transparency of hybrid materials is strongly affected by the type and nature of the filler and matrix, the size distribution of the filler particles, as well as their dispersion, in correlation with the processing parameters. It is known that fillers having micrometric particles scatter the incident light, reducing the transmittance and the optical clarity of composites. On the other hand, nanometric fillers, such as clays, in totally or preponderantly exfoliated composites grant them high optical transparency. Still, when these nanometric clay particles coalesce in large aggregates (i.e., the secondary aggregation as result of processing conditions), they diminish the transparency of the material.<sup>1,2</sup>

In the case of the thermoplastic ternary copolyamide-clay hybrid materials selected for this study, the matrix was an aliphatic semicrystalline copolyamide patented by ICMPP Iasi, Romania, while three different clays, namely K10, I.30P and a native Romanian bentonite BTN, were employed as nanometric fillers (filler content was 5% in all formulations). The electronic absorption spectra evidenced that the hybrids transmittance in the visible range is slightly altered by the filler, which may be explained taking into consideration the penetration of the polymer between the clay platelets, due to their wettability as result of the strong copolyamide-clay interfacial interactions. This complex of phenomena yielded in composites with highly exfoliated structure, as proved by SEM and XRD data as well. Thus, these results come to further confirm the exfoliated structure of the selected composites, along with information from other characterization methods.

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## P15. Physico-chemical methods research of the old documents recovered in border crossing

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The documents represent the most virile proof of existence of a civilization, all of these being protected since antiquity. 3000 years ago, in Europe, after each rainy season, scrolls of papyrus were dry or unroll to see if the rain did not affect the writing.<sup>1</sup> Moreover, for protection against insects, moisture and dust, Egyptians, Greeks and Romans introduced the scrolls written in cylindrical boxes of wood or ivory.<sup>1</sup> Destroying or damaging documents and records of the national cultural heritage cultural identity means damage to cultural identity of a state or civilization, consequently, the inability to transmit this heritage to future generations. The article presents, based on experimental protocols performed in research laboratory of the University, a series of documents, selected and extracted from the evidence rooms and taking into custody for dating, conservation and restoration. For this purpose, using identification data commonly used in retention, in conjunction with different information from scientific investigation through modern system assisted (SEM-EDX, micro-FTIR Analysis Graphics and Graphoscope, Optical Microscopy) has resulted in a number of characteristics specific to the paper and inks, for authentication, restoration and their museum exploitation.<sup>2</sup> Therefore, the dating was managed by identify of some archaeometric features, and preservation of documents in order to be returned in the museum circuit. Also in the article there are presented a number of security features that exists in illicit documents compared with genuine documents used for crossing the border.

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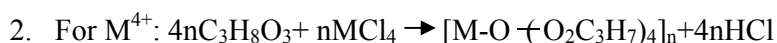
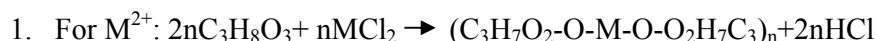
## P16. A new method for obtaining perovskites

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Various methods are used for preparing perovskite compounds including: solid oxide synthesis, sol-gel synthesis, hydrothermal, high-pressure synthesis, mechanically-activated synthesis.<sup>1</sup> The first technique developed for the synthesis of these oxides is the so called ceramic route: a mixture of oxides and / or carbonates subjected to heat treatments at high temperatures. The compound is then processed with the conventional techniques and transformed to powder.<sup>2</sup> CaTiO<sub>3</sub>, BaTiO<sub>3</sub>, BaCeO<sub>3</sub> and PdCeO<sub>3</sub> mixed oxides were synthesized by reaction of M<sup>II</sup>Cl<sub>2</sub> (M<sup>II</sup>=Ca, Ba, Pd) and M<sup>IV</sup>Cl<sub>4</sub> (M<sup>IV</sup>=Ti, Ce), in the 1:1 ratio, with glycerol.



The obtained gel was heated at 120°C for 12h in order to reduce traces and then thermally treated at 300°C, 500°C and 700°C till 24h/step. The intermediate and final compounds were subjected to XRD and FTIR analyses that revealed the formation of M<sup>A</sup>M<sup>B</sup>O<sub>3</sub> compounds type where M<sup>A</sup> = Ca, Ba, Pd and M<sup>B</sup> = Ti, Ce .

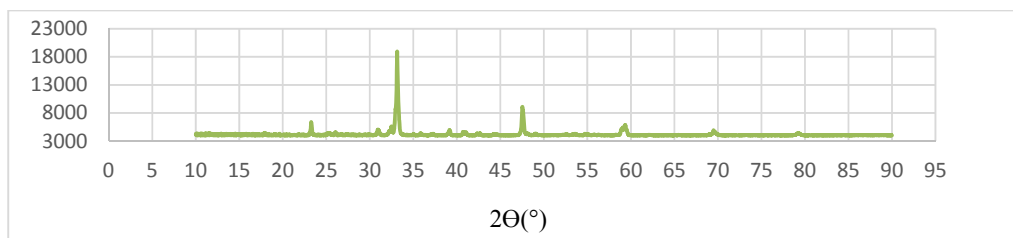


Figure.1. Xray of CaTiO<sub>3</sub> treated 700°C

PdCeO<sub>3</sub> presents photochemical properties in the presence of methyl blue at irradiation with 100W UV lamp. The 0.2mL<sup>-1</sup> dye solution is total depredated after ≈ 5h of irradiation.

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## P17. Study on caloric capacity of fermented and unfermented sewage sludge

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The objective of development for this study is the identification of the best elimination options for the sewage sludge in the Waste Water Treatment Plant of Galati.

For this purpose, several tests were conducted to establish the chemical composition, structure, caloric capacity and ash quantity (after incineration) of the sewage sludge. The methods used for analysis were SEM, EDAX, XRF and DSC.

The researched sewage sludge can be used as fuels with low caloric power (9.5 9,5MJ·kg<sup>-1</sup>mean) in preheated systems of technological materials, for warm water and central heating mixed with coal. Studied sewage sludge can also be burnt in cement fabrics' ovens. The listed procedures present the economic inconveniences regarding preparation, transport, etc.

In siderurgy, in steel making processes, casting and rolling, the sewage sludge usage is not recommended to be used. Sewage sludge is possible and recommended to be used in the process of overcrowding in furnaces, as it creates heat by burning fuel substances out of their own composition. The mix of silicon oxides, aluminium, calcium, magnesium, sodium, potassium, favour the vitrification or overcrowding processes.

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## P18. New ionophores for anion-selective electrodes

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Ion selective electrodes (ISE) are used for detecting various ions important in clinical, environmental and industrial areas, because they offer advantages such as high selectivity, sensitivity, good precision, simplicity and low cost. Ion-selective polymeric membranes usually contain about 30 % (m/m) polymer, 65 % plasticizer and a few % of ionophore and ion exchanger.<sup>1</sup> Ionophores are complexing agents that are capable of reversibly binding ions and transporting them across organic membranes by carrier translocation. Because of the importance of developing new synthetic receptor molecules in the construction of poly(vinyl chloride) membrane ion-selective electrodes, many carboxylates have been introduced as ionophores. The analytical and functional parameters (concentration range where the potential changes with pA linearly, the slope of the calibration curve, selectivity, response time and life time) have been determined.<sup>2</sup> The interference of other species on these parameters and behaviour of the electrodes in policomponent systems were studied.

*Table* Response characteristics of the proposed ion-selective electrodes

ISE	Slope, mV/-lg a	Detection limit, M	pH range	Interference
ISE-perchlorate	57 - 59	$2 \cdot 10^{-6}$	2 - 10	$\text{BF}_4^-$ , $\text{I}^-$ , $\text{SCN}^-$
ISE-nitrate	54 - 56	$3 \cdot 10^{-6}$	2 - 11	$\text{ClO}_4^-$ , $\text{I}^-$ , $\text{SCN}^-$
ISE-thiocyanate	56 - 58	$2 \cdot 10^{-6}$	4 - 11	$\text{I}^-$ , $\text{ClO}_4^-$ , $\text{NO}_3^-$
ISE-salicylate	56 - 58	$1 \cdot 10^{-6}$	7 - 11	$\text{SCN}^-$ , $\text{I}^-$ , $\text{C}_9\text{H}_7\text{O}_4^-$
ISE-dodecylsulfate	58 - 60	$3 \cdot 10^{-6}$	4 - 9	$\text{H}_2\text{C}_6\text{H}_5\text{O}_7^-$ , $\text{C}_2\text{H}_3\text{O}_2^-$ , $\text{NO}_3^-$
ISE-tetraphenylborate	52 - 54	$6 \cdot 10^{-6}$	3 - 11	$\text{ClO}_4^-$ , $\text{I}^-$ , $\text{NO}_3^-$
ISE-perrhenate	56 - 59	$6 \cdot 10^{-6}$	4 - 7	$\text{SCN}^-$ , $\text{ClO}_4^-$ , $\text{I}^-$

The presented electrodes have chemometric parameters good enough for the analysis of these species in real objects.

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## P19. Synthesis, structure and biological proprieties of some Cu(II) complexes with imidazole thiosemicarbazone derivatives

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Thiosemicarbazones are currently well established as an important class of sulphur donor ligands particularly for transition metal ions. These compound containing thione (C=S) and thiole (C-S) groups occupy an important position among organic reagents as potential donor ligands for transition metal ions.<sup>1-3</sup>

In this work we report the syntheses, structure and characterization of copper(II) coordination compounds with thiosemicarbazones 2-methyl -1H-imidazole-4-carbaldehyde (**1**) and thiosemicarbazones 4-methyl -1H-imidazole-5-carbaldehyde (**2**) containing dichloroacetate anion (Fig.1). The complexes were synthesized by reacting ligand with the metal ions in 1:1 molar ratio in an ethanolic medium. The complexes were identified and characterized by elemental analyses, IR and electronic spectral studies also by X-ray diffraction. Copper (II) ions are coordinated via NNS donor atoms at the thiosemicarbazone fragment and O from carboxylate ligand. The mononuclear unit is assembled in dimer via O from carboxylate ligand. The complexes have pyramidal geometry.

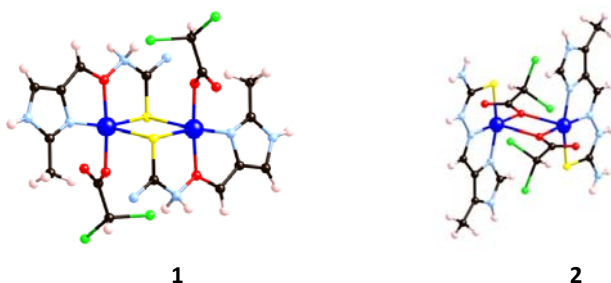


Figure 1. Crystal structure of the synthesized compounds.

The antimicrobial activity against gram-negative and gram-positive bacteria have been determined for this compounds. Newly synthesized molecules exhibited good antimicrobial activity against bacterial species.

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## P20. Investigation of a spin crossover mechanism in an iron(II) compound

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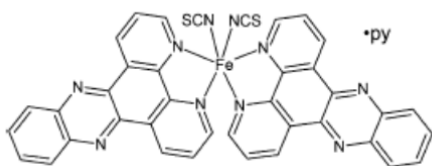
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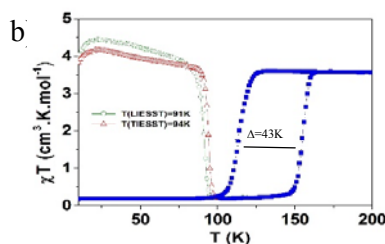
The design of iron(II) spin crossover (SCO) complexes which exhibit wide thermal hysteresis have attracted much attention lately, since their bistable nature could allow their use as molecular switches in new electronic devices. In this aim, it is crucial to understand the main factors which control the spin crossover phenomenon.

We were interested in investigating the cooperative effects in the  $[\text{Fe}(\text{dpp})_2(\text{NCS})_2]\cdot\text{py}$  (dpp = dipyrido[3,2-*a*:2'3'-*c*]phenazine and py = pyridine) compound (Figure 1a) described in 1998<sup>1</sup> which presents a fairly abrupt spin transition at 123 K in the cooling mode and 163 K in the heating mode, with a resulting hysteresis of 40 K (Figure 1b).

In this study we used high-pressure single-crystal X-ray diffraction and Raman spectroscopy to study the spin crossover (SCO) between high spin (HS) and low spin (LS) states in the mentioned above compound. A single geometrical mechanism is responsible not only for the strongest negative linear compression (NLC) behaviour yet observed in a molecular material, combined with negative thermal expansion (NTE) and extreme positive linear compressibility, but also for the high cooperativity of the SCO in  $[\text{Fe}(\text{dpp})_2(\text{NCS})_2]\cdot\text{py}$ . The scissor-like motion of individual molecules is propagated through the lattice via the physical intercalation of ligands and is also responsible for suppressing the expected HS→LS SCO under pressure.<sup>2</sup>



a) Structural formula of  $[\text{Fe}(\text{dpp})_2(\text{NCS})_2]\cdot\text{py}$ .



b)  $\chi_M T$  vs  $T$  for  $[\text{Fe}(\text{dpp})_2(\text{NCS})_2]\cdot\text{py}$  compound.

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## P21. Identification and differentiation of metal ions sorption mechanism onto an ion exchanger functionalized with triethylenetetramine

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Synthetic resins are very promising to preconcentrate and to separate metal ions from complex matrices, invariably needed in the quality control of many materials as well as in the analysis of environmental and biological samples.<sup>1</sup> Understanding the sorption mechanism is an important step in the development of effective technology for treatment of heavy metal contaminated industrial wastewater.<sup>2</sup> The study was conducted on a weak basic ion exchanger of acrylic type copolymer functionalized with triethylenetetramine (TETA), cross-linked with 2% divinylbenzene. The base dissociation constants of the functional group were determined by pH-metric titration using the Gran method. Previous studies in solution were carried out to establish the optimal sorption conditions for eight metal ions Ag(I), Co(II), Cd(II), Cu(II), Mn(II), Ni(II), Pb(II), and Zn(II). The metal loaded resins, after air drying, were analysed by IR spectroscopy, diffuse reflectance UV-VIS spectroscopy, and thermogravimetric degradation. The changes in the IR spectra of the ion exchanger and of the ion exchanger loaded with metal ions suggests the involvement of nitrogen in newly formed metal - ligand chemical bonds. UV-VIS spectra analysis before and after saturation with metal ions suggest complexes of distorted octahedral type. The allure of the obtained TG and DTG curves (in N<sub>2</sub>) and the characteristic parameters determined from thermogravimetric analysis under non-isothermal conditions showed that the degradation is specific to each type of ion, suggesting the involvement of different strong enough chemical bonds. The presence of metal ion affects polymer degradation by improving heat transfer and catalytic action at the temperatures above 200 °C. Oxidative degradation is also dependent on the ion type; the thermostability series is:  $T_{i(R-Zn)} > T_{i(R-Co)} > T_{i(R-Pb)} > T_{i(R-Ni)} > T_{i(R-Cu)} > T_{i(R)}$ . Thermogravimetric stabilizing level indicates oxides as residue.

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## P22. Ultrasound-assisted synthesis of the mesoporous titania photocatalyst

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Nowadays, lot of researchers pay attention to a semiconductor of great value with a huge potential for applications in various areas of nanotechnology of important technological reason (energy, environment, built environment, biomedicine). Titanium dioxide is a semiconductor having a strong oxidative potential due to the positive holes that are capable to oxidize water or various organic molecules to create hydroxyl radicals. Titanium dioxide, in the nanoparticles form has potential for use in energy production, as a photocatalyst. Because of its great photocatalytic properties, an increasing attention has recently been focused on the simultaneous achievement of high specific surface area and the formation of mesoporous TiO<sub>2</sub> frameworks. Today, many researches are still looking for various synthetic method to obtain mesoporous titania photocatalyst. It is well known that its textural properties promote the diffusion of reactants to the reactive sites enhancing the photocatalytic activity of the titania material. Thus, the porosity of TiO<sub>2</sub> nanoparticles has been demonstrated to play an important role in the photocatalytic protection of the environment.

The present work describes an ultrasound-assisted synthetic method of mesoporous TiO<sub>2</sub> nanoparticles. During synthesis, one parameter have been modified and the obtained results are great and comparable with others obtained by conventional synthetic method. The varied parameter is the weight ratio between the used structure directing agent and titania source. In order to understand the exact function of structure directing agents under ultrasound conditions in the proposed synthesis method, surfactant F127 of different weights was used. According, the photocatalytic activity will be discussed, concerning the influence of the used synthesis method and used structure directing agent/titania source weight ratios.

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### **P23. Study on the thermal degradation of brominated flame retardants: computational thermochemistry, kinetics and degradation mechanism**

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The extensive use of flame retardants (FRs) in various materials has led to the widespread and substantial contamination of the indoor environment, e.g. indoor air and dust.<sup>1</sup> Given their relatively low volatility, high elution temperatures are needed when applying conventional chromatographic techniques leading to thermal degradation that generate under-estimation of human exposure to such compounds.<sup>2</sup> Conventional chromatographic techniques suitable for the determination of such compounds are not satisfactory for their determination, especially for higher brominated congeners such as decabromodiphenyl ether (BDE 209).<sup>2</sup> Throughout this study, pathways to thermal decomposition of BDE 209 were investigated by thermochemical computations at the density functional theory level. Therefore we computed bond dissociation energies (DEs) relevant to the initial steps in thermal degradation of BDE 209, one of the most prominent brominated FR reported from Romanian samples. Computed C-Br and C-O DEs foresee a 10 kcal/mol lowering for BDE 209 compared to the nona-brominated compound, whereas the former DE varies within 1-2 kcal/mol with the position on the phenyl ring (ortho>meta>para). We have also investigated thermal degradation behavior of BDE 209 by simultaneous thermogravimetry and differential thermal analysis under different conditions (atmosphere and heating rates). Degradation onset was found to occur at rather low temperatures, around 310 °C. Non-parametric kinetic analysis method was applied to experimental data and the investigation of the obtained isoconversional and isothermal vectors allowed for two parallel major degradation pathways to be identified, corresponding to two different bond breakage patterns.

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## **P24. Functionalization of a natural material towards applications in water depollution**

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Recent trends in the treatment of polluted waters see a shift towards the use of natural and inexpensive products. One of the materials which have been successfully applied in the decontamination of polluted waters are clays. They present numerous advantages such as the lack of toxic by-products, low obtaining costs, easy purification and the possibility of boosting local economy. A difficulty imposed by the use of clays, when applied to a larger, industrial, scale is their removal from the aqueous mixture. Their very small particle dimensions makes their separation from the solution more difficult, and a considerable amount of material is lost. A solution to this problem is functionalizing the clays by combining them with magnetic nanoparticles. This enables the facile recuperation of the new product after depollution by using an exterior magnetic field.

The present study is focused on the insertion of a polymetallic oxide, namely a ferrite, into the structure of a kaolin type clay obtained from a Romanian deposit. Sol-gel autocombustion method was employed to synthesize the material, using glycine as the chelating/combustion agent. The newly created compound was characterized by FTIR spectroscopy, X-ray diffraction, and nitrogen adsorption-desorption analysis. It was then tested in the removal of an organic dye, Basic Blue 41, from aqueous solution. UV-Vis spectroscopy was used to determine dye concentration before and after conducting the adsorption tests.