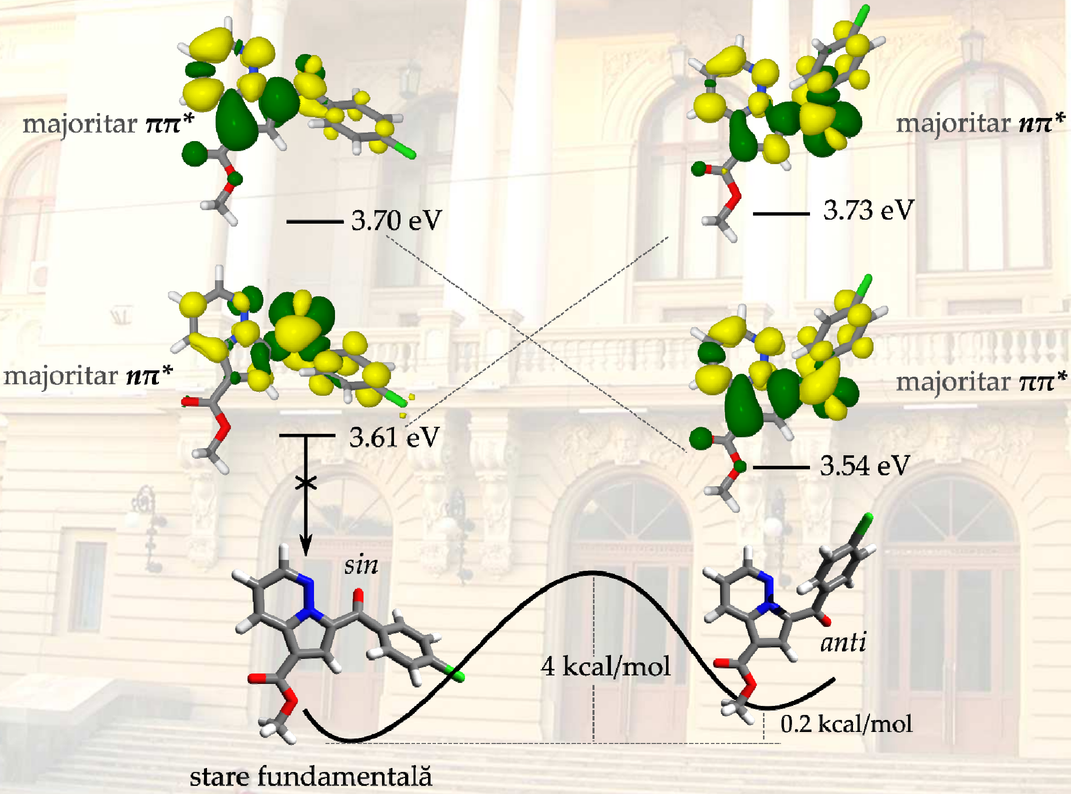
“Alexandru Ioan Cuza” University Days

Faculty of Chemistry Conference

Book of Abstracts



Iasi,
October 31 – November 01, 2014

S. C. ROFAROM
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C1. The separation of biosynthetic products by pertraction

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This presentation is based on our group experience on separation of natural/biosynthetic compounds by free, facilitated and synergic pertraction.

Pertraction, also defined as the extraction and transport through liquid membranes, is a new separation technique and consists in the transfer of a solute between two aqueous phases of different pH-values, phases that are separated by a solvent layer of various sizes. The pertraction efficiency and selectivity could be significantly enhanced by adding a carrier in the liquid membrane, such as organophosphoric compounds, long chain amines or crown-ethers, etc., the separation process being called facilitated pertraction and facilitated transport. Compared to the physical or reactive liquid-liquid extraction, the use of pertraction reduces the loss of solvent during the separation cycle, needs small quantity of solvent and carrier, owing to their continuous regeneration, and offers the possibility of solute transport against its concentration gradient, as long as the pH-gradient between the two aqueous phases is maintained.

Beside the separation conditions and the physical properties of the liquid membrane, the pertraction mechanism and, implicitly, its performance are controlled by the solute and carrier characteristics, respectively by their ability to form products soluble in the liquid membrane. Among the mentioned factors, the pH-difference between the feed and stripping phase exhibits the most significant influence, this parameter controlling the yields and selectivity of the extraction and reextraction processes, on the one hand, and the rate of the solute transfer through the solvent layer, on the other hand.

In this context, the proposed topic will include the methods for obtaining and stabilizing the liquid membranes, and the main results of our experiments on individual or selective separation of some biosynthetic products (antibiotics, carboxylic acids, amino acids, vitamins) by free, facilitated or synergic pertraction. In this purpose, the involved pertraction mechanisms and influencing factors will be discussed.

The main subjects will be as follows:

1. Pertraction of antibiotics (Penicillins G and V, Gentamicins, Erythromycin)

2. Pertraction of carboxylic acids obtained by mixed acids fermentation (carboxylic acids obtained by citric acid, succinic acid and propionic acid fermentations)

3. Pertraction of cinnamic acids (individual and selective separation of cinnamic and p-methoxycinnamic acids from fermentation broths or vegetable extracts)

4. Pertraction of vitamins (nicotinic acid, folic acid)

5. Pertraction of amino acids (fractionation of mixture containing amino acids obtained either by fermentation or protein hydrolysis)

From this very short presentation, it can be concluded that pertraction has a considerable potential for biosynthetic products separation and purification, being required for further development of many biotechnologies, and represents a very attractive research domain for chemical and biochemical engineering.

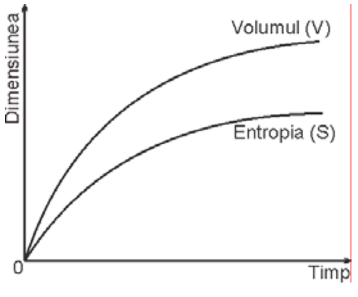
C2. Condițiile inițiale şi legile naturii

G. Bourceanu

Lucrarea îşi propune să analizeze următorul aspect: Evoluția Universului în care trăim, cu o coerență perfectă între milioanele de fenomene cosmice şi cele atomice, este rodul hazardului sau, mai degrabă, această evoluție a fost impusă din condițiile inițiale, înainte de naşterea Universului? Pentru a răspunde la această întrebare se face o incursiune succintă asupra teoriilor despre Univers ce s-au formulat de la Copernic, Kepler şi Newton până în zilele noastre. In acord cu legea fundamentală a dinamicii lui Newton, mişcarea mecanică este reversibilă. Rezultă că *sensul de curgere a timpului nu are nicio preferință. Dinamica clasică nu poate distinge viitorul de trecut.* Mecanica lui Newton, dezvoltată mai târziu de Lagrange, Hamilton şi Laplace a dobândit succese remarcabile în mecanica cerească. Mişcarea aştrilor fiind conservativă, întăreşte imaginea unei mişcări repetabile, reversibile, a unei mişcări ce se reia în mod etern. Aceste aspecte au condus la viziunea unui Univers infinit în timp şi spațiu, a unui Univers fără de început şi fără de sfârşit, a unui Univers static şi etern . Evident, un astfel de Univers, fără de început şi fără de sfârşit, nu avea nevoie de condiții inițiale. După 1915, Einstein, Friedmann şi Lemaitre dovedesc teoretic că Universul are un început.Între 1924-1931, Edwin Hubble, astronom american, realizează măsurători spectrale asupra luminii ce venea de la galaxiile care se găseau la distanțe de milioane de ani lumină față de Calea Lactee. Acesta pune în evidență faptul că lumina, emisă de galaxii, captată de un telescop, suferă o *deplasare a lungimii de undă spre valori mai mari, adică spre roşu.* Pe această cale, Hubble realizează cea mai teribilă descoperire şi anume că Universul este în expansiune. Sursa de lumină, galaxiile, se îndepărtau de observator. Observațiile lui Hubble erau în acord total cu teoriile lui Einstein, Friedmann şi Lemaître.O altă dovadă extraordinară cu privire la expansiunea Universului este creşterea entropiei acestuia. Entropia Universului creşte nu numai datorită degradării energiei ordonate dar şi datorită creşterii volumului acestuia în acord cu relația:

$$\Delta S \approx R \ln(V_p / V_t)$$

unde, V_p şi V_t reprezintă volumul Universului la timpul prezent, respectiv la timpul trecut.



Totul a pornit, aşadar, dintr-un singur punct (originea) printr-o explozie, Marea Explozie, ceea ce a condus la formularea modelului standard al Universului, modelul Big-Bang.

Teoria Big-Bang nu implică numai un început al Universului dar şi faptul că acest Univers este unic. *Dacă Universul este unic atunci condițiile inițiale sunt la rândul lor unice şi devin ele însele legi ale naturii.*

C3. Macrocyclic coordination compounds of some metals based on 2,6- diformyilthiophenol

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The chemistry of container molecules has developed extensively over the past two deca-des.By adjusting the size and form of the binding cavity it is often possible to complex co-liga-nds in unusual coordination modes, to activate and transform small molecules, or to stabilize re-active intermediates.One subclass are the metallated container molecules, in which metal ions and clusters are used as both a point of recognition and to give the container a well-defined structure. Much less is known of ligand systems that encapsulate polynuclear core structures and the chemistry of such systems is not well explored. The ligand H2L (L2¯ = represents a macrocyclic hexaaza-dithiophenolate ligand) is effective dinucleating ligand towards various divalent metals ions and can formed a series of complexes with compo-sition [LMII2(μ-L')]+ (M = MnII, FeII, CoII, NiII, ZnII) (Fig.1).

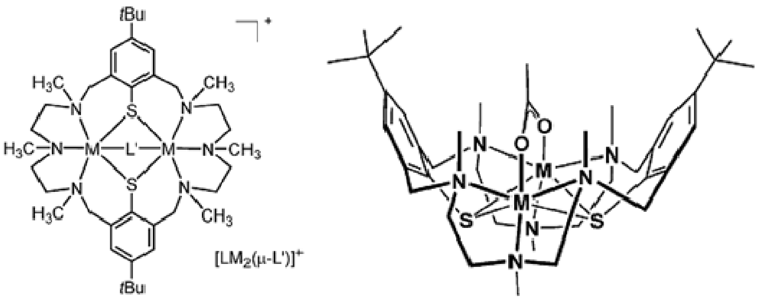

Fig.1.Schematic representation of the complexes$[LM^{II}_2(L')]^+$ (M = Fe^{II}, Co^{II},Ni^{II}, Zn^{II})

These complexes have a rich coordination chemistry since the $[(L)M^{II}_2]^+$fragments are able to coordinate a large variety of coligands as azoligands, carboxylates, which feature unusual ligand coordination modes.Several unusual transformations within the pocket of the $[LM^{II}_2(\mu\text{-}L')]^+$ complexes will be reportd. These include fixation of CO $_2$, *cis*-bro-mination of ***α,β-*** unsaturatedcarboxylate ligands, reduction of S_8 to S_6^{2-} by encapsulated BH_4^-. A series of novel tri-, tetra- and pentanuclear complexes composed of dinucle-ar $[(L)M^{II}_2]^+$units and($CpFeC_5H_4CO_2^-$), ($Fe(C_5H_4\text{-}CO_2)_2^{2-}$),acetylene-dicarboxylate, terephthalate, and naphthalene diimide dicarboxylate groups will be reported.

C4. Supramolecular chemistry: The effect of permodified cyclodextrin encapsulations in photophysical and morphological properties of conjugated polymers for organic electronics applications

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Interest in the area of conjugated polymers for organic electronics applications has intensified during the last few decades, as a consequence of their multiple advantages compared to conventional inorganic materials, such as their solubility and good film-forming properties, of the improvements in the electronic properties through chemical structure modification of the conjugated backbones, of the possibility of preparation on both rigid and flexible substrates, facile synthesis, and low-cost processing. Unfortunately, the use of these materials is often affected by several limitations including undesirable aggregation, which leads to low oxidation stability, charge-transport properties and the ability to self-assemble into ordered nanoscale architectures at the surfaces. As a result, several approaches have been undertaken for the preparation of these materials with enhanced photophysical properties. Currently, in the field of supramolecular chemistry, the construction of mechanically interlocked molecular architectures, such as rotaxanes and polyrotaxanes, is considered an emerging challenge and these supramolecular architectures could provide insight into the design and synthesis of chemical systems for molecular recognition.[1-4]

Our study relies in the investigation of the optical, electrochemical, morphology, surface free-energies, as well as transport properties of the encapsulated conjugated polymers into permodified cyclodextrin derivatives. Their photophysical characteristics will be compared with to those of the non-rotaxane counterparts.

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CO 1. Profesor Lucia Odochian - Contribuții aduse la dezvoltarea tehnicii de analiză termică cuplată cu spectrometria de infraroșu în vederea studiului compușilor micro- și macromoleculari

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This paper is dedicated to the memory of Professor Lucia Odochian, who was born on December 13, 1938 at Botosani, Romania and passed away on August 11, 2014.

Education and scientific degrees: Chemist, Faculty of Chemistry, “Alexandru Ioan Cuza” University of Iasi (1955-1960); Ph.D. (1973); Professor (1992).

Workplaces: Faculty of Chemistry, “Alexandru Ioan Cuza” University of Iasi (1960-2005); Sci. Advisor (2005-2014)

Main fields of interest:

- ✓ Nonisothermal kinetics – Thermal behavior of micro- and macro-molecular compounds;
- ✓ Isothermal kinetics – Chain reactions.

Relevant categories in thermal analyses:

- fields: inorganic, materials, organic, polymer, biology, ceramics.

- method: TG, DTA, DSC, kinetics, specific heat, calorimetry, TG-FTIR, TG-FTIR-MS.

Professional activities: Member of the Chemical Society of Romania (SChR); member of Scientist from Romania Association; member of International Confederation of Thermal Analysis and Calorimetry (1997-2000);

Publication record: number of papers (110; 42 in thermal analysis), books (9), patents (5), citation index (167), h-index (8).

5 most important publications:

- L. Odochian: *J. Thermal Anal.*, **45 (1995)** 1437.
- M. Dumitras, L. Odochian: *J. Thermal Anal.*, **69 (2002)** 599.
- L. Odochian, A.M. Mocanu, C. Moldoveanu, G. Carja, C. Oniscu: *J. Therm. Anal. Cal.*, **93 (2008)** 907.
- L. Odochian, C. Moldoveanu, A.M. Mocanu, G. Carja: *Thermochimica Acta*, **526 (2011)** 205.
- L. Odochian, C. Moldoveanu, G. Carja: *Thermochimica Acta*, **558 (2013)** 22.

From the datasheet submitted to “Who is Who in Thermal Analysis and Calorimetry” book.

CO2. Gas-phase absorption cross sections of selected aromatic hydrocarbons in the IR spectral ranges

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Absorption cross sections of selected volatile and semi-volatile derivatives of benzene in the infrared (IR) regions of the electromagnetic spectrum have been determined using a quartz cell reaction chamber. IR spectra were recorded with an FT-IR spectrometer (with a spectral resolution of 1 cm-1). Absorption cross sections, integrated band intensities and the technical procedure are given for the IR spectral range.

The study focused primarily on the atmospherically relevant (methylated)-1,2-dihydroxybenzenes (1,2-dihydroxybenzene, 1,2-dihydroxy-3-methylbenzene, 1,2-dihydroxy-4-methylbenzene) and some gas-phase ring retaining oxidation products from phenol and cresols isomers (1,4-benzoquinone methyl-1,4-benzoquinone, 2-nitrophenol, 4-nitrophenol, 6-methyl-2-nitrophenol, 3-methyl-4-nitrophenol, 3-methyl-2-nitrophenol, 5-methyl-2-nitrophenol, 4-methyl-2-nitrophenol).

The IR absorption cross sections determined can be used either for the evaluation of IR spectra for measurements of the above compounds in the atmosphere and in laboratory studies on atmospheric chemistry, where FT-IR spectrometry is an important tool.

Acknowledgments: R.I. Olariu and C. Arsene acknowledge the financial support provided by UEFISCDI within the PN-II-PCE-2011-3-0471 Project, Contract No. 200/05.10.2011. CERNESIM Center is also gratefully acknowledged for the infrastructure used in this work.

CO3. Structure – rheological properties relationships in thermo-sensitive polymers

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Thermoresponsive polymers are a class of "smart" materials that have the ability to respond to a change in temperature. This property makes them useful materials in a wide range of applications and for this reason attracts much scientific interest [1]. The synthesis of novel polymers obtained by grafting poly(dimethylsiloxane) with N-isopropylacrylamide (NIPAM), N,N'-dimethyl acrylamide (DMA) and copolymers of NIPAM with DMA and butyl acrylate using SET-LRP technique is presented [2]. The presence of clorobenzyl side-groups allowed both the easy bonding of hydrophobic or hydrophilic groups and good control of the coil to globule transition temperature [3-5]. The lower critical solution temperature (LCST) and the aggregation phenomena (figure 1) during phase transition are evidenced by dynamic light scattering (DLS) and rheology coupled with small angle light scattering (SALS). Good correlation was found between rheological, rheo-SALS and DLS data [2].

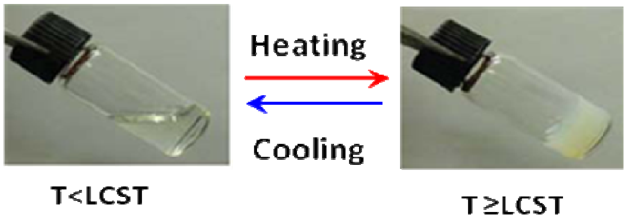

Figure 1. The aggregation phenomena in polymer solutions

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CO4. Influence of TiO_2 and Ag/Au nanoparticles on morphological, thermal, mechanical and catalytic properties of some hybrid composites

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In recent years, the attention of researchers of all over the world was focused on preparing and studying polymer composites with various inorganic components (Si-O-Si moieties, Ag, Au, Pt, CuO, ZnO, TiO_2 nanoparticles and so on) because their potential applications, ease processing ability and potential for large-scale manufacturing. Besides, these materials combine the advantages of organic polymers (flexibility, good impact resistance) with those manifested by the inorganic components (high mechanical strength, enhanced thermal stability, rigidity, good chemical resistance and particularly, optical properties). In this communication we present the synthesis and characterization of hybrid materials incorporating titania and Si-O-Si units achieved through the sol–gel and photopolymerization processes together with photoinduced formation of noble metallic nanoparticles (Ag/Au) in polymer networks. Also, we investigated the effect of the TiO_2 and Ag/Au nanoparticles precursors on the morphological modification of the hybrid materials. Other major characteristics that depend on the TiO_2 amount as well as on the presence of noble metallic nanoparticles are the thermal and mechanical behaviour of the sol-gel hybrid composites. It is well known that the materials incorporating titanium dioxide are widely used as photocatalysts due to their high activity, low cost, long-term stability, non-toxic nature, and excellent photoelectric properties. Preliminarily, we have tested the photocatalytic activity of some hybrid composites in degradation experiments of phenol derivatives under UV irradiation. It was established that the catalyst efficiency is improved by the increase of the content of TiO_2 NPs formed *in situ* in the sol-gel composites and through the existence of noble nanoparticles (Ag/Au) photogenerated *in situ*.

Acknowledgments: A. L. Chibac is thankful for the financial support offered by European Social Fond – " Doctoral and postdoctoral programs – support for increasing research competitiveness in the field of Exact Sciences" - ID POSDRU/159/1.5/S/137750, Sectoral Operational Programme Human Resources Development

CO5. Distribution of mixing efficiency in a split-cylinder air-lift bioreactor for *Y. lipolytica* suspensions

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The biomass or high weight molecular products accumulation usually induces the continuous change of the rheological characteristics or behavior of the broths during a fermentation process. In the case of internal-loop gas-lift bioreactors, the heterogeneity and, implicitly, complexity of the broth hydrodynamics are even more pronounced, due to the cyclic pattern of the fluid flow.

The aim of this study is to establish the distribution of mixing efficiency inside a split-cylinder air-lift bioreactor, as well as the influences of biomass concentration and bioreactor operating parameters on the interchange of active and stagnant positions. The results obtained for *Y. lipolytica* suspensions with cells concentration varying between 10 and 50 g/L d. w. indicate important variations of the mixing efficiency and behaviors of suspensions circulation for the riser and the downcomer regions.

The riser region is associated with the most intense mixing and the highest rates of mass and heat transfer. The broth hydrodynamics in the downcomer region is more complex and is determined by the number and behavior of bubbles entrapped in the fluid circulating downward. The less intense mixing for the upward flow is located at its bottom, as the result of biomass deposition and hindrance of broth circulation. The aeration rate exhibits a continuous positive influence on the ascending circulation for the superior positions, whereas its positive effect on downward circulation is limited only for air superficial velocity up to $1.35 \cdot 10^{-3}$ m/s. The intermediary positions of the downcomer region are associated with the less intense mixing, due to the buoyancy tendency of the bubbles and stratification phenomena.

The influences of the considered parameters were included in three mathematical correlations that allow predicting the mixing time, for both examined regions. The general expression of these models is $t_m = \alpha \cdot C_x^{\beta} \cdot v_s^{\gamma} \cdot h^{\delta}$.

CO6. Heterometallic aminopolycarboxylates as molecular precursors for mixed-oxides

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With respect to physical characteristics that are important for advanced technology, a major target has become heterometallic oxides, which performances are generally determined by the preparative method. An alternative synthetic strategy is the single-source molecular precursor (SSMP) method [1], which allows mixing of the metal species on an atomic scale and considerably reduces the reaction time and temperature. It has been shown that the use of SSMP often favours the formation of heterometallic oxides at conditions even milder than what can be achieved by sol-gel or co-precipitation routes [2]. Aminopolycarboxylate (APC) complexes have been demonstrated to be promising SSMP candidates due to a wide variety of available ligands with high coordination capacity and variable charge which afford an easy adjustable stoichiometry of the target metals. In that context, three series of heterometallic complexes of general formula $BaM(APC)X\cdot nH_2O$ (M = $Co^{2+(3+)}$, Mn^{2+}; X = no specie, H^+ or CH_3COO^-); $M(L)_y\{Bi(APC)\}_2\cdot nH_2O$(M = VO^{2+}, Cu^{2+}; L = 2,2'-bipyridine; y = 0, 1, 2; n = 5 – 16); $Ln\{Bi(APC)\}_z(X)_y\cdot nH_2O$ (Ln^{3+} = lanthanide; X = no specie or NO_3^-; y = 0, 1 or 2; z = 1 or 3; n = 6 – 8) have been synthesized and probed as SSMPs for the preparation of $BaCoO_{3-\delta}$, $BaMnO_3$, $Bi_4V_2O_{11}$, Bi_2CuO_4 or $Bi_{2-x}Ln_xO_3$mixed-oxides. Here, APC stands for nitrilotriacetate (nta^{3-}), ethylenediaminetetraacetate ($edta^{4-}$), 1,2-cyclohexanediaminetetraacetate ($cdta^{4-}$) or diethylenetriaminepentaacetate ($dtpa^{5-}$) ions. The optimal working conditions under which the precursors could be converted to the corresponding heterometallic oxides are heating at low rates under air or oxygen flows. The conditions required to produce heterometallic oxides from the corresponding SSMP are significantly milder than what has been previously reported.

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Acknowledgements: This work has been carried out with the financial support of Erasmus Mundus Ianus II project.

CO7. Activation of the thiosemicarbazide fragment through coordination with transition metals

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The coordination chemistry of the transition metal coordination compounds containing thiosemicarbazide derivatives has been widely investigated due to their attractive chemical, physical and biological properties. Using various thiosemicarbazide derivatives and different metal ions with a variety of oxidation states allows preparing a large number of coordination compounds with original structure and properties.

In this work we present a new area of activation of the thiosemicarbazide fragment and its condensation product with different carbonyl - thiosemicarbazone by coordination to the transition metals. For example, for manganese chemistry it is necessary to obtain a precursor in the strong basic medium and afterwards promoting the oxidation reaction in different solvent. For copper compounds important is the role of the pH value, in order to obtain materials with protonate, molecular or deprotonate thiosemicarbazone present in the crystal structure. All these parameters present in thiosemicarbazide fragment permit to predict the composition and structure of the final products of a metal promoted or templated reaction. The influences of the carbonyl group, pH-value, and derivatives of thiosemicarbazide (Figure 1) on the crystal structure, magnetic and biological properties were studied for each type of compounds.

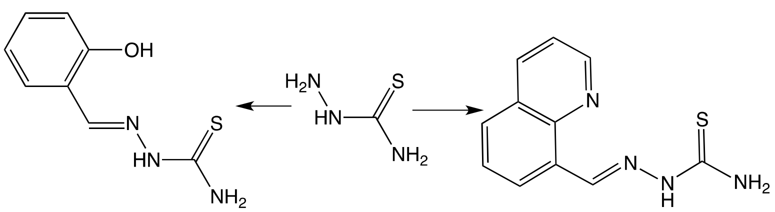

Figure 1. Derivatives of 4-thiosemicarbazide

Acknowledgements: The authors thanks Erasmus Mundus EMERGE scholarship program, AUF Eugen Ionesco postdoctorate grant, CIM- Centre for International Migration and Development and ASM, USM and Supreme Council for financial support, projects: 11.817.08.42F, 14.819.02.15F and 14.518.02.01A.

CO8. New investigations on the gas phase reactions important for Atmosphere

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The oxidation process in the atmosphere is very complex and despite years of research studies is still poorly understood. There are two important environments which catch mostly the attention: urban atmosphere characterized by high NOx environments and remote atmosphere characterized by low NOx environments.

Among the different classes of anthropogenic VOCs emitted to the atmosphere, aromatic hydrocarbons are of particular interest to urban atmosphere. They contribute appreciably to photooxidant and SOA formation and are associated with human health problems. Nitroaromatics, which are important intermediates in the chemical industry, possess carcinogenic and phytotoxic properties and have been implied to play a role in forest decline. In a recent study in our laboratories formation of nitrous acid (HONO) from the photolysis of nitrophenols has been shown for the first time.

HONO is of major significance in tropospheric chemistry since the photolysis leads to the formation of OH radicals, the key atmospheric oxidant in the degradation of most air pollutants and a crucial intermediate in the formation of photochemical smog in the troposphere. Recent field studies have demonstrated that the contribution of HONO to the oxidation capacity of the atmosphere has been underestimated and point to the existence of yet unknown daytime sources of HONO.

Formation of HONO in the gas phase was studied in a flow tube photoreactor upon irradiation (300-500 nm) of ortho-nitrophenols and ortho-nitrotoluenes and derivatives, using a selective and very sensitive instrument (LOPAP) for the detection of HONO. Photochemical formation of HONO was observed upon irradiation for the first time, which was linear correlated to the gas phase concentration of the nitrocompounds. Variation of the surface to volume ratio and the nitrocompounds concentration showed that the photolysis occurred in the gas phase. The huge difference on the HONO formation between 2- and 3-nitrotoluene supports that HONO formation is initiated by intramolecular hydrogen transfer from the ortho-alkylic CH_3 group to the nitro group. Contribution of photolysis of nitroaromatic compounds to the oxidation capacity of the urban atmosphere will be discussed.

CO9. The identification of the materials used in a panel painting icon

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This paper presents a study on pigment identification of the panel painting icon "Saints Constantine and Helen", which comes from an important church in Iasi, Romania. The icon is painted in the Byzantine style, characteristic for the Orthodox Church. As a cultural heritage monument, the iconostasis of the church has an artistic and historic value. In time it suffered a great deal from earthquakes, floods, wars and fire. In the XXth century a large fire burned big parts of the iconostasis and the original painting needed to be replaced. Using modern techniques of investigation, important information about the icon painting technique, the materials used and about the period in which the icon was made, were found. The aim of this study is to gather useful information about the icon to make a suitable conservation and restoration of the artifact. For the analysis of the icons components (preparation layer, paint layer and varnish), the Optical Microscopy (OM), the scanning electron microscopy connected with X-ray spectrometry (SEM-EDX) and the Fourier transformed infrared spectrophotometry (μ-FTIR), were used. It was concluded that the paint layer is made of tempera (pigment with emulsion), and gold leaf for the halos. From the style of the painting and of the conservation state, it is presumed that it was painted in the XIXth century. The corroboration between the analytic techniques, highlighted different details of the painting process and of the used materials. Thus, mineral pigments, colored earths, gold leaf and calcium based gesso, were identified.

Keywords: panel painting icon, wood specie identification, OM, SEM-EDX, μ-FTIR.

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CO10. Effect of temperature on aliphatic–aromatic polyimides

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The effect of temperature on six semiaromatic polyimides was investigated. The structures thermal decomposition processes had been conducted using dynamic thermogravimetry in nitrogen atmosphere and up to 700 ^{o}C. Comparative thermal stability studies of the samples were conducted. The thermostability of the studied structures was dependent on the nature of the entities linking the benzophenone–3,3′,4,4′–tetracarboxylic dianhydride (BTDA) moieties. Such aromatic entities were found to greatly increase the thermal stability of the polyimides, compared to cycloalkyl and linear alkyl linkers. The analyses of evolved gases were monitored *via* dynamic thermogravimetry coupled to a quadrupole mass spectrometer and a Fourier transform infrared spectrometer equipped with external modulus for gas analysis. Evolved gases analyses showed a complex gaseous mixture. The Ozawa–Flynn and Wall (OFW) and non–linear regression methods were applied for the kinetic study. There was observed a decrease in kinetic parameters values with conversion degree, suggesting the occurrence of a change in the rate determining step.

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CO11. Polymeric adsorbents with covalently immobilized ionic liquid-like fragments for retention of metal ions

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Metals and their compounds are essential to economic development due to their applications in a variety of domains. However, heavy metals make a great impact on environment quality and human health because of their high toxicity and also because they are conservative pollutants, bioaccumulating in organisms and ecosystems. Usually, these metals and their compounds are introduced into natural water resources by wastewaters dumped from industrial activities; therefore, their removal from contaminated waters is an absolute necessity.

The purpose of this work was to investigate the possibility of employing polymeric materials containing covalently immobilized ionic liquid-like fragments for the retention of heavy metal ions from aqueous salt solutions. The adsorbents were synthesized by a stepwise method using gel-type (microporous) styrene-divinylbenzene copolymers with different divinylbenzene contents, as primary polymeric precursors, and an imidazolium-based ionic liquid. The utilization for the adsorption of heavy metal ions of these materials consisting of supported ionic liquid-like phases was investigated by carrying out batch experiments. It was evidenced that the adsorption behavior is dependent on the initial pH of the salt solution: the less acidic the solution, the better the adsorption capacity. At the optimal pH value, the adsorption capacity increased with the increasing of the initial metal ion concentration. The higher content of ionic liquid-like fragments resulted in improved adsorption performance for the retention of metal ion species. The equilibrium adsorption data were analyzed using different isotherm models, and the model which simulates better the experimental results was determined. On the basis of the obtained results, the adsorption mechanism and the structure of the resulting compounds were suggested. It was revealed that these adsorbents have potential to be employed for the removal of heavy metal ions from aqueous solutions, and hence could find applications as adsorbents in wastewater treatment.

CO12. Metallopolymeric systems based on polyesterurethane and iron ions: Synthesis and characterization

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The study of the interactions taking place in polymer-metal ions systems gains increasing importance since it provides valuable information on the capability of polymers to retain metal ions and the influence of the latter on the synthesis, processing and properties of the former. Metallopolymers suitable for a variety of applications may be tailored by selecting the appropriate reactants and preparation conditions. Polyurethanes are an important class of industrial polymers; therefore it is of great interest to establish the way in which they are affected by the presence of metal ions.

The present work deals with the investigation of polyesterurethane/iron(III) ions systems in order to determine the influence of this ion species on the polymer structure and properties. A series of four metallopolymers whose iron content ranges from 0.06 to 0.82% were synthesized from a linear segmented MDI-based polyesterurethane and ferric chloride hexahydrate, $FeCl_3 \cdot 6H_2O$, by using different molar ratios of urethane groups to iron ions in the initial reaction systems. The metallopolymers were characterized in comparison with the parent polymer by spectroscopic (AAS, UV-vis absorption spectroscopy and FTIR spectroscopy) and thermal (DSC, DMA and TGA) methods. As compared with the polyurethane, the metallopolymers exhibit a characteristic colour, as well as enhanced adherence to different substrates and improved solvent resistance. Iron(III) ions form complexes with polymer functional groups, the intermolecular complexation resulting in coordination crosslinking of the polymer chains. As a consequence, the interurethane hydrogen bonding existing in the hard-segment domains is disturbed. The complex formation interferes with the packing of the hard segments inducing modifications in hard segment crystallinity. An interplay of factors leads to the viscoelastic behaviour of metallopolymers. All processes involved in polyesterurethane thermal decomposition are favored by the presence of iron (III) ions. Generally, the higher the iron content of the metallopolymers, the more pronounced the differences between their properties and those of polyurethane.

CO13. Magnetic Nanocomposites PLGA/Magnetite

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The study presents the synthesis of some new materials with magnetic properties, achieved by the double-emulsion (w/o/w) method, based on PLGA copolymer and magnetite (Fe_3O_4). The low molecular weight PLGA copolymer used to obtain the magnetic nanocomposites was synthesized by the copolymerization of lactic acid (LA) with glycolic acid (GA), molar ratio LA/GA (80/20) in the presence of tin octanoate [$Sn(Oct)_2$] as catalyst, by polycondensation procedure. Magnetite was obtained by co-precipitation from aqueous salt solutions $FeCl_2/FeCl_3$ (molar ratio 1/2). The particles size of magnetite measured by DLS-technique was 420 nm, and the saturation magnetization 62.78 emu/g, while the PLGA/magnetite nanocomposite size was 864 nm and the saturation magnetization 39.44 emu/g. The polymer matrix, magnetite and magnetic nanocomposite were characterized by infrared spectroscopy (FT-IR), scanning electron microscopy (SEM), dynamic light scattering (DLS) technique, and vibrating sample magnetometer (VSM). The thermal properties and evolved gases analysis by thermal decomposition of the PLGA copolymer has been determined by simultaneous thermal analyses TG/DTA-FTIR-MS, and a possible degradation mechanism was proposed.

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SC1. Controlled synthesis of water-soluble HPAM-NAS copolymer via RAFT polymerization and post-polymerization modification reactions

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The reactivity ratios of N-(2-Hydroxypropyl) methacrylamide (HPMA) with N-Acryloxysuccinimide (NAS) were determined in DMSO with free radical polymerization and in DMSO and DMF with reversible addition-fragmentation chain transfer (RAFT) polymerization. Furthermore, RAFT mediated copolymerizations were conducted at two different feed compositions of NAS (20 mol % and 30 mol %) in DMSO and respectively DMF. In the second case, size exclusion chromatography of the polymers was used to confirm the RAFT control over the copolymerization. By selecting an appropriate monomer feed ratio and conversion during the polymerization, we show that we can prepare compositionally uniform copolymers.

In the structure of the synthesised copolymer, the NAS units provide reactive functional groups, which can be further post-modified. Modification of the polymer with an amino-functionalised crown ether demonstrated the ability of the pendant NAS groups to be functionalised without the formation of any cross-linked products. In short the direct RAFT-mediated polymerization of the HPMA/NAS co-monomer system has been demonstrated, followed by the post-polymerization modification of the final product with functional crown-ether moieties, in order to obtain a water soluble precisely controlled copolymer bearing crown ether moieties as lateral substituents, with possible applications in building quartz crystal microbalance (QCM) sensors for Pb(II). The QCM modified sensor was evaluated for the determination of Pb(II) in aqueous solutions, as a promising alternative for the lead detection and quantification.

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SC2. Maleic acid copolymers for the preparation of stimuli-sensitive microparticles

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Thermo- and pH-sensitive copolymers based on maleic acid and N-vinyl caprolactam were synthesized and their composition was determined by ^{1}H NMR spectroscopy and conductometric titration. The behavior of the poly(N-vinyl caprolactam-co-maleic acid) (VCL-MAc) in aqueous solution is a result of the interplay between electrostatic, hydrophobic and hydrogen-bonding interactions. Thus the copolymer precipitates from aqueous solution with the increase of the temperature, with the decrease of the pH or with the interaction with hydrophobic drugs. The lower critical solution temperature is influenced by the copolymer composition, ionic strength and pH of the solution.

VCL-MAc copolymers were cross-linked with hexamethylendiamine in order to obtain stable stimuli-sensitive microparticles (Fig. 1). The water retention of the microparticles is strongly influenced by the pH (Fig. 2), but only a slight influence of the temperature was observed. When the microparticles were loaded with model drugs (dyphenylhydramine, metoclopramide), a burst release of the drugs were obtained in buffers, independent of the pH, due to the fact that the salt determines the screening of the electrostatic interactions.

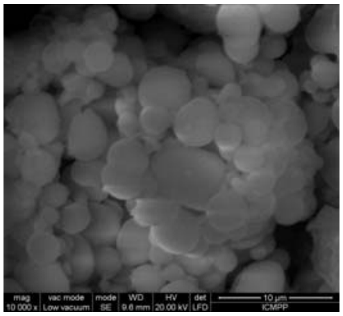

Fig. 1. SEM image of VCL-MAc microparticles

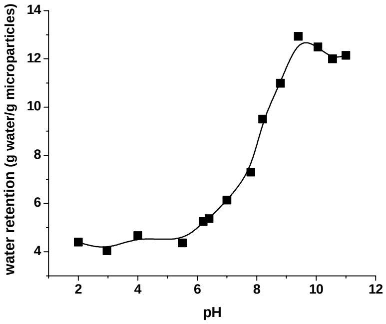

Fig 2. Influence of the pH on the swelling characteristics of VCL-MAC microparticles in water

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SC3. Cationic polysaccharides: Synthesis, characterization and application of quaternary ammonium salts of curdlan

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Polysaccharides with quaternary ammonium groups have some important properties as for example: hydrophilicity, biodegradability, biocompatibility, and bacteriostatic properties very useful for bio-applications. These derivatives are widely used in different fields including waters treatment, papermaking, food, pharmaceutical, and cosmetic industries. These derivatives can be obtained by the reaction of the native polymers with reagents with ammonium groups such as glycidyltrimethylammonium chloride, 3-chloro-2-hydroxypropyltrimethylammonium chloride.

The aim of this work was to synthesize of some novel quaternary ammonium salts of curdlan. Curdlan, a bacterial polysaccharide formed by pure culture fermentation of *Agrobacterium biobar 1*, is a polysaccharide with a linear structure composed entirely from D-glucose linked by β-glicosidic bonds in (1→3) positions. New curdlan derivatives with quaternary ammonium groups were synthesised using etherifying agents such as 2, 3-epoxypropyl trialkylammonium chloride or (3-chloro-2-hydroxypropyl) trialkylammonium chloride. The obtained derivatives with good water-solubility were characterized by FTIR and NMR spectroscopy. The viscosity behavior and the complexation capacity of these new polysaccharide derivatives were also studied. In order to obtain polyelectrolyte complexes (PECs) for further biologically active principles incorporation and delivery, the obtained cationic curdlan derivatives were used as cationic partners, while the monobasic curdlan phosphate was used as anionic partner. The interaction between curdlan derivatives was in situ investigated by turbidimetric measurements and the resulted PECs were characterized after 24 hours of equilibration by optical density and dynamic light scattering methods. The morphology of the PECs particles in dry state was investigated by atomic force microscopy.

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SC4. Lysosomal Storage Disease. Characterization and Diagnostics of MPS II and MPS VI

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Lysosomal storage diseases (LSDs) are a group of rare and inherited diseases that lead to accumulation of glycosaminoglycans (GAGs) in different organs and tissues. People with one of this disease do not produce enough of the specific lysosomal enzyme required to break down this long sugar chains in small pieces. Accumulation of GAGs within lysosomes can produce progressive cellular damage leading to skeletal malformations, pulmonary deficits, short stature, retarded growth, hepatic and cardiac abnormalities and sometimes neurological abnormalities[1].

MPS II, known as Hunter disease, is one of the most common MPSs and is caused by a deficiency of the lysosomal enzyme iduroate-2-sulfatase (I2S), which catalyzes the removal of the sulfate group at the 2 position of L-iduronic acid in dermatan sulfate and heparan sulfate. MPS VI, known as Maroteaux-Lamy syndrome is determined by the absent activity of the enzyme arylsulfatase B (ASB) also named N-acetylgalactosamine 4-sulfatase. ASB is required for degradation of the glycosaminoglycans dermatan sulfate and chondroitin 4-sulfate[2].

In this report we describe a specific and sensitive diagnostics on dry blod spots (DBS) for single and multiplexing assay from MPS II and MPS VI patients by multiple reactions monitoring mass spectrometry (MRM-MS). We optimized enzyme reaction condition and procedure for the assay, including concentration of substrates and internal standard, composition of extract buffer and mass spectrometer parameters. Clinical diagnostics assays were developed by MS-MRM determinations with an Esquire 3000 ion trap mass spectrometer (Brucker, Germany). 7

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SC5. Photopolymerizable hybrid composites containing silver nanoparticles

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A popular route toward the preparation of advanced functional materials for applications in nanoscience and nanotechnology is focused on fabricating nanoparticle assemblies [1] and polymer-nanoparticle composites, which may have various novel and improved properties originating from the synergism between organic and inorganic components. As a consequence, these hybrid nanocomposites have a large applicability in many important areas such as coatings, [2] inks, [3] dental materials, [4] optical elements, [5, 6] photoresits, [7, 8] and so on. One of common methods used for the obtaining of hybrid composites involves a photochemical approach for the *in situ* synthesis of metal nanoparticles and particularly, noble metals (silver, gold), created during the photopolymerization of some liquid monomers incorporating metal salt precursors. [9] To this end, we studied the synthesis of hybrid composites using a mixture of photopolymerizable monomers and silver nitrate witch exposed to UV irradiation leads to organic/inorganic polymer networks. Characterization of the formed materials was done by UV-Vis spectroscopy, FTIR and FotoDSC, fluorescence measurements, EDX and TEM analysis.

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SC6. In vitro testing of polyvinyl alcohol/chitosan hydrogels as systems for controlled delivery of bisoprolol fumarate

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Biodegradable polymeric materials have a great impact on the science of controlled drug delivery due to their simplicity, cost effectiveness, reduced risk of systemic toxicity, being good carrier for both small molecules and bioactive macromolecules. In this study, we reported the synthesis of hydrogels based on poly (vinyl alcohol)/chitosan, by repeated freezing and thawing cycles. Prior analysis, the obtained materials were dried by two methods, respectively lyophylization and vacuum drying.

The freezed-thawed obtained membranes based on poly (vinyl alcohol) and chitosan were thermally characterized by means of thermogravimetric (TG), differential scanning calorimetry (DSC) and dynamic thermo-mechanical analysis (DMTA); the morphological aspects were followed by scanning electron microscopy (SEM) completed by swelling measurements and drug released tests. The hydrogels were characterized by swelling measurements in bidistilled water because the swelling capacity may significantly influence the drug release profile. The aim was to determine the influence of chitosan concentration on the degree of water absorption. Also, the load/release behavior of bisoprolol fumurate on the obtained systems was tested under physiological conditions.

The swelling degree was depended of the polymeric material morphology, according to the drying mechanism and the chitosan content. Thus, the swelling degree increases with decreasing the chitosan content in case of lyophilized hydrogels and the variation is opposite in case of vacuum dried hydrogels. It was observed that the drying method has influenced the drug loaded/release process of hydrogels. The poly (vinyl alcohol)/chitosan materials loaded with bisoprolol fumarate could be proposed as drug delivery systems and promise to have a great impact in human health care.

SC7. Molecular characterization of eosinophil peroxidase peptide by mass spectrometry

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Eosinophil peroxidase (EPO) is an haloperoxidase enzyme, whose structure is composed of two chains: glycosilated heavy chain of aproximatively 53 kDa and a light chain of aproximatively 13 kDa. The two consituing chains are bound by strong non-covalent forces. Human eosinophil peroxidase is a secreted hemoprotein and plays an important role in the defense mechanism of the organism against multicellular parasites [1]. In its primary structure EPO presents several tyrosine residues that can be modified by oxidation, in particular by nitration. Nitration at the tyrosine residue occurs in normal physiological conditions,but it is more intense in disease conditions such as inflammations[2]. Eosiniphil peroxidase was extracted from human eosinophil granule suspensions, derived from hypereosinophilic patients with marked eosinophilia and purified by chromatographic methods[3]. Further the obtained peptide was analyzed by 1D electrophoresis. The sample was prepared both in presence and absence of a reducing agent. A band corresponding to intact EPO and two bands corresponding to heavy and light chain were observed in gel. Western Blot experiment realised using anti 3-NT monoclonal antibody showed that only the intact EPO and the heavy chain were 3NT-positive. The bands were exicesed from gel and digested with trypsine. All the peptides resulted from digest mixture were measured by MALDI-FT-ICR and the corresponding monoisotopic masses were used for database search using Mascot peptide mass fingerprinting search engine. As a result eosinophil preperoxidase (AA-127 to 575) was identified with a high probability.

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SC8. The in vitro testing of xanthan/lignin hydrogels as carriers for controlled delivery of bisoprolol fumarate

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Many hydrogel - based delivery matrices have been designed and fabricated to fulfill the ever-increasing needs of the pharmaceutical and medical fields. The objective of this study was to develop novel matrix for sustained-release of drugs based on highly water-soluble natural gums, like xanthan, as cost-effective, non-toxic, easily available, and suitable hydrophilic systems. Xanthan and epoxy-modified lignin resin (LER) mixture were crosslinked using epichlorohydrin as crosslinking agent leading to superabsorbant hydrogels with high swelling rate in aqueous mediums. These hydrogels were tested as carries by the loading / delivery behavior of bisoprolol fumarate in physiological conditions and based on the obtained results these hydrogels may show interest for application in medical and pharmaceutical areas. The amount of drug loaded in polymer networks was found to be ranging between 14.4 % and 19.2 % increasing with lignin content of hydrogels. The drug release was retarded and mechanism was found to depend on matrix composition.

Table I. The drug loading degree for hydrogels

Sample code	Drug loading degree determined by UV-Vis
90X/10LER	14.4 %
80X/20LER	14.8 %
70X/30LER	16.4 %
65X/35LER	19.2 %

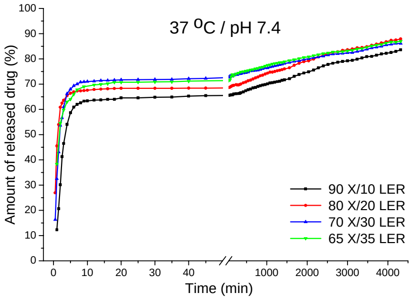

Figure. 1. The drug release profiles of BF from X/LER hydrogels with different composition

The hydrogels based on X/LER loaded with bisoprolol fumarate may show interest for application in medical and pharmaceutical areas.

SC9. Synthesis and characterization of poly(arylene ethynylene)s containing indol[3,2-b]carbazole moieties

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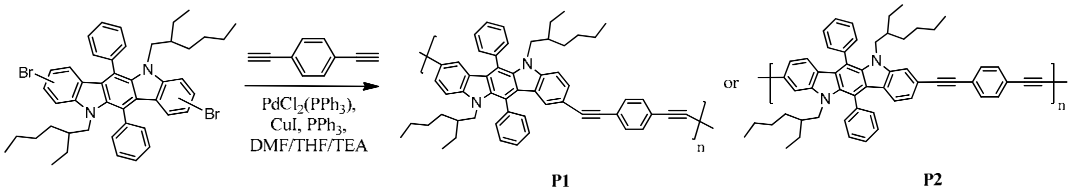
Poly(arylenen ethynylene)s are an interesting class of conjugated polymers that have potential uses in the field of thin film transistors, sensors, organic LEDs, molecular wires and photovoltaic cells [1, 2]. Indolo[3,2-b]carbazoles represent an important class of ladder-type N-heteroacenes, which have various applications in the area of organic electronics and biology. The indolo[3,2-b]carbazole core has an advantage compared to that of carbazoles because of a larger resonance structure that includes three phenyl rings [3]. In this study, we report the synthesis, characterization and opto-electrochemical properties of two polymers containing 2,8- or 3,9-disubstituted indolo[3,2-b]carbazole moieties, spaced by 1.4-phenylene ethynylene groups (P1 and P2). The polymers were synthesized *via* Sonogashira coupling polymerization (Scheme 1).



Scheme 1: Synthesis poly(arylene ethynylene)s by Sonogashira coupling reaction

The polymers have been characterized via Fourier-transform infrared spectra (FTIR), ^{1}H and ^{13}C-NMR spectroscopy, gel permeation chromatography (GPC), UV-vis absorption and fluorescence spectroscopy and cyclic voltammetry, respectively. The dependence of optical and electronic properties on the connection positions of indolo[3,2-b]carbazole units in the polymer chain is discussed.

Acknowledgments: Authors thank the Romanian National Authority for Scientific Research (UEFISCDI) for the financial support (grant PN-II-ID-PCE-2011-3-0274, contract 148/2011).

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SC10. Phenothiazine derivatives. The influence the of substituent upon optical and electrochemical properties

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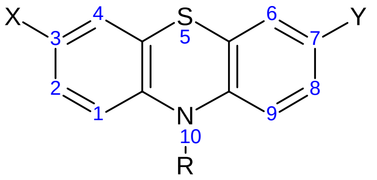
A new series of phenothiazine derivatives have been obtained by introduction of different substituents having electrono-acceptor or electrono-donor character, in order to create push-pull systems. Formyl, carboxyl and cyanoacryl units were used as electron acceptor units, and bromine atomwas used as electrono-donor moiety (Figure 1.).



R = $C_{12}H_{17}O$ (n-hexyloxyphenyl)

Figure 1. General structure of phenothiazine derivatives

Cod	**X**	**Y**
Fh	-H	-H
FhBr	-H	-Br
$FhBr_2$	-Br	-Br
FhA	-CHO	-H
FhABr	-CHO	-Br
FhAc	-COOH	-H
FhBrAc	-COOH	-Br
FhCA	-CH=C(CN)COOH	-H
FhBrCA	-CH=C(CN)COOH	-Br

Thecompounds under study were structural characterized by FTIR and ^{1}H-NMR spectroscopy and single crystal X-ray diffraction. Besides, the single crystal X-ray diffraction brings information regarding the supramolecular architecture of the compounds.

Photophysical properties indicated that the absorption maxima vary in a large range(322-455 nm), reflecting the different electronic delocalization degree, depending by the substituent nature. In a similar manner, the emission spectra reveal different colours of emited light, a red shift being evident for the groups with higher electron withdrawing ability (Figure 2.).

Figure 2. Light emission when using a UV lamp

Electrochemical study show reversible oxidative and reduction processes for all the compounds, and a close correlation of the HOMO-LUMO band gap with substituent nature.

SC11. Poly(vinyl alcohol) copolymers biodegradation with Trichotecium roseum fungi

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The study presents the biodegradation of poly(vinyl alcohol) (PVA) and some PVA copolymers using *Trichotecium roseum* fungi. The samples were examined after several days of innoculation, up to maximum 24 days. Structural modifications of the biodegraded samples were investigated by FTIR-ATR spectroscopy, the surface morphology by scanning electron microscopy (SEM). The static light scattering (SLS) study revealed that the weight average molecular weight (Mw) of the copolymers increased after biodegradation, due to the destruction of the fractions with low molecular weight. The thermal characteristics of the biodegraded samples were analysed by differential scanning calorimetry (DSC) and thermogravimetry analyses (TGA). The DSC results concluded that biodegradation took place in the amorphous domains of the investigated samples.

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P1. Physico-chemical forensic expertise in the analysis of soil samples by graphite furnace atomic absorption spectrometry

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Atomic absorption spectrometry (AAS), in physico-chemical forensic expertise, as in many other research areas, is characterized by accuracy, reliability and precision to determine the exact concentrations of metals and nutrients of very low concentrations in a sample, regardless the fact the sample is contaminated or not with other elements.[1] Graphite furnace atomic absorption spectrometry (GFAAS) technique, on a solid module, was used in the present work to investigate soil samples collected from two different locations (Ciric-Venetia and Dobrovat) in Iasi county, north-eastern Romania. Four soil samples were collected and analysed from each single interest location. For the sampling procedure strategic "forensic trace" points, distributed along the routes identified as belonging to "crime scene scenarios", have been chosen for further investigations. Specific protocols have been rigorously followed for investigating the forensic evidences in the interest samples. Heavy metals, i.e. Pb, Cd, Cr and Ni, at trace levels (mg kg^{-1}, μg kg^{-1}), have been measured. Among the quantified elements, lead was tracing a specific behaviour at both Ciric-Venetia and Dobrovat locations. Higher concentrations of lead were determined in particular in samples characterised by the influence of intense traffic (Ciric-Venetia) or in samples from areas where geographical features would enhance accumulation of this element in time (valleys). The results obtained within the present work allow us suggesting that lead can be included in the category of potential "tracers" for possible forensic trace identification. Moreover it can constitute very good evidence to state the possible presence of a suspect at the crime scene.

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Acknowledgments:CERNESIM, is gratefully acknowledged for the infrastructure used in this work.

P2. Water soluble organic carbon in aerosols from Iasi, north-eastern Romania

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Within the Convention's Cooperative Programme for Monitoring and Evaluation of the Long-range Transmissions of Air Pollutants in Europe (EMEP) a number of different particulate matter (PM) parameters are part of a well developed monitoring strategy.[1] Two levels of the EMEP strategy are mandatory while the last is voluntary. However, it is generally admitted that the monitoring strategy is far from fully implemented. Organic carbon (OC) speciation, related to both water-soluble and water-insoluble OC, is included within level 3 of the monitoring programme strategy, since it scatters the solar radiation finally influencing aerosol climate direct forcing. In the present work chemical characterization was performed on water soluble organic carbon (WSOC) fraction of aerosol total carbon (TC) from Iasi. Sampling has been undertaken during the cold season in an urban environment with less exposure to anthropogenic emission sources, i.e. Botanical Garden from Iasi, Romania. Aerosol samples were collected on prebaked quartz filters (600 ^{o}C) loaded on a Stacked Filter Unit (SFU). Samples were continuously collected for 72 h. For the measurements of WSOC, one quarter of the filter was soaked in 20 mL ultrapure water (18.2 MΩ.cm rezistivity), with ultrasonic treatment for 40 min. The analyses of WSOC concentrations were performed on a 3100 Multi N/C Analyzer, Analytic Jena, Germany, by a technique based on the IR detection of the CO_2 formed after the hot chemical oxidation of the carbon content of the liquid sample. The WSOC concentrations, in this study, varied from 0.78 to 6.93 μg C m^{-3} (average: 3.03 ± 1.53 μg C m^{-3}). The values are in agreement with other reports[2] but in the present study the WSOC fraction is ~99% of the total soluble carbon.

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P3. Multicriteria analysis applied to bioplastics and bioenergy production from waste

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One of the greatest global challenges facing the world today is to minimize the production of waste and obtain new products from recovered materials, mainly from waste.

Starting from the premise of the 7th Environmental Action Programme "Turning Waste into Resources", which proposes waste conversion into valuable materials and energy resources so as to achieve "zero waste", the purpose of this study is to find out the most efficient method for obtaining materials and energy from potential recoverable waste based on specific criteria, by using ELECTRE multicriteria analysis method.

ELECTRE method is able to work with both quantitative and qualitative discrete criteria, and provides a ranking of all alternatives. All the steps included in this multicriteria method are followed. The problem to be solved is formulated according to the goal of the research in order to select the alternatives which are preferred to several criteria and not generate undesirable levels of dissatisfaction for one criterion. For this evaluation we have used concordance and discordance indicators and threshold values.

During the application of ELECTRE method, we have selected a number of methods to obtaining a secondary raw material and energy from waste with potential renewable and a coherent family of criteria, assessing the performance of each material on each criterion, which resulted in a performance matrix. The results showed that the production of bioplastics is the most suitable method for obtaining new materials, while mechanical biological treatment process is the most efficient method to obtain energy.

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P4. Analysis of environmental impacts of municipal solid waste

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Human activities always produce waste, whose generation rates increase with population expansion and economic growth. The impact of waste on the environment, resources and human health depends on its quantity and nature. Municipal solid waste management (MSWM) systems consist mainly of three main parts: temporary storage in containers, collection and transportation, and waste treatment processes. The difference between these systems lies in the type of collection management (selective, mixed), and methods of treatment applied to different fractions of waste depending on the composition and quantity of waste generated. In this paper we have chosen for evaluation two municipal solid waste management systems: 1) MSWM system existent in 2008 (municipal solid waste was landfilled in a non-compliant landfill) and 2) the MSWM system from 2013 which includes: temporary storage; collection and transport; sorting of paper, plastic, glass, metals; composting of biodegradable waste and landfilling. Life cycle assessment (LCA) methodology was used to evaluate the environmental impacts of these two systems. All four steps (goal definition and scoping, inventory analysis, impact assessment, and interpretation) included in a LCA study were followed. The data obtained in the inventory analysis phase (quantities of waste generated in Iasi, number of containers, number of vehicles, emissions in air, soil, water from different phases etc.), along with other collected data were introduced by us in the LCA software (GaBi) in order to achieve the impact assessment phase. The results reveal that environmental impacts are lower for certain categories of impact (abiotic depletion, global warming) in the case of the system existent in 2013 compared to 2008. Results showed that the waste management system existing in Iasi, Romania has to be improved.

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P5. Induced processes in cellulose derivative systems

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The synthesis, properties, and application of polymer liquid crystals have recently become a promising trend in the chemistry of high molecular weight compounds. It has gained significant importance, along with an intensive development of low molecular weight liquid crystals science. Cellulose and its derivatives can form liquid crystalline solutions in a variety of solvents. The present work summarizes results from research concerning the liquid crystal behavior in a series of blends from cellulose acetate phthalate (CAP)/hydroxypropyl cellulose (HPC) and cellulose acetate phthalate (CAP)/ethyl cellulose (EC) in N,N-dimethylacetamide at different mixing ratios and concentrations. Flow behavior is the most studied rheological property which describes the liquid crystal polymer state. Existence of three universal flow regimes to describe the viscosity of liquid crystal polymers is proposed in the literature [1]. For CAP/HPC and CAP/EC systems two and three flow regimes, respectively, were observed in the present work (Figure 1). The lyotropic liquid crystal behavior of these systems was influenced by the specific interactions, such as hydrogen bonding which occur between CAP and the liquid crystalline components (HPC or EC), the chemical structure of components, mixture composition, solution concentration and used solvent. A better understanding of the interactions occurring within the interest cellulose systems significantly will enhance the knowledge required to improve/optimize the design of novel structures with potential application in biomedical or electronic field.

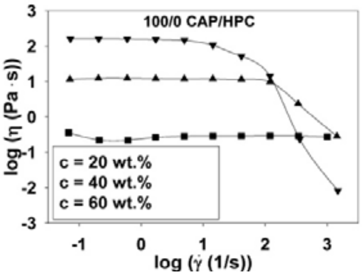

Figure 1. Log-log plots between dynamic viscosity and shear rate for CAP/HPC blends at different concentrations in N,N-dimethylacetamide.

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P6. Polyimide/iron oxide composites. Synthesis and characterization.

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Partially aliphatic polyimide/iron oxides (IO) composites based on the poly (amic acid) from 5-(2,5-dioxotetrahydro-3-furyl)-3-methyl-3-cyclohexene-1,2 dicarboxylic anhydride (DOCDA) and 4,4'-oxydianiline (ODA) with iron oxide in different weight percentages have been obtained. The structural phases transition of magnetite to maghemite in these composites, at different temperatures, has been discussed. The physical characteristics including magnetic, thermal, structural and morphological properties, evaluated by using X-ray diffraction (XRD), scanning electron microscopy (SEM) and thermal analysis (DTA/TGA/DSC), are influenced by the interplay of the filler content and the structural changes of the composite. The X-ray diffraction patterns of all samples show a cubic structure indexed as both magnetite (Fe_3O_4) or maghemite (γ-Fe_2O_3). Quantification of these two phases has been evidenced by Rietveld method. The presence of agglomerates in all polyimide/iron oxide (IO) composite films could be correlated with the electrical, dielectric and humidity sensing response for all investigated sample. From all composite films was observed that the permittivity of the material increases with increasing of relative humidity and decreases with increasing of frequency, being in agreement with Maxwell-Wagner model which was derived for the permittivity of a homogeneous two-phase system. Variation of electrical resistivity with frequency for all polyimide/iron oxide (IO) composite films and the electrical resistivity-humidity characteristics were also investigated. The electrical conduction in this samples is attributed to the electron hopping between Fe^{2+} and Fe^{3+} ions distributed on the octahedral sites (Vervey mechanism). The measurements show a decrease of electrical resistivity (ρ) as the frequency increases in the relative humidity range 0-100 RH for all investigated sample. The reduction of ρ under the influence of humidity depends on the composition changes and the microstructure being independent by the concentration of filler content into the amorphous poly(DOCDA-ODA) matrix where the decrease of electrical resistivity could be correlated with the beginning of the transition from Fe_3O_4 to γ-Fe_2O_3 phase.

P7. Thin gold layers sputtered on quaternized polysulfone substrate modified by low pressure plasma treatment

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Continuous gold layers sputtered on modified polysulfones (PSF) with different tertiary amines - N,N-dimethylethylamine (DMEA) and N,N-dimethyloctylamine (DMOA), providing to be applied in microelectronic domain, were characterized by atomic force microscopy (AFM). Low pressure plasma treatment for adhesion improvement was performed on PSF-DMEA and PSF-DMOA surfaces at various times. The results were discussed according to the chemical structure of polysulfones and to their different properties, such as flexibility, hydrophobicity and surface morphology. It has been showed that the obtained parameters, controlled by the interactions occurring in the polysulfone systems, can be correlated with the adhesion/cohesion of sputtered gold and plasma treatment.

Force-distance spectroscopy DFL (Height) from AFM data was used to measure the adhesion forces between polysulfone samples' surface and the silicon cantilever. In contact mode, the adhesion forces have a significant effect on the cantilever during its withdrawal from the sample. These forces cause deflection of the cantilever before it interrupts the contact with the surface. With the z-scanner length being reduced, the DFL (normal deflection distribution of the cantilever) first falls below its value, observed well away from the surface, and then abruptly reaches the free-state value, thus forming a specific dip. Analysis of the occurrence of the retraction curves evidences differences between the surface properties of the polysulfone films before and after plasma treatment and with and without gold deposition. Assuming that the cleaned and dried silica surface of the cantilever is hydrophobic, the interactions between a hydrophobic tip and a hydrophobic substrate will be higher than those between a hydrophobic tip and a hydrophilic substrate, respectively. The higher or lower values of the mean adhesion force obtained for polysulfone films can be explained by its more hydrophobic or hydrophilic properties induced by plasma treatment of substrate films and gold deposition time.

P8. Phosphorus-containing polysulfones for high-performance applications in advanced technologies

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Among the high-performance polymers with specific macromolecular structures, unique morphologies and special properties, polysulfones have drawn attention due to their versatile reactivity and participation to a wide range of technological applications. The paper addresses key features of phosphorus-containing polysulfones and how they can be optimized for applications in advanced technologies. New trends in biomedical uses of phosphorus-containing polysulfones are based on their specific properties (*i.e.* biodegradability, compatibility with blood compounds and structural similarities to the naturally nucleic and teichoic acids), these characteristics making them suitable for applications like drug delivery, dental uses, tissue engineering or protein adsorption (Figure 1).

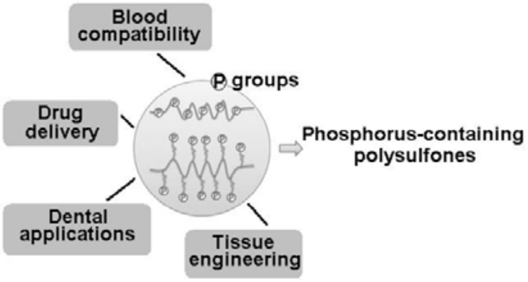

Figure 1. Main applications of phosphorus-containing polymers

Recent studies have focused on the synthesis and characterization of new polysulfones containing phosphorus in the side chain, following the effect of the chemical structure on the rheological behavior and topography, and establishing the relation among their processing, morphology and specific properties. Assessments like shear thinning behavior, good film-forming properties, viscoelastic characteristics and appropriate surface topography make these materials suitable for applications in medicine.

P9. Packaging influence on coffee quality through measurements of relevant physico-chemical parameters

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Packaging materials and storage conditions are among the most important parameters directly affecting the quality of a final product. For coffee, a well known agricultural product, the quality controls the price. Maintaining product's quality for longer storage periods ensures a longer selling time for the manufacturers and guarantees better prices. The present study was aimed to identify the best packaging material that preserves better the physical, chemical and sensorial qualities of the stored coffee beans. Sensorial analysis and physico-chemical determination of some parameters were used to investigate the influence of three types of packaging materials on the coffee quality. Marks ranking from 0 to 10 have been assigned accordingly to the coffee quality by using sensorial analysis. Flavor, uniformity, sweetness, acidity, impression after long term taste accounted for the given score. Physico-chemical investigations have been undertaken in order to measure mineral substances, the fat content and the humidity. Parchment paper padded with polyethylene negatively influenced coffees quality which obtained the lowest score 14.988 (assigned as a second grade coffee). Use of metallic cans enhanced coffees score to 18.844 which could be considered as a first grade coffee. The coffee packed in a double layer packaging system, made of aluminum foil and laminated paper, obtained the highest score, i.e. 24.056, being assigned as a high class quality coffee. The coffee beans stored in the metallic cans have higher water content till the sixth storage month. Water content increased with about 6.60%, however, it remained in equilibrium with the relative temperature and humidity of the ambient air. In the waterproof package (firstly ranked) the water content remained stable at ~10% during the entire storage time. Use of improper packaging material highly affects the flavor loss. Volatilization, oxidation, hydrolysis or interaction of various chemical constituents can be prevented by using appropriate packaging materials which should be air free after applying vacuum or inert gas packing. However, the best packaging material is that made of two layers, i.e. aluminum foil and laminated paper, which act as an efficient barrier.

P10. Evaluation of Optical and Dielectric Properties of Polystyrene/$BaTiO_3$ nanocomposites

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Introduction of inorganic fillers into polymer matrix opens new perspectives in various industrial sectors ranging from aeronautics to microelectronics since it leads to hybrid materials with improved thermal, separation, mechanical and electrical properties. The resulting thermo-physical characteristics of the composite are dependent on both the polymer and the particles properties and their state of dispersion. When at least one of the phases shows dimensions in the nanometer range the surface to volume ratio is increased and consequently enhancing some of the thermo-physical of interest in applications. In this context, the nanocomposites have emerged as suitable alternatives to overcome limitations of microcomposites, while posing preparation challenges related to the control of elemental composition and stoichiometry in the nanocluster phase. The increasing need of materials for new applications requires polymers with diverse architectures, leading to specific properties. Polystyrene is a widely investigated polymer owing to its good mechanical resistance and high transparency in some organic solvents. Many studies have been focused on improving the dielectric properties of this macromolecular compound by introduction of various types of nanofillers [1]. In order to evaluate and predict the applicability of the reinforced polystyrene in microelectronic industry, a deep theoretical analysis should be performed. The formalism developed by Bicerano [2] utilizes connectivity indices defined via graph theoretical concepts as its main structural and topological descriptors. The present paper describes the evaluation of the optical and dielectric properties of some polystyrene/$BaTiO_3$ nanocomposites. The characteristics of the polystyrene matrix are determined using the connectivity index formalism. The dielectric constant values of the nanocomposites are estimated from the Maxwell relationship, while the optical features are evaluated using some mathematical approaches.

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P11. Evaluation of untreated biomass of Phaseolus vulgaris L. as potential biosorbent for organic dyes

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The objective of the present work was to conduct preliminary study on the evaluation of *Phaseolus vulgaris* L. biomass as biosorbent material for azo and xanthene dyes. Acid orange 7 (AO7) and Erythrosine B (Ery B) were selected as model pollutants due to their extensive use in textile, food and cosmetic industry. The effects of operational parameters on the biosorption yield of dyes removal, including contact time, initial pollutants concentration and biosorbent dose have been investigated.

The solid agricultural waste was characterized using Fourier Transform Infrared Spectroscopy (FTIR) and Scanning Electron Microscopy (SEM-EDX) analysis. The obtained results show that the amount of dye uptake was found to increase with the increase of contact time and initial dye concentration for both classes of dye. The maximum biosorption capacity at 20°C was found to be 0.827 mg g^{-1} for AO7 and 0.913 mg g^{-1} for Ery B, respectively. The removal efficiency of the dyes is increasing with the increase on biosorbent dose, in the range of studied concentration (5-50 mg L^{-1}). The biosorption of Acid Orange 7 and Ery B was observed to be rapid at the primary stages of process.

For evaluating the mechanism involved in the biosorption process a detailed analysis using a set of kinetic equations was carried out to describe the biosorption of AO7 and Ery B onto *Phaseolus vulgaris* hull. Based on the regression coefficient values, the biosorption dynamic behavior of AO7 and Ery B onto *Phaseolus vulgaris* L. hull agreed very well with the pseudo second-order kinetic model, which indicate that the main biosorption mechanism is probably a chemisorption reaction. The results of the intraparticle diffusion model in the case of AO7 and Erythrosine B suggested that intraparticle diffusion was not the single rate-controlling step, the process is more complex, it can be inferred that external mass transfer and intraparticle diffusion occurred simultaneously.

The experimental biosorption results indicated that agricultural waste - *Phaseolus vulgaris* hull can be considered an economic and eco-friendly material, due to their unique chemical composition, availability in abundance, renewable nature and low cost and is a viable option for industrial effluents pollution control.

Acknowledgement

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P12. Green composites comprising starch and natural fillers: structure and properties investigation

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Natural fillers derived from renewable sources offer significant advantages over the traditional synthetic ones in terms of environmental protection (these fillers being biodegradable and non-toxic), low cost, and suitability for various applications through the obtainment of composite materials with improved properties.

In the present paper, preparation and characterization of new green composite materials (obtained as films by solution casting processing method) comprising chitin, industrial pulp cellulose, and wheat straws as reinforcing fillers within glycerol plasticized starch matrix are reported. Structural features of individual components and resulted composites were investigated by FTIR spectroscopy.

The surface properties, such as the contact angle values, transparency, and water sorption behavior, as well as mechanical properties of composite films (tensile strength, Young's modulus, and elongation at break, respectively) were also evaluated and discussed. The water resistance was improved by addition of natural fillers in composite formulations, while the opacity properties were negatively affected.

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P13. Wood treatment with vegetable oils and its protective effect under environmental factors action

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Wood preservation through chemical treatments (i.e. copper compounds) is restricted for more applications due to both their pronounced toxicity and their harmful effects to the environment. Preservative systems based on vegetable seed oils from natural and renewable sources may confer protection to wood under the action of various environmental factors. Vegetable oils, as non-toxic substances, can form an environmental friendly and efficient protective layer on the surface of the wood samples, thus improving water resistance of wood and its dimensional stability.

In present paper, fir tree wood samples, prepared as dried discs (25-30 mm diameter, 8-10 mm thickness), were treated with *Asclepias syriaca* seed oil (ASSO), and soybean oil (SBO), respectively. Structural properties, biodegradation under controlled and simulated natural conditions, and water sorption behavior of wood samples were investigated. FTIR spectroscopy, X-ray diffraction analysis, and scanning electron microscopy (SEM) investigation methods were used for wood samples characterization before and after treatment with vegetable oils, as well as under biodegradation process in soil burial tests.

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P14. Polymers with biopassive and bioactive properties

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Bacterial infection onto implanted materials and devices (catheters, pacemakers, knee and hip implants) is a major problem with negative impact on the quality of life of patients and their recovery. Bacterial adherence to implant surfaces occurs in two phases: (i) first, bacteria compete with host cells for binding to the extracellular matrix or plasma proteins on the surface of the device ("race for the surface"); (ii) adherent bacteria proliferate and cluster in multilayers of exo-polysaccharides into biofilms, which have a low metabolism with low toxicity. The use of an implanted device increases the susceptibility towards infection due to the damages caused to epithelial and mucosal barriers upon implantation.

Many concepts have been investigated in order to prevent bacterial adhesion to and biofilm formation on implants. One effective approach is including both biopassive and bioactive surfaces [1-4], either with a covalently attached moiety or one that is released into the environment. Preventing protein binding to the implanted surfaces by using polymeric materials may be reached through various strategies, such as surface modification by hydrophilic polymers or block copolymers consisting of highly hydrated, flexible chains having low values of polymer–water interfacial forces. In the case of short chain polymers, the surface hydration seems to be the driving force. For the long chain polymers, the surface hydration and steric repulsion act synergistically.

This paper presents a few polymers with bioactive and biopassive properties, some aspects concerning their development, as well as some limitations.

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P15. Composite scaffolds with interconnected pores

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Scaffolds with interconnected pores are one of challenges in nowadays tissue engineering. This is the reason why knowledge from fundamental and applied sciences are put together in order to design and develop and artificial structures to replace or regenerate human tissues.

A fundamental requirement for scaffolds in tissue engineering is a controllable interconnected porosity to direct the cell growth and to support vascularization of the new grown tissue. A typical porosity of 90%, as well as a pore diameter of 100 mm, is required for cell penetration and proper vascularization [1].

Porous scaffolds are currently made of natural or synthetic polymers, such as polysaccharides, poly(α-hydroxyester)s, hydrogels or thermoplastic elastomers (polyamides and copolyamides). Other relevant groups of materials are bioactive ceramics, such as calcium phosphates, and bioactive glasses or glass-ceramics. At the same time, polymer composites filled with ceramics are being under study in order to achieve porous scaffolds with increased mechanical strength and improved tissue compatibility, and with the ability to deliver compounds with biologic activity at the implantation site: antibiotics, anti-inflammatory drugs, growth factors, immune-suppressors, gene therapy agents, etc. Polymer composites filled with bioactive ceramic particles having nanometric dimensions (such as nano-hydroxylapatite) [2] appear to be a solution that responds to most requirements in the field, due to the combination of advantageous properties of polymers and bioactive fillers, and their synergistic action.

This paper reviews some relevant achievements in this domain, with highlights on design and manufacture strategies.

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P16. Tansfection capacity of PEI-based nanovehicles depending on their molecular architecture

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Polyethylenimine (PEI) is one of the most investigated cationic polymers as a non-viral vector for gene delivery. PEI molecule itself, although very effective in DNA or RNA packaging and release, shows a highly cytotoxicity when tested in cell cultures. PEI < 2 kDa molecular weight (Mw) has been proved to be non-toxic while PEI with Mw = 5 ÷ 25 kDa are suitable for gene transfer but leading to increased cytotoxicity.[1] A strategy to increase transfection efficiency with decreased cytotoxicity is to couple low molecular weight PEIs to form conjugates of 14–30 kDa.[2] Fullerene C60, β-cyclodextrine (β-CD) and cyclic siloxane (D4) used as compact cores, covered by hiperbranched PEI (Mw=2kDa) within certain polymeric architectures, are able to form polyplexes with nucleic acids via electrostatic interaction. Polyethylene glycol (PEG) molecule is also considered to increase the biocompatibility of the system and avoid the immune system.[3] This work displays the ability of polyethylenimine-based vehicles such as: C60-PEI, C60-PEG-PEI, D4-PEI and β-CD-PEG-PEI to bind plasmid DNA (pEYFP) and their transfection capacity. The formation of expected polyplexes was evaluated by: particle size and zeta potential measurements, gel retardation assay and atomic force microscopy. The transfection efficiency was investigated using *in vitro* tests on HEK 293T cells, treated with vehicle/pEYFP complexes by fluorescence microscopy as a qualitative evaluation, and flow cytometry for a quantitative determination of the cells that express the fluorescent protein encoded by pEYFP. As a conclusion, all tested PEI-based vehicles were proved appropriate carriers for gene delivery. PEG molecule may reduce the rate of transfection with the benefit of a lower cytotoxicity.

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P17. Mesoporous silica (SBA-15) as adsorbent for removal of dyes from wastewaters

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Dyes are considered important water pollutants and are generally present in the effluents of different industries, because of that their removal has been the subject of attention of environmental specialists. The negative dyes impact is due to their possible toxicity and carcinogenicity, heightened by the fact that many dyes were formerly made of known carcinogens (i.e. benzidine).

Nowadays, a large number of methods for dyes removal, such as oxidative destruction via UV/ozone treatment, photocatalytic degradation which have certain efficiency (but their initial and operational costs are so great), are known and applied.

Adsorption (inexpensive, simply designed, easy to handle and providing sludge-free cleaning operations), represents an attractive alternative compared to the conventional wastewater treatment technologies. One of the main advantage of this method is the possibility to use like adsorbent a vast category of materials for wastewaters treatment: materials with ion exchange properties, activated charcoal, natural or synthetic zeolite, lignin-cellulose materials which are presented in nature or are by-products from industrial or agricultural transformation, or the active or inactive biomass which is special produced or resulted from industrial fermentative technology (food and pharmaceutical industry).

This paper presents the preliminary results in the study regarding the use of mesoporous silica materials like SBA-15, in the discoloration of aqueous solutions. The adsorption of cationic dye Methylene Blue from its aqueous solution has been studied in order to establish the optimum conditions of adsorption on SBA-15 powder. The effect of various experimental parameters such as adsorbent dose, temperature, initial dye concentration and solution pH were investigated. The SBA-15 mesoporous material synthesized in this preliminary study was characterized by X-ray diffraction (XRD) and nitrogen physisorbtion. The adsorption equilibrium concentrations were determined by UV-VIS spectrophotometry as an analytical method.

P18. New mechanistic insights on the cycloaddition of the benzimidazolium ylides with alkynes

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A widely but also disputed method used for the synthesis of the pyrrolo[1,2-a]quinoxalinone derivatives is the cycloaddition reaction of the benzimidazolium ylides to dipolarophyles.[1-4] Even if this method was used since 1972, there are still some unsolved issues regarding the way that the cycloaddition products (dihydropyrrolo[1,2-a]benzimidazole derivatives) are stabilized. Some authors claim the formation of the pyrrolo[1,2-a]benzimidazole derivatives,[3,4] while others indicate the formation of pyrrolo[1,2-a]quinoxalin-4(5H)-one derivatives.[1,2]

Having in view the above consideration and our background in the cycloimmonium ylides area,[5-8] we decide to investigate the cycloaddition reaction of the benzimidazolium ylides, with dimethylacetylene dicarboxylate (DMAD) as dipolarophile in order to elucidate the reaction mechanism.

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P19. Microwave assisted synthesis of benzofuran derivatives

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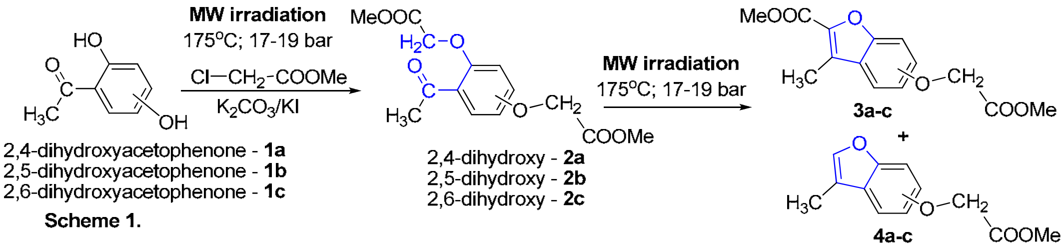
The synthesis of benzofuran derivatives has attracted a special attention thanks to their appearance in large number of natural products [1] and synthetic pharmaceuticals [2]. MW irradiation became in organic chemistry a powerful tool offering a versatile and facile pathway in a large variety of syntheses [3,4].

Under MW irradiation, the reaction was carried out at a higher temperature (165 ºC) and higher pressure (17-19 bars). Reactions have occurred very slowly (5-8 h), but instead of obtaining only compounds (**3a-c**), were obtained a mixture of benzofuran derivatives (**3a-c** and **4a-c**). Scheme 1.



Scheme 1.

The structures of all compounds were proved unambiguously by spectral analysis (IR, ^{1}H-NMR, ^{13}C NMR, two-dimensional experiments 2D-COSY, 2D-HETCOR (HMQC), long range 2D-HETCOR (HMBC).

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P20. New complexes of 5-(3-Pyridyl)-4H-1,2,4-triazole-3-thiol with Co(II), Ni(II), Mn(II), Cu(II) ions: Synthesis, structure and magnetic properties.

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In transition metal coordination chemistry, 1,2,4-triazoles are versatile ligands due to their different binding modes. In this work, 5-(3-Pyridyl)-4H-1,2,4-triazole-3-thiol (LH) was investigated as suitable ligand for preparation of new Co^{2+}, Ni^{2+}, Mn^{2+} and Cu^{2+}complexes. The complexes were prepared at metal to ligand 1:2 ratio and were characterized using elemental analysis, mass spectrometry, magnetic susceptibility measurements, XRD methods (Fig. 1), FT-IR and DR-UV-Vis spectroscopy and thermal analysis. The FT-IR spectra of LH and $[M(L)_2(H_2O)_2]$ complexes show characteristic stretching (ν) bands assigned to NH, C-S and C = N groups. The band of S-H group disappeared after coordination process and $\nu_{C=N}$ of complexes shifted to a lower energies compared to the LH. Also, the ν_{NH} bands were shifted due to complexation. The DR spectra of ligand and complexes show characteristic π-π* and π-π* bands due to intraligand transitions.

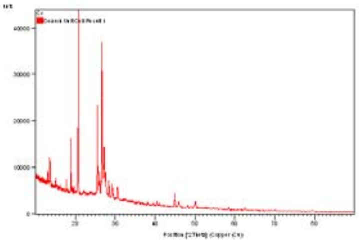

Figure 1. Diffractogram of $[Cu(L)_2(H_2O)_2]$ compound

For complexes, in visible and near infrared regions the d-d electronic transitions were observed. All complexes showed paramagnetic properties lower than of the same aquocations. The triazole compound acts as bidentate ligand that coordinates to the metal ions by thiol and amine groups. The coordination centers of $[M(L)_2(H_2O)_2]$ (M = Co^{2+}, Ni^{2+}, Mn^{2+} and Cu^{2+}) have a distorted square planar geometry.

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P21. Influence of Pb substitution with Sr on the magnetic/crystalline structure and transport properties of $La_{0.5}Pr_{0.2}Pb_{0.3}MnO_3$ manganites

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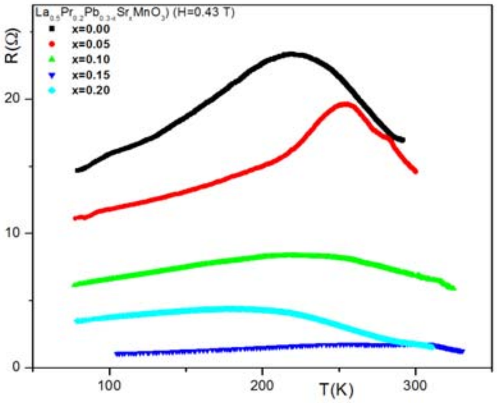
The rare earth manganites with general formula $RMnO_3$ are the most interesting studied materials for practical applications of colossal magnetoresistance effect. The coexisting of competing phases in manganites, such as metallic ferromagnetic, charge ordered, antiferromagnetic insulating and ferromagnetic insulating phases, determines an important change of magnetic and transport properties with the microstructure.



Variation of the resistance *vs* temperature and Pb concentration. The samples were cooled and measured in a magnetic field of 4300 Oe.

We report on the correlations between microstructural, magnetic and transport properties at temperatures ranging from 263 to 343 K of $La_{0.5}Pr_{0.2}Pb_{0.3-x}Sr_xMnO_3$ manganites synthesized by ceramic technology. The structure and microstructure is studied using X-ray diffraction (XRD) and small-angle neutron scattering (SANS). The $La_{0.5}Pr_{0.2}Pb_{0.3-x}Sr_xMnO_3$ manganites crystallize in cubic structure Pm-3m (for x = 0.00 and 0.05) and rhombohedral structure R-3c (for x = 0.15 and 0.20). The magnetic and transport properties were studied between 77 and 350 K. SANS data reveal the shape and concentration of magnetic nanodomains and their dependency on temperature, especially at higher temperatures than T_C.

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P22. The study of oxygen mass transfer in tetraphasic systems: gas-liquid-liquid-solid in stirred bioreactors

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The oxygen supply into the broths constitutes one of the decisive factors for aerobic microorganism's growth, playing an important role in the scale-up and economy of large-scale fermentation systems. The aeration efficiency depends on the bioreactor capacity to generate high rate of oxygen diffusion from air to the broths, as well as of its transfer through the liquid phase to the microorganisms. Therefore, one of the priorities in designing and operating aerobic bioreactors is to ensure the optimum oxygen transfer from the gaseous phase to the microbial cells which could be improved by the presence of oxygen-vectors, without intensification of mixing or aeration.

For this reason, the aim of this study is to analyze the distribution of the oxygen transfer rate in broths - oxygen-vector dispersions, for a stirred bioreactor and different fermentation broths without biomass (simulated broths) and with microorganisms (bacteria, *Propionibacterium shermanii*, and yeasts, *Saccharomyces cerevisiae*), using a large domain of operating variables.

The experimental results for simulated, *P. shermanii* and *S. cerevisiae* broths indicated the significant increase of k_La (oxygen mass transfer coefficient), by adding *n*-dodecane, but the magnitude of this effect depends mainly on the cells affinity for hydrocarbon droplets. Therefore, due to the higher affinity of yeasts cells for hydrocarbon droplets during their entire growth cycle, the increase of oxygen mass transfer rate was lower and the influence of specific power input was different than those recorded for simulated or bacterial broths.

By means of the experimental data, mathematical correlations describing the influences of the main parameters on k_La have been proposed for each studied fermentation systems at different positions on the broths height, offering an average deviation between ±6.72% and ±6.93%.

P23. Study on synergic reactive extraction of vitamin B_9

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The folic acid, also called pteroylglutamic acid or vitamin B_9, is one of the important members of vitamins B group, being a growth factor, essential for making genetic material. This study focused on separation of vitamin B_9 by synergistic reactive extraction with a mixture of two extractants, one acidic (acid di-(2-ethylhexyl) phosphoric acid, D2EHPA) and one with basic character (Amberlite LA-2).

The influence of extractants concentrations and solvent polarity on the efficiency of vitamin B_9 separation by synergic extraction with Amberlite LA-2 and D2EHPA mixture have been analyzed. The results indicated the formation of an interfacial compound which includes one molecule of folic acid and one of D2EHPA, the hydrophobicity of this compound being increased by solvation with Amberlite LA-2 molecules.

The synergistic coefficient was calculated with the following expression:

$$C_S = \frac{K \cdot \left[HP_{(o)}\right] \cdot \left[A_{(o)}\right]^n}{\left(D_{D2EHPA} + D_{LA-2}\right)}$$, the synergism appearing for $C_S > 1$.

By maintaining the D2EHPA concentration at a constant value, and increasing the concentration of Amberlite LA-2, the synergistic coefficient could become higher than 1, its highest values being reached for n-heptane. The extractants role in promoting the synergic effect is different. Therefore, the organophosphoric extractant reacts with vitamin B_9 and forms an interfacial compound soluble in organic phase, while the aminic extractant increases the hydrophobicity of this compound by solvation. The chemical structure of aminic adduct depends on the concentration of D2EHPA and solvent polarity. The number of aminic molecules included in the interfacial complex is reduced from 3 to 1 by increasing the solvent polarity and D2EHPA concentration. The most important synergic effect is obtained for the combination extractants mixture - n-heptane, the organic phase containing 5 g/l of D2EHPA.

P24. Selective separation of acetophenone and methylbenzylamine from their mixture by extraction

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Acetophenone (AP) is the simplest aromatic ketone that can be found naturally in many vegetables and fruits. Industrial production of AP is based on chemical synthesis but recent studies focused on microbial and enzymatic production. An important drawback of enzymatic production is the difficult separation of AP from methylbenzylamine (MBA), the main substrate for enzymatic reaction. MBA is a chiral amine that is a key building block for many new pharmaceuticals.

The aim of this study was the separation of AP and MBA from their mixture by extraction.The experiments have been carried out using an extraction column with vibratory mixing, which offers high interfacial area andrapid attainment of equilibrium state. The initial concentrations of MBA and AP in aqueous solution were 3 g/l with the pH-values of 5, 7, and 9.The experiments were performed in three extraction systems: (1) with n-heptane, (2) n-heptane + 1-octanol as phase modifier, and (3) n-heptane + di(2-ethylhexyl)phosphoric acid (D2EHPA) as extractant.

Regardless of the extraction system, the results indicated that, the yield of MBA extraction was below 33%, this value corresponding only to the reactive extraction with n-heptane and D2EHPA at pH = 9. Moreover, the extraction yield was almost 0 for the physical extraction with n-heptane and 1-octanol, at pH = 5 and pH = 7. These data suggest the modification of the organic phase (n-heptane or n-heptane + 1-octanol) ability to induce the solvation of MBA and, consequently, to extract it. This phenomenon could be the result of the change of the intermolecular interactions inside the organic phase, due to the presence of AP. For AP extraction the highest yield (94.5%) was reached for the system with n-heptane + 1-octanol and for a pH =7 of aqueous phase. In conclusion, AP can be efficiently removed selectively from the mixture with MBA by physical extraction with n-heptane and 1-octanol, usingan aqueous phase pH equal to 7.

P25. Synthesis and structure of new 1,10-phenantroline derivatives

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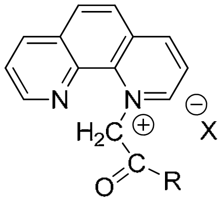
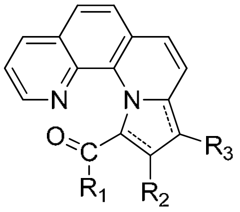
Phenanthroline derivatives attracted attention in the last years especially due to their biological effects [1], materials science applications, crystal engineering [2], their unique π-electrons delocalization, and complexation properties [3].

Phenanthrolines polycyclic skeletons are also present in sterols, sex hormones, cardiac glycosides, bile acids and morphine alkaloids. Recently, compounds with phenathroline skeleton have been synthesized and biologically evaluated as analogs of benzo[c]phenanthridine alkaloids (e.g. nitidine, fagaronine, sanguinarine) that attracted attention due to their interesting biological properties [4].





Inspired by our previous results obtained on the synthesis and properties of polycyclic indolizine derived from 1,10-phenanthroline (pyrrolo[1,2-a][1,10]phenathrolines) [5], the main goal of this work was to synthesize new similar derivatives using the strategy involving cycloimmonium ylides as 1,3-dipol intermediates, in order to comparative study their biological, optical and electrical properties.

The structures of the newly compounds were proven by elemental and spectral (IR, NMR, MS, X-Ray) analysis.

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P26. High yield photocatalytic degradation of pesticide contaminants by ferrite nanoparticles

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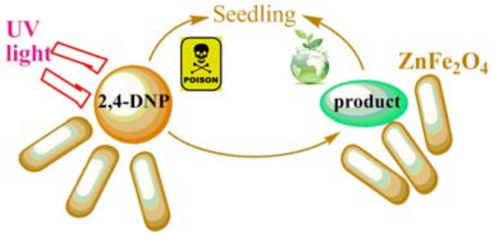
Pesticide residues could be extremely hazardous to the environment[1]. Among various treatment methods employed to remove refractory pollutants from contaminated water, photocatalytic processes have generated a great interest in the last decade[2]. A special issue is DNP toxicity to the environment, which is manifested during production, conditioning, transportation, storing and especially the consumption of treated plant products[3]. Photocatalytic degradation of these contaminants could be an alternative method decontamination pathway.

Here a zinc ferrite, $ZnFe_2O_4$, as a catalyst to degrade photocatalytically 2,4-dinitrophenol (DNP) has been used. The contaminant removal efficiency was enhanced up to 82% for photocatalytic degradation after 15 min of UV light irradiation, with first order kinetic rate constant k_1 of $3.4 \cdot 10^{-2}$ min^{-1}. When treated wheat seeds within germination experiment a dramatically decrease in the toxicity of the resulting photodegraded DNP solution was observed.



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Acknowledgements: Partnership project Metafore PN-II-PT-PCCA-2013-4-1149. Also, M Z acknowledges the financial support by the strategic grant POSDRU/159/1.5/S/137750.

P27. Metal-organic frameworks based on pyridine-2,6-dicarboxylic acid as ligand

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Metal-organic frameworks have attracted considerable attention in last years due to their possible application in different field such as: magnetism, luminescence, catalysis. The versatile coordination mode of the pyridine-2,6-dicarboxylic acid has been established with the synthesis of some metal-organic complexes with different metal ions, Co(II), Ni(II), Fe(II) and Cu(II). These metal-organic complexes have been characterized by single crystal X-ray analyses, thermal analyses, UV-Vis and FT-IR spectral techniques.

Pyridine - 2,6-dicarboxylic acid, partially or completely deprotonated, coordinates to the 3d or 4f transition metals, by both carboxylate groups which results in getting the complex dimers or polymers, or ligand acts as bidentate (N, O) from transition metals which results in obtaining the metal-organic networks (MOFs) with different configurations and specific properties, either by the two carboxylate groups and the nitrogen atom (ONO) to a single metal ion.

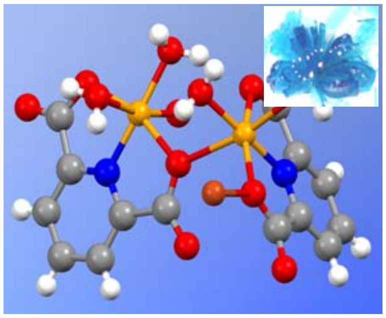

Figure 1. Cristals and DRX structure of coordinative compounds of Cu(II).

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P28. Synthesis and structure particularities of two new coordination polymers of Zinc(II) and Cobalt(II) with 1,2,3- benzenetricarboxylic acid and 1,4-bis((1H-imidazoyl-1-yl)methyl)benzene

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Metal-organic networks attract much attention because of topology design and potential properties in gas adsorption and separation, catalysis, magnetism, luminescence, micro sensing, etc. [1-2]

A hydrothermal synthesis comprising 1,4-bis((1H-imidazoyl-1-yl)methyl)benzene (BIB), 1,2,3-benzenetricarboxylic acid (1,2,3-BTC) as ligands, and Zn(II) and Co(II) as metal centers leads to the formation of new two- and three-dimensional polymers with intriguing structures (Fig.1).

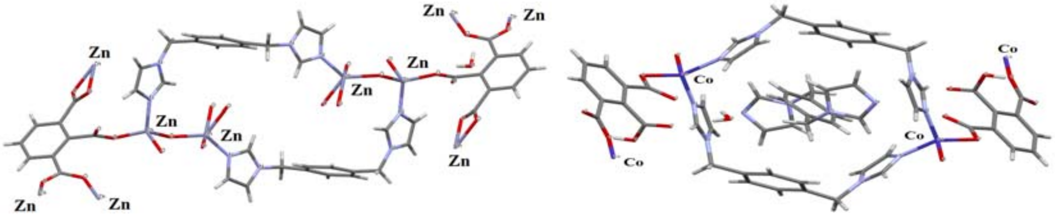

Figure. 1. The structural unit of $\{[Zn_2O(1,2,3\text{-BTC})(BIB)](H_2O)_{0.5}\}_n$(left) and $\{[Co(1,2,3\text{-BTC})(BIB)](BIB)_{0.5}(H_2O)_{0.5}\}_n$ (right).

In the dinuclear zinc compound metal ions link together through μ_2-oxo bridges and manifest different coordination numbers 4 and 5. The carboxylic groups of the acid are mono- and bidentate or have a chelate function.

The cobalt compound is mononuclear, the metal centers exhibit coordination number 4 having a tetrahedral geometry. Inside the pores formed in the structure there are inclusion compounds – one molecule of BIB and one molecule of water for two complex units that are capped in the "cage" via intermolecular interactions.

Although the two structures are bulky, they can show interesting sorption properties that are now on the way.

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Acknowledgements: Present work was supported by the Moldova State Project Nr. 14.518.02.05A and bilateral Moldovan-German Project Nr. 13.820.08.03/GF.

P29. Preparation by citrate combustion and characterization of the double perovskite oxides Ca_2BMoO_6 (B = Cr, La, Sm)

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The aim of this work was to obtain a series of double perovskite oxides Ca_2BMoO_6 (B = Cr, La, Sm) for the first time. Also, a study on the effect of these three trivalent B-site cations on the phase formation by the sol–gel autocombustion method, structural characteristics, and magnetic properties are presented.

Samples of Ca_2BMoO_6 were prepared using the sol–gel autocombustion method by mixing $Ca(NO_3)_2{\cdot}4H_2O$, $Cr(NO_3)_3{\cdot}9H_2O$, $La(NO_3)_3$, $Sm(NO_3)_3{\cdot}6H_2O$, $(NH_4)_6Mo_7O_{24}{\cdot}4H_2O$ with citric acid as the combustion agent. The precursors were pre-sintered and sintered at different temperatures.

The synthesis progress was monitored by IR spectra obtained by using a JASCO 660 PLUS spectrophotometer. All the spectra present the typical band pattern characteristic of the perovskite structure. The differences between the three spectra appear to be due to the cation from the position B or to the symmetry of the crystal cell.

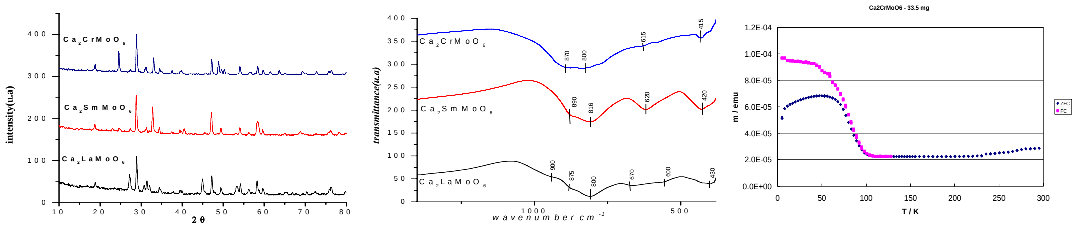

Figure 1. a) X-ray diffraction patterns of Ca_2BMoO_6 b) FTIR spectra of Ca_2BMoO_6
c) Variation of the specific magnetization with temperature of Ca_2CrMoO_6

X-ray diffraction (XRD) patterns of the sample were recorded with a SHIMADZU LabX6000 diffractometer equipped with a graphite monochromator and CuKα radiation. The strongest reflection peak at 2θ of around 30º, assigned to (112) XRD diffraction plane, was identified in the pattern for each sample, confirming the formation of the double-perovskites phase

Magnetization measurements were made with a SQUID magnetometer. All compounds are ferimagnetics and magnetic properties are indirectly influenced by the distorsion degree of the lattice and degree of ordering cations B/B'.

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P30. Synthesis and structure of new compounds with 1,10-phenantroline and 2,2'-bipyridine skeletons

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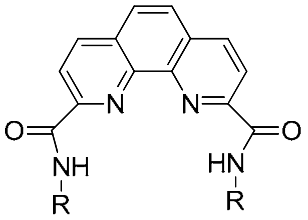
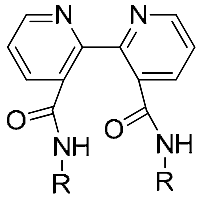
Phenanthroline derivatives attracted attention in the last years not only because of their pharmacological effects in many drugs, but also because of their functional role in DNA ligands. Thus, the extended aromatic structure of a 1,10-phenanthroline scaffold provides a basis for efficient π-π interactions with the terminal G-quadruplexes (secondary structures that can be formed by nucleic acid sequences rich in guanosine residues). Targeting G-quadruplex DNAs with small molecules is emerging as a rational and promising strategy for anticancer drug design, since they might inhibit telomerase activity and block transcription or translation of a particular gene by stabilizing G-quadruplex DNAs.

The recent results in this field, prompted us to develop and synthesize new compounds with 1,10-phenanthroline and 2,2'-bipyridine scaffold, as potential G-quadruplex ligands.





The general synthetic route for 1,10-phenanthroline derivatives involves the oxidation of neocuproine to 1,10-phenanthroline-2,9-dicarboxylic acid and its derivatization. For the synthesis of 2,2'-bipyridine derivatives, 1,10-phenanthroline has been oxidized to the 2,2'-bipyridine-3,3-dicarboxylic acid followed by its transformation in diverse diamides. The structures of the newly compounds were proven by elemental and spectral (IR, NMR, MS, X-Ray) analysis. The anticancer activity of these compounds is under investigation.

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P31. DNA interactions with tannic acid and its titanyl complex

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Tannic acid is a form of tannin, which is a plant polyphenol composed of a glucose molecule derivatized with 2 to 12 galloyl residues, depending on the biological source. The tannic acid complex with titanyl (TiO^{2+}) is used in the modern leather industry as an alternative of chromium tannage and it is nowadays an attempt to replace the synthetic dyes with natural ones trying, in this way, to decrease the level of allergic impact by produced leather. Both compounds display an antioxidant and antimicrobial character. Supplementary, it has been found that tannic acid has antimutagenic and anticarcinogenic behavior.

In the present study, we have investigated the effects of tannic acid and its titanyl-tannin complex (TiO^{2+}-TA) on herring DNA at various pH and buffer conditions. Since there was no concluding information in the literature about a possible interaction between these two compounds and DNA, some UV-Vis measurements were performed in order to prove this binding. Therefore, during the titration of these compounds with the herring DNA, bathochromic shifts were observed. Moreover, the second derivative spectra offer valuable information regarding this interaction.

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P32. Metal heterocyclic complexes in polysiloxane matrix

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Dielectric elastomers with improved electrical properties constitute an important class of materials with applications in medical devices and energy harvesting. Fillers are used for improving the mechanical and dielectric properties of elastomers.

In this paper we report the synthesis, structural data and some properties for four clusters with Cu(II), Ni(II), Co(II) and triethanolamine and the preparation of composite materials with silicones that were processed as thin films.

The properties of the obtained materials were tested for future use in the structure of dielectric elastomer devices for actuation and energy harvesting.

The introduction of metal complexes in the polymer matrix, even at low percentages, increases the values for the dielectric constant and for the breaking strain of the samples. The hydrophobic character of the siloxane-based elastomers was preserved, as was determined from water vapor sorption curves, making these films suitable for applications in wet environments, such as biological implants and sea waves. The data obtained from DSC analysis confirm the degree of crosslinking determined by solvent swelling. The degree of crosslinking has specific values for each type of metal complex sample, but it increases with the content of metal complex for every metal used. This shows the microparticles of metal complex act as centers for crosslinking in radical condensation.

Sample	Solvent uptake capacity ($g \cdot g^{-1}$)[a]		Crosslinking yield, C_y[b]	Weight loss, L_w[c]	Heat capacity, C_p ($cal \cdot g^{-1} \cdot K^{-1}$)	Crosslinking density, ρ_c ($mol \cdot cm^{-3}$)[d]
	Water	Chloroform				
GC00	0.010	-	0	1	0.100	-
GC0	0.007	7.26	0.852	0.148	0.115	0.15
GC1	0.012	5.62	0.943	0.057	0.152	0.52
GC2	0.126	8.00	0.750	0.250	0.105	0.05
GC3	0.300	12.03	0.867	0.133	0.068	0.32
GC4	0.091	6.04	0.941	0.059	0.119	0.19
GC5	0.200	7.22	0.934	0.066	0.087	0.13
GC6	0.472	6.92	0.951	0.049	0.123	0.23
GC7	0.114	6.53	0.948	0.052	0.097	0.03
GC8	0.045	5.75	0.952	0.048	0.087	0.13

References:

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P33. New compound of Ce(III) with Keggin monolacunary polyoxometalate

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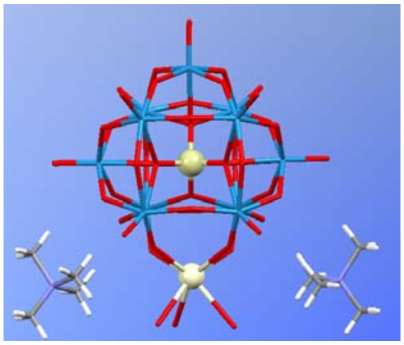
POMs interest in molecular magnetism is determined by the ability of this class of inorganic compounds to be good examples of magnetic clusters. Due to the rigidity imposed by the ligands heteropoly-, this class of complexes is a unique example in coordination chemistry where the sign, intensity and nature of the exchange interactions can be easily changed.

They can serve as model systems for understanding the magnetic exchange interactions.

Rational synthesis of polyoxometalates usually follows a self-assembly mechanism involving lacunary precursors. In the final polyanion, these vacant subunits can incorporate functionalities that are appropriate for the construction of miniaturized molecular devices.

An example of this class of materials is the complex of Ce(III) with monolacunary Keggin structure $[XW_{10}O_{36}]^{n-}$ in presence of tetrabutyl-ammonium (TBA^+) cations. The structure was solved by the direct method and refined by the full-matrix least squares method on F^2 using SHELXTL 97 crystallographic software package.



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P34. Cobalt influence on crystalline structure and transport properties of $La_{0.9}Sr_{0.1}Cr_{1-x}Co_xO_3$

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The system of $LaCrO_3$ perovskite has drawn up an interesting picture that, depending on the alkali-earth and transitional metals-doping. The partial replacement of La^{3+} with Sr^{2+} and Cr ions by Co ions increases concentration of Co^{4+} ion and introducing more chemical disorder which permits to figure out how much effect the structural behavior and electronic phases concentrations. A row of $La_{0.9}Sr_{0.1}Cr_{1-x}Co_xO_3$ (x=0, 0.05, 0.1, 0.2, 0.3 and 0.5) perovskites were obtained by sol-gel method. XRD analysis and IR spectra indicated the formation of only perovskite phase. The compounds with a low Co content have an orthorhombic (Pnma) structure. For x=0.3 and 0.5 LSCCO sample a rhombohedral transformation take place. Such behavior can be attributed to the increase of $Co^{3+/4+}$ concentration or/and of the appearance of an important voids concentration.

Magnetic properties and transport characteristics were investigated between 77 and 400 K. A non-monotonous variation of the magnetic moment with the increase of the Co concentration can be observed in LSCCO case. A mixture of electronic phases is present in the investigated perovskites: a AFM (at low temperature) phase, an orthorhombic FM phase, which determine the magnetoresistive behavior, and an orthorhombic AFMI/PI phase, insulator in the investigated range of temperatures.

The influence of structure and Cr/Co concentration on electrochemical response was studied by cyclic voltametry. The anodic and cathodic current signals are present and cathodic peak shifted to high potential with x. The $La_{0.9}Sr_{0.1}CrO_3$ could be effectively used as cathode active material in the formation of electrochemical power sources, while $La_{0.9}Sr_{0.1}Cr_{0.9}Co_{0.1}O_3$ can be used both as anode and cathode active material, multiple cyclization current values increase from 94.6 to 161 μA.

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P35. Atmospheric deposition of copper and zinc in Maramures county

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The need to reduce pollution to levels that minimize adverse effects on human health involve the monitoring of air quality, including dry depositions and their metal content[1-2]. The analysis of these parameters aims to investigate the air quality in Maramures County (with nonferrous mining activities) and in the Romanian -Ukraine transboundary area. The present paper presents the experimental results obtained for dry atmospheric deposition of copper and zinc using atomic absorption spectrometry (AAS).The samples were collected from four location of Maramures County (Baia Mare, Sighet, Viseu and Borsa) during May-October 2014. The highest average values of copper concentrations in the dry depositions were found in Baia Mare (199.88 µg/g), that is the most important industrial center followed by Borsa (111.49 µg/g), that is a nonferrous mining center. In Viseu and Sighet the average concentrations of copper in the dry depositions were lower: 75.63 and 64.26 µg/g. Zn average concentrations in the dry depositions were 6.4 -12 times higher than Cu concentrations. No correlation between copper and zinc were found in Baia Mare and Sighet. In Viseu and Borsa relative high values of Person correlation coefficients between copper and zinc content in the dry deposition were found: 0.688 respectively 0.702 estimating that both pollutant in the ambient air have the same sources probably due to the re-suspension of the deposed dust from tailing ponds.

References:

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P36. Synthesis and characterization of new mutant peptides used for understanding the conformational changes related to Alzheimer disease

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Neuropeptides are biomolecules which have biological activities such as antimicrobial, antioxidant, as well as in neuroprotection and immune regulation; therefore, they are important candidates for future drug development. Metal ions have been implicated in multiple pathologies, but neurotoxicity is believed to be their most common manifestation.[1] Thus, the binding of metals to peptides, such as amyloid-β peptide was found to be dependent on the Aβ conformation.[2] The amyloid β-peptide (Aβ) is the major component of senile plaques, which are considered to play an important role in Alzheimer's disease pathology.[3] Short peptides have been used to study the structures and mechanisms that are also relevant for the native and longer peptides involved in the neurodegenerative diseases.[4]

Here, we report the experimental results that are focused on the synthesis and characterization of normal Aβ1-16 peptide and modified peptides such Aβ1-16 Ala and Aβ1-16 Ser, where hystidine was replaced with alanine, serine respectively. These are residues 1-16 of the full-length β-amyloid peptide (Aβ1-40) associated with AD and were obtained with an automated peptide synthesizer using solid phase peptide synthesis method. The interaction between metal ions and synthesized peptides have been studied using Fourier transform infrared spectroscopy (FT-IR), AFM measurements, as well as NMR spectroscopy. NMR technique has already become an important device in studies of the binding properties of metal ions to peptides and proteins. Therefore, the conformation of the synthesized peptides can be deduced from ^{1}H-NMR spectra, according to the results obtained by FT-IR.

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Acknowledgements: C.-I. Ciobanu is thankful to the grant POSDRU/159/1.5/S/137750, for financial support. For NMR experiments,we thank to the POSCCE-O 2.2.1, SMIS-CSNR 13984-901, CERNESIM.

P37. Optimal tosylation parameters for *β*-cyclodextrin functionalization

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Cyclodextrins are desired hosts for a wide range of applications, starting from microencapsulation to enzyme mimics. The *β*-cyclodextrin is especially studied and even has found real life applications due to the appropriate size of the cavity that may accommodate various organic species. Further development of *β*-cyclodextrin derivatives is therefore needed for better, more efficient and specific applications. One attractive compound is mono-6-amino-6-deoxy-*β*-cyclodextrin which can be used to create new sensors and new polymers with absorption capabilities. To synthesize this derivative, a regiospecific tosylation of *β*-cyclodextrin is needed in order to obtain mono-6-deoxy-(*p*-toluenesulfonyl)-*β*-cyclodextrin. This regiospecific tosylation is the only stage that lowers the yield of the overall reaction and restricts the industrial applications of this compound. In order to simulate technical applications, food grade *β*-cyclodextrin (95%) was used and 4 different literature tosylation approaches were attempted [1],[2],[3],[4]. The synthesis with the highest yield has proven to be a mixture of mono-, di-, tri- tosylated-*β*-cyclodextrin after MS analysis. After varying synthesis parameters, guidelines have been obtained in order to decrease the high tosylation degree. After the complete parameterization this type of reaction is suitable for obtaining polymers.

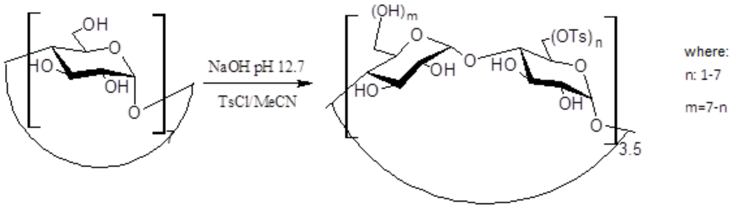

Figure 1. General tosylation reaction scheme.

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P38. ATR-FTIR, a non-invasive tool to investigate keratin from human fingernails

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In recent studies, infrared (IR) spectroscopy was used to detect common contaminants, molecular deformations and complexities in biological fluids such as serum, plasma hemoglobin molecule, tears, saliva, and some other components such as nails, skin, and hair [1]. Also, IR has been used as a tool to optimize topical drug delivery systems to treat nail disease [2], or to monitor chronic fatigue syndrome [3], and diabetic patients by analyzing the amide I region of the IR spectra of nails.

The purpose of this study is to investigate keratin, the major component of the fingernails, from patients diagnosed with nail psoriasis in comparison to healthy donors, using the ATR-FTIR technique in order to highlight modifications in the molecular structure. ATR-FTIR provides qualitative and quantitative information about the secondary structure of proteins by analyzing the amide I, amide II and amide III bands.

Besides the structural information obtained by ATR-FTIR spectroscopy, the elemental composition variations were monitored by EDX, in healthy and psoriatic nails.

by the European Social Fund Operational Programme "Human Resources Development" for 2007-2013.

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Acknowledgement: This work received financial support through the "Program of Excellence in multidisciplinary doctoral and postdoctoral research in chronic diseases", contract no. POSDRU/159/1.5/S/133377, beneficiary U.M.F. "Gr. T. Popa" Iasi, project co-financed

P39. New Tetrathiafulvalene Derivatives Substituted with [2.2]Paracyclophanes

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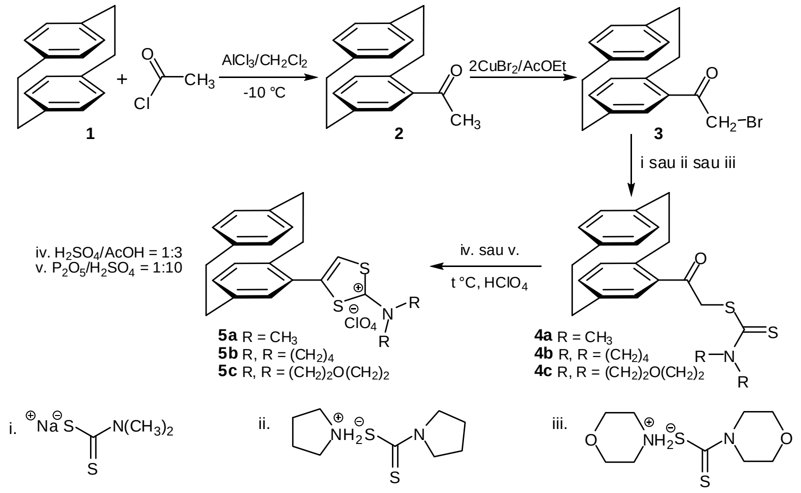
Tetrathiafulvalene (TTF) derivatives belong to the group of the most intensively studied strong organic electron donors, employed as components for conducting ion-radical salts (IRS) and charge transfer complexes (CTC). [1, 2] The charge-transfer salt of TTF with tetracyanoquinodimethane (TCNQ) displays metallic-like behavior over a wide temperature range and exceptional electrical conductivity.[3, 4]

We report the synthesis of new tetrathiafulvalene (TTF) derivatives containing [2.2]paracyclophane units. The increasing of the donor properties of TTF should results in complexes with application in material chemistry. The synthetic route involves the preparation of the corresponding 1,3-dithiolium perchlorates **5a-c**, their conversion to 1,3-dithiol-2-thione **6**, followed by its dimerization using trimethylphosphite.[5]



Scheme 1. Synthesis of 1,3-dithiolium perchlorates **5a-c**

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P40. X-Ray evidence of cyclic and acyclic phthalazinic derivatives with vinyl chain

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A thorough study on the chemistry of fused *N*-azaheterocyclic compounds have revealed many practical applications, due to their extended π-conjugation, being used like sensors, biosensors, electroluminescent materials, lasers, and other semiconductors devices.[1-4] Compounds with pyrrolo-pyridazine skeleton represents such a class, this unit being a pure blue-emitting moiety. [1,3,4]

Taking in view these considerations we desired to synthesize new pyrrolo-phthalazinic compounds with a vinyl chain (**I**), using two steps only: quaternization and cycloaddition reactions. The second step was done at 40^{0}C, when the cyclic compound (**I**) was obtained, but in case of lower temperature, it was obtained besides the other the acyclic compound (**II**). The structures of new compounds were proven using X-Ray diffraction and NMR spectroscopy. The NMR spectra were recorded on a Bruker Avance III 500 MHz spectrometer. The X-Ray experiments were performed using a SuperNova Dual diffractometer.

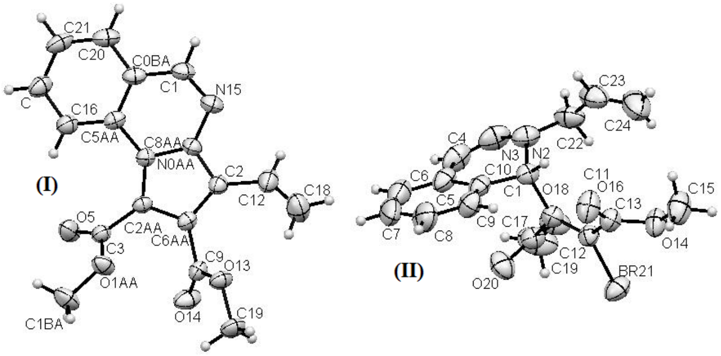

Figure. 1. X-Ray structures of cyclic (**I**) and acyclic (**II**) pthalazinic derivatives.

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Acknowledgements: The present work was supported by PN-II-DE-PCE-2011-3-0038, no.268/05.10.2011 We also thank to the POSCCE-O 2.2.1, SMIS-CSNR 13984-901, Project no. 257/28.09.2010, CERNESIM, for X-ray experiments.

P41. Synthesis and characterization of new anthracene-based imidazolium salts

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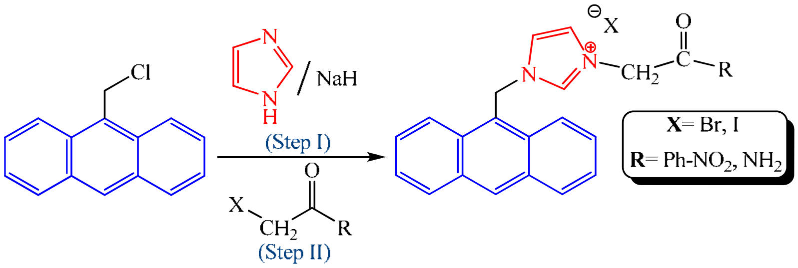
Due to its strong π-π* emitting properties, anthracene scaffold is a well known chromophore, inducing versatile photophysical and photochemical properties to the anthracene-based compounds[1,2]. On the other hand, anthracene-based imidazolium salts have been reported as compounds with fluorescence properties as well as biological properties, especially when varying the nature of anion[3-5].

In the present work, we realize the synthesis of new anthracene imidazolium salts, in order to test their fluorescence properties. Thus, in the first step the *N*-alkylation of imidazole was performed, using 9-chloromethilantracene, followed by quaternization reaction at the *N^3* position of imidazole.



The structure of all new compounds was proved by spectral analysis (IR, ^{1}H NMR, ^{13}C NMR, 2D-COSY, 2D-HMQC, 2D-HMBC). Also, preliminary UV-Vis measurements have been done, in order to test the emission properties of the synthesized compounds.

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Acknowledgements: to CNCS Bucharest for financial support, project PN-II-DE-PCE-2011-3-0038, no. 268/05.10.2011 and to the POSCCE-O 2.2.1, SMIS-CSNR 13984-901, No. 257/28.09.2010 Project, CERNESIM, for NMR measurements.

P42. The antifungal activity and cytotoxicity of MXP-4509, a new compound with pharmaceutic potential

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The antifungal activity of MXP-4509 (MXP) was compared with that of two commercial compounds, fluconazole (FLC) and voriconazole (VOR). A preliminary assessment of the cytotxicity of MXP is also included.

The antifungal activity was assessed by using the EUCAST 7.1 method on 265 *Candida* spp. pathogenic isolates identified with the ID 32 C® *Candida* strips (BioMerieux). The minimum inhibitory concentrations (MIC) were spectrophotometrically determined at 405 nm.

The cytotoxicity of MXP was tested on normal dermal human fibroblasts using the Promega „CellTiter 96® Non-Radioactive Cell Proliferation Assay" kit with an inoculation density of 6×10^3 cells/well. Absorbance was read at 570 nm.

The new compound, MXP-4509, showed a very good antifungal activity, comparable to VOR and much superior to FLC. The MIC_{50} and MIC_{90} values and the geometric mean of the MICs were equal or close to those of VOR and much lower than those of FLC.

In relation to the 4 μg/mL maximum level reached by the MIC values, MXP has a very low citotoxicity. An over 20 fold concentration of the compound caused a cellular growth inhibition of only 22%.

In conclusion, MXP-4509 has a high pharmaceutic potential due to its very good antifungal activity and its low citotoxicity.

Acknowledgements: "This publication benefited from the financial support of the project "Programme of excellency in the multidisciplinary doctoral and post-doctoral research of chronic diseases", contract no. POSDRU/159/1.5/S/133377, beneficiary "Gr. T. Popa" University of Medicine and Pharmacy of Iasi, project co-financed from the European Social Fund through the Sectoral Operational Programme Human Resources Development (SOP HRD) 2007-2013".

P43. Optimization of catalytic degradation of organic dyes in the presence of nanoferrites

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The nanoparticles were synthesized using the co-precipitation method in basic media using food grade Palm Oil, a cheap, easily available reagent as surfactant. The as synthesized materials have been characterized using X-ray diffraction, UV-Vis and FT-IR spectroscopy, SEM imaging as well as regarding the magnetic properties (VSM) and surface characterization using BET theory.

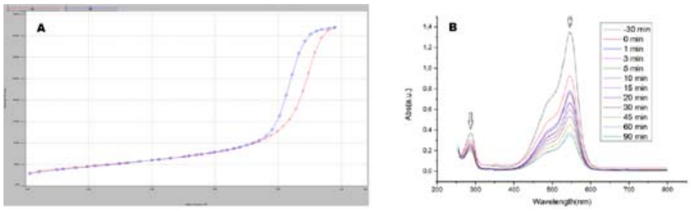

Figure 1: A) Adsorption isotherm for $MnFe_2O_4$
B) Time dependence of BF concentration in the presence of Mg ferrite

The catalytic activity was studied using the decolouration of dyes in the presence of H_2O_2 as oxidizing agent. This process is based on the so called Fenton process where the metal cations react with the hydrogen peroxide to generate HO• radicals that decompose the dyes.

Results indicate that the most important parameter affecting the efficiency of the catalyst is the specific surface of the nanoparticles as the nanoparticles with the highest specific surface offer the best results for the dye degradation.

Cation distribution is also of great importance due to the fact that the reaction takes place on the surface of the nanoparticles. It is well known that mainly octahedral sites are on the surface of the NP's therefore the cation distribution in octahedral sites is important. This characteristic is especially visible when considering $CuFe_2O_4$ which is a inversed spinel with almost all copper cations in the octahedral sites and despite its smaller specific surface has a high catalytic activity, reacting through both the Cu^I-Cu^{II} and Fe^{II}-Fe^{III} pairs.

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P44. Synthesis and characterization of $Mn_xCo_{1-x}Fe_2O_4$ by co-precipitation route and absorption of AuBSA NCs on the surface of magnetic NPs

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In the last few years, multifunctional magnetic nanoparticles have attracted great attention for their biomedical and industrial application like: hyperthermia, resonance imaging (MRI) and as targeted drug delivery.

Multifunctional nanoparticles (NPs) $Mn_xCo_{1-x}Fe_2O_4$ series have been prepared using co-precipitation method, and as surfactant, carboxymethylcellulose. Magnetic NPs were coated three times with oppositely charged polyelectrolytes (PEs) using a layer-by-layer technique. Last step was the absorption of gold nanocrystals on the surface of magnetic nanoparticles, coated with PEs. XRD patterns for $Mn_xCo_{1-x}Fe_2O_4$ series are present in figure 1. The patterns were found to match well with those of cubic spinel crystalline structure without secondary metal oxide phase.

Formation of gold nanocrystals, in BSA matrix, with size smaller than 3 nm is presented in figure 2. EDX analysis confirms the presence of gold.

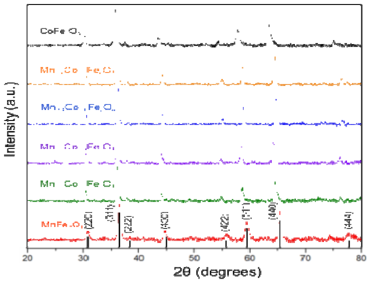

Figure. 1 XRD patterns for $Mn_xCo_{1-x}Fe_2O_4$.

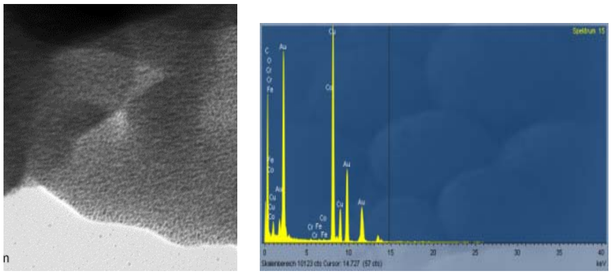

Figure. 2 Micrograph for gold particles, and EDX.

ATR-FTIR analysis confirms that the noparticles surface is activated with hydroxyl and carboxyl groups after thermal treatment. The results from ATR-FTIR shows that polyelectrolytes were absorbed on the surface of nanoparticles.

These results confirm formation the gold nanoparticles, smaller than 3 nm and absorption of these on magnetic NPs-PE system.

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P45. Stiffening porous inorganic materials in particulate form for polymeric composites

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Our study aims to obtain composites with a polymer matrix including granular porous inorganic materials. The polymer matrix is an epoxy resin, and AAC (autoclaved aerated concrete), the extruded carbon, activated alumina, silica gel and glass fiber were used as reinforcing beads. The comparative study of the properties of the obtained composites was intended to determine the structure with the lowest cost, increased mechanical strength and the development of manufacturing technologies in the laboratory.

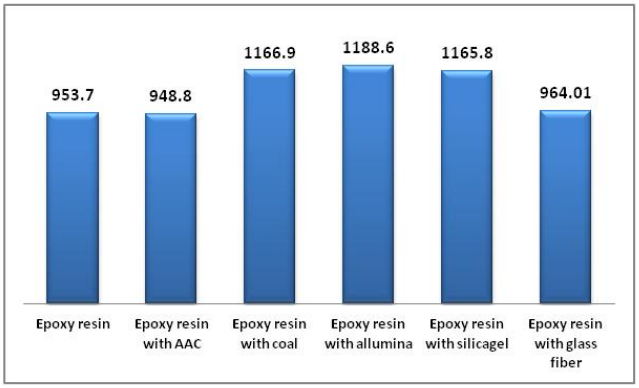

Figure 1. *Density of the composite samples, kg/m*^{3}

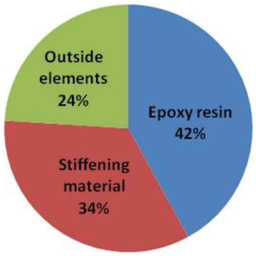

Figure 2. *Structure of the composite with AAC granules*

The composites containing AAC or extruded carbon had adequate mechanical strength, low density (Figure 1), and in the manufacturing process there were no problems with cross-linking of the resin. In economic terms, the use of AAC is desirable because this material results as waste from construction activity and can replace up to 45% (Figure 2) of the polymer matrix.

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P46. Multifunctional sandwich composites with possibilities to control the flexibility degree

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Laminated sandwich composite materials are used especially for their thermo-insulating properties; the usual form is a polyurethane foam layer inserted between two rigid walls. This paper aimed to increase the flexibility of the product and diversification of their properties. To this end, we have made in laboratory multi-layer laminated composite of different materials. Polyurethane foam, cellular polyethylene and mineral wool were used for the core. For sides, we used laminated cardboard, polyester fabrics and cellular polyethylene.

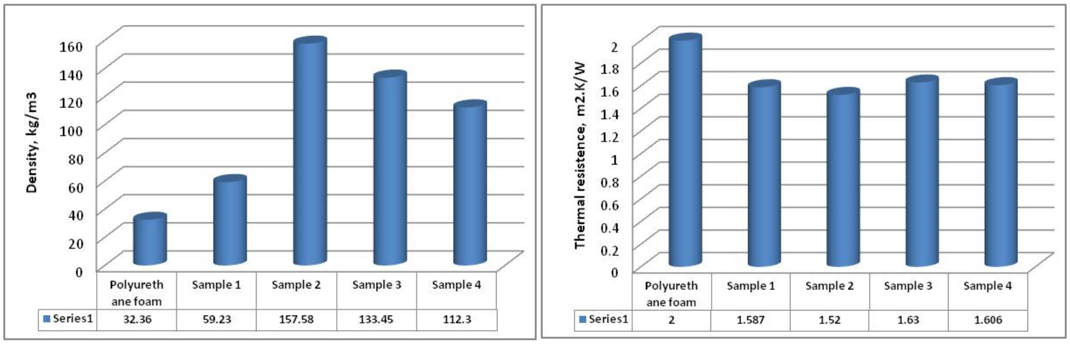

Figure 1. *Properties of the composite samples*

The analysis of the obtained composite samples showed multilayer structures of polyurethane foam, mineral wool and cellular polyethylene (samples 3 and 4), with properties of sound insulation, thermal insulation and high flexibility. In order to reduce the degree of flexibility, internal metal structure of the aluminum sheet has been introduced into the foam layer.

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P47. Dinamica reacției Dushman în prezența ionilor Ce^{3+} şi Mn^{2+}

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Reacția Dushman se realizează între ionul IO_3^- şi ionul I^- în mediul acid. Reacția constă în două etape şi anume:

$$IO_3^- + 5I^- + 6HClO_4 \rightarrow 3I_2 + 3H_2O$$
$$I_2 + I^- \Leftrightarrow I_3^-$$

Dinamica formării I_2 şi I_3^- s-a studiat spectral la lungimile de undă λ=350nm şi λ=460 nm, în absența şi în prezența ionilor metalici. Rezultatele sunt date în figurile de mai jos.

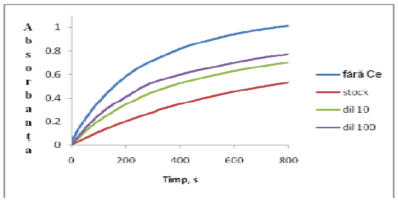


Fig. 2. *Evoluția $[I_2]$, $\lambda = 350$ nm în prezența ionilor de Ce(III)*

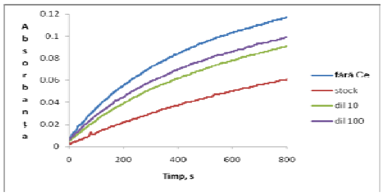


Fig. 3. *Evoluția $[I_3^-]$, $\lambda = 460$ nm în prezența ionilor de Ce(III)*

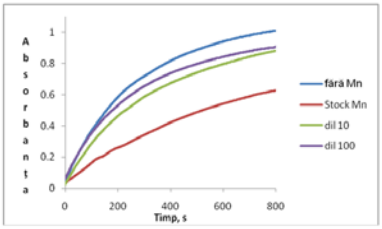


Fig. 1. *Evoluția $[I_2]$, $\lambda = 350$ nm în prezența ionilor de Mn (II)*

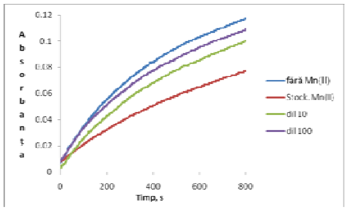
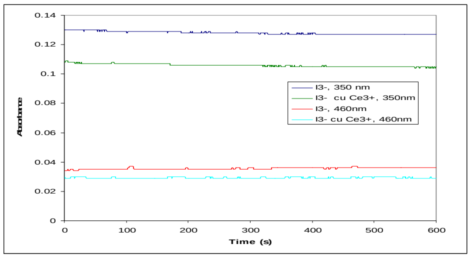


Fig. 4. *Evoluția $[I_3^-]$, $\lambda = 460$ nm în prezența ionilor de Mn(II)*

Din aceste reprezentări rezultă că în prezența ionilor metalici, concentratiile de I_2 şi I_3^- descresc. Această scădere s-ar datora fomării unor compusi între: $\{Me^{z+},IO_3^-\}$,$\{Me^{z+},I^-\}$, $\{Me^{z+},I_2\}$sau $\{Me^{z+},I_3^-\}$.

Folosind metoda punctului izobestic si metoda JOB am dovedit că nu se formează compuşi de tipul $\{Me^{z+},IO_3^-\}$,$\{ Me^{z+},I^-\}$,$\{ Me^{z+},I_2\}$. Evolutia temporală a amestecului $\{I_3^- ,I_2 ,I^-\}$ respectiv $\{I_3^- ,I_2,I^-,Me^{z+}\}$ dovedeşte indubitabil că se formează un ion molecular de forma $[Me(I_3^-)]^{z-1}$ sau $[Me(I_3^-)_2]^{z-2}$



(Figura.5). Absorbanța amestecului $\{I_3^- ,I_2 ,I^-\}$este mai mică în prezenta Me^{z+}atît la λ=350nm cat şi la λ=460 nm (liniile doi si patru).

P48. Molecular studies of some azobenzene derivatives

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Azobenzene and its derivatives represent versatile structures with unique trans (E) to cis (Z) izomerization properties when submitted to irradiation upon UV light. The reverse cis to trans izomerization is mainly carried out by light or occurs thermally in the dark [1].

During the process of photoizomerization, four possible mechanisms have been proposed up to now: rotation, inversion, concerted inversion and inversion assisted by rotation [2].

Despite numerous studies, research of azobenzene photochemistry, mainly of the isomerization mechanisms, remains still a topic open to investigation. Additional substituents (in the present work, derivatives containing maleimide moieties) on the azobenzene ring structure can change the izomerization mechanism.

The main goal of the present study was to investigate the influence of substituents concerning the azobenzene structure (Fig. 1) by theoretical calculations, based on Density Functional Theory (DFT) [3].

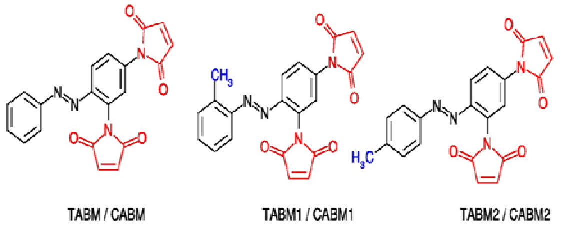

Figure 2 Additional substituents on the azobenzene structure

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P49. Compliance with the Romanian regulation of the quality indicators for the indoor swimming pool water samples: potential risks for human health?

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This study aimed on assessing the water quality for randomly selected indoor swimming pools located in Iasi city in order to determine its compliance with the Romanian regulation (order no. 119/2014). Therefore, physical and chemical parameters, including free and combined chloride, $KMnO_4$ consumption, total hardness, pH, temperature and turbidity together with microbiological characterization (*Escherichia coli*, Coliforms, *Pseudomonas aeruginosa*, *Enterococci*, *Staphylococcus aureus)* was carried out for a total of 30 samples, using standard analytical protocols. The obtained results of the present study showed significant correlations ($p<0.05$) between the investigated parameters. However, in order to determine the compliance with the Romanian regulation, after evaluating the obtained results it could be concluded that only 20% of the total analyzed samples correspond within the regulatory limits. The parameters which were mostly outside of the legal limits were free chlorine and water pH. Therefore, 80% of the analyzed samples presented higher values for the free chlorine and 30% presented lower pH values when compared with the Romanian regulation. Additionally, 17% of the samples included in our study were declared unacceptable after the microbiological investigation. The results of the present study suggest the need of continuously monitoring of the indoor swimming pool water quality in order to increase bather hygienic practices and awareness of the risks.

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P50. Linear and nonlinear isotherm models for adsorption of heavy metal ions on functionalized polymeric materials: A comparative study

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A variety of adsorption isotherm models (Langmuir, Freundlich, Dubinin-Radushkevich, Temkin, Sips, Redlich-Peterson, Koble-Corrigan etc.) may be employed to evaluate the adsorption process at equilibrium. The method of least squares with linearly transformed isotherm equations is the most widely used technique to find the best fitting of equilibrium experimental results. For achieving this objective, the nonlinear regression method, in which the error distribution between the experimental data and the predicted isotherm is minimized by an iterative procedure, has been considered lately to be better than the linear one.

In this investigation, linear and nonlinear forms of several isotherm models were compared to determine which one provides the best fit of experimental results for the adsorption of some heavy metal ions onto functionalized polymer beads. The experimental data for the adsorption of different metal ion species onto crosslinked polystyrene resins containing ionic liquid-like fragments covalently attached were obtained by performing batch equilibrium tests. Four two-parameter (Langmuir, Freundlich, Dubinin-Radushkevich and Temkin) and one three-parameter (Sips) isotherm models were employed in their linear and nonlinear forms to analyze the equilibrium data; in the case of Langmuir model, several linear equations were considered. It was revealed that the nonlinear regression model is not always the best way for predicting the isotherm parameters. Also, it was evidenced that, of all isotherm models in both linear and nonlinear forms, the Langmuir model in a certain linear form best describes the experimental data. The obtained results support the assumption that chemisorption is the dominant adsorption mechanism taking place by monolayer coverage of the adsorbent surface. It seems likely that adsorption process occurs mostly by the formation of coordination compounds involving the metal ions, their counterions and the ionic liquid-like fragments.

P51. Synthesis, structure and biological activity of Cu(II) coordination compounds with imidazole thiosemicarbazide derivatives

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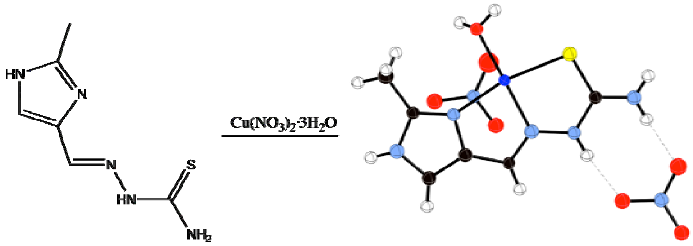
Recent expansion of antimicrobial drug research has occurred because there is a critical need for new antimicrobial agents to treat these life threatening invasive infections. Imidazole and its derivatives have gained remarkable importance due to their widespread biological activities and their use in synthetic chemistry. [1] The synthesis of transition metal coordination compounds with thiosemicarbazone ligands have been received considerable attention due to the pharmacological properties of both ligands and complexes [2,3].

We report here the synthesis, structure and biological studies of a new copper(II) coordination compound with 2-methyl-1H-imidazole-4-carbaldehyde thiosemicarbazone. The organic ligand (HL-TSC-4-IM) was prepared by condensation of 2-methyl-1H-imidazole-4-carbaldehyde with tiosemicarbazide. Copper(II) nitrate and TSC-4-IM in equimolar ratio were dissolved separated in ethanol, and mixed together.



The antimicrobial activity against gram-negative and gram-positive bacteria has been determined for this considered compound.

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P52. A study about some parameters regarding the quality of water of Suceava River

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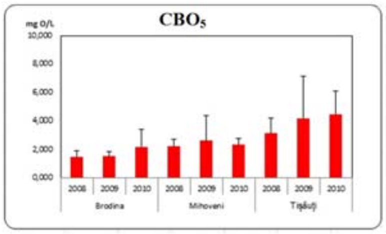
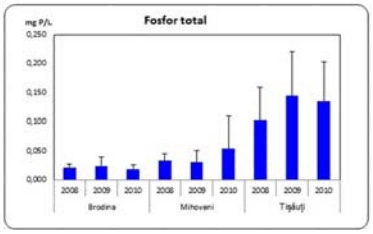
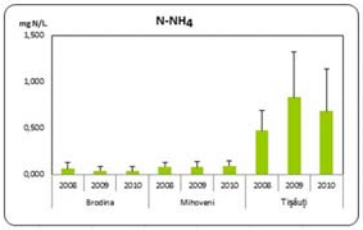
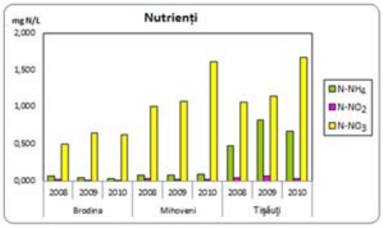
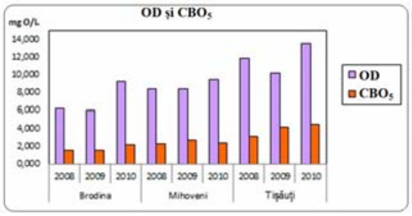
This article presents a study about the quality of water of Suceava River closed to parameters CBO5, CCO-Cr, phosphates, total phosphorus, nitrites, nitrates, nutrients, dissolved oxygen and ammoniacal nitrogen. Three distinct sections of the river, Brodina, Mihoveni and Tisauti were monitored during three years, between 2008 and 2010. Although the correlations between parameters seem to be chaotic, some correspondences were established and the activity of some possible pollutants was emphasized.

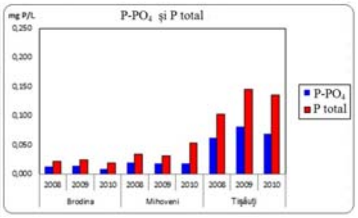












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P53. Research on the use of ceramics in the process of drinking water

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Since ancient times it is known antimicrobial effect of ceramics, and later, their great capacity of ion exchange. The two effects are much studied today for their application for the purification and treatment of water.

The main advantage of ceramics used in the purification and treatment of water is due to theirs mechanical strength, acid-base and redox stability, the thermal and photochemical stability as well as a large number of important characteristics as specific gravity under 1500Kg/m^3 and compressive strength, which varies between 50 and 200daN/cm^2; maximum amount of water absorbed varies between 8-20%; chemical and biochemical processes and specific loads due to water treated. In addition, another technical advantage of industrial ceramics is the minimum concentration of components soluble in aqueous systems.

In this paper work we studied a large group of industrial ceramics and traditional ceramics (pottery fragments) different caustic module Si (Ti) / Al and in terms of composition of the Ca, Mg and Fe and morphology. Chemical composition obtained by means of SEM-EDX acid was coupled with ceramics and their ability to retain cations of Fe (II).

Keywords: Ceramics, potable water, ion exchange capacity, analysis SEM /

P54. SEM characterization of photocatalytic ZnO for air purification applications

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TiO_2 and ZnO are most widely used semiconductor photocatalysts because of their high photosensitivity, photochemical stability, large band gap, strong oxidizing power and non-toxic nature. In particular, anatase TiO_2 has been reported as the most extensively used semiconductor photocatalyst for industrial applications and pollution clean-up since 1970s. Recent researches highlight ZnO to show an even better activity than TiO_2 in the photodegradation of some dyes in aqueous solutions, since it can absorb more light quanta. The successful exploitation of such catalysts requires the development of techniques for controlling their size, morphology, structural and surface characteristics, as well as efforts to enhance their photochemical response to visible/solar illumination.

Up to date, there are quite few reports in the literature presenting state of art approaches of use of ZnO material onto textile substrates for several applications as antibacterial [1], deodorizing [2] and UV protection [1,3], and none regarding any systematic approach of direct growth and optimization with respect the textile support. More than that, up to our knowledge, there is no available study in the literature about ZnO coated textiles used as photocatalytic active support for gaseous compounds decomposition. The present contribution brings in the attention the structuring in various morphologies of photocatalytic ZnO grown onto textile supports for air purification applications.

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P55. Nanostructured metal oxides for advanced applications

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Metal oxides are the key ingredients for the development of many advanced functional materials and smart devices. Nanostructuring is one of the best ways to exploit their properties. Metal oxides can be prepared in various sizes and geometries, but one of the greatest challenges remains the precise control of the particle size, shape, crystalline structure and processing properties. Tungsten oxide (WO_3) is a material that have been mostly studied for its electrochromism, photocatalysis, and sensing capabilities. The present contribution presents preliminary results of chemical synthesis and characterization of nanostructured WO_3 and ZnO for potential applications in organic solar cells application as a charge injection layer and electrochromic devices.

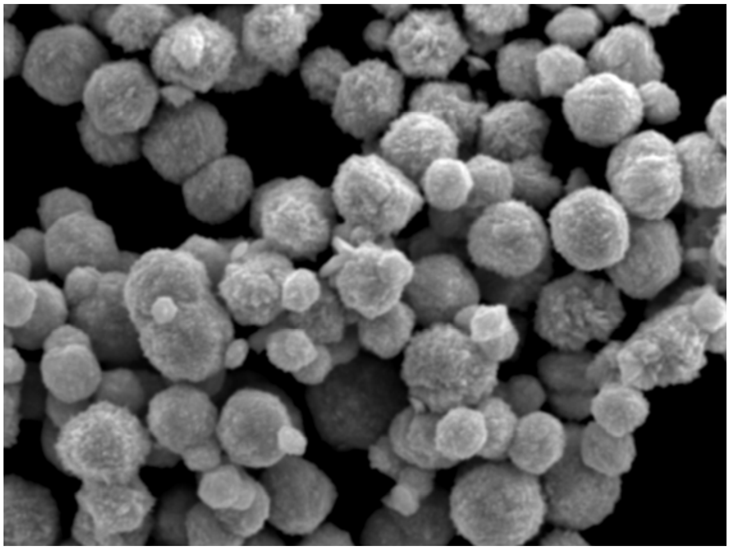

Figure.1 Chemical synthesized nanostructured WO_3.

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