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ABSTRACTS

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CI 1. Spin coupling and magnetic anisotropy in mn(iii) complexes: weighing the fine balance of ligand field, spin orbit and lattice effects

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Aiming for systems behaving as magnet at molecular or nano scale, must consider molecular bricks carrying magnetic anisotropy. Therefore, the Mn(III) building blocks are valuable pieces in the puzzle of molecular magnetism, combining the specifics of magnetic anisotropy of the units with the variety resulting from the riches of possible assembling manners, various bridging modes and agents tuning the exchange effects.[1] We discuss the synthesis, structure and magnetic properties of a new series of Mn(III) salen complexes with acetate ion as bridging ligand.[2] The manganese salen complex form oxo-bridged dimers whose further assembling by acetate groups, leads to zig-zag chains. There are two alternating types of dimeric {Mn_2O_2} units, each of them intrinsically ferromagnetic and anisotropic, but mutually coupled antiferromagneticaly along the chain. Magneto-structural analyses were done with the help of ab initio calculations understanding the subtle factors of local magnetic anisotropy combined with the exchange effects. A new qualitative explanation of ferro- vs. antiferro- coupling, in terms of orthogonalized magnetic orbitals (OMOs) is outlined, shifting the customary paradigms of the domain, to meet the technical realization of ab initio calculations.

Since the magnetic anisotropy is due to the interplay of Ligand Field and Spin Orbit effects it is also important in spin conversion phenomena. The spin transition is driven by Ligand Field balance and the communication between the two spin states is possible by spin orbit, so we meet a common mechanism.[3]

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CI 2. Back to the basis! A critical revision of gaussian basis sets

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It is well acknowledged that the Gaussian Type Orbitals (GTOs) are not natural primitives to build approximations of the atom electronic structure, first of all, because of the exp($-\alpha r^2$) pattern, while Slater Type Orbitals (STOs), with exp($-\alpha r$) exponential components are more appropriate to this goal. However, the GTOs are accepted as compromise for easier calculations of the atomic and molecular integrals, since the dawn of quantum chemistry.

At the same time, a hidden drawback, overlooked by the quasi-unanimity of users and developers of quantum chemistry programs, stays in the fact that the standardized GTO bases have drastic limitations in the radial polynomial co-factors. Thus, all the s-type GTOs are exclusively collections of exp($-\alpha r^2$) functions, all the p-type ones consist in r•exp($-\alpha r^2$) components, while the d-type sets based on r^2•exp($-\alpha r^2$) sets, and so on. Then, for instance, the lack of any r-type factor for the s-orbitals makes very problematic the retrieval of correct long range dependence of medium and high quantum numbers. The situation is similar for all types of GTO-based atomic orbitals.

A easy alleviation of the situation can be achieved introducing general r^{n-1}•exp($-\alpha r^2$) primitives for all the types of atomic shells, in analogy to the well-known r^{n-1}•exp($-\alpha r$) pattern of STO bases. Thus, in spite of the tacit belief that all the methodologic backgrounds are nowadays clarified, it seems that there is yet room to rework some essential issues on in the mathematical blueprints of the applied quantum chemistry.

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CP 1. Polymetallic oxide-based composite materials obtained through sol-gel method

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A composite material is created by combining two or more materials – often ones that have very different properties. The two materials work together to give the composite unique properties. However, within the composite we can easily distinguish each of the different materials, as they do not dissolve or blend into one another. Inorganic-inorganic or inorganic-organic polymetallic oxide-based composite materials were synthesized using the sol-gel method.

$CoFe_2O_4$-Nb-Pb(Zr,Ti)O_3 multiferroic composites. Di-phase magnetoelectric composites formed by the magnetic $CoFe_2O_4$ and the ferroelectric Nb–Pb(Zr,Ti)O_3 were prepared through citrate–nitrate combustion method, using Nb–Pb(Zr,Ti)O_3 template powders prepared by mixed oxides. Pure di-phase powder composites with good crystallinity were obtained after the calcination stage. The dielectric and magnetic investigations performed at room temperature confirmed the formation of composite ceramics which exhibited both dielectric and magnetic properties, at room temperature, with the resulting permittivity and magnetization being the sum of the properties from the parent Pb(Zr,Ti)O_3 and ferrite phases.

Spherical Alumina Pellets Coated with $BaTiO_3$. For the first time a spherical deposit of a dielectric compound ($BaTiO_3$) was obtained by an adapted sol–gel method.

Nanosized $NiFe_2O_4$/kaolinite composite as adsorbent for organic dyes. A magnetic inorganic/inorganic composite material was synthesized by sol-gel autocombustion method, using tartaric acid as fuel. Experiments on methyl orange dye removal in the presence of the composite materials showed very good adsorptive/catalytic behavior.

Composite materials based on hydrogels and $NiFe_2O_4$. Nickel ferrite was obtained by the sol–gel autocombustion method using citric acid as chelating/fuel agent, while the hydrogels and the ferrite–hydrogel composites were prepared by an original polymerization-crosslinking simultaneous method using a monofunctional crosslinking agent. The microbiological activities of composites were determined against the *Staphylococcus aureus* test strain. Kinetic studies of drug delivery efficiency were performed.

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CO 1. Efficient removal of Methylene Blue from aqueous solution using ionic biocomposites: Sorption and reusability studies

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Dyes are broadly utilized in various industries, such as paper, textile, leather, cosmetics, pharmaceuticals, and others. The considerable amount of colored effluents resulting from these industrial domains cannot be disposed without an adequate treatment.[1] Accordingly, concentrated efforts have been undertaken for the treatment of industrial dye-laden effluents on a large scale using various methods including oxidation, biological treatment, flocculation, coagulation and adsorption, respectively. Among these techniques, adsorption is especially attractive due to its simplicity of design, high efficiency and ease of exploitation.[2,3] In this context, ionic biocomposites based on sodium alginate and clinoptilolite (Alg/CPL) were fabricated by a dual ionic cross-linking strategy and applied for the removal of Methylene Blue (MB).[4] The structural and morphological characterization of the ionic biocomposites were performed by FT-IR, energy dispersive X-ray spectroscopy (EDX) and SEM. The influence of CPL content, contact time, sorbent dose and initial MB concentration on the sorption capacity was also studied. To get insights into the sorption mechanism, the kinetics and sorption isotherms were analyzed.

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CO 6. Aromatic hydrocarbon contribution to the secondary organic aerosol formation in urban atmosphere

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Aromatic hydrocarbons (AHs) are ubiquitous volatile organic compounds in the urban atmosphere. They have an important contribution to the formation of atmospheric photooxidants (30% of total) and are responsible up to 10% of global secondary organic aerosol (SOA) formation with mankind origin (Seinfeld and Pandis, 2016).

This study explores the SOA formation pathways from two important classes of AHs (hydroxy- and nitroaromatics) in two simulation chambers (Wuppertal, Germany and Cork, Ireland) using state of the art techniques (Fourier Transform Infrared Spectroscopy (FTIR) and Scanning Mobility Particle Sizer (SMPS)).

SOAs formation yields from nitrophenols photolysis have shown the dependency with OH radical scavenger and concentration of NOx.

SOA formation yields from photooxidation of 2,6-dimethylphenol (26DMP) (~ 17-35%) (Fig.1) have been measured in various experimental conditions. Yields of SOAs have been found dependent of the presence of preexisting seed aerosol, relative humidity (RH), NOx and HOx concentration, etc. For the first time in these studies have been used four different sources of OH radical (HONO, H_2O_2 and methyl nitrite photolysis and alkene+O_3). The experimental SOA yield has been fitted using Odum model considering one major component for the partition between gas and particle phase.

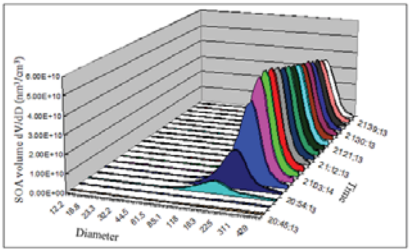

Fig. 1. Instantaneous aerosol formation 26DMP/alkene /O_3/seed/dry)

The results contribute significantly to the understanding of chemistry of urban atmosphere.

Acknowledgements

This work was supported by IRCSET project and by UEFISCDI within the PN-II-TE-2014-4-2461, PN-III-P2-2.1-PED-2016-1621, and PN-III-P4-ID-PCE-2016-0807.

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CO 8. Rational design of coordination compounds based on thiosemicarbazide ligands – synthesis, structure and application

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The coordination chemistry of the transition metal complexes containing thiosemicarbazide derivatives are investigated due to their attractive chemical, physical and biological properties. Using various thiosemicarbazide derivatives and different metal ions with different oxidation states, allows the preparation of a large number of coordination compounds with original structures and properties.

In this work we present a new way of activation of the thiosemicarbazide fragment and its condensation product with salicylaldehyde - thiosemicarbazone by coordination with manganese metal ions. It is known that the manganese chemistry with thiosemicarbazide-based ligands is not so much investigated. Mn(II) is not known to be an efficient templating ion for this type of condensation. Nevertheless using Mn(II) precursors, we were able to successfully synthesize polynuclear manganese complexes. The single crystal X-ray study of these compounds shows the formation of deca- and hexa- nuclear Mn species containing two different ligands: one initial ligand, and the second is the additional product between 2-formylpyridine and salicylaldehyde S-methyl-isothiosemicarbazone. The non-alkylatedsalicylaldehydethiosemicarbazone in strongly alkaline solutions allows the formation of the compounds with composition $Mn(L)\cdot 3H_2O$. The X-ray investigation of its structure demonstrated the formation of a binuclear complex of the composition $[(MnL_2)(Mn(H_2O)_4)]\cdot 2H_2O$. The compound is not soluble in any solvent in inert atmosphere. In the presence of the air oxygen, in methanol solutions the Mn(II) compounds are oxidized to Mn(III). As a result, the formation of a new hexadentatebicompartimental ligand coordinated to two different Mn(III) ions by O_2N_4 donor atoms has been observed. The Mn(III) units $[(Mn_2L)(CH_3O)_2(CH_3OH)_2]$ are assembled in polymer *via* μ_2-oxo bridges provided by methoxy groups coordinated to the metal ions. Low-temperature magneticinvestigations show ferromagnetic interaction and a slow relaxation in *ac* susceptibility, confirming the SMM behavior of the complexes.

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SC 2. Theoretical study of the effects of heteroatom substitution on electronic spectra of selected heterocyclic compounds

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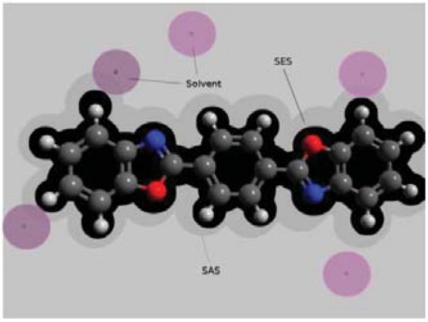
The effects of the nature of the heteroatom in the selected heterocyclic compounds containing benzimidazole, benzoxazole and benzothiazole moities, have been evaluated by using a time-dependent density functional theory approach, explicitly taking into account bulk solvent effects through the PCM model.[1]

All calculations have been performed with the Gaussian 09 program package and a methodological study using the CAM-B3LYP functional with the 6-311G(d) atomic basis set was implied. The performance of the continuum solvation model has been analyzed and the scheme of choice was the corrected linear response approach (cLR).

The visible absorption and emission spectra of selected heterocyclic compounds have been evaluated and they are in good agreement with the experimental values.

The software package FcClasses[2] had a major role in the computation of the final form of the electronic spectra.



General representation of the Solvent accessible surface (SAS) and the Solvent excluded surface (SES) in relationship with the solvent cavity

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SC 7. Synthesis and characterization of spinel type compounds ACr_2O_4 (A= Ni, Zn, Co and Cu)

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Chromites of transition metals ACr_2O_4 (A= Ni, Zn, Co and Cu) are oxidative compounds with a spinel structure, which have important applications in modern technologies such as catalysis or as gas sensors in the chemical industry.[1-3]

In this study, chromites were synthesized by sol-gel autocombustion method using fructose as a complexing/combustion agent. Metal nitrates $A(NO_3)_2$ (A=Ni, Zn, Co and Cu) were used as cation source. A graphic representation of the synthesis protocol is shown in Figure 1.

The synthesis was monitored by infrared absorption spectroscopy. In the IR spectra the vibrations corresponding to spinel structure are visible.

X-ray diffractograms indicate the existence of a pure spinel phase with crystallization in the cubic system, in the case of cobalt and zinc chromites. In the case of copper and nickel chromites, XRD analysis revealed that the samples had a spinel structure, crystallizing in the tetragonal system. Additionally the XRD patterns revealed traces of impurities, identified from the databases as $CuCrO_2$ and Cr_2O_3, respectively. The dielectric properties of the samples were also measured.

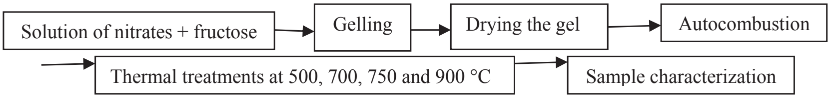

Figure 1. Synthesis protocol of chromites

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SC 8. Synthesis of zinc oxide (ZnO) particles for glucose sensing applications

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Diabetes is a worldwide public health issue affecting millions of people all around the world and causing more than 3 million deaths every year due to complications, such as hypoglycemia and other severe diabetes-related disorders, as well as degenerative associated diseases (diabetic neuropathy, retinopathy, breast cancer, etc). A crucial problem in preventing diabetes complications in the retina, heart, kidneys, and neural system is that of frequent testing of blood glucose concentration and timely insulin administration. Nowadays, millions of diabetic patients need their glucose level tested every day, most of them using the fingertip prick method for collecting the blood sample. There are two common approaches for monitoring the glucose levels: (a) the enzymatic technique and (b) the non-enzymatic technique.[1-3] Glucose monitoring without enzyme is simpler, has a higher stability than the enzymatic method and, at the same time, and is reusable. Scientists studied and confirmed the use of ZnO nanoparticles based sensors in both enzymatic and non-enzymatic methods.[4] All reports evidenced the high sensitivity of the new material, as it can detect glucose at millimolar (mM) concentrations. The objective of this research was the synthesis and characterization of ZnO particles, as well as testing the new ZnO particles for glucose sensing applications.

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SC 10. Catalytic and fluorescence properties of new double hydrophilic imidazole-based copolymers

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Temperature and light-sensitive polymeric materials are receiving increasing interest these days because of their ability to modulate their physical properties to environmental perturbations when they are excited with corresponding physical external stimuli. For sure, thermoresponsive polymers are among the most investigated “smart” entities. Among these systems, thermosensitive poly(*N*-isopropylacrylamide) (PNIPAm) is a commonly studied polymer which demonstrate a well-known volume phase transition at its LCST (lower critical solution temperature, around 32-33 ºC)[1] and a characteristic miscibility gap in aqueous solutions, too.

On the other hand, the imidazole ring is another interesting system which offers high chemical stability and attractive biological and sensor applications,[2] while imidazole-containing polymers demonstrated wide optical absorption, high thermal stability, as well as catalytic activity in buffer solutions.[3] Thus, the incorporation of the imidazole ring into polymeric systems is particularly advantageous due to its facile chemical modification and relevance to many biomacromolecules (drugs and proteins).

In this contribution we explore the advantages of both PNIPAm and imidazole-based systems and we describe the synthesis of two new double-hydrophilic copolymers containing the thermosensitive NIPAm and the imidazole based-monomer taken in different molar ratios. Final copolymers were investigated according to their characteristics since they showed stimuli-responsive behaviour against changes in temperature (impart by the PNIPAm component), improved catalytic activity in aqueous solution (*via* the presence of the imidazole-based counterpart) and fluorescence properties (applied for future fluorescence detection of various metal ions).

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SC 12. „Grey” water: characteristics, treatment methods and reuse/recycling possibilities

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Considering the development of current concept of ‘waste as a resource’, the segregation of domestic wastewater in ‘grey’ and ‘black’ water components becomes important, mainly associated with its individual treatment (not mixed, transported in a sewer system, and after treated jointly in a wastewater treatment plant) and further applications (*e.g*., few possible applications for ‘grey water’: irrigation water of lawns at cemeteries, golf courses, and college campuses (caused of valuable nutrients contained), vehicle washing, fire water protection, boiler feedwater, industrial water in concrete production and preservation of wetlands).[1]

A sustainable management of all types of water resources is recommended in actual times at national and also international level. Therefore, a special attention is according to the ‘grey water’, considering the main important aspects of: (*1*) characteristics and its produced flow; (*2*) treatment systems and reuse technologies, together with (*3*) the recycling standards and guidelines.[2]

Therefore, this paper proposes a short review devoted to the presentation of ‘grey’ water characteristics, including appreciation on its biodegradability, as well as current technologies used for grey water treatment (based on *(i) pre-treatment*; *(ii) treatment* based on physical, chemical, biological, or extensive advanced processes; *(iii) final treatment* by disinfection) and final discharge in natural aquatic receptor, reuse or recycling, when this option is indicated. Moreover, a few information on the potential residuals and its risks to environment health and increasing of pollution level (local or regional ones) of aquatic environment are presented and discussed.

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SC 13. Professor Petru Poni's contributions to the establishment of major educational and research institutions: the United Institutes and the Institute of Chemistry

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Petru Poni is considered the founder of the Romanian chemistry school. He established the terminology and chemical nomenclature in Romanian language, he held the first chemistry course at the University of Iasi, he wrote and printed the first general chemistry and physics textbooks and he was also the first to deal with the chemical study of the Romanian oil.

He has also set up prestigious educational and research units: the United Institutes and the Institute of Chemistry.

The United Institutes represented a model of school because of the elite's professorial staff, but also very good organizations. Among the illustrious professors of the United Institutes we mention: Titu Maiorescu - Professor of Literature and Philosophy, Petru Poni - Professor of Chemistry and Physics, Grigore Cobălcescu - Professor of Natural Sciences, A.D. Xenopol - Professor of History, Stefan Vârgolici - Professor of Latin Language, Aron Densuşianu and Alexandru Philippide - Romanian Language and Literature Professors, Neculai Culianu - Professor of Mathematics, Grigore Mezincescu and Eduard Caudella - Professors of music, as well as Mihai Eminescu - a German and logic teacher.

The Chemistry Institute was a research institution founded by Petru Poni in 1885 (originally called the Laboratory of Chemical Analytical Chemistry) and was located on Carp Street at number 4. In the institute's laboratories, Poni analyzed several samples of natural wines, coming from different vineyards of the country, he made chemical-legal expertise, mineral water analysis at Fundata, Amara, Slatina, two sources from Cozia, two sources from Oglinzi.

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P 1. Synthesis and characterization of a novel composite based on poly(2,2-dimethyltrimethylene carbonate) with carboxylic end-groups and hydroxyapatite

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Aliphatic polycarbonates are extensively studied in the field of resorbable medical materials due to their biodegradability and biocompatibility. In this respect, poly(trimethylene carbonate) derivatives are much considered for their slow degradation profile and can be used as organic matrix in composites in order to provide suitable properties for tissue regeneration applications.[1] The aim of our work was to synthesize and characterize a biodegradable polymer – hydroxyapatite ($Ca_{10}(PO_4)_6(OH)_2$, HAp) composite, through a modified colloidal non-aqueous chemical precipitation method, at room temperature.[2,3] The composite matrix was a star-shaped four arms poly(2,2-dimethyltrimethylene carbonate) containing carboxylic end-groups [PDTC-$(COOH)_4$]. Polymers with different molecular weights (Mn_{NMR} = 5000, 20000, 35000 Da) were obtained by the ring-opening polymerization of 2,2-dimethyltrimethylene carbonate and further functionalization with succinic anhydride. The reagents chosen for HAp synthesis, in the absence or in the presence of PDTC-$(COOH)_4$, were $Ca(NO_3)_2 \cdot 4H_2O$ as source of calcium ions and H_3PO_4 as source of phosphate ions. It is supposed that the presence of carboxylic end-groups of PDTC derivative has the ability to chelate calcium ions and to influence the size of the HAp particles during the synthesis in moderate alkaline medium. The composite with initial content of 30 wt.% HAp was characterized by FT-IR, XRD, TGA, DSC and SEM, and the results were compared with those of the HAp particles obtained in the absence of the PDTC-$(COOH)_4$.

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P 2. Atmospheric behavior of water soluble organic anions in fine and coarse particulate matter from Iasi, Romania

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Organic compounds account for a significant fraction of the particulate matter mass in the atmosphere.[1] Carboxylic acids, as ubiquitous constituents of organic fraction, can affect the global radiation balance of the Earth since they have a strong influence on the physico-chemical properties of atmospheric particles.[2,3] The atmospheric behavior of water soluble organic anions including acetate, formate and oxalate are investigated in the present work in fine and coarse particulate matter collected in Iasi, north-eastern Romania. Aerosol samples were collected over a time period of 36-hour at the Air Quality Monitoring Station (AMOS) of CERNESIM, from the "Alexandru Ioan Cuza" University of Iasi, on polycarbonate hydrophilic membranes (of 8.0 and 0.4 μm) and quartz filters appropriately disposed on a Stacked Filter Unit (SFU). More than 160 samples have been investigated by ion chromatography for their water soluble ionic content. Acetate, formate and oxalate ions showed significant statistical correlation with potassium ion (Pearson coefficient, r, higher than 0.60). For the investigated period ($C_2O_4^{2-}$, SO_4^{2-}) and (CH_3COO^-, $HCOO^-$) pairs showed statistically significant correlations (i.e., $r = 0.84$, and, respectively, $r = 0.57$) suggesting possible common sources in fine fraction of particulate matter collected at Iasi. An important contribution of organic anions within fine fraction (9.4%) may indicate a possible important role of organic acids in the formation of secondary organic aerosols.

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P 5. Efficient adsorption of Cr(VI) ions from synthetic aqueous solution using novel composites with strong base anion exchangers embedded into chitosan/poly(vinyl amine) cryogels

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Removal of chromium (VI), from the polluted waters, represents an important problem which requires efficient and, preferable, reusable sorbents. Novel macroporous composite sorbents were used in this work consisting of a combination between the chitosan (CS) and a synthetic polycation, poly(vinyl amine) (PVAm). The effect of contact time, initial concentration of solutions, sorbent mass, pH value and temperature on the adsorption capacity of the sorbents was investigated. The sorption kinetics was well described by pseudo-first order kinetic model, and the sorption at equilibrium data were well fitted by the Sips, Langmuir and Temkin isotherms. The positive values of enthalpy confirmed the endothermic nature of the adsorption and the negative values of Gibbs free energy suggested the spontaneity of the adsorption process. As a result of desorption studies it was found that the recovery of Cr (VI) ions from sorbent can be successfully done using a solution of NaOH 0.1 M.

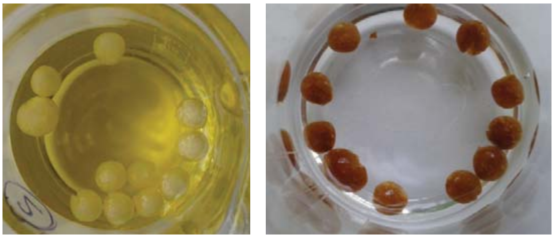

Fig. 1. Sorbent before and after adsorption process.

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P 7. Pedologic, atmospheric or anthropogenic contributions as driving forces for aquaculture water quality. A case study for an artificial lake from the north-eastern Romania

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Water body quality, affecting organisms health and aquaculture production costs,[1] has a chemical composition which is highly dependent on various factors[2] among which atmospheric deposition of both nutrients[3] and toxic substances[4] are the most important.[5] The present work reports about results on the analysis of water soluble ions in both water (44) and sediment (14) samples collected on the July 16th, 2017, from Podu Iloaiei Lake, Iasi, north-eastern Romania. Measurements of H_3CCOO^-, $HCOO^-$, F^-, Cl^-, NO_2^-, Br^-, NO_3^-, PO_4^{3-}, SO_4^{2-}, $C_2O_4^{2-}$, Li^+, Na^+, NH_4^+, K^+, Mg^{2+} and Ca^{2+} chemical species were performed by ion chromatography using Thermo Scientific Dionex ICS-5000$^+$ DP (Thermo Scientific, SUA) system. In water samples SO_4^{2-} and Na^+ are the most abundant ions, with averaged values of 254.8 mg L^{-1}, and, respectively, 153.7 mg L^{-1}. In sediment samples most identified ions showed concentrations in the μg g^{-1} range, except for Ca^{2+} whose concentration varied in the 0.926-3.624 mg g^{-1} range. In sediment samples NH_4^+ (pollutant) concentration varied between 80.8 μg g^{-1} and 284.3 μg g^{-1}. High total water hardness was estimated at the investigated site (minimum of 245.3 and maximum of 406.0 mg L^{-1} $CaCO_3$). Within the geospatial distribution of the identified species attempts will be given to discriminate to some extent between potential pedologic, atmospheric or anthropogenic sources origin contributions.

Acknowledgements: The authors acknowledge the financial support provided by UEFISCDI within the PN-III-P4-ID-PCE-2016-0299 Project (AI-FORECAST). CERNESIM Center is gratefully acknowledged for the infrastructure used in this work.

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P 8. FT-IR gas-phase products study of OH radicals initiated photooxidation of phenol

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Smog chamber FT-IR measurements have been performed in order to study the formation yield of 1,2-dihydroxybenzene from the gas-phase OH radicals initiated photooxidation of phenol. Experiments have been undertaken by using the ESC-Q-UAIC chamber facilities at a total synthetic air pressure of 1000±10 mbar and at a temperature of 298±3K. Photolysis of CH_3ONO at 365 nm has been used as OH radicals source. Additionally, certain amount of NO has been added to the gas mixture in order to avoid ozone formation. Some test experiments have been performed in order to determine both, the phenol and 1,2-dihydroxybenzene wall deposition. To evaluate the OH radicals initiated photochemical degradation of phenol additional kinetic experiments have been performed in this study. The obtained results are in good agreement with published data.[1] Rate coefficient of gas phase OH radicals reaction with 1,2-dihydroxybenzene needed for the formation yield correction was taken from literature.[2] Preliminary results from this product study highlights the formation of 1,2-dihydroxybenzene at 82÷91% yield under the present experimental conditions, in good agreement with previous studies.[3] No other products have been quantified. However, some IR spectral data support also the formation of other products such as 2-nitrophenol and 1,4-benzoquinone. Further investigations are in progress to elucidate the full photooxidation of phenol under the ESC-Q-UAIC chamber conditions.

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P 9. Non-conventional heavy metals remediation methods of Tarnița site

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The rationale for this research is that mine tailings and metals pollution of soils is a major problem globally, and it has been identified as a primary research priority task for the forest polluted areas in Romania.[1] Mine tailings and heavy metal polluted soils around the closed mines are the world's largest waste streams, and they often contain high concentrations of toxic elements that can have severe effects on ecosystems and humans.[2] Noxious heavy metals may accumulate in plant tissues and inhibit most physiological processes at all metabolism levels.[3] Tarnita site in the Eastern Carpathians is a much polluted area especially with **arsenic** and **heavy metals** and represents a persistent ecological disaster. Here, the topography, soil, vegetation, hydrology, fauna, microclimate and landscape were altered or even destroyed.[4]

Therefore, this work envisages the use of bioremediation, which can be used in Romania and abroad. The main innovation of this research relies on eco-friendly precipitation-, electrolysis-, and microbiological-based methods for heavy metals removal from contaminated forests with mining waste. Our results showed that the improved methods seem to be suitable for heavy metal and arsenic removing from Tarnita area, depending on the concentrations of pollutants. Germination tests confirmed that the decontaminated solutions are safe to plants.

ACKNOWLEDGEMENTS

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P 10. Experimental data of functionalized nanocrystalline ferrites MFe_2O_4 (M = Co, Mg, Mn, Ni, Zn) adsorption capability for Congo red dye

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Nanocrystalline ferrites are knows to be used in different type of applications, one of them including the industrial wastewater management due to their adsorption capabilities. Congo red (CR) and other cationic dyes are generating eco toxic hazards when released in water. In order to study the retention of CR on the surface of magnetic nanoparticles for a wide domain of concentration and to generate adsorption kinetics models, experimental data for 5 different types of ferrites exposed to several initial concentrations of CR solutions were obtain. Visible differences were observed in time for the CR solutions, most efficient adsorption was determined for $MgFe_2O_4$ nanoparticles with a maximum of adsorption of 29.37ppm when exposed to a 75ppm initial solution of CR. By the calculation of Langmuir isotherm model, the maximum adsorption capacity of the ferrites was determined. Also, the total uncertainty was calculated depending on the errors included by the pipes, weighting process and equipment errors.

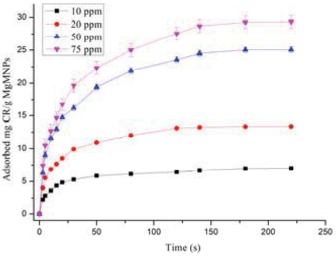

Figure 1. *Adsorption rate of different initial solution of CR (10, 20, 50 and 75 ppm) on coated $MgFe_2O_4$ MNPs.*

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P 13. Synthesis of new imidazolium/benzimidazolium salts: conventional *versus* nonconventional methods

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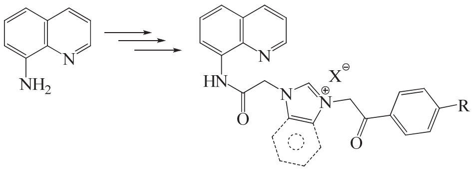
Nitrogen heterocyclic compounds are invaluable structures, with a great importance in many domains.[1] Particularly, quinoline and imidazole/benzimidazole derivatives are used as "parental" compounds in a large variety of syntheses, providing new entities with a broadened spectrum of biological properties.[2,3] On the other hand, nonconventional methods are widely used in the organic synthesis in order to activate and promote different chemical transformations.[4]

Our goal was to synthesize new imidazolium/benzimidazolium salts by both, conventional and nonconventional methods, using ultrasound irradiation, and to establish the optimal conditions for the quaternary salts synthesis. Thus, starting from 8-aminoquinoline, in the first step an *N*-acylation was performed, followed by an *N*-alkylation of imidazole and benzimidazole. In the last step, quaternization reactions of imidazole/benzimidazole derivatives with different *p*-substituted phenacyl bromides were performed.



The quaternization reactions were performed both under classical conditions and US irradiation. A comparative analysis demonstrated superior yields and shortening reaction time for quaternizations under US irradiation.

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P 17. Dynamic azo-polymeric surfaces for cell culture application

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Research regarding azo-polymer use in cell culture application has grown from one year to the next.[1-3] In this context we developed azo-materials capable of dynamic modulation of surfaces under aqueous media. This kind of materials opens a whole new area of study in biological domain. Different behavior type of dynamic surfaces can be obtained depending on the chemical structure of the azo-polymer. Chemical structure of azo-polysiloxanes and properties can be controlled by changing the p-substituent of phenyl-azo-phenol compound (Tg, surface energy, contact angle, dipole-moment).[1,2] The degree and speed modification of dynamic surfaces were studied with the help of AFM technique. We also noticed behavioral patterns of the dynamic surfaces according to the thickness of the azo-polymeric film.

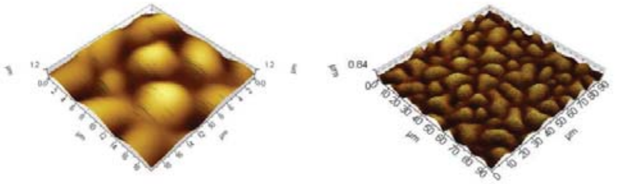

Figure 1. 3D-AFM images of dynamic surfaces under aqueous media for sample PM 2(left) and PM 15 (right)

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P 23. Synthesis and mesomorphic properties of 1,3,5-trisubstituted benzene derivatives containing azo-aromatic units as the peripheral arms

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Five new symmetrical trimeric liquid crystalline compounds comprising 1,3,5-trihydroxybenzene (phloroglucinol) as a central core have been synthesized and characterized. To the 1,3,5-positions of the benzene central ring three linearly extended semi-flexible mesogenic triphenyleneazobenzene arms with long alkyl chains as peripheral units were linked to, via esteric linkage. The compounds differ in the even-parity terminal alkyl chain length (R= $-OC_nH_{2n+1}$), with n= 6 ÷ 10. Synthesis was carried out following a convergent strategy, where the arms 4-(4-alkoxyphenylazo)-benzoic acid chlorides prepared by using diazotization/coupling/Williamson etherification/acylation reactions were attached to the resorcinol, providing the target star-shaped molecules.

Their molecular structures were confirmed by spectroscopic techniques (FT-IR, H^1-NMR and C^{13}-NMR). Thermal and liquid crystalline properties were investigated by DSC and POM studies. All the compounds showed liquid crystalline behavior of enantiotropic and monotropic type with characteristic textures.

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P 24. Synthesis of novel luminescent and paramagnetic 2,6-bis(5-aryl-1,3,4-oxadiazol-2-yl)phenols

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Among many methods for dyes removal, such as oxidative destruction *via* UV/ozone treatment, photocatalytic degradation that have certain efficiency but relative high initial and operational costs, **adsorption** is positioned as an attractive alternative,[1,2] being characterized by the following advantages: increasing of processing sensibility and selectivity; reducing of matrix effects and possibility of simultaneous achievement the pre-concentration and proper estimation. One of remarkable advantages 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, celluloses, lignin-cellulose-based materials which are presented in nature, or are secondary products from industrial or agricultural transformation.[2,3]

The aim of this paper is to present a review of our results performed in study of a new versatile cellulose-based product (Cellets), which has interesting properties (e.g. perfect sphericity, narrow particle size distribution, low friability, low solubility, and inertness), as adsorbent for removal of some dyes (Brilliant Red HE-3B, Methylene Blue, Orange 16, Rodhamine) from their aqueous solutions. Operating variables (initial dye concentration, adsorbent dose, dye concentration, pH, temperature) were studied in batch conditions, in order to establish the adequate conditions of adsorption process onto Cellets.

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P 28. Synthesis and characterization of new heterocyclic polydentate ligands

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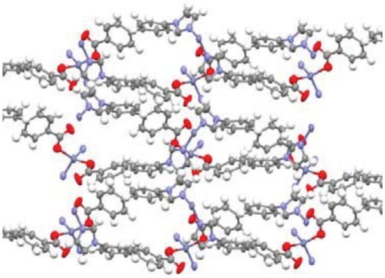
Nitrogen containing heterocycles are widely used in the design and synthesis of Metal Organic Frameworks (MOFs),[1,2] a relatively new class of porous materials with many applications in heterogeneous catalysis, gas storage and separation or controlled drug release.[3]

Our interest focuses, amongst others, on the design of new ligands which can be used in the synthesis of MOFs. Three new heterocyclic ligands, containing either an imidazole or a tetrazole ring, were thus obtained, through the use of Ullmann and Suzuki coupling reactions. All three products were characterized by proton and carbon NMR spectroscopy and will further be used in the synthesis of MOFs.



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P 29. QuEChERS and ultrasound-assisted extraction as preparative tools for various secondary metabolites analysis by GC-MS technique

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Nowadays is clearly established that higher plants chemical composition is dominated mainly by the existence of various secondary metabolites in the form of phytochemicals among which alkaloid (27%), terpenoid (55%) and phenolic (18%) compounds are the most important.[1] Within secondary metabolites detection, identification and quantification processes a very important role is played by the selected preparative techniques which are still very challenging in terms of improved efficiency.[2] The present work reports result on a comparative study regarding the relationship between extraction efficiency and gas chromatography-mass spectrometry (GC-MS) analysis for secondary metabolites from *Datura inoxia* structural units (*i.e.*, flowers, seeds, leaves). Ultrasound-assisted extraction (UAE)[3] and QuEChERS (quick, easy, cheap, effective, rugged and safe) extraction technique were under scrutiny for their efficiency under different organic solvent conditions (*i.e.*, methanol, ethanol, butanol, acetonitrile, ethyl acetate, chloroform, *n*-hexane). Extracts generated both by the UAE and QuEChERS techniques supplied samples for which GC-MS signaling revealed the existence of secondary metabolites such as alkaloids (*e.g.*, scopolamine), sterols (brasicasterol, fucosterol, campesterol, stigmasterol), tocopherols (α- and γ-tocopherol), etc. In terms of extraction efficiency QuEChERS, although seen as a state-of-the-art preparative technique, seems to be overwhelmed by UAE technique (e.g., 34.73 μg scopolamine g^{-1} dw versus 432.87 μg scopolamine g^{-1} dw in seeds).

Acknowledgements
CERNESIM Center is gratefully acknowledged for the infrastructure used in this work.

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P 31. Biologic properties of 5-sulfonate-salicylaldehyde thiosemicarbazone derivatives in copper(II) compounds

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The thiosemicarbazone-based ligands have an important role for compounds withchemical, analytical, catalytic and biologic properties.[1,2] A series of water-soluble sodium salts of 3-formyl-4-hydroxybenzenesulfonic acid thiosemicarbazone (or sodium 5-sulfonate-salicylaldehyde thiosemicarbazone) containing different substituents at the terminal nitrogen atom (H, Me, Et, Ph) and their copper(II) complexes have been prepared and investigated their biologic properties (Fig. 1).[3] The copper(II) complexes exhibited moderate anticancer activity in established human cancer cell lines (A2780, A2780cis and MCF-7) relative to their toxicity in healthy embryonic kidney cell line, while their parental proligands were devoid of cytotoxicity. The anticancer activityof the copper(II) complexes correlated with their ability to induce ROS (Reactive Oxygen Species) accumulation in cells, consistent with their redox potentials within the biological window, triggering the activation of antioxidation defence mechanisms in response to the ROS insult. The results clearly demonstrated the role of copper(II) center in the mechanism of action of new complexes.

These studies pave the way for the investigation of ROS-inducing copper(II) complexes as prospective antiproliferative agents in cancer chemotherapy.

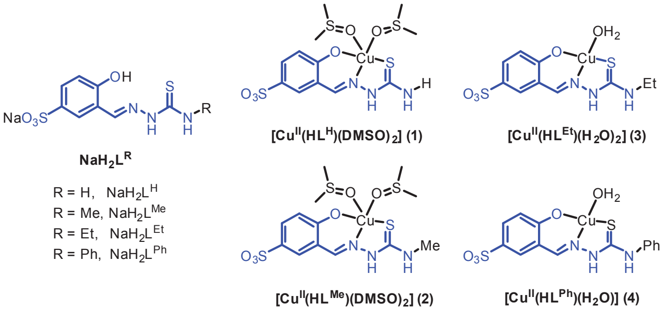

Fig. 1. Line drawings structures of thiosemicarbazones NaH_2L^R, as well as of their copper(II) complexes

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P 32. Modelling of photocatalytic degradation processes of organic compounds in the presence of TiO_2

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In this work, it was studied the process of photodegradation of Levetiracetam (LEV), in the presence of two photocatalysts: TiO_2 Aeroxide® P25 and TiO_2 Kronos uvlp 7500.

The importance of reducing water pollution with organic compounds has led to the intensification of experimental studies, of which photocatalysis using TiO_2 is a recommended method due to: the high photocatalytic activity, high chemical stability, thermal stability, non-toxicity and low costs.

TiO_2 is well known as an excellent photocatalyst, which allows degradation and, ultimately, the mineralization of organic compounds. In literature, there are insufficient papers regarding the photodegradation of LEV using TiO_2, and the modeling of the process, respectively.

The experiments were carried out in a batch reactor (BR EXT), mechanical stirred with 300 rpm, with external irradiation with UVA lamps (λ=365 nm). LEV concentration in solution was determined by HPLC method. It was studied the influence of different parameters: initial pH, the effect of catalyst dosage, type of TiO_2, LEV concentration, the effect of UV irradiation and irradiation intensity.

The study of the catalyst type has shown that, after 140 min of irradiation, the degradation yield of 75% was obtained for P25, while with Kronos 7500 the degradation yield was only of 20%. Increasing TiO_2 concentration in the range of 0.5-2g/L provides improved degradation efficiency from 68% to 93%. For the study of pH influence, tests were conducted in the range of 2.5-10.5. The experimental results have shown that the degradation yield was 76.4% at pH=10.5, and increase up to 99% for pH=2.5. Experimental data have shown that the degradation yield decreased from 99% to 74% with increasing LEV concentration from 4.5 to 24.78 mg/L. Kinetics studies indicates that the photocatalytic degradation of LEV is well described by Langmuir-Hinshelwood kinetic model.

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P 36. Determination of acidity, moisture and NaCl content in bread

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Bread has been used as a form of currency, has provided millions of jobs for hundreds of years, and overall has evolved itself over the span of thousands of years to become a surviving staple, as well as a daily food source for humans living in the world today.

We wanted to analyze white bread, graham without salt. For each type of bread we assayed by titration following physical and chemical parameters such as humidity, the amount of salt and acidity. The acidity of the flour is a measure of freshness, varying depending on its type. This is higher in black flours and old.[1]

Determination of acidity can be achieved by: the method with ethyl alcohol 67% vol., with ethyl alcohol 90% vol. and most commonly, by the method of suspension in the water. The acidity of the flour is expressed in degrees of acidity and is between 2 and 4 degrees of acidity.[2] Moisture of the flour was determined by the method of drying to constant weight. The sample was dried in an oven at 103 °C for 16 h. After cooling in a desiccator, the dried sample was weighed and the total water content was determined and expressed in g water/g dry matter. The measurements were conducted in triplicate.

Salt Quality Controll is established by organoleptic salt, following the taste, smell, color and foreign bodies. All values obtained should be compared with standard values tabulated.[3]

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P 37. Study of siloxanic schiff bases as ionofores for cation selective electrodes

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Ion-selective electrodes provide a convenient and rapid analytical procedure for estimating content of ions in solutions that may be heterogeneous, colored and contain additives ranging from simple cations to large organic molecules. Due to their simplicity, reduced costs, improved precision, applicability under unusual or extreme conditions, their properties and characteristics make the sensors suitable for various areas of analysis such as pharmaceutical analysis, plant and vegetable analysis, seawater analysis,etc. The functional parameters of ion-selective electrodes depend essentially on the nature of the ionophore. In this paper we intend to study for this purpose a Siloxanic Schiff base, synthesized in the process of preparing the polymeric membrane. The polymer film was prepared from 1,3-*bis*(3-aminopropyl)-tetramethyldisiloxane, salicylic aldehyde, 2-nitrophenyl ethyl ether, tetrahydrofuran and polyvinyl chloride. For cations of Ni^{2+}, Co^{2+}, Cd^{2+} and Cu^{2+} were assembled electrodes and preconditioned in solutions containing the same cations. As a result of the first experimental data, in order to block the membrane anionic function, sodium tetraphenylborate was added in the polymer membrane. The best performance parameters were recorded for Cu^{2+} selective electrode: slope 30 ± 2 mV/decade of activity, detection limit 10^{-5} mol/L and optimal pH range 2,00 – 4,67.The values of the selectivity constants, determined by the separate solution method,[1] indicate interference of cadmium ions for potentiometric analysis of copper(II) with this electrodes. The sensor lifetime is three months, then the measurement error is greater than that allowed for potentiometric analyzes.

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P 38. Intelligent molecular materials

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bistability. This phenomenon is observed in materials based on transition metals with 3d4-3d7 electronic configuration as: Fe(II), Fe(III), Co(II), Co(III), Mn(II), Mn(III) and Cr(II).1 Among the wide range of SCO compounds, those based on Fe(II) are the most studied. Generally, these compounds have a coordination sphere FeN6. In some cases anions as NCS-, NCSe-, etc. are used for neutralising the Fe(II) ion charge. The literature studies show that coordination modes as FeN_4O_2, $FeC_2N_3O_2$, FeP^2N^2X (X = Cl, Br) are also present for SCO compounds.[2]
In terms of application of SCO compounds those based on Fe(III) shows have higher advantage over Fe(II) SCO compounds because of their air stability. Regarding this fact the Fe(III) SCO materials are actively developed in the last years.[3] The Schiff based ligands and thiosemicarbazone ligands are the most employed.

In this work we investigate the pH influence on crystal packing and properties of thiocarbohidrazide derivatives and salicylaldehydeligands with Fe(III). The crystallographic studies revealed an octahedral coordination sphere for the Fe ion formed by two bideprotonated ligands. The ligands are linked to the metal ion by ONN set of atoms. The tetramethylammonium salt was used to compensate the positive charge in the outer sphere of the compound.

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P 39. The preparation and characterization of some copper(II) complexes of 2-methyl-imidazole-4-carbaldehyde thiosemicarbazonederivatives

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Thiosemicarbazones are a diverse class of organic compounds that still attract researcher's attention due to their wide spectrum of biological activity. Copper(II) coordination compounds with thiosemicarbazone are intensively studied due to their structural, biological, magnetic, electron transfer and catalytic properties.[1-3] Changing the composition and structure of the thiosemicarbazide fragment and/or the carbonyl component offers a means for modelling new molecules. After, monitoring the influence of the parameters on the properties of the synthesized organic reagents.

In the present work, we report the synthesis, structures and antibacterial properties of copper(II) complexes derived from 2-methyl-imidazole-4-carbaldehydethiosemicarbazone. The complexes were obtained by the reactions of the cooper(II) nitrate with the corresponding organic ligands (HL^1- 2-methyl-imidazole-4-carbaldehyde thiosemicarbazone; HL^2- 2-methyl-imidazole-4-carbaldehyde phenylthiosemicarbazone; HL^3- 2-methyl-imidazole-4-carbaldehyde metylthiosemicarbazone). It was observed that regardless of the reactant ratio, only compounds with a metal to ligand ratio of 1:1 are formed. The organic ligands are coordinated to the metal ion through the NNS set of donor atoms.

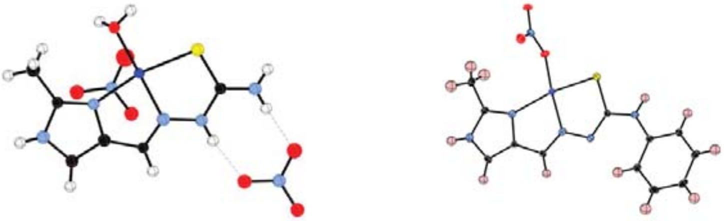

Fig.1 Example of crystal structure of the synthesized compounds

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P 40. Kinetic analysis of the thermal degradation of decabromodiphenylether

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This study aims to investigate the thermal degradation behavior of decabromodiphenyl ether (BDE 209) by simultaneous TG/DTA under various conditions. Due to low volatility, high elution temperatures are needed when applying chromatographic techniques for this class of flame retardants (FR), resulting in thermal degradation affecting analysis results, but no systematic study has been reported. Kinetic analysis was performed by the non-parametric (NPK) method, and in correlation with evolved gas analysis (EGA) information and molecular modeling results, provided valuable insight into the kinetics and mechanism of BDE 209 thermal degradation. The conclusions were aimed at designing proper specific GC analytical methods for the selected FRs and serving for a better estimation of the human exposure to such compounds.

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P 41. Reducing the energy consumption for anodizing process of aluminium alloys

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The anodization of aluminium is a well-known and attractive electrochemical method leading to the formation of a porous oxide film on aluminium and its alloys surfaces. For this process, sulphuric acid electrolytes are commonly used. The anodic oxidation of aluminium is a complex process, characterized by low values of the current yield and high consumption of materials, electric energy. All these drawbacks lead to the increase of the cost of the finished product.[1] The additional energy consumption and, implicit, the deceased value of the energy yield are caused by the simultaneous development of the specific electrode processes and to the secondary process that involves hydrogen and oxygen release because of water electrolysis. In practice, for a certain electrolyte with specified functioning parameters, the reduction of the specific consumption of electric energy is possible through the rigorous control of the actual voltage at the terminals of the electrolyte.[2,3] In this work, the analysis of the voltage balance for the process of aluminium alloys anodizing, in order to establish the mathematical relationship of the voltage drop through the electrolyte, the voltage at the terminals of the electrolysis cells and the distance between the electrodes is carried-out. Based on these dependences are established the mathematic relationships of dependence of the electric energy specific consumption in function of the voltage at the terminals for different thickness of the oxide aluminium layer and for a typical anodizing electrolyte. The results of this study present a peculiar practical importance, facilitating a fast and relative exact calculus concerning the real terminal voltage and the practical electric energy consumption in function of the distance between the electrodes.

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P 42. Copper recovery from galvanic effluents

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The copper recovery from galvanic effluents associated with electrolytes waste and wastewater from metal finishing industries, is a very important part of most of the current research in the environmental integrated production and recycling management. Different treatment methods employed to recover or remove the copper is chemical precipitation, adsorption onto different adsorbents or biosorbents, ion exchange, cementation, membrane filtration, electrochemical methods, photocatalysis.[1]

The first part of this work focuses on reviewing the most the methods used to recover copper from galvanic effluents. Cementations is an important process used in galvanic industry in order to recovery of copper, removal of copper ions from dilute wastes and for purification of solutions. The cementation reaction consists of heterogeneous and spontaneous reduction (cathodic reaction) of a relatively noble metal ion, contained in a liquid phase, with a sacrificial solid metal (anodic reaction) according to their electrochemical potential values.[1,2] The sacrificial metals such as iron,[2,3] zinc,[3,4] aluminium,[5] alone or in mixture.

In the second part, we have comparatively investigated the copper separation from cupric chloride solutions by cementation process using iron bars and zinc powders. The effect of the different experimental factors on cementation rate were determined. The copper cementation yield increased with initial copper concentration, temperature, stirring speed. The reaction follows the first-order kinetics, and the reaction rate is controlled by diffusion. The cementation of copper by zinc is more effective than cementation with iron because the oxidation potential of iron is lower than that of zinc.

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