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CP 1. Oligomers, Layers and 3D supramolecular architectures in organopnicogen (M = Sb, Bi) chemistry

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The chemistry of organoantimony and –bismuth compounds is concerned to different topics *i.e.* fundamental research, biological activities, uses in organic syntheses or preparation of precursors in advanced material science, catalysts etc. Therefore continuous efforts are concentrated to develop studies related to these topics.

The structural chemistry of the organometallic species of heavy pnicogens in oxidation state +3 is controlled by the Lewis acidic character of the metal atom. This results in intra- or intermolecular contacts (*"secondary bonds* or *interactions"*), in addition to the normal covalent bonds (*"primary bonds"*). Usually such interactions are established in presence of donor molecules or ions, and the results are increased coordination numbers and different degrees of association (oligomers or polymers) of the molecular units. The degree of oligomerization can be controlled, at least in part, by two strategies: (*i*) the use of bulky substituents, which affords steric protection of the metal atom, and (*ii*) the use of one pendant arm ligands such as 2-(MeOCR₂)C₆H₄ (R = Me, CF₃) and 2-(Me₂NCH₂)C₆H₄, or "pincer" ligands like 2,6-(Me₂NCH₂)₂C₆H₃, 2,6-[MeN(CH₂CH₂)₂NCH₂]₂C₆H₃ and 2,6-(ROCH₂)₂C₆H₃ (R = Me, ^tBu). Such ligands protect the metal centre both sterically, by increased coordination, and by significant reduction of the Lewis acidity through their (*C*,*E*) or (*E*,*C*,*E*) (E = O, N) coordination pattern.

In addition to intermolecular interactions between the metal and heavy atoms (halogens, chalcogens, nitrogen, etc.), further associations through hydrogen bonding, $C \Box H \cdots \pi$ (Ph_{centroid}) or $M \cdots \pi$ (Ph_{centroid}) contacts have also to be taken into account. All these types of intermolecular interactions are common in the organometallic chemistry of heavier pnicogens (Sb, Bi) and various examples of resulted oligomers, chain polymers, layers or 3D supramolecular networks will be discussed.



 $[\{2-(Me_2NCH_2)C_6H_4\}Ph_2Sb]_n$

CP 2. Magnetic anisotropy in lanthanide complexes: Synthesis, Structure, properties

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Occurring in specific d^n and f^n configurations, the anisotropy is a key effect to design magnets at molecular and nano-metric scale, being the causal determination for stable poles of the magnet with respect of given molecular frame. Taking several examples of lanthanide^{1,2} complexes, from the synthetic outcome of our group, we illustrate the interplay between magnetic anisotropy and exchange effects in the magnetic properties of considered systems, and the structural determinations of these manifestations (Fig.1.)

We present methodological advances which enable, at ab initio level, the full decryption of the structure-property relationships in its basic determinants: exchange and spin orbit couplings, Ligand Field and long range effects.



Figure 1. Synopsis of anisotropy molecular magnets made of d-f complexes. (a) the magnetic anisotropy (non-spherical, e.g. bilobal, magnetization polar surfaces) and the energy barrier between opposed spin projections states are the sine qua non premises of building systems behaving as magnets; (b) the state-specific magnetization functions for Gd(III) ion in the coordination sites of the

 $[Fe_{LS}^{II}(\mu-bpca)_2Gd(NO_3)_2(H_2O)]NO_3$ compound.

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CP 3. New Models on Fullerenes and Carbon Materials. Both Paths to the Experiment: Interpretation and Prediction.

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The tableau of various special properties of fullerene and graphene systems rises challenges for theoretical and computational explanation of the underlying mechanisms. We present several advances continuing previous contributions to the interpretation of vibrational shifts in filled fullerenes,¹ thermal negative expansion of C60 cage,² and spin distribution in triangular graphene systems.³

Besides, taking polyacene systems as case studies, new molecular models on conduction are presented, establishing conceptual links between relevance for application purposes and heuristic ideas of aromaticity and resonance structures.



Figure 1. (a) Synopsis of vibration shifts of Raman frequencies in noble gas endohedral fullerenes. (b) Synopsis of topology determined spin distribution in triangular graphene systems.

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CO 1. Synthesis and photochemical investigations of poly[(D/L),(-/+)N-methacryloyloxyethyl-N'-2-buthanol[urea]-co-N-acryloyl-(D/L),(+/-)-phenylalanine] copolymers

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In last years, the synthesis and structure of copolymers with phenylalanine and urea groups [1] is of great interest because these materials can be used for chemosensors applications owing to a wide range of properties such as biocompatibility, biodegradability, increased solubility, good mechanical properties, a.s.o. The present study is focused on the synthesis of new optically active monomers (D/L),(-/+)-N-methacryloyloxyethyl-N'-2-buthanol[urea] and their copolymers poly[(D/L),(-/+)-N-methacryloyloxyethyl-N'-2-buthanol[urea]-*co*-N-acryloyl-(D/L),(+/-)-phenylalanine] prepared via free radical polymerization to be tested as potential fluorescent chemical sensor able to sense pH variations after a chemical modification with fluorescein-isothiocyanate. The structure and thermal properties of the synthesized polymers were investigated by FT-IR, ¹H-NMR, circular dichroism, UV and fluorescence spectroscopies.



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CO 2. When is mass spectrometry combined with affinity approaches essential? A case study of Tyrosine nitration in proteins

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Oxidative modification of proteins may cause substantial biochemical changes as well as pathophysiological changes, both by chemical reactions and specific enzymatic pathways; however, the identification of corresponding fine- structure modifications is often tedious and requires methods of high sensitivity and molecular specificity. In particular, nitration of Tyrosine residues has been associated to pathophysiological effects in proteins related to neurodegeneration such as in Alzheimer's disease, atherosclerosis, and broncho-alveolar diseases^{1.2}. While immuno-analytical methods suffer from low detection specificity of antibodies, mass spectrometric methods for identification of Tyrosine nitrations are hampered by low stabilities and levels of modification, and by possible changes of structure introduced by the nitro group. High resolution FTICR mass spectrometry (FTICR MS) using electrospray (ESI) in combination with immuno-affinity procedures have been developed as powerful tools for unequivocal and sensitive identification of Tyr-modifications in proteins which is hampered, by low levels of modifications³.

Recent studies reveal (1) specific Tyr-nitration substrates in blood eosinophils proteins and (2) unexpected Tyr-hydroxylation in human sputum sample. Model peptide containing specific modifications of Tyrosine residues were synthesized by solid phase peptide synthesis and used for mass spectrometric and immuno-analytical characterization.

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CO 3. Facile synthesis method for the preparation of CMC capped MFe₂O₄ (M=Co, Mg, Mn, Ni) nanoparticles

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Magnetic mixed oxides with chemical formula of MFe_2O_4 (where M = divalent metal), are known to be technologically important materials, because of their properties such as high specific heating, high thermodynamic stability, high electrical conductivity, high corrosion resistance, low magnetic transition temperature, and low melting point making them suitable in many technical applications like semiconductors, catalysts, photoelectrical devices sensors, nanodevices, microwave devices, pigments and biomedical applications [1].

In the present work we report the synthesis of MFe_2O_4 (M= Co²⁺, Mg²⁺, Mn²⁺, Ni²⁺) nanoparticles by co-precipitation method, using metal chlorides as precursors and as capping agent, carboxymethylcelullose (CMC) solution at different NaOH concentration.



Figure 1. FT IR spectrum of MFe₂O₄ annealed at 500°C

The presence in the FTIR spectra of characteristic absorption bands of CMC indicates that some functional groups of the surfactant are grafted on the surface of the nanoparticles. This indicate that the NPs obtained are capped with molecular groups of surfactant provides [2]. The experimental studies show that the NaOH concentration does not influence significantly the size and morphology of nanoparticles.

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CO 4. Synthesis and biological evaluation of new 1,4-disubstituted 1,2,3,tiazole derivates

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Inhibition of protein farnesyltransferase (FTase) prevents membrane localization of Ras proteins which plays a fundamental role in the cellular signalling that allows cell division. Thus, the inhibition of the farnesylation process can constitute a potential target for anticancer therapeutics.¹

We have recently reported three novel families of phenothiazin-triazole derivatives with general structure 1^2 , potential inhibitors of farnesyltransferase, some compounds showed IC₅₀ values in the micromolar range.



The goal of our research was to identify new 1,2,3-triazole derivatives, potential inhibitors of farnesyltransferase. We brought structural modifications in the 1 and 4 positions of the triazole moiety with the aim to observe if the modification leads to compounds with similar biological profile as the reported families.





The biological evaluation of the new potential inhibitors of protein farnesyltransferase revealed that the inhibition ratio can be increased when bulky heterocycles are used, linked at the 1st position of the triazole moiety, respectively, when alkyl groups are linked in the 4th position.

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CO 5. Thermotropic and optical behaviour of new PDLC systems based on a polysulfone matrix and a phosphorous-containing smectic-A liquid crystal

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The thermotropic and optical characterisations of novel polymer dispersed liquid crystal (PDLC) systems based on polysulfone UDEL-3000 (PSU) or its derivatives (chloromethylated polysulfone or polysulfone containing lateral phosphaphenanthrene substituent) as polymer matrix and a phosphorus-containing liquid crystalline polymer (LCC) which displays isotropic/nematic/smectic-A mesophase transition (Figure 1) were investigated. The PDLC samples were prepared by solvent-induced phase separation technique (SIPS) using various weight ratios of the both components (polymer matrix vs. LCC copolyester). Information on the morphology and phase structure was obtained by polarising optical microscopy, differential scanning calorimetry and X-ray diffraction measurements. The samples revealed a multiple melting behavior in the first heating scan due to the presence of the liquid crystalline aromatic-aliphatic polymer in the polymer matrix. PLM observations enlighted the appearance of fine grainy textures – nematic (Figure 2a) upon heating and birefringent droplets growing from isotropic state upon cooling (Figure 2b). The X-ray patterns evidenced the ability of organizing in more ordered phases (smectic) in the case of the samples having a higher content of liquid crystal. TGA results showed that 5% weight loss temperatures were greater than 337°C for all the samples, and the residue at 700°C was generally dependent on the amount of phosphorus-containing heterocycle in the macromolecular system.



Figure 1. Chemical structure of phosphoruscontaining liquid crystalline copolyester (LCC).



Figure 2. Optical micrographs of PDLC systems with 10% wt LCC.

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CO 6. Complexation of 4- (4'- pyridyl) pyridinium disubstituted monoylides with palladium (II)

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Disubstituted cycloimmonium ylides have a great potential for use as analytical reagents¹ and semiconducting materials,² and some of them have shown biological activity.³ The 4-(4'pyridyl) pyridinium disubstituted monoylides were investigated for DNA binding properties. It was found that Y_{NIC} and Y_{FITC} ylides ligands hydrolysis compete to the DNA binding. In order to stop the hydrolysis, we investigated the complexation of these ligands with palladium (II). The UV-VIS spectroscopy (Figure 1) shows that the ligand Y_{NIC} forms a complex with Pd(II) with a molar ratio of 1:1 ligand Pd(II)



Figure 1. UV-visible absorbance spectra for Y_{NIC} in the presence of $Pd(CH_3CN)_2Cl_2$ in DCM at 25°C (left) and absorbance at 481 nm (blue triangles), 525nm (red circles) and 570nm (black squares) as a function of $Pd(CH_3CN)_2Cl_2$ concentration, solid lines gives the molar ratio(1:1 in this case) (right)

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CO 7. Application of ecological footprint as a measure of sustainability in construction building

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Construction materials have environmental impacts at each stage of the construction process, from raw material extraction, processing, manufacturing, transportation, construction, until the end of utility lifecycle of the building. Application of sustainable development principles in the construction of buildings tends to reduce consumption of resources (materials and energy) and waste production impact on the environment and guarantee the high quality of construction and utility areas built. In this study we sought ecological footprint methodology application in construction of buildings consisting of centralizing data from LCA involving the consumption of raw materials and energy (input) and all waste generation (output). As a case study, it was considered a dwelling structure built out of wood and straw bales to achieve high energy performance with low environmental impact by implementing sustainable solutions.

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CO 8. Influence of aluminium ion substitution on magnetic and dielectric properties of zinc ferrite

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Spinel oxides with formula $ZnFe_{2-x}Al_xO_4$ ($0 \le x \le 2$) were synthesized by sol-gel process, using nitrat as precursors and tartaric acid as complexing - combustion agent. Infrared spectroscopy was used for monitoring solid phase chemical reactions and the dissappearence of the organic phase. XRD data confirm the formation of cubic spinel structure.



Fig.1. σ -H hysteresis loop of the ZnFe_{2-X}Al_xO₄ **Fig.2.** Plots of real (ϵ ') parts of dielectric constant versus frequency

Fig.1. shows that all compounds produced a narrow σ – H cycle, with a behavior characteristic of soft magnetic materials (easy magnetization and demagnetization) [1]. According with Fig.1., can be observed that the saturation magnetization and the coercitive field decreased with increase of aluminium content. Fig.2. shows that dielectric constant goes on decreasing with increase of non magnetic Al³⁺ content and it decreases steeply at lower frequencies and remains constant at higher frequencies, indicating the normal dielectric dispersion [2]. The electrical analysis showed very low values of dielectric loss at frequencies over 10⁵ Hz.

Acknowledgements

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CO 9. Luminescent phenothiazine-azomethines with tuned morphology

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The thermotropic symmetric dimers formed by two identical rigid cores linked via a single non-conjugated bridge, usually a flexible spacer, are interesting compounds from the academic and technological point of view, investigated as models for polymers and for their special behavior, different from that of corresponding monomers.

New Schiff base dimers based on phenothiazine heterocycle have been obtained with high yield and purity, by condensation of 3-formil-10-methyl phenothiazine with various amines. The structural characterization was performed by FTIR, 1D and 2D-NMR spectroscopy and single crystal and powder wide angle X-ray diffraction. The obtained compounds have high thermal stability and some of them present cubic mesophase and molecular glass states. The thermotropic study performed by polarized light microscopy and differential scanning calorimetry revealed the possibility to control the compound morphology by blending and thermal annealing. The photophysical characterization shows green light emission, with good absolute fluorescence quantum yield, large Stokes shift and high purity and fully saturated color. The special thermal behavior and photophysical properties appear to be significantly dependent on the special supramolecular architecture generated by the hockey-stick shape of this mesogenic core.

Collectively, the properties of these azomethines provide the basis for interesting compounds with great advantages for optoelectronic applications.

CO 10. Effectiveness of an alcohol assay in establishing uncoupling activity of some pollutants

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Although, the dinitrophenols and other related compounds are deeply poisonous, they are still used as pesticides, drugs or even weight loss agents¹. Today, DNP is used by bodybuilders, often illegally, to rapidly lose body fat before contests². It is thought that they uncouple the oxidative phosphorylation by carrying protons across the mitochondrial membrane, leading to a rapid consumption of energy without generation of ATP³.

Since the level of toxicity of dinitrophenyl derivatives depends on their property of uncoupling the respiration from ATP synthesis, leading to anaerobic metabolism and alcohol formation in plant tissues, we have investigated their relationship with wheat roots. First, we have introduced and characterized a micro-method for determining the production of ethanol by roots (1 g) in the presence of dinitrophenyl derivatives. The procedure is based on alcohol reaction with dichromate ions, which induce a proportional decrease in Cr^{6+} absorbance at 350 nm, with the corresponding increase in that at around 600 nm due to the formation of Cr^{3+} ions. Alcohol is evaporated at 50° C in a Conway cell and kept in a solution containing potassium dichromate and sulfuric acid. Second, the micro-method was applied to characterize various uncoupling agents, and its analytical parameters have been studied.

This micro-method was tested using dinitrophenols and related compounds, the method is reproductible, sensitive and selective. It can be used to test new compounds in order to discovery new properties of chemical compounds based on alcohol production by fermentation.



Fig 1. Dish Conway

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CO 11. Synthesis of poly(vinyl acetate-co-4-acryloyloxybenzilideneiminepyrene) and fluorescence study

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Nowadays, photosensitive materials containing a highly sensitive aromatic fluorophore to external stimulus have attracted increasing attention mainly for their specialized applications as chemosensing, optical switching and molecular computation. On this line, poly(vinyl acetate-co-4-acryloyloxybenzaldehyde) (PVAc-co-PAB) was synthesized to be further grafted with 1-aminopyrene. The resulting copolymer poly(vinyl acetate-co-4-acryloyloxybenzilidene-iminepyrene) (PVAc-co-PABPy) was tested as a potential chemical sensor for the detection of metal ions and nitroaromatic derivatives in DMF solutions. The fluorescence study was conducted at $\lambda = 344$ nm. For instance, in the presence of Co²⁺ the fluorescence intensity of PVAc-co-PABPy decreases as the concentration of 39.48 x 10⁻³ mol/L a quenching efficiency of 76% was achieved.



Fluorescence spectrum of PVA-co-PABPy in the absence

and presence of Co²⁺ at different concentrations a), and Stern–Volmer plots, b).

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CO 12. The corrosion behavior of mild steel in water from Bahlui River

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The current paper presents the experimental data of the corrosion tests of mild steel alloys immersed in river water, for a short time, in laboratory conditions. As steels occupy the first place in industry as engineering material, the water is the most important medium among terrestrial environments and in industry.

Using both electrochemical methods (cyclic voltammetry, method of polarization resistance, Tafel extrapolation method and electrochemical impedance spectroscopy) and non-electrochemical methods (scanning electron microscopy and IR spectroscopy) was followed the evolution of the rust layers by maintaining the steels immersed for different periods of time. The electrochemical methods were used to study the variation of the corrosion parameters by increasing the immersion time and to follow the development of the corrosion product layers formed on mild steels surfaces.

The non-electrochemical methods were used for the identification of the rust phases and the morphological and compositional study of the corrosion products.

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CO 13. Electrosynthesis of copolymers based on water-soluble Nsubstituted aniline derivatives: structural characterization and electrochemical stability

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Copolymerization of aniline with different N-substituted aniline derivatives was considered the most effective and promising way to improve the properties of polyanilines. Copolymers containing N-(3-sulfopropyl) aniline acid (AnPS) or 3-[(anilinephenyl)amino]propane-1-sulfonic acid (DAnPS) and 2-anilinoethanol (AnEtOH), were electrochemically synthesised as thin green layers deposited on working electrode surface, from electrolyte solutions with different pH values. The surface morphologies were analyzed by AFM and SEM, which revealed that the roughnesses and the surface topographies of the layers depend on the ratio between the monomers and the nature of the electrolysis medium. The electrochemical stability of the copolymers layers was also investigated. Copolymers having AnPS units in their structure are stable and preserve their redox activity during the voltammetric measurements, even at high number of cycles, while the layers containing DAnPS units are not stable. It was noticed that only aniline-AnPS (1:1) molar ratio copolymer layer, preserves its electrochemical activity in bidistilled water. These layers of copolymers were characterized by Raman, UV-Vis, XRD and XPS spectroscopies.

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CO 14. (Bio)Active Layers Deposition by Electrospraying

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The coating of polymeric surfaces with multifunctional layers plays an important role in many applications such as: biomedical (creating biocompatible/hemocompatible materials for catheters, cardiovascular stents, skeletal prostheses, endotracheal tubes, synthetic vascular grafts, intraocular lenses, adjustment of protein adsorption), tissue engineering, elaboration of sensors and biosensors for diagnosis techniques, food packaging (by creating (bio)active packaging), printing (improving dye adhesion), (micro)electronics, etc.

Chitosan (CHT) and vitamin E (VE) based formulations deposited on various substrate surface provide antibacterial (CHT) and antioxidant (VE) properties, and also permeability improvement to different gases. In this regard, the CHT and CHT/VE-based coatings were made by electrospraying onto polyethylene (PE), poly(vinyl chloride), poly(vinylidene fluoride), glass and aluminium. The stability of the bioactive layer was achieved by covalent linking of the formulation to the plasma treated substrates. The electrospraying experimental conditions were optimized. The corona treatment effects as well as surface properties modification have been established by goniometry, ATR-FTIR, XPS, potentiometric and polyelectrolyte titration, SEM, AFM and antibacterial tests.

Substrates surface chemistry and roughness influence the organization and wettability of CHT/VE-based coatings. IR spectra revealed the chemical interactions between chitosan and corona treated PE and activated with coupling agents. The potentiometric and polyelectrolyte titrations proved that after reaching steady state the covalent immobilized CHT/VE layer is stable. Depending on the substrate nature the coatings presents different morphologies and manifest expected antibacterial activity.

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CO 15. Electrospin coatings for antioxidant food packaging

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Nowadays, the development of advanced formulations used for food packaging applications, which behave as protection or preservation materials, multifunctional (active or bioactive) are able to improve products' quality, extend the shelf-life and subsequently consumers' health becomes a challenging research task.

The present study deals with investigation on the possibility of obtaining by electrospinning of new functionalized coatings, as materials with antioxidant properties for food packaging. Electrospun fibres based on polycaprolactone a synthetic biodegradable polymer were obtained and characterized. Polycaprolactone can improve the performance of coatings, adhesives and elastomers giving materials with special properties, such as good resistance to abrasion or at UV irradiation, smooth aspect, hydrolytic stability, enhanced adhesion or flexibility at low temperatures. Films containing polycaprolactone can be used for packaging in direct or indirect contact with food. The obtained coatings have both good properties and act as bioactive layer for packaging material by effect of vitamin E, selected as plant phenolic antioxidant and bioactive agent. The electrospinning conditions required for obtaining fibres were optimized both in respect with device parameters and the solutions properties. The obtained electrospun fibres were analysed by ¹H-NMR and scanning electron microscopy. The quality of coating and antioxidant properties were evaluated by radical scavenging activity and it has been shown that vitamin E imparts good antioxidant characteristics.

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CO 16. Interaction of CoA-SH with metal ions

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Sulfur containing biomolecules are easily involved in complexes with gold. CoA is an important cofactor for many enzymes involved in metabolic processes. Fatty acyl-CoAthioesters, substrates of mitochondrial β -oxidation, are sulfur containg compounds and potential gold ligands. The CoA-mercury-gold complexes can be easily assessed by UV-Vis spectroscopy or indirectly by antibacterial tests that reconfirmed the protective role of CoA on *Ecoli*. The characteristics of these complexes were determined by means of FTIR spectroscopy. The interaction of gold with CoA in borate buffer was also proved by cyclic voltametry. These complexes were observed by AFM studies. The complexes stability is strongly influenced by pH. Our study clearly shows that CoA-mercury complex is formed even at pH 8 while CoA-gold complex at pH >10.

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CO 17. Crosslinked structures based on cellulose and siloxane derivatives

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Cellulose acetate, easily soluble in common solvents was converted to allyl cellulose by using two methods, i.e. the method proposed by Takano¹ and the method proposed by Kondo². The allylated product was reacted with either telechelic (1,1,3,3)tetramethyldisiloxane) or side Si-H functionalized siloxanes, (poly[dimethyl(methyl-Karstedt catalyst (Pt-bis[1,3-bis(vinyl)-1,1,3,3-H)siloxane]), in presence of tetramethyldisiloxane] complex), when crosslinking occured by hydrosilylation reaction (Scheme 1). The products were processed as films and studied by different techniques. Thus, surface (static contact angle, water vapor sorption capacity and swelling in different solvents), mechanical and thermal properties of the films were investigated and the results were correlated with the reactants ratios and preparation conditions. Crosslinking density was determined based on differential scaning calorimetry (DSC) records.



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CO 18. Functionalized polyurethanes as valuable supports for biomolecules conjugation

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Polyurethane-based materials (PU) are widely used in various biomedical applications due to their relative good biocompatibility and low toxicity, versatile synthesis, and high flexibility in acquiring the most appropriate physical properties for a peculiar use. However, a major drawback in obtaining bioconjugates and bioactive materials starting with this type of polymers is given by the lack of reactive groups available for post-synthetic chemical modifications. Moreover, the use of free isocyanate groups from PU prepolymers, and surface functionalisation through physical means do not usually provide enough control, efficiency and reproducibility in the processes of obtaining bioconjugates constructs. A recent approach to overcome the absence of reactive groups consists in bulk functionalisation of PUs by using appropriate polyols or chain extenders. In the present work, the dimethylolpropionic acid was used as chain extender in order to obtain free carboxyl-bearing PUs susceptible to post-synthetic functionalisation and subsequently bioconjugation. The resulting polyurethanes were tested with good results as supports for papain immobilization. The examination of relevant surface and bulk properties strongly suggests that such approaches do not only open the way of preparing new bioconjugate derivatives, but also could afford better and more versatile biomaterials.

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CO 19. Metal-peptide complexes involved in the neurodegenerative diseases

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Heavy metal ions are known to interact with peptides and proteins in the cells, being thus involved in the conformational diseases, which represents an intriguing but devastating class of neurodegenerative disorders that includes prion disease, Alzheimer's disease (AD), Parkinson's disease and Huntington's disease.¹ The interaction between metal ions and peptides has been investigated by using mass spectrometry, atomic force microscopy, and circular dichroism techniques at various pH values. Cu²⁺, Zn²⁺, Fe³⁺, Al³⁺ and other ions bind amyloid beta peptide (A β) to induce aggregation and form reactive oxygen species. These reactions may play a deleterious role in the disease state, because high concentrations of iron, copper, and zinc have been located in amyloid proteins in diseased brains. Here we show conformational changes of A β peptide and its fragments in the presence of metal ions at various pH. The competitive role of various peptides for metal ions was also investigated. In addition, we show that metal binding to peptides within the neurodegenerative processes is complex and some other factor should be more investigated.²

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CO 20. Non-covalent interactions in some supramolecular aromatic systems

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Non-covalent interactions are of great importance in determining the reactivity and structural properties in many important chemical or biological systems and are nowadays considered as cornerstones in supramolecular chemistry and materials science. The multitude of these types of interactions and their involvement in various systems required some detailed of experimental and theoretical studies. Non-covalent interactions encountered in aromatic systems can be established between pi-electronic system and a metal, an ion, a molecule, or other pi-electronic system. The most common non-covalent interactions are metal - pi electronic, polar - pi electronic pi donor - acceptor interactions, ion - pi interactions and aromatic - aromatic interactions or pi-pi stacking. Pi-pi stacking interactions are usually considered as occurring between aromatic rings and such interactions along with ion (anion or cation) - pi interactions are often collectively called as aromatic interactions. The present study shows a theoretical investigation of the aromatic interactions in some supramolecular systems as results of *ab-initio* and DFT levels of quantum chemistry.



Electrostatic potential contour (isoval=0.003) for benzene molecule in nanotube fragment.

CO 21. Dinitrophenols and Cyanide: Analytical and Toxicological Approach

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Numerous hazardous chemicals enter the environment from various industrial or agricultural sources daily.¹ Among them, cyanide and dinitrophenols are known to inhibit ATP production at the respiratory chain level, although by different mechanisms. This work reports on the determination of such compounds in the environment by using spectrophotometric assays. The use of cyanide to identify dinitrophenols and dinitrophenols to identify cyanide is also discussed. Besides, ninhydrin was demonstrated to be effective color reagent for spectrophotometric determination of trace levels of cyanide. We show here that reading of the absorbance at 485 nm could be more suitable and reliable than that at 590 nm, where the pH-dependent blue colored cyanide-ninhydrin adducts are less stable. The new color reagent was applied for cyanide determination in real samples of water, cigarette smoke, urine and cyanogens in plants. In addition, the mechanism of toxicity of both classes of pollutants is reconsidered. Especially dinitrophenyl derivatives admit a radiation-based toxicity mechanism, which differs much from that proposed by Peter Mitchell and those scientists that support the chemiosmotic hypothesis and proton translocation in production of ATP.² All these findings show that such major pollutants might be of interest to young scientists. Another present-day topic is the biodegradation and environment protection from such pollutants.³

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CO 22. Synthesis and characterization of oxide compounds with general formula Mg_{1-x}Cu_xFe₂O₄

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Ferrites with spinel structure, which have nanometer particles size, represent the major interest to researchers because of applications as: data storage devices, microwave devices, catalysts, biomedical applications [1]. The $Mg_{1-x}Cu_xFe_2O_4$ samples, with x = 0, 0.17, 0.34, 0.5, 0.67, 0.84, 1, have been prepared by sol-gel self-combustion method, using corresponding nitrates metal and glycine as chelating / combustion agent. The synthesis progress was followed by IR spectroscopy.



Fig.1 FT-IR samples at 900^oC

Fig. 2 XRD samples at 900^oC

The spinel phase formation was investigated and confirmed by X-ray diffraction patterns [2]. The lattice parameter and crystalline size values were calculated from X-ray diffraction data. Lattice parameter value is influenced by substitution of Mg^{2+} with Cu^{2+} , due to the difference of ionic radii and increase with increases in copper concentration. It can be seen that there is a transition from the cubic structure of magnesium ferrite to tetragonal structure of copper ferrite. The morphology and microstructure was investigated using scanning electron microscopy.

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CO 23. Influence of nanoparticles on the thermal decomposition of hybrid nanocomposites based on starch/poly(vinyl alcohol) montmorillonite

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Polymer-montmorillonite (MMT) hybrid nanocomposites are one of the significant developments of modern technology because of their capability to generate materials with selectiv properties. Incorporation of small amounts of nanoclays in polymer matrices (<5%) leads to significant improvement of mechanical properties, thermal and flame resistance, decrease the gas permeability, etc. These behavior modifications can be explained by the formation of a barrier that inhibits heat and mass transfer from the polymer that degrades to vapor, thus the volatile products release during the thermal decomposition are delayed. The present paper show the effect of the type and content of nanoparticles Nanocor I28, Peruvian clay and bentonite on the thermal behavior of polymer matrix based on poly(vinyl alcohol) and starch.

The thermal study of hybrid composites was performed on a simultaneous thermal analysis (Netzsch STA-409) coupled to an infrared spectrophotometer and a mass spectrometer. *In situ* detailed analysis of gaseous phase during the thermal decomposition of nanocomposites allowed the identification of volatile compounds, time and temperature of emission and their mechanism of decomposition was enabled. It was established that for a content of 2-4 wt% Nanocor I28, the thermal stability is enhanced, the thermal decomposition was delayed while the Peruvian clay and Bentonite nanoparticles act as catalysts. This behavior is attributed to the dispersion way of the clay nanoparticles in polymer matrix (exfoliation, intercalation), the presence of structures assembled head-to-head and to the Si-O-C bonds formed between clay and polymer compounds. Nanocor I28 nanoparticles, organically modified nanoparticles, present better compatibility with the polymeric matrix.

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CO 24. Synthesis and study of catalytic properties of bulk and supported LaCrO₃

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The main objective of this work was to investigate the catalityc activity of LaCrO₃ and LaCrO₃ supported on ZrO₂, SiO₂, TiO₂ and Al₂O₃. The synthesis was performed by using sol-gel auto-combustion method¹ and citric acid as combustion agent. Those materials are used as catalysts for the hydrogen peroxide decomposition. Synthesized catalysts were structurally characterized by FT-IR spectroscopy and X-ray diffraction (XRD). The presence of pure phase of perovskite oxide was confirmed at 700°C by XRD and is suitable to impregnate the support. The formation of LaCrO₃/suport can be followed by less intense reflections of the perovskite phase. The activity of the oxide catalysts for hydrogen peroxide decomposition was evaluated at room temperature². The reaction rate of hydrogen peroxide decomposition was determined by measuring the volume of evolved O₂ as a function of time, as show in Fig.1A) LaCoO₃/ZrO₂ and B)LaCoO₃/Al₂O₃. The optimal catalityc activity among all the samples is belonging to the LaCoO₃/ZrO₂.



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CO 25. Photocatalytic activity study of Metal - SnO₂ for the degradation of Eosin Y in aqueous suspension

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Three coupled Metal/SnO₂ nanocomposites (Ag/SnO₂, Ce/SnO₂ and Co/SnO₂) were prepared in different molar ratios situations implying a co-precipitation method[1,2]. Their

properties were evaluated by using different techniques: XRD, N_2 adsorption, SEM and IR. The photocatalytic activity samples were tested for removing eosin Y in different UV conditions [3]. One of the best photocatalyst properties is related to Ce/SnO₂.



Figure 1. Effect of irradiation time in the degradation of eosin Y (initial concentration of eosin Y $20mgL^{-1}$; pH 6; catalyst amount =2g /L).

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CO 26. Green synthesis of silver nanoparticles with sodium lignosulphonate

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Silver nanoparticles (AgNPs) are one of the first and most extensively studied materials at the nanoscale, with a wide range of applications, from catalysis, biosensors, biolabelling and bioassays to photovoltaics and enhanced optical spectroscopies. The AgNPs properties, uses and potential toxicity strictly depend on their size, shape, polydispersity and stability, which are in turn conditioned by the parameters of synthesis. There are many ways to synthesize AgNPs, but most of them require complex, strict synthetic conditions, and harsh reducing agents. Moreover, the recently published reports regarding the environmentally friendly synthesis of AgNPs present different issues related to size, polydispersity, stability, and require preliminary operations. Unlike previously reports, we present a very convenient and green synthesis of stable, crystalline AgNPs of about 20 to 40 nm by using a biodegradable, low toxic sodium lignosulphonate (LS) as both reductant and capping compound. The influence of different factors (i.e. reactant concentrations, temperature, and pH) on resulting AgNPs was assessed from UV-VIS spectra. The AgNPs size, shape, and crystallinity, as well as LS-AgNPs interactions were furthermore analyzed by the means of dynamic light scattering (DLS), transmission electron microscopy (TEM), X-ray photoelectron spectroscopy (XPS) and X-ray diffraction patterns (XRD).

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CO 27. Hydrolytic degradation of some poly(vinyl alcohol) copolymers for biomedical applications

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The continuous demand for environmentally degradable polymers has initiated the synthesis of new poly(vinyl alcohol) copolymers. In this research the hydrolytic degradation of some graft copolymers: poly(vinyl alcohol)-co-lactic acid (PVA-g-LA) and poly(vinyl alcohol)-lactic acid-aspartic acid (PVA/LA/Asp) has been studied. The copolymers were synthesized utilizing PVA/LA molar ratios (1.5/1 and 1/1) and PVA/LA/Asp molar ratios (1/1/0.75 and 2/1/0.75), respectively. The *in vitro* degradation was conducted in phosphate buffer solution (KH₂PO₄ 0.2M and NaOH 0.2M), pH=7.4, at 37 ^oC by immersion of the samples in the solution for 164-211 h. Different techniques: FTIR-ATR, DLS, SEM, DSC were used to monitor the changes of the chemical structure, average molecular weight, and thermal properties of the copolymers after hydrolytic degradation. By DSC could be noticed that the hydrolytic degradation determined Tg increase and Δ Cp decrease, as a result of free volume decrease due to graft chain scission. The results demonstrated that all the studied copolymers are hydrolytic degradable, as the ester bonds have been broken, resulting degradation products with a low weight average molecular weight.

P 1. New "SWS" (Solid Water Sorption)

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In this paper we focus on the characteristics of some new composite materials synthesized by impregnating granular activated carbon with CaCl₂ solutions of different concentrations. The properties of water sorption of the novel composite materials were analyzed and it was found that the water amount adsorbed increases when the CaCl₂ concentration in matrix increases too. The sorption properties and structure of the new composites were investigated by XRF, XRD, TG, BET, and SEM techniques. In order to realise XRF determinations we used an Axios Panalytical X-ray Fluorescence Spectrometer and for the phase composition of the confined salt was used an X-ray diffraction analysis by the AD- 500 Diffractometer (Siemens) with a graphite reflected beam monochromator The thermogravimetric (TG) technique was applied to measure water content in the sorbents using a STA 6000 Perkin Elmer Thermal Analyzer. Nitrogen adsorption isotherms were carried out at -196°C on a Micromeritics ASAP 2020 volumetric adsorption analyzer. The BET specific surface area was calculated based on nitrogen adsorption data in the range of relative pressure from 0 to 1. SEM images were realised using The Jeol 6330F Field Emission equipment.



Fig.1. SEM Image for the Ca²⁺ activated carbon impregnated with 30% CaCl₂ solution



Fig. 2. SEM Image for the Cl⁻ activated carbon impregnated with 30% CaCl₂ solution

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P 2. Preparation and characterization of a new composite material used for the water vapour adsorption

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This paper presents the preparation and characterization of a new composite material named MCC1 which was obtained by impregnating the active carbon with a 15 w% solution of calcium chloride.

The granular activated carbon with an average of 3.5 mm was used as "host matrix", and then the impregnation was realized for 2 hours under agitation conditions

Firstly the activated carbon was dryed at 200° C in an oven and then was cooled down in a vacuum desiccator. The dried carbon was immersed into an aqueous solution of calcium chloride with concentration of 15 w% and 30 w% for 2h. The activated carbon was impregnated under stirring conditions at 260 rpm, and the ratio solid to solution volume was 1:2. After 2 h, the prepared materials obtained were heated to 200° C for 4 h to remove water.

To measure the conductivity of solutions and determine their salt concentrations was used a high precision WTW Cond 315i conductometer.

A series of analyses were performed in order to establish the physical and chemical characteristics of the prepared composite sorbents.

This material was analyzed by XRF, XRD, TG, BET and SEM techniques in order to determine some properties.

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P 3. Preliminary data on contribution of Eastern Romania to the monitoring of atmospheric heavy metal deposition in Europe using bryophytes (2010 Survey)

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The European moss survey provides data on concentration of heavy metals, nitrogen and selected persistent organic pollutants in naturally growing mosses and is being repeated at five-yearly intervals (1990, 1995, 2000, 2005, and 2010). The main purpose of the survey is: to provide maps of spatial distribution of heavy metal concentrations in mosses in Europe; to identify main polluted areas; to develop the understanding of long-range transboundary pollution; to establish the effectiveness of air pollution abatement policies within Europe, based on temporal trend of pollutants concentration.1 The European moss network has expanded greatly since 1990, from 4661 sites in 1990 to about 6000 sites and twenty-eight European countries in 2005. First data from Eastern Romania were included in the report on 2000/2001 survey. As concerns heavy metals, the survey provides data on As, Cd, Cr, Cu, Fe, Hg, Ni, Pb, V, Zn. In addition, Al and Sb should be determined to indicate contamination of the samples by soil/the contribution of windblown dust and to indicate anthropogenic origin respectively.

Moss samples (of species Hylocomium splendens, Pleurozium schreberi and Hypnum cupressiforme) were collected across Eastern Romania in September – October 2010, at 78 sampling sites. The moss sampling procedure was according to the guidelines of the monitoring manual in the protocol for the 2010 survey.1 Al, As, Cr, Fe, Ni, Sb, V and Zn were determined by instrumental neutron activation analysis and Cd, Cu, Pb by atomic absorption spectrometry. At the moment data are only available for Al (mean 3566 mg kg-1) and V (mean 5.45 mg kg-1). Strong linear relationship was found between these two elements concentrations (R2 = 0.98), indicating possible common sources of these metals in mosses.

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P 4. Synthesis of new aza-analogues of pyrimidines bases

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A series of 2,4,6-tris(N,N-dialkylamino)-1,3,5-triazines has been studied for their antitumoral activity[1-3]. Among these derivates, hexamethylmelamine (1), an alkylating agent, is very efficient against ovarian, breast, and lung cancers but it generates side effects limiting its use in clinic. Thereafter, similar compounds such as 2-alkyl-4,6-diheteroalkyl-1,3,5-triazines (2-4) demonstrated a significant cytotoxicity towards various tumor cell lines *in vitro*.



It was suggested that the antitumoral activity of some triazinic derivatives is related to the fact that these compunds represented antimetabolites wich are able to accumulate in tumor cells. Currently, the chemical reactivity of these triazines attached in position 5 to *N*-benzylpyroglutamic or *N*-phenylpyroglutamic derivatives **5** has been explored under different conditions in order to access to new aza-analogues with potential bioactivity.



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P 5. Micro and mesoporous materials for heavy metals removal from wine

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Browning and loss of color, aroma and taste are the main oenological problems for wine producers during the storage.The wine browning is a result of phenols oxidation to quinones (catalyzed by Fe2+/Fe3+ or Cu2+ and oxidative enzymes) and of condensation reactions between phenol compounds with the formation of stable yellowbrown colored polymers [1]. The OIV method (MA-E-AS322-05-ERF) was used to measure the total content of iron in wine, based on the colorimetric method with orthophenantroline [2].

This paper presents the impact of some nanoporous materials: mordenite, AlMCM-41, MCM-41, on the iron content of a white wine, after contacting the wine with the solids.

Silica MCM-41 mesoporous material was synthesized using a gel with molar composition: 1SiO2: 0.2C16TMABr: 5.7NH3: 113 H2O. For the synthesis of AlMCM-41 (Si/Al = 16) material, a gel with composition: 1SiO2: 0.033Al2O3: 0.2C16TMABr: 100H2O was used.

The partial substitution of Si4+ in the walls of mesoporous silica MCM-41 with Al3+, leads to the negative charge of the network, which can be compensated by metal cations or by H+. The mesoporous material Al-MCM-41 can be used as an acidic ion exchanger with a higher efficiency. The comparison between the three materials (mordenite, Al-MCM-41, MCM-41) showed that the most efficient material in Fe2+ ions capturing.) is Al-MCM-41.

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P 6. Synthesis and biological evaluation of new propargyl derivatives containing phenothiazine moiety

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Recent studies have shown that propargyl derivatives are potential agents for neuroprotection in Alzheimer's, Parkinson's and other neurodegenerative diseases. N-propargyl-containing compounds such as rasagiline, pargyline, clorgyline, and deprenyl show high MAO inhibitory activity. Experiments revealed that propargylamine itself possesses the neuroprotective activities of rasagiline and other propargylamines.¹ These derivatives are also known for their in vitro antimicrobial activity², cardioprotective agents³, etc.

Starting from these previous considerations, a series of easily affordable phenothiazine derivatives bearing a propargyl chain were synthesized and tested by our research team, in order to evaluate their inhibitory activity against human farnesyltransferase protein (FTase).



Figure 1. Structure of propargyl derivatives

The synthesized compounds where tested on human FTase. Among the tested compounds at 100 μ M, derivative **d** emerged as the most active compound of the series, with IC₅₀=24,498±2,3268 μ M. To establish the activity for the rest of the derivatives, the percent inhibition was calculated. This evaluation revealed that compound **c** has no activity, while derivatives **a** and **b** have a modest inhibitory activity against FTase.

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P 7. Testing of antioxidative and antimicrobial activity of some new food packagings

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The objective of this study was the comparative analysis of some new food packaging based on low density polyethylene, chitosan and vitamin E in respect with those commonly used in specific conditions of the commercialization of food products such as poultry meat. With this aim the particula exams have been applied such as senzorial appreciation, chemical and microbiological analysis monitoring the changes during self - service of products of 48 hours.

The meat and meat products alteration depends on the nature and concentration of microorganisms, meat type, relative humidity from storage space and temperature of conservation. The process of the meat putrefaction starts with activity of the bacteria of the aerobic putrefaction (*Pseudomonas, Bacillus, Proteus, Streprococcus*), firstly at surface then the muscular mass is affected by proteazes (mainly *Proteus*) and continue by anaerobic putrefaction intermediated by facultatice anaerobic bacteria (*Escherichia, Staphylococcus, Clostridium*). This process is accompanied by organoleptic changes as: aspect, color, consistence and odour.

Testing was done by standard methods such as: SR EN ISO 5495:2007, SR ISO 6658:2007, SR ISO 2917:2007, SR 9065-11:2007, SR ISO 7031:2008. From all performed tests it has been established that packaging containing both chitosan and vitamin E show superior properties in respect with common method used for poultry meat preservation.

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P 8. New derivatives of 5-nitroindazole with potential antitumoral activity

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The remarkable pharmacodynamic properties of numerous chemical compounds with large practical usage result from the interactions of certain groups of atoms within their molecules with the biological environment¹. Among the intensely researched functional groups, which are present within certain drug molecules with biological activity, the N-mustards stand out.

New 5-nitroindazole derivatives substituted in 1^{st} position with radicals that contains the di(β -chloroethyl)-amine group grafted on the pyrazol ring of the substrate have been synthesized in order to obtain compounds with enhanced antitumoral activity. Thus, a novel method of synthesizing N-mustard compounds was developed to link di(β -chloroethyl)-amine by ethylene, ester or acetyl bonds.

The chemical structure of the new derivatives has been confirmed by elemental and spectral analysis (¹H-NMR and FT-IR). The potential cytostatic action of the compounds studied on Guerin experimental tumours proved that the new alkylating agents significantly suppressed the proliferation of the neoplastic cells, close to the reference cytostatic-endoxan.

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P 9. Synthesis and characterization of new hydrazides derived from N-(p-aminobenzoyl)-L-glutamine with potential tuberculostatic and their immobilization on polymer support of poly (N-vinylpyrolidone-alt-itaconic anhydride)

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New hydrazide derivatives from N-(p-aminobenzoyl)-L-glutamine have been synthesized having oxazolones as intermediates.

R-CH-COOH	(CH ₃ CO) ₂ O	R-CH-C	NH2-NH2	R-CH-CO-NH-N	H ₂
HŃ		N=c>0	>		
$\dot{C} = 0 0$ $C_{cH_4} = NH - \ddot{C} =$	- 2 CH ₃ COOH R ₁ (p)	C ₆ H ₄ -NH	$-\overset{O}{C}-R_{1}$ (p)	C_6H_4 NH- C_8H_4	e ₁ (p)
I, II		III, IV		V, <mark>VI</mark>	

I, III, V: R = - (CH₂)₂ -CO-NH₂; R₁= -H si II, IV, VI: R = -(CH₂)₂-CO-NH₂; R₁= -CH₃

New drug-polymer conjugates were prepared by chemically linking the hydrazides to polymer support, based on co-polymer poly (N-vinylpyrolidone-itaconic anhydride).



The structure of all new compounds has been confirmed by elemental and spectral analysis (FT-IR and ¹H-RMN). The biological activity of the active principles and polymer conjugates was evaluated by registering acute toxicity and tuberculostatic activity against Mycobacterium tuberculosis.

Acknowledgement This work is realized with the support of the program POSDRU/89/1.5/S/49944 financed by the European Social Found and the Romanian Government.

P 10. New phenothiazine and carbazole derivatives as inhibitors of human farnesyltransferase. Design, synthesis and biological evaluation

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Many biological properties have already been described for phenothiazine and carbazole derivatives,¹ some of phenothiazine derivatives display anthelmintic activities,² and others are (reversible) inhibitors of trypanothione reductase,³ inhibit lipid peroxidation⁴ or tubulin polymerization⁵, and some carbazole derivatives are inhibitors of human adipocyte fatty acid-binding protein.⁶

Compounds with the phenothiazine moiety were reported by our research group in the field of human farnesyltransferase⁷ and we have now modified the carbazole and phenothiazine scaffolds by using chains often encountered in the field.

The biological activity of all the synthesized derivatives was evaluated on human FTase and the results obtained were in micromole fields. These results allow us to establish structure-activity relationships and targeting research to improve biological activity. Compounds I and II constitute starting points for further investigation of new potential inhibitors of protein farnesyltransferase.



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P 11. Synthesis and Antimicrobial Activity of New Amidic Derivatives of 5-Nitroindazol-1-yl Acetic Acid Encapsulated into Alginate/Pectin Particles

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New amidic compounds with biologic activity, derived from 5-nitroindazol-1-ylacetic acid have been synthesized using as intermediate the ethyl ester of 5- nitroindazol-1yl-acetic acid (I) ¹, which was condensed with various amines: monoethanol amine, diethanol amine, diethanol ethyl amine, isopropyl amine and alyl amine (Fig.1). Their chemical structure was confirmed by elemental and spectral analyses (FT-IR, ¹H-NMR, ¹³C-NMR and mass spectrometry).



Figure 1. Synthesis of amides of 5-nitroindazol-1-yl-acetic acid

The incorporation of some of the amides into sodium alginate and pectin based microcapsules, prepared by polymer ionotropic gelation in O/W emulsion determined the augmentation of their antibacterial potential against bacterial strains.

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P 12. Gas permeability of some biocomposites

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The environmental concerns and the need for more versatile polymer-based materials has led to increasing interest on the polymer composites filled with natural organic fillers, i.e. fillers coming from renewable sources and biodegradable.

Cellulose-based polymer composites are characterized by low cost, desirable fiber aspect ratio, low density, high specific stiffness and strength, biodegradability, flexibility during processing with no harm to the equipment, and good mechanical properties.

The permeability of different gases through a material is a critical factor when it concerns the ability of a package to prolong the self life of packaged food. The permeation is affected in a complex way by a number of parameters within the material, like the flexibility of the polymer chains, morphology including orientation effects, crystallinity and interaction between the permeant molecules and the polymer, and interaction with an eventual filler. The relative humidity has also a great influence on certain materials.

The aim of this work was to prepare biocomposites by melt mixing and to investigate the influence of the unbleached and bleached cellulose Kraft pulp fibers, unmodified and modified with oleic acid, on gas permeability and crystallinity changes in comparison with neat LDPE. It has been established that the modification of the fibres with oleic acid does not increase the permeability because of the improved compatibility of components.

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P 13. Segmented polyurethane and poly(urethane-urea) elastomers based on heterocyclic moiety: relaxations phenomena

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Polyurethanes are polymeric materials characterized by a wide range of physical and chemical properties and are suitable for many applications.

Dielectric spectroscopy provides information about dipole reorientation, rotations of the main and segmental chains of the polymers when an electric field is applied. The main objective of this study is to find a relationship between the relaxation parameters and chemical structure of the synthesized polyurethane and poly(urethane-urea) elastomers.

The polyurethanes and poly(urethane-urea)s synthesized are based on a aliphatic prepolymer containing poly(ether) soft segment and two chain extenders containing 2,3-substituted pyridine moiety. Dielectric properties were evaluated on the basis of dielectric constant, dielectric loss and electric modulus. Their variation with frequency and temperature was studied.

Polyurethanes usually exhibit three relaxation processes under the electric field, γ , β and α in order of increasing temperature. The temperature of alpha relaxation is in good agreement with the DSC results. At temperatures higher than α relaxation temperature, dielectric loss increases abruptly especially at the lower frequencies, this behavior being attributed to the increasing conductivity. In order to analyzed the conductivity process, dielectric relaxation data was interpreted by means of the electric modulus. The activation energy for dc conduction is higher for polyurethanes than for the poly(urethane-urea) samples. The introduction of urea linkage facilitates the relaxation mechanism.

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P 14. Aspects of thermal behavior in air of casein investigated by FTIR and calorimetry

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In the present paper the thermal behavior of casein was studied by the TG – FTIR and Differential Scanning Calorimetry (DSC) techniques.

The casein is the main protein in milk being of great interest due to its many uses in the cosmetic, food and pharmaceutical industries. The casein under study (99% purity and bovine nature) was supplied by Lancaster Company (England).

Study by TG, DTG, DTA specifies the range of temperature in which casein is thermally stable with some applications in cosmetics, food and pharmaceuticals containing casein [1,2].

The thermal methods (TG, DTG, DTA) were coupled with the FTIR analysis in order to obtain supplementary information which are crucial in the prediction of the thermal degradation. By analyzing the gaseous species resulted (CO₂, CO, NH₃, HNCO) from thermal degradation this method gives useful information regarding the possible impact over the environmental pollution.

Calorimetric studies confirms the results obtained by thermal methods, namely casein is totally degraded in air.

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P 15. Synthesis and characterization of some lanthanide polioxomolybdates

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Polyoxometalates of lanthanides ions have remarkable properties which make them to be used in different fields, such as: photochemistry, catalysis, material science, magnetism, medicine, etc.

The aim of our study is to investigate the new synthesis method for polyoxometalates. In present work we studied the clusters between Nd^{3+} and Ho^{3+} , respectively, with paramolybdate, $[Mo_7O_{24}]^{6-}$ obtained by hydrothermal method.

The characterization of the systems Ln^{3+} -POM was accomplished by means of FTIR and UV-Vis spectroscopy, thermal analysis and structure was confirmed by X-ray single crystal analysis. The structure was solved by the direct method and refined by the full-matrix least squares technique on F² using SHELXTL 97 crystallographic software package. The IR bands spectra of the newly compounds present some modification by comparison with those associated to (iso)polioxomolybdate ligands, especially because of the structural changes caused by coordination of lanthanide cations.

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P 16. Fluorescence compounds in biosystems: a first step study

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Fluorescence measurements may be used to reveal the conformational changes of biological active peptides especially the tryptophan-containing ones¹. Fluorescence changes of some fluorophores bound to amyloid- β peptides have been associated with their conformational changes. In this work, we investigate the fluorescent properties of two important fluorofors, glycyltryptophan peptide (GW) and salicylic acid, as well as the adducts of GW with various metal ions, such as copper(II), nickel (II) and mercury (II). The excitation wavelength was 265 nm, whereas fluorescence maxima were found at 691 nm, 530 nm, and 350 nm. On increasing concentration of metal ions, the fluorescence pattern changed accordingly, depending on the type of metal. Both nickel and copper ions influenced the fluorescence of peptide GW; however, copper ion reduced the fluorescence intensity of peptide, while nickel ion has an adverse effect.² On adding GW to amyloid- β peptide in the presence of heavy metals, a decrease by 30% of fluorescence intensity was observed in the case of copper and by 50% when mercury was studied. Since metal ions influence also peptide conformation, GW might be a candidate to investigate A β conformational changes. When studied the fluorescence of salicylic acid (SA) and the influence of 2,4-DNP, we observed that dinitrophenol compunds quench the fluorescence of salicylic acid, acting as inhibitors of fluorescence, depending on the concentration, as expected. Salicylic acid had an emmission maximum at 405 nm, with an intensity of 65.8 in the absence of 2,4-dinitrophenol. In the presence of 2,4-DNP the intensity of SA decrease to 52.9 for 50 µL of 10⁻² M added to 3 mL of SA solution. Finally, the decrease reached a value of 6 when 1000 µL added. Our results revealed that fluorescence spectroscopy could be an important tool to reveal novel properties of the biological active compounds.

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P 17. Synthesis under ultrasound irradiation of new pyrrolodiazinic compounds with acetophenonic chain

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During the last decades, ultrasound (US) irradiation has became an increasingly valuable tool in organic chemistry, since it is a versatile and facile technique applicable to a large variety of syntheses¹⁻⁴. In particular, for the chemistry of nitrogen heterocycles, literature data indicates that Huisgen [3+2] dipolar cycloaddition has been done under ultrasound irradiation in nitrogen ylide classes except for the cycloimmonium ylides, our group being the first to investigate this aspect².

In this respect we synthesize new pyrrolo-diazinic compounds with acetophenonic chain, using a general and straightforward strategy (quaternization and cycloaddition reactions) under classical conditions and nonconventional methods.



Scheme 1. Synthesis of new pyrrolo-diazinic compounds with acetophenonic chain.

Ultrasound assisted reactions were carried out using a SONICS (130 W, Newton, CT USA) processor; comparative studies classical *vs* US were done.

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P 18. Photo-induced grating formations on polysiloxanes modified with azobenzene derivates

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The aim of this work is to investigate the nanostructuration capacity of azopolysiloxanes for application in biological field (cell culture development and nanomanipulation of biomolecules) [1]. Formation of gratings is possible due to photoisomerization properties of azobenzene groups capable to generate nanostructured surfaces under laser UV/Vis irradiation process [2]. Azo-polymers were synthesized starting from a linear polysiloxane with chlorobenzyl groups in the side chain using a Williamson substitution reaction (figure 1a).





The geometry of modulated azo-polymeric surfaces was study with AFM technique (figure 1b). By changing the p-substituent of phenyl-azo-phenol compound we succeed to obtain amplitude of modulation between 10-800nm, using the same thickness film and condition of irradiation. The most efficient mass transport we obtain in the case of polysiloxane modified with 4-naphtalene-azo-phenol groups.

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P 19. X-ray studies of some unexpected fused azaheterocycles

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Nitrogen heterocycles have gained much interest over the time, actually being the basis of many significant pharmaceuticals, physiologically-active natural products and synthetic compounds¹. Among them, 1,2-diazines are important constituents in some drugs already in use for different human diseases² or agrochemical products³. In this respect, the main objective of the present work was to synthesize new



hydrazides/hydrazones starting from some N^2 substituted/unsubstituted pyridazin-3(2*H*)-ones and hydrazine hydrate, by adapting the literature procedures. Thus, varying the reactant ratio and using ethanol as solvent, we obtained the desired hydrazides, but also some unexpected fused azaheterocycles, as products of cyclocondensation reactions.

Figure 1. X-ray structure of 7-(4-bromophenyl)-4-methyl-8,9-dihydro-2*H*-pyridazino[6,1-*c*][1,2,4]triazin-3(4*H*)-one.

The structure of compounds was proved by spectral

analysis (IR, ¹H-NMR, ¹³C-NMR) and X-ray diffraction (using a X-ray diffractometer: *Xcalibur, Eos diffractometer*).

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P 20. One-pot synthesis of new pyrrolo-diazine compounds with sulfonamide chain (classical versus ultrasound)

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It is well known that sulfonamide, with particularly structure, are inhibitors of carbonic anhydrase isozymes 1,2 . The compounds containing 1,2-diazinic moiety have demonstrated versatile biological activities, such as antiviral, anticancer, antituberculosis³.

In the present work we have synthesized new pyrrolo-phthalazinic compounds with sulfonamide chain. The synthesis of dimethyl 3-(4-sulfamoylphenylcarbamoyl)-pyrrolo[2,1-a]phthalazine-1,2-dicarboxylate (D) was performed by an efficient *one-pot* reaction, from three-components: phthalazine (A), 2-chloro-*N*-(4-sulfamoylphenyl)-acetamide (B) and dimethyl acetylenedicarboxylate (C) (scheme). This *one-pot* reaction was performed under ultrasound and classical conditions. Ultrasound assisted reactions were carried out using a Sonics reactor (Sonics VCX-130,USA).



The structure of new pyrrolo-diazinic compound (D) was proved by spectral analysis: IR, ¹H NMR, ¹³C NMR, and 2D-experiments (COSY, HMQC, HMBC).

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P 21.Influence of Fe/Ta substitution on the structural and physical properties of $Sr_2Fe_{1+x}Ta_{1-x}O_6$ double perovskite

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The interesting physical properties of the new perovskites are primarily due to the electronic interactions of B-site cations [1]. In this paper we purpose to study the influence of Fe/Ta substitution in the structural and physical properties on the perovskites $Sr_2Fe_{1+x}Ta_{1-x}O_6$. Polycrystaline samples $Sr_2Fe_{1+x}Ta_{1-x}O_6$ (x = 0,÷0.5) were obtained by conventional solid state reaction. The resulting powders was sintering at $1300^{\circ}C$ /48h.

X-ray diffraction measurements at room temperature, used to investigate the purity of the perovskite powders. Note that with increasing degree of substitution the tolerance factor decrease and the symmetry of the crystalline cell. FT-IR transmission spectra were obtained using a spectrophotometer with wave number range 4000 cm⁻¹– 400 cm⁻¹ used to complete the structure studies. All the spectra present the typical two band pattern characteristic of the perovskite structure.

The complex impedance in the frequency domain of $20 \div 2 \times 10^6$ Hz at room temperature was determined and the perovskite with x = 0.5 has low dielectric losses and low relative permittivity.

We are investigating the catalytic properties of perovskites in water splitting process, under gamma-rays irradiation emitted by a ⁶⁰Co source. It was noticed that the perovskite with x = 0.5 had a higher catalytic effect.

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P 22. Crosslinked silicones functionalized for metal retention

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Poly(dimethylmethyl-3-aminopropyl)dimethylsiloxane-a,w-diols were endcrosslinked with tetraethylorthosilcate (Scheme 1a) and processed as films. These were characterized and used as such for the retention of the metal ions (Cr^{3+} and Ni^{2+}) from aqueous or alcoholic solution by immersion procedure. The metal ions absorption capacity was evaluated by FTIR, UV-Viz and XRF spectroscopy. $Cr(NO_3)_3$ ·9H₂O and NiCl₂·6H₂O were used as metal salts. In this order, the measurements were made at different concentrations and different period of time. Based on the obtained results it was possible to appreciate the $Cr3^+$ ions are faster retain than Ni²⁺ ones.



Scheme 1

In another approach, a polydimethylsiloxane- α , ω -diol (M=43000) was crosslinked with 3-aminopropyltrietahoxisilane and free amine groups were condesed with 2,6-diformyl-4-methylphenol to form supplementary bis-azomethine bridges between polysiloxane chains.

The resulted film was tested for the retention of cupper ions in methanolic solution. The process was monitored by FTIR, UV-Vis and XRF spectroscopies.

P 23. Kinetic study of the penicillin g degradation in the presence of a penicillinase with attenuated activity

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The degradation or stability study of β -lactam antibiotics has been of paramount importance not only due to their market availability, but also due to their potential to be use in the evaluation process of their pharmacokinetic properties and adverse reactions. Penicillinase is the enzyme that inactivates the antibiotic, hydrolyzing β -lactam nucleus and leading to the inactivation of the biological product.

Linearization procedures of the Michaelis-Menten model, respectively the Lineweaver-Burk, allowed us to calculate the characteristic constants of the action of a penicillinase with attenuated activity on a substrate of penicillin G.

Comparing the experimental results with those obtained in the absence of a penicillinase with attenuated activity we found that, in the beginning of the experiments, the slope of the antibiotic concentration decreases more, and in the final part of the degradation process, the chemical reaction speed exceeds that of the enzymatic process.

P 24. Oxidative modification in proteins: synthesis and structural characterisation of tyrosine modified peptides

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Oxidative modification of Tyrosine residues in proteins may occur in cells upon oxidative stress and inflammation processes mediated through generation of reactive nitroxyl from peroxynitrite. Tyrosine nitration and hydroxylation from oxidative pathways may generate cytotoxic species that cause protein dysfunction and pathogenesis. A number of protein nitrations from *in vivo* and *in vitro* studies have been reported and some specific Tyrosine modified sites have been recently identified using mass spectrometric methods [1]. Following the identification of oxidative modified sites of tyrosine residue in proteins we synthesised several model peptides. The peptides were synthesised by solid-phase peptide synthesis (SPPS), purified by reversed phasehigh performance liquid chromatography (RP-HPLC) and characterised by electrospray (ESI) and matrix-assisted laser desorption-ionisation (MALDI) mass spectrometry [2]. Binding affinities and specificities of synthetic peptides with different Tyr-modified sites were determined by evaluation of anti-nitrotyrosine antibodies using immunoanalytical determination as dot-blot and ELISA [3]. The results showed that the antibodies may discriminate in the recognition of peptides with different N-terminal adjacent sequences to the nitrotyrosine residues, depending on the type of immunogen employed.

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P 25. Morphological and surface studies of some new supramolecular polymers containing dimethylsilane groups

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Three supramolecular polymers assembled by hydrogen bonds between a dicarboxylic acid, bis[N-(4-carboxyphenyl)phtalimidyl]dimethylsilane, and bipyridyl derivatives, 4,4'-bipyridyl, 1,2-bis(4-pyridyl)ethylene, and 4,4'-azopyridine, have been prepared [1]. The resulted structures were investigated by FTIR, ¹H NMR spectroscopy and X-ray single crystal diffraction. The morphology of the films spin coated from THF solution was emphasized by AFM, being evaluated in terms of average roughness (Sa), root mean square roughness (Sq), core fluid retention index (Sci), developed interfacial area ratio (Sdr) and texture direction index (Stdi). The porosity, internal surface and sorption capacity were determined by water vapor sorption analysis in dynamic regim. The capacity to retain different gases was estimated on the basis of structures as determined by single crystal X-ray diffraction, using Mercury program.



Chemical structure and AFM images of the supramolecular polymers, SP1, SP2, and SP3

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P 26. Studies on water-soluble ionic species in atmospheric particulate matter and lichenized fungi populations of Xanthoria parietina and Phaeophyscia orbicularis in Iasi urban area

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Lichenized fungi are nowadays known as popular biomonitors of air pollution and bioindicators of air quality. Many references give details concerning lichenized fungi potential to be used in air pollution studies or in research areas dealing with the past, present and future climate changes [1].

Analysis of water soluble cationic species (Na⁺, NH₄⁺, K⁺, Mg²⁺, Ca²⁺) present in Xanthoria parietina and Phaeophyscia orbicularis lichenized fungi samples, was performed on a *Dionex ICS 3000* ion chromatograph, using methane sulfonic acid (6 mM) as eluent. Lichenized fungi samples were collected from Tudor Vladimirescu, Podul Ros and Bucium locations. At each site the temporal distributions in the concentrations of the identified cationic species ($\mu g/g$ dry weight), showed variability from one month to another. Significant statistical correlations were observed for $(K^+,$ Mg^{2+}) and (K⁺, Na⁺) pairs. The above mentioned aspects corroborated with data from the literature, allow us to emit the suggestion that these elements most probably are involved in mechanisms occurring at the cellular level.

Since particulate matter (PM), which may affect human health and play an important role in climatic changes, represents an important component of urban air pollution in Iasi [2], in the present work investigations were performed on the relative contributions of water-soluble ionic species identified in coarse and fine fractions, from a typical urban to rural site, i.e. "Anastasie Fatu" Botanical Garden of Iasi. The identified and quantified water-soluble ionic species in the analysed particulate matter samples have highlighted the existence of a complex chemical composition in these matrices.

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P 27. Adsorbtion capacity study of cationic dyes on several magnetic nanoparticles

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The aim of this study is to obtain a clear comparison of the adsorption capacity of cationic dyes on magnetic nanoparticles in relation to the cation present in the ferrite as to find the best material fit for wastewater treatment.

The preliminary step was the synthesis by the coprecipitation method and characterization by X-ray diffraction, UV-VIS and FT-IR spectroscopy of magnetic nanoparticles. The nanoparticles used in the study were MFe₂O₄ (M=Mg, Mn, Co, Ni) on which was studied the adsorption of basic fuchsine and methylene blue by UV-VIS spectroscopy at specific time intervals for a total time of 50 minutes.





The results of this study indicate a correlation between the adsorption capacity and the metal's group number. $MgFe_2O_4$ showed the best results compared to any other investigated ferrites showing adsorbing capacities approximately three times lower in the same time interval. A possible explanation for this may be that the Mg ferrite has a less occupied surface with –OH groups as shown in FT-IR spectra. The nanoparticles have a high adsorption speed in the first 10 minutes followed by a decrease in efficiency most probably because of the surface saturation.

In conclusion the materials used in this study are sitable for use as adsorbents for wastewater treatment and posses the ability to extract even highly concentrated dyes with the help of magnetic fields. Another important property is their potential to be reused.

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P 28. Influence of NaOH concentration on coprecipitation synthesis, morphology and particle size of cobalt ferrite nanoparticles

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Cobalt ferrite (CoFe₂O₄) nanoparticles were prepared by coprecipitation method. The ferrite precursors were produced from aqueous mixtures of cobalt chloride and ferric chloride by coprecipitation, using sodium hydroxide aqueous solution as precipitant agent. Six different concentration of NaOH (1-6 M) were used in the synthesis, and the influence on the properties was studied. The ferrite precursors are first calcined in the furnance at 500°C for 6 hours and then, the samples were characterized by X-ray powder diffraction (XRD), Fourier transform infrared spectroscopy (FTIR) and scanning electron microscopy (SEM).

Powder XRD profiles of the cobalt ferrite nanoparticles precipitated with different concentration of NaOH and annealed at 500°C under air are presented in Figure 1.



different concentration of NaOH

For all patterns the diffraction peaks exhibit Bragg reflections perfectly indexed to the cubic spinel structure (space group Fd-3m) which indicating the formation of the single-phase cobalt ferrite.

Acknowledgements

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P 29. Ultrasound assisted synthesis of new imidazoilum salts

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Imidazole and its derivatives are well known biologically active and medicinally potent anticancer agents¹, anti-HIV², antibacterial and antifungal^{3,4}, or used in the treatment of cardiovascular diseases⁵, etc. Moreover, imidazolium salts are potent room temperature ionic liquids of current great interest in industry⁶.

The aim of this work was to synthesize new azaheterocyle salts derived from 1,3diazoles, which are possible ionic liquids, via conventional heating and ultrasound irradiation. In this respect we performed the alkylation of some five-member rings *N*heterocyles derived from imidazole and benzimidazole.

Thus, imidazolium salts were obtained in two steps: initially we carried out the *N*-alkylation of the acidic nitrogen of imidazole derivatives (imidazole and benzimidazole) via Michael addition of acrylonitrile; in the second step we carried out the quaternization of the second nitrogen atom with iodoacetamide and methyl- or ethyl bromoacetate, respectively.

The structure of the newly synthesized compounds was proven by elemental (C, H, N) and spectral analysis (IR, 1H NMR, 13C NMR, 2D-COSY, HMQC, HMBC). All the elemental and spectral data are in accordance with the proposed structure.

Aknowledgements: To CNCS-UEFISCDI, grant PN-II-TE/ 0010 -79/05.10.2011 (director conf. dr. Costel Moldoveanu) for financial support.

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P 30. Synthesis of new coronands and spiro-derivatives using ultrasonic irradiation

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Supramolecular chemistry [1,2], a branch of modern chemistry, designs chemical compounds with pre-established structures and properties. Coronands [3,4] are targets of interest in supramolecular chemistry, being used as host molecules for cations, anions and organic molecules.

The syntheses of oxaazacoronands based ligands occur were carried out under conventional conditions: with stirring at room temperature and atmospheric pressure. Thus, α -chloro-3,4-dihydroxyacetophenone **1** was treated with 1,3-phthaloyl dichloride **2a**, or 1,4-phthaloyl dichloride **2b**, respectively, to give the desired symmetric 18- and 20-membered ring coronands **3a** and **3b** (Scheme 1).



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P 31. Contributions to the Thermal Degradation Mechanism under Nitrogen Atmosphere of PTFE by TG-FTIR Analysis. Influence of the Particle Size.

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The thermal behavior of polytetrafluoroethylene (PTFE) with different particle size was studied under nitrogen atmosphere by the thermogravimetric analysis coupled with Fourier transform infrared analysis (TG-FTIR analysis) in comparison with the synthesized PTFE.

The goal of this work was to find the best degradation conditions having in view the monomer (C_2F_4) recovery from polymer residues due to the highly cost both of the polymer obtaining and especially to the monomer synthesis^{1,2}.

The characteristic amounts from the TG-DTG-DTA analysis afforded the study of thermal stability giving also some information about the particle size influence on the thermal degradation.

The TG-FTIR analysis of the gaseous products evolved by thermal degradation of the samples under nitrogen atmosphere was applied for the first time with the different particle size PTFE leading to results regarding the obtaining of the monomer (C_2F_4) from residue resulted on PTFE mechanical processing, in view of its recovering.

The obtained results afforded the optimum degradation conditions which lead to a profitable monomer recovery (almost 99%).

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P 32. Synthesis, structural analysis and magnetic properties of low Pbdoped LaMnO₃ manganites

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The La_{1-x}A_xMnO₃ manganites have a rich electronic diagram: for x<0.25 the manganites behave as ferromagnetic insulator ($T_C \in (100 \div 180 \text{ K})$), for 0.25<x<0.5 as ferromagnetic metal ($T_C \in (180 \div 270 \text{ K})$) and for x>0.5 as charge ordered insulator. A new type of manganites, with La_{1-x}Pb_xMnO₃ (x=0.03, 0.06 and 0.10) chemical composition, was obtained by sol-gel method. The synthesized manganites contain only the perovskite phase, (GS R -3 c) (Fig 1.). A small variation of the lattice constant was observed despite the difference between the radii of La³⁺ (1.216 Å) and Pb²⁺ (1.35 Å).

The molar magnetization is close to 3.7 μ_B /f.u., with a maximum for x=0.06, near to maximum theoretical value for molar magnetization, while the Curie temperature is about 250 K for all investigated samples. Transport properties, determined between 7 and 350 K, indicated a metallic behaviour for the samples with x \leq 0.10. The transition temperature between metallic and insulator behaviour have a minimum with increase of Pb concentration in the samples.



Figure 1 Diffractograms of La_{0.97}Pb_{0.03}MnO₃: bottom-Bragg position of calculated maxima (vertical segment) and the difference between observed and calculated diffractograms, FullProf code

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P 33. Characterization of certain metalloporphyrins using dynamic thermal methods and molecular modeling

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Porphyrins and metalloporphyrins have a wide range of applications, and optoelectronics is one of them¹⁻³. It is absolutely vital that materials used for these applications reach good thermal stability since the liquid crystalline structure ordering property occurs within a specific temperature range and involves a system temperature increase². The paper tackles the characterization of certain metalloporphyrins using dynamic thermal methods and molecular modeling.

The thermal analysis was done on a Mettler Toledo derivatograph in nitrogen atmosphere and at various heating rates. The molecular modeling was carried out on Hyperchem 7.5 software, which provided optimized shapes and revealed a series of changes in the position of the phenyl groups in relation to porphyrin, changes that are dependent on the type of metal. The correlations established between the thermal, kinetic and structural characteristics enabled us to draw conclusions about thermal stability and the degradation mechanism. Metalloporphyrins are stable until they reach about 480°C, depending on the nature of the metal. The degradation includes a single stage and provides a compound that is thermally stable up to 900°C. The apparent activation energy determined by the Flynn-Wall⁴ method depends on the conversion degree, i.e. the energy consumption is dictated by the position of the phenyl groups and by the type of metal.

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P 34. Uranium removal from aqueous solutions by new materials based on power station ash

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Abstract: Uranium is one of the most important heavy metals because of the chemical toxicity and radioactivity. Excessive amounts of uranium have entered into environment through the activities of nuclear industry. For this reason, removal of uranium from wastewater is of great importance [1, 2]. The removal of uranium from aqueous solutions (concentration range: 125-2000 mg U/L, initial pH 3) by power station ash in raw modified form was investigated using a batch technique. Two types of modification were tested, an ultrasonic one (for 1 hour at 70° C) and a direct activation (4h using 5M NaOH at 70° C). The sorbents were characterized by electron microscopy/energy dispersive spectroscopy (SEM/EDS), X-ray diffraction (XRD) and Fourier Transform Infrared Spectroscopy (FT-IR). The determination of uranium was performed by means of the Arsenazo III method. Sorption isotherms were determined and modeled using the Langmuir and Freundlich equations. The U-uptake by raw and ultrasonic modified ash was better reproduced by the Freundlich equation, where as the one by the directed activated ash by the Langmuir equation providing a maximum sorption capacity (Q_{max}) of 186 mg/g. The direct activated ash seems to be the most effective compared with the other two sorbents (s. Figure) and could present application potential for the U-removal from aqueous media.



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P 35. Wood-polymer composites: effect of the thermal pre-treatment of wood filler on the composites stability towards water

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Despite of some advantages (such as low cost, low density, renewable nature, high specific strength and modulus), natural fibers are hydrophilic because of their cellulosic and hemicelluloses constituents preponderant in the fiber composition. When used as filler for wood-polymer composites (WPCs), their hydrophilic behaviour can cause weak interfacial adhesion between fibers and the hydrophobic matrix. Moisture sorption can also promote the biological attack and, subsequently, degradation.

Thermal pre-treatment of wood prior to blending with the polymer is one of the most interesting approach and can potentially be used as a solution to reduce the water sorption of WPCs. Pre-treated wood showed an increased dimensional stability probably due to the loss of constitutional water and enhancement of crosslinking reactions between formaldehyde (generated during the decomposition of organic acids from wood) and phenol units from lignin.

Measurements (water sorption, thickness swelling) indicated a significant increase of the composites stability towards water. Further use of a coupling agent (maleated polypropylene) yielded in even more improved properties (water sorption and mechanical resistance).

P 36. Effect of chemically modified cellulosic fibres on the properties of novel polypropylene composite materials

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The use of natural fibres as reinforcement in composite materials, similar to glass fibre reinforced composites, requires adequate adhesion between filler and matrix, whether the matrix is a conventional polymer (thermoplastics or thermosets) or a biodegradable polymer, or even a cement. In addition, processing conditions also influence the properties of these materials. Composite materials based on thermoplastic matrices and high content of natural reinforcement (such as ligno-cellulosic fibres) are increasingly used in a wide variety of industrial and domestic applications.

The two main drawbacks of cellulose fibres as reinforcement for thermoplastics are the relatively low degradation temperature (approx. 200°C) and the high values of water sorption. The first criterion limits the variety of thermoplastics that can be used as matrix, because it limits the processing temperatures at lower values, below cellulose fibres degradation temperature. The second one has negative effect on the adhesion to hydrophobic matrices, yielding in a poor dispersion of the filler within the matrix and a defective wetting of the filler surfaces by the polymeric matrix.

This paper describes the characteristics of novel polypropylene-straw fibres composites. The filler was chemically modified using a coupling agent, such as polymethylhydrosiloxane (PMHS), in order to change the nature of its surface, from hydrophilic to hydrophobic. Experimental data obtained during tests indicated a significant decrease of water sorption characteristics, while adhesion and mechanical properties improved.

P 37. Ternary thermoplastic blends based on block-copolymers, recycled polyethylene and polyamide fibers

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Plastic waste management is one of the major environmental concerns worldwide. For the last 30 years many studies have been conducted in order to assess the feasibility of using industrial by-products and waste materials in civil engineering applications.

Among the most voluminous polymer waste, thermoplastic polymers (polyolefins, polyamides, PET) and scrap automobile tires are in great abundance. One of the promising ways to up-cycle plastic waste is to obtain multicomponent polymeric materials with competitive properties. A good compatibility in these blends made of immiscible polymers is very difficult to obtain. Their properties are strongly affected by several factors: the ratio of the melt viscosities of components, interfacial tension and adhesion, processing parameters. Several studies were performed to overcome this barrier to expanding markets for waste in material composites.

In this work, the influence of two copolyamide-dienic rubber block copolymers (BCPs) on the properties of a series of new blend formulations based on polyamide fibres recovered from worn tires and recycled polyethylene films was studied. The blends were processed by extrusion-compression molding and their morphological and mechanical properties were investigated in correlation with the nature and amount of BCP used for each formulation.

Based on our experimental results and literature data, due to these new BCPs properties, it will be possible to open new opportunities for recovery and recycling polymer waste.

P 38. Blends based on a nylon copolymer and EPDM rubber. Compatibilizer influence on their properties

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Thermoplastic elastomers (TPEs) are a relatively new class of materials which combine the excellent processability characteristics of thermoplastics and the physical properties of elastomers. TPEs from blends of rubbers and plastics have attracted much interest in recent years because the required properties of blends can be easily achieved by the careful selection of components (rubber and plastic), the blend ratio and processing conditions

Polyamides (PAs) are materials widely used in engineering applications due to their superior mechanical properties and good chemical resistance. But, PAs have some limitations: poor impact strength and high yield cost. These limitations can be alleviated by blending with suitable polymers.

Blends of PAs and ethylene/propylene/rubber (EPM) are a new class of TPEs which combine the excellent processability characteristics and engineering properties of PAs with elastic properties and low water sorption of EPM. However, they are highly immiscible and incompatible due to the high difference of polarity between the components.

The main objective of the present study is to analyze the effects of a maleated ethylene-propylene rubber (EP-g-MA) on the micro- and macroscopic properties of the copolyamide/ethylene propylene diene terpolymer (coPA/EPDM) blends. Blends were prepared by melt blending in a Haake Rheocord mixer. Individual components and polymer blends with different compositions were characterized by dynamic rheology, and differential scanning calorimetry (DSC).

The results suggest immiscible mixture in the entire range of the blend's compositions. However, the presence of EP-g-MA in the blend leads to the enhancement of the interfacial viscosity and adhesion due to the intermolecular interaction between the functional groups of components during processing.

P 39. Multivariate statistical analysis on size dependent thermal behavior of CoFe₂O₄ nanoparticles

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Cobalt ferrite $CoFe_2O_4$, with a partially inverse spinel structure, is one of the most important and most abundant magnetic materials [1]. Cobalt ultrafine powders and films have attracted considerable attention for their wide range of technological applications such as transformer cores, recording heads, antenna rods, memory, ferrofluids and biomedical application [2]. The phase transformation of cobalt ferrite during annealing under air, are influencing by the factors such as preparation methods, size, reaction media and heating rate [3].

This study proposes a multivariate statistical treatment to establish the variation of crystallite size as a function of thermal annealing.



Figure 1. (a) In situ high temperature X-ray diffraction (HTXRD) pattern of CoFe₂O₄ heated from room temperature to 850°C in steps of 50°C, and (b) variation of crystallite size against thermal treatment

As seen from the plot (Figure 1.b), the crystallite size increases significantly when the sample is heated above 850 $^{\circ}$ C

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P 40. Performances of implicit (PCM), explicit and mixed solvation models in computing UV-Vis spectra of fluorescein in aqueous solution

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Electronic absorption (UV-Vis) spectra of the prototropic forms of fluorescein in aqueous media (protonated, neutral quinoid, neutral lactone, mono and dianionic species) are computed at the time-dependent density functional theory (TD-DFT) level using the widely-used B3LYP and the parameter-free PBE0 local hybrid functionals in conjunction with various Pople basis sets. To account for solvent effects, two conceptually different solvation models are used, including the implicit Polarisable Continuum Model (PCM) and an explicit solvation model in which discrete solvent molecules (water). In implicit PCM, electronic absorption spectra were computed by TD-B3LYP and TD-PBE0 on optimized ground-state geometries in both linear-response and state-specific approaches. The latter, in conjunction with the B3LYP functional is shown to be the most appropriate for computing the lowest excitation energies of all the molecules species being investigated. To construct solute-water complexes, in both discrete and mixed solvent models, molecular dynamics (MD) simulations were performed on fluorescein species solvated in a 30x30x30 Å water box. Force-field parameters for fluorescein and fluorescein-water interaction, including force constants and partial atomic charges, were derived from B3LYP/6-31G(d) computations. A corresponding number of Cl⁻ or Na⁺ ions were also added to the simulation box to ensure charge neutrality needed in MD simulations using periodic boundary conditions. To compute electronic absorption spectra, several snapshots taken from the MD runs were considered. The solute molecule surrounded by an increasing number water molecules were subjected to TD-DFT computations, without any further geometry optimization. Excitation energies computed in our discrete solvation approach show a rapid convergence when increasing the number of water molecules. Further consideration of implicit solvent effects on solute-water complexes has little effect on the computed spectra.

P 41. Ab initio and DFT studies on keto-enol tautomerism and fluorescence emission of 7-acetyl pyrrolopyridazine

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Computational investigations at the *ab initio* (RHF and CIS) and density functional theory (DFT and TD-DFT) levels are performed on a model compound (7-acetyl pyrrolopyridazine) to account for the effects of keto-enol tautomerism on the electronic absorption and fluorescence properties. CIS and TD-DFT computations predict the title compound to be fluorescent in it's enol form and nonfluorescent in it's ketone tautomer due to a $n\pi^*$ nature of the first electronic excited state. Computed barriers for acetyl torsion are 6-8 kcal/mol, about half of the value reported for nitroso-pyrrolopyridazine and denote larger steric effects and little electron π -electron delocalisation over the exocyclic bond. Equilibrium geometry and free energy computations performed in gas phase and in PCM water reveal two transition states on the reaction path leading from the ketone form to the most stable geometry of the enol. The highest free energy barrier on the reaction path (corresponding to proton transfer from methyl to carbonyl group) is about 62 kcal/mol in gas phase and show no significant difference when solvent effects are included using an implicit model. In contrast, explicit consideration of two water molecules to mediate the proton transfer lowers the barrier to ~ 31 kcal/mol.



P 42. Titaniumsilsesquioxane synthesis and use as filler for silicone polymers

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Titaniumsilsesquioxane, a cage-like metallosiloxane was synthesized by cocondensation of phenylsilanetriol with $Ti(OiPr)_4$ (Scheme 1) and characterized by elemental analysis and spectral techniques (IR, NMR, ED-XRF). The compound is stable in solid state.



Scheme 1

Having the structure similar to that of polyhedral oligomeric silsesquioxane, abbreviated as POSS, that is thought of as the smallest particles of silica possible, the titaniumsilsesquioxane was used as nanofiller for a polydimethylsiloxane matrix. The aim was to reinforce and to increase the dielectric constant of the resulted composite. The presence of the siloxane sequence similar with that in polymeric matrix and of titanium with high dielectric constant constitutes a premise for this. The moisture sorption capacity and electromechanical response of the film composite were measured.