OVIDIUS UNIVERSITY of CONSTANTA
Faculty of Applied Sciences and Engineering

Romanian Chemistry Society (SChR)
Constanta Branch

Eurachem Romania

INTERNATIONAL CONFERENCE
CHIMIA 2014
"NEW TRENDS IN APPLIED CHEMISTRY"

Book of Abstracts

May 23 – 24, 2014
Constanța, Romania

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Foreword for the 6th Conference "Chimia" 2014

The sixth in the cycle "Chimia", this conference was organized by our department starting with 2000 every three years until 2012, since it is organized every two years.

Chimia 2014 is part of an on-going Conference series which focuses on applied chemistry problems. The conference's proceedings were and continue to be published in Ovidius University Annals of Chemistry, which is indexed in Chemical Abstracts, in Index Copernicus starting with 2009 and in Polymer Library, Pirabase, Paperbase starting with 2013. From 2012 the journal is published in Versita OPEN system with de Gruyter partner.

At this meeting you can present your most recent research achievements and ideas. The organizers intend to create a warm and friendly atmosphere for stimulate the scientific discussions and confrontations.

Chimia 2014 is conducted at the University Ovidius of Constanta and Royal Hotel. Conveniently located, Royal Hotel offers excellent facilities for conferences. The meeting halls and poster area are designed to facilitate interactions among Conference participants.

Constanta is the second largest city in Romania and the biggest port at the Black Sea, an important cultural and economic centre, worth exploring for its archaeological treasures and the atmosphere of the old town centre. The name of Constanta dates from the Byzantine ruling when Tomis appears in Byzantine and later Italian documents, as Constantia, after an important imperial Roman family.

We wish you all a fruitful conference in Constanta with many new ideas and contacts all over Europe. We look forward to meet each of you at the Chimia 2014!

Sincerely,
Viorica Popescu
Conference Chairperson
Chimia 2014 Organizing Committee

FACULTY OF APPLIED SCIENCES AND ENGINEERING OVIDIUS UNIVERSITY OF CONSTANTA

Flagship of scientific research in the entire region

The Faculty of Applied Sciences and Engineeringis well-known for the team of teachers and research, recognized in recent years for the most significant research results of all the Ovidius University and the entire Constanta district. The academic staff has published in the last five years 137 papers in ISI journals and over 130papers in BDI journals, which represents about 2/3 of the scientific production of the entire university. The faculty is now known in the country and abroad for the research in the field of electron microscopy and nanostructured materials, physics of plasma, ultraacustic microscopy, alternative energy sources, environmental quality control and petroleum and petrochemical technologies. Many research grants funded by government institutions or economic agents, amounting during the last five years nearly 2.900.000 Euros, strengthened the infrastructure with modern and highly performant equipment. Some of these contracts led to the filing of some internationally awarded patents, which were subsequently followed by technologies applied in refineries throughout the country.

Academic programs revised together with employers

The Faculty of Applied Sciences and Engineeringtook advantage of the changes brought about by the reform of the European educational system and revamped all the programs of study. The new curricula were developed together with the major employers, such as Rompetrol, Petrom, Oil Terminal, RAJA, Romtelecom, Cernavoda Nuclear Power Plant, Constanta Shipyard, to provide the graduates with all the skills needed for immediate employment.

The educational offer of the facultyconsists in 5 fields of study with 5 programmes of study at undergraduate level and 4 fields of study with 4 programmes of study at postgraduate level.

The bachelor and master academic programs are based on the European Credit Transfer System, ECTS, fully compatible with the current standards of European education under the Bologna process. The areas of specialization are modern, in accordance with the requirements on the local job market and the national employment requirements. The graduates are prepared to face a highly competitive environment, where great emphasis is placed on creativity, flexibility, adaptability, interdisciplinarity, in line with the requirements of the knowledge-based society of the future.

The faculty offers bachelor programs in Physics, Chemistry, Chemical Engineering, Electronic Engineering and Telecommunications and Applied Sciences Engineering. In the case of the **Physics** program, with a major in **Physics** (3 years) and the **Applied Sciences Engineering** program, with specialization in **Applied Physics** (4 years), there are two directions of concentration: *Physics and technology of advanced materials* and *Physics and technology of nuclear reactors*. The **Chemistry** program, with the study area **Chemistry** (3 years), allows the graduates to be employed as chemists in both education and industry, in environmental monitoring and food safety agencies, in chemical analysis laboratories, as well as in the field of pharmacy, medicine, environmental chemistry, food chemistry etc. The **Chemical Engineering**, program has a major in **Petroleum Processing and Petrochemistry**, which this year reaches 37 years of activity, prepares engineers for the oil refineries and petrochemical complexes, for the transportation, storage and distribution of petroleum and natural gas, in after extraction oil preparation units, etc. The three directions of concentration are *Petroleum and gas processing*, *Petrochemical technologies* and *Biofuels*. In the same field a new major starts in the 2009-2010 academic year: **Food Chemistry and Biochemical Technologies**, focusing on the *Quality and analysis of food* and *Food technologies*. In the field of **Electronics and Telecommunication Engineering**, the **Applied Electronics** major gives students a general training in electronics, as well as in depth knowledge and practical skills in *Industrial and medical electronics* and *Electronics in telecommunications*. The graduates gain useful skills in automation, IT systems, the command of electrical power systems, in mobile communications, modern television systems, GPS systems, radars, etc.

Academic programs at the master's level are available in Physics, Chemistry and Chemical Engineering. In the field of **Physics** the major is **Condensed matter physics and technology** (2 years), which provides the students with unique skills in areas such as the *Physics and technology of advanced materials* and *Physics and technology of materials for nuclear reactors*. The master's program called **Chemistry and management of**

quality of chemical products and the environment (2 years) provides deeper knowledge in quality assurance of consumer products (food animals and plants, detergents and cosmetics) and the environment. The master's program in **Technology and management of petroleum processing** (2 years) continues according to the Bologna process a traditional master's program in place since 2000, concentrating on the design as well as the economic management in the oil industry, being addressed both to chemical engineers in the oil industry who want to be familiar with concepts of economics and management and to economists who look for some technical knowledge.

Generous merit-based and need-based scholarships. International study opportunities

The students of the Faculty of Applied Sciences and Engineeringbenefit annually of about 130 seats subsidized by the state budget. The beneficiaries of these tuition waivers, as well as the best students who pay for their studies may receive generous merit-based scholarships of about 250-350 lei per month. On the other hand, students with special family conditions may be eligible for social, need-based scholarships. Moreover, students can take advantage of numerous international relations to study for one semester at partner European universities under the Socrates-Erasmus bilateral agreements schemes. Bachelor and master's students can compete for an individual mobility grant in universities such as University of Besancon, University of Nice-Sophia Antipolis, Nisa, France, University of Barcelona, Spain, University of Bologna and University of Ferrara, University of Calabria, University Catolica del Sacro Cuore, Milan, Italy, Kavala Insitute of Technology, Greece, etc. Additionally, CEEPUS projects have enabled student training stages at the Institute of Ionic Systems and Plasma Physics in Innsbruck, Austria, the Comenius University in Bratislava, Slovakia, Franz Josef University in Ljubljana, Slovenia, Charles University in Prague, Czech Republic, etc.

Graduates can have high incomes in the country or abroad

Graduates in physics and applied physics at both bachelor and master's level work primarily in industry, services and research but also in education. Another important employer is the Nuclear Power Plant in Cernavoda, and the companies that provide services for it. Other areas of interest are metrology, quality control of products and environment, medical equipment and advanced technologies with plasma and lasers, automation, etc. Outstanding graduates with research interest pursue doctoral studies in the country or abroad. Chemists are employed in companies active in the field

of environment monitoring and food security, such as the Environmental Guard, the Environment Agency, the Office for consumer protection, in chemical analysis laboratories, as well as in companies in the field of pharmacy, medicine, environmental chemistry, chemistry food, etc. The graduates of the petroleum and gas major work at companies that deal with the drilling, extraction, transport, storage and disposal of petroleum products, such as Rompetrol Refining SA, Rompetrol Petrochemicals, Rompetrol Quality Control, Petrobrazi SA, Lukoil TeleajenPetromar Constanta (WCO), INCERP (WCO), ICERP Ploiesti Oil Terminal Constanta, Constanta RPT Oil. The graduates in Electronics work for famous industrial companies, such as the shipyards in Constanta and Mangalia, Rompetrol, CNE Cernavoda, communication companies (Romtelecom, Vodafone, Orange), cable television and data communications companies (RDS-RCS, UPC), and also for small and medium enterprises with various objects of activity, such as science and computers, office equipment and peripherals, security and surveillance, electronics repair, etc.

Nationally and internationally recognized academic staff

Continuing a tradition of over 45 years of higher education in Constanta, the Faculty of Applied Sciences and Engineering is one of the most prestigious of the "Ovidius" University. The last ten years have proved to be the most dynamic, the faculty reached a total of about 600 students, of whom nearly 100 at master's level, over 32 full time academic staff and about 15 associated faculty members.

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PLENARY LECTURES

PL1. THE POTENTIAL OF SENSORS AND BIOSENSORS FOR INTEGRATED PROCESS CONTROL IN REAL-TIME. CAN THEY SURVIVE THE ENVIRONMENT?

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Combined dot sensors are new tools in sensors' technology. Different scenarios regarding the innovation, development, design, behaviour, implementation and application of dot sensors will be outlined. They were designed for food, pharmaceutical or biological analysis. Food additives such as colorants and ascorbic acid were determined directly from food and beverages, folic acid from food, pharmaceutical and biological samples, sildenafil citrate in pharmaceutical formulations and dopamine from pharmaceutical and biological samples. The working dot sensors were based on diamond or carbon paste modified with different porphyrin base or metal-porphyrin complexes, using different electrochemical techniques such as, differential pulse voltammetry (DPV) were used for the assay of the samples. The lower limits of detection obtained allowed the assay of these analytes at levels which do not need preconcentration of the samples.

Acknowledgements
The present work was supported by the Romanian National Programme PN II, Ideas, Contract Nr. 100/27.10.2011.

PL2. NANOSTRUCTURED MATERIALS FOR SOLAR HYDROGEN PRODUCTION

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One of the main requirements for a future Hydrogen Economy is a clean and efficient process for producing hydrogen using renewable energy sources. Hydrogen is a promising energy carrier because of its high energy content and clean combustion. In particular, the production of hydrogen from water and solar energy, i.e., photo-electrolysis, is one of the few methods for both renewable and sustainable energy production. While water splitting can be carried out with coupled solar cell – water electrolysis systems, the direct photo-electrolysis with a semiconductor photo-electrode is a more elegant and potentially cheaper approach and the direct photo-electrolysis is the Holy Grail of electrochemistry, using the power of light. Here, the photo-active semiconductor is immersed in water and the photo-generated electrons and holes are directly used to reduce and oxidize water, respectively, in a PhotoElectroChemical cell (PEC cell).

Here, we will present the principle of the PEC cell for water splitting, along with advanced photo-electrode materials and their requirements for application in a PEC cell. Defect chemical aspects in relation to charge transport in doped materials will be high-lighted. To date, the decreasing length scale to the nano-scale of the functional materials for photo-electrochemical applications attracts widespread attention and a variety of synthesis routes has been designed to manufacture nano tubes, nano-flake surface structures, and fractal surface morphologies of photo-electrodes. It will be shown, how the nano-structure is beneficial in case diffusion lengths of the photo-generated charge carriers are substantially different.

PL3. ON-LINE REVERSED PHASE SUPPORTED LIQUID EXTRACTION (RP-SLE) AS A BASIC SCENARIO FOR EXPLAINING LARGE VOLUME INJECTION (LVI) OF IMMISCIBLE DILUENTS IN RPLC

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The topic of large volume injection in liquid chromatography should be considered in direct relationship with the continuous quest for increased sensitivity. Although the subject of LVI in RPLC was extensively discussed and already reached an "axiomatic" level, some "exotic" approaches referring to LVI of stronger or even immiscible diluents with respect to the mobile phase appeared in the literature during the last decade. The LVI of non-miscible diluents in RPLC was pertinently explained and consequently applied by our team in the pharmaceutical control and bioanalytical areas. However, the theoretical basis of the process remained only superficially covered. It appears that the process may be modeled through a reversed phase supported liquid extraction (RP-SLE) process on-line coupled to the chromatographic column. The stages of such a process are: (I) the transfer of the diluent plug in the head of the chromatographic column; (IIa) inflation of the diluent plug produced by the penetration of the mobile phase (formation of channels); (IIb) the liquid-liquid extraction (LLE) of the analyte from the diluent in the mobile phase until the diluent/mobile phase front interface is reached; (IIIa) reinjection of the virtual sample volume of the analyte contained in the mobile and continuation of the LLE process; (IIIb) the regular chromatographic process arising in the remaining portion of the column. The compliance of the theoretical model to experimental observations was tested by using data collected for LVI of a homologous series of para-hydroxyalkylbenzoates (methyl, ethyl, propyl, butyl, pentyl, hexyl and octyl congeners) in liquid alkanes (hexane, heptane, iso-octane, decane and dodecane) on a stationary phase consisting in a octadecyl chemically modified silicagel eluted with a mixture of acetonitrile:water 4:6 (v/v). Although the model mainly focus on explaining the linear reduction of the retention time with the injected volume, some aspects relating to front spreading and thermodynamic aspects are also qualitatively discussed.

PL4. NOVEL MATERIALS FROM TRIGYLCERIDES AND FATTY ACIDS: SYNTHESIS AND MATERIALS PROPERTIES

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The use of plant metabolites to make monomers, polymers or composite materials is a growing area of research.[1] Recent research has focused upon the use of vegetable oils,[2] carbohydrates[3] and lignins[4] among others. These natural products may be polymers themselves (e.g. lignin) or molecules which can be made into polymers (e.g. vegetable oils, flavanoids). In this paper we illustrate how triglycerides and fatty acids can be manipulated using green chemistry into a range of surface coatings, poly(urethane), poly(ether),5 and poly(methacrylate) materials.

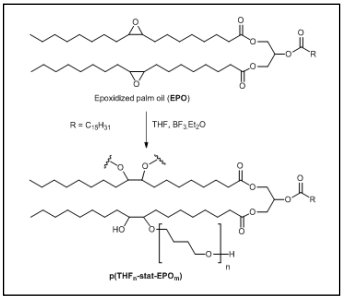

Fig. 1. Poly(ethers) from palm oil

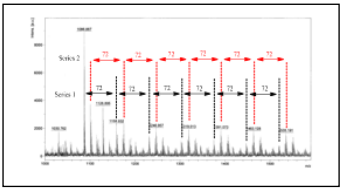

Fig. 2. MALDI-TOF mass spectrum

In addition, the introduction of functionality into vegetable oils suitable for use in azide-click and other non-classical click reactions will be will be described and the polymerisation of these monomers into new classes of material will be illustrated. Materials thermal and mechanical properties will be presented and the effect of different vegetable oils starting upon the materials properties will be described.

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PL5. ANALYTICAL CHEMISTRY IN FORENSIC SCIENCE

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Chemistry is the science that studies the composition, the structure, and the properties of the matter, as well as the reactions by which a substance is transformed into another one with completely different characteristics. Consequently, it has a very broad application area. The forensic chemist, by analyzing the findings from the crime scene, tries to define a "*scientific truth*" in order to support the achievement of the "*legal truth"*. The more careful and informative data will be collected at the crime scene, evidence will become more and more clues, and the legal truth will get closer to the objective truth. The term "*legal truth*" defines a truth substantially similar to the objective one, which arose out of a debate among the reasons for the prosecution and for the defense, preceded by surveys conducted carefully, using the facts found in our case on chemical analysis, and listening to the actors and witnesses. The term "objective truth" means the actual knowledge of all the facts of an event with all internal and external causes that led to the development and real conscious and unconscious motivations behind the actions of all actors of the offense.

The Analytical Forensic Chemistry must have in mind some fundamental needs and concepts of a legal procedure. The sampling of analytes (substances to be determined) must be representative; the verbalization of all sampling procedures must be accurate and detailed; the preparation of a sample for the analysis of first instance and, where possible and when required by law, of corresponding samples available to the counterparty and/or to the judiciary when further investigation are needed.

In conclusion, the terms Forensic Chemistry and Analytical Forensic Chemistry mean all the activities related to the classical definition of Chemistry and Analytical Chemistry, however carried out keeping in mind that the implications and the interpretation of analytical data must be evaluated from the legal point of view.

S.Girotti, A.Montoya, S.Eremin, M.J.Moreno, P.Caputo, M.D'Elia, L.Ripani, F.S.Romolo, E.Maiolini. "Development of a chemiluminescent ELISA and a colloidal gold based LFIA for TNT detection". Analytical and Bioanalytical Chemistry, 396 (2), 687-695, 2010.

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PL6. NEW SYNTHESES OF USEFUL CHEMICALS STARTING FROM AGRICULTURAL ROW MATERIALS

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We report here some of our results concerned with exploration of new pathes devised to obtain useful chemicals and materials starting from renewable agricultural products.

Thus, naturally available aminoacids were subjected to degradation by anodic non-Kolbe oxidation to afford high yields of N,O-acetals which are valuable synthons due to their high and versatile reactivity. When starting aminoacids contain a second stereocenter (e.g. L-isoleucine, L-hydroxyproline) resulted optically pure N,O-acetals are suitable for enantioselective syntheses. We have demonstrated high potency in asymmetric induction of natural aminoacids derivatives by performing enantioselective reduction of 2-hydroxyaryl ketons. Reaction was mediated by an aluminium hydrade-type reagent synthesized from L-valine and grafted onto a Merrifield resin (solid-phase regenerable system). Apart from aminoacids other naturally occuring compounds were transformed into useful synthons by anodic oxidation: glucose (degradation to inferior monosaccharides); ketalized tartaric acid monomethyl ester (monodecarboxylation to hemialdehyde of hydroxymalonic acid); malic acid (good yield of succindialdehyde).

Taking as raw material vegetable oils, the aim of our work was to create modified fatty acids by grafting on aliphatic chain some structural motifs, e.g. antioxidizing (polyhydroxy phenols) or dyeing (azo-type chromophores) moieties. The syntheses, tested on methyl oleate as model substrate, consisted in bromination (allylic substitution mediated by NBS, or bromine addition respectively) followed by graft coupling using a Williamson-type reaction. All modified fatty acids were structurally and stereochemically characterized (NMR, FTIR,MS) and are available for biological tests in view of their potential uses in cosmetics or medicine. Due to relatively non-expensive access to large amounts of linseed oil we used this raw material to obtain macromolecular resins by epoxydation followed by acid catalized ($BF_3.OEt_2$) polycondensation. Interesting polyhydroxy fatty acids were also prepared from epoxydated linseed oil (by acid or base catalyzed hydrolysis) and from sun-flower oil (by Baeyer oxidation).

KEYNOTES

KN1. STOCHASTIC SENSORS - NEW TOOLS FOR BIOMEDICAL ANALYSIS

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Electrochemial micro and nanosensors based on nanostructured materials were developed for *in vitro* biomedical analysis. The evolution of the performances and design of the sensors is directly related to the evolution of material science, and the performance of the analytical instrumentation. Carbon and diamond paste are recognized as the most reliable matrices for sensors' design; they also improved the selectivity and sensitivity of the sensors. Introduction of nanostructured materials in sensors' design enhanced their response characteristics. While amperometric sensors, and potentiometric sensors are used for the direct analysis of substances of biological importance, for biomarkers there is a need for development of selective sensors. Stochastic sensors were used for both qualitative and quantitaive analysis of biomarkers and simultaneous assay of substances of biological importance such as dopamine and ascorbic acid directly in the biological fluids. Examples of utilization of new micro and nanosensors based on nanostructured materials (e.g., maltodextrins, porphyrins, inulins) for biomedical analysis and enantioanalysis will be shown.

Acknowledgements
This work has been supported by the Romanian National Programme PN II, Ideas, Contract Nr. 123/2011 and PNII Program Capacity, 2012-2014, Contract nr. 3ERC-like/2012

KN2. WASTE MANAGEMENT TRENDS IN OIL PROCESSING INDUSTRY

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The waste management is one of the major challenges for oil processing industry. The waste diversity, the continuously hardening legislation, the costs of waste management, all create a complex problem to be solved by every refinery coping with narrow profit margins.

This keynote presents the new trends in waste management, starting with mitigation of waste by proper process design, continuing with emissions reduction, the neutralization of wastes and the recovery in new products, always having in view the integration of waste management in the general management of the refinery.

An ample discussion on the different wastes recovery or neutralization is given, pointing out the best practices at this moment and the research contributions of our staff in the management of sludge, slurry, slime, industrial wastewaters, spent caustic, spent mineral oils and residual petroleum fractions.

KN3. CHEMICALLY MODIFIED ELECTRODES BASED ON POLYAZULENE FOR HEAVY METAL IONS DETECTION

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Determination of trace levels from heavy metal ions in the environment is a highly important, yet challenging analytical problem. Numerous health problems are associated with exposure to high levels of metal ions (e.g., Cd^{2+}, Pb^{2+}, Hg^{2+}) because of their tendency to be accumulated in the body, toxicity and low rate of clearance.

In the last years the electrochemical methods for detection of trace metals become very important since these methods offer several advantages, including remarkable sensitivity, inherent miniaturization and portability. Electrochemical analysis using chemically modified electrodes represents a promising method for metals determination at trace levels. Also, conducting polymers have attracted great attention due to their wide fundamental interest and potential industrial applications.

Being formed by fusing a seven-membered ring with a five-membered ring, the azulene shows low ionization energy and a high electron affinity, which makes it a very interesting building block among the monomers for the synthesis of advanced materials. New complexing polymer-coated electrodes have been synthesized by oxidative electropolymerization of azulen substituted with malonamide-like complexing groups in acetonitrile solutions. The novel electrodes were used for the electrochemical detection of heavy metal ions by means of the chemical preconcentration-anodic stripping technique. The DPV curves recorded at glassy carbon modified electrode in 0.1mol L^{-1} aqueous acetate buffer (pH 5.5) after an optimum preconcentration time in Pb(II), Cu(II) and Hg(II) buffered solution and electroprecipitation to zero valent metals performed at −1 V in metal-free electrolyte allowed simultaneous detection of Pb(II), Cu(II) and Hg(II) metal ions.

Acknowledgements
The authors are grateful to UEFISCDI - Exploratory Research Projects PN-II-ID-PCE-2011-3, project ID 15/2011.

KN4. THE CHEMISTS' NMR APPROACH ON MONITORING DISEASES

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During its rather brief history, NMR spectroscopy was initially used by physicists. It was only in the 1960's when the chemical shift was discovered that the chemical community started to use it and the field took off. NMR became an indispensable tool in structure elucidation of pure compounds and until late 1980's this remained the most important type of application. Once the high field NMR spectrometers entered the chemical community the method started to be used also for complex mixture analysis, penetrating new fields like medicine or food sciences.

Today we see a rather balanced use of the NMR spectroscopy between the structure elucidation of pure compounds and analysis of complex mixtures.

When it comes to applications of NMR to complex systems, like biological ones, one should carefully balance between the excitement of the "potential" of the technique and claims of "ultimate diagnosis tool capabilities". Thus, one should be always aware which techniques and protocols are valuable but restricted to advanced medical research and which ones can be already extended to clinical practice.

The present paper starts with examples of structure elucidation of isolated compounds, and moves to spectra of complex body fluids, discussing some experimental factors, reproducibility, and data interpretation via either biomarker identification approach or blind statistical classifier approach.

Section A: Natural and Synthetic Compounds

PA1. PHYSICO-CHEMICAL AND BIOLOGIC CHARACTERISATION OF SOME Cu(II) COMPLEXES BEARING BIOACTIVE LIGANDS

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Recent studies evidenced a good anti-inflammatory, antimicrobial, and antitumor activity for some polyfunctional ligands with oxygen and nitrogen donor atoms. As result several complexes with this kind of ligands were studied and some of that demonstrated ability to mimics or to inhibit metal-enzymes. The anticonvulsant, antitumor, anti-inflammatory, antimicrobial or neurological activity was also evidenced for such complexes.

Having in view these aspects, we extended this field in synthesis of new complexes of Cu(II) with carboxylic derivatives (acetate, aspartate or glutamate). The features of complexes have been assigned from elemental analyses, IR, UV-Vis-NIR, NMR, EPR spectra, magnetic susceptibility at room temperature as well as thermogravimetric analysis. The ligand behaves as bidentate deprotonated species resulting in distorted square pyramidal stereochemistry in all cases.

The *in vitro* screening of the antimicrobial activity were performed against Gram positive (*S. aureus*, *B. subtilis*), Gram negative (*E. coli*, *P. aeruginosa*, *K. pneumoniae*) and fungal (*C. albicans*), both reference and clinical isolates multidrug resistant strains. In all cases it was evidenced that overall antimicrobial potency of ligand was enhanced upon coordination, regarding both resistant planktonic and biofilm embedded pathogenic strains.

PA2. PHYSICO-CHEMICAL AND BIOLOGIC CHARACTERISATION OF SOME Ni(II), Pd(II) AND Pt(II) COMPLEXES WITH *o*-TOLYLBIGUANIDE

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The increasing incidence of bacterial drug resistance imposes an improvement of the known antimicrobial drugs and also the development of new ones. In the last years the attention in this field was oriented to inorganic species among the organic ones. Although many complexes showed a good antimicrobial activity until now only a few are used as metalloantibiotics (antiseptics and antimicrobial) or disinfectants. So far a good antimicrobial activity was observed for complexes bearing a biocation and a multidentate ligand and/or having a proved antimicrobial activity.

In order to obtain new antimicrobials new complexes of type $[M(HTBG)_2]Cl_2$ and $[M(TBG)_2]$ (M: Ni, Pd, Pt and HTBG: 2-tolylbiguanide) were synthesised and characterised. The features of complexes have been assigned from microanalytical, IR and UV–Vis data.

The *in vitro* qualitative and quantitative antimicrobial activity assays performed against Gram positive (*S. aureus, B. Subtilis, E. faecalis*), Gram negative (*E. coli*, *P. aeruginosa*) and fungal (*C. albicans*) strains showed that the complexes exhibited variable antimicrobial activity against Gram-negative and Gram-positive strains both planktonic and biofilm embedded. In all cases it was evidenced that overall antimicrobial potency of ligand was enhanced upon coordination, concerning both resistant planktonic and biofilm embedded pathogenic strains. The Pt(II) and Pd(II) complexes were the most active species.

PA3. ANTIOXIDANT ACTIVITY EVALUATION OF SOME NOVEL SALICYLAMIDE DERIVATIVES

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A series of new salicylamide derivatives, esters, hydrazides and hydrazones were synthesized in order to evaluate their biological activity. Antioxidant activities of the synthesized compounds were studied by *in vitro* DPPH scavenging method, ABTS radical scavenging capacity assay and ferric reducing antioxidant potential (FRAP) assay. In all cases, the antioxidant reference compound was Trolox, and the antioxidant activity values were expressed as mmoli/L equivalents Trolox. The DPPH method seemed to be not very suitable for this kind of compounds, or for the concentration we used, because of the too slow reaction kinetics between DPPH and the tested compounds. This could explain the much lower values obtained for the antioxidant activity determined by this method. In case of ABTS and FRAP assay, the results are comparable, higher antioxidant capacity was obtained for hydrazides derivatives (between 10.2-12.6 mmoli/L Eq. Trolox), followed by those obtained for hydrazones. The scavenging activity of the compounds which showed antioxidant effect is possible due to the presence of an N-H group in the hydrazino moiety, which can donate a hydrogen atom and became a radical.

PA4. ELECTROCHEMICAL BEHAVIOR OF SOME NEW 2-HYDROXY-BENZAMIDE DERIVATIVES

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A series of novel 2-hydroxy-benzamide derivatives, esters, hydrazides and hydrazones were synthesized and their electrochemical behavior was investigated via cyclic voltammetry using a glassy carbon working electrode (GCE) and $NaClO_4$ 0.1M in methanol as supporting electrolyte, which is the most versatile electro analytical technique for the study of electroactive species. The cyclic voltammograms were recorded at different scan rates (100-500 mV/s), in the range 0-1300 mV. Three parameters, the oxidation potentials ($E_{1/2}$), the anodic peak current (I_a) and the area under the anodic wave (S_a) were studied, in order to evaluate the reducing capacity of the tested compounds. To achieve a proper correlation between electrochemical results and antioxidant activities determined by chemical methods (DPPH, ABTS and FRAP), the area under the anodic curves (S_a) was converted to Trolox equivalents based on the calibration curve. The hydrazides derivatives proved higher antioxidant capacity, followed by those obtained for hydrazones. Cyclic voltammetry proved to be a simple and fast technique for the antioxidant properties evaluation of the organic compounds.

PA5. *Agrimonia eupatoria* L. – GOOD SOURCE OF ANTIOXIDANTS

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Agrimonia eupatoria L. (agrimony, *Rosaceae*) was used in traditional medicine to treat especially gall bladder, gastrointestinal tract, diseases of the liver and was less investigated concerning the chemical composition and antioxidant capacity.

Alcoholic extracts from *herba* agrimony tea from four different Romanian producers were obtained by reflux, ultrasounds and maceration methods. By LC/MS/MS analysis gallic acid, ferulic acid, caffeic acid, chlorogenic acid, apigenin, quercetin, rutin, and catechin were quantified in analyzed vegetable extracts. Total antioxidant capacity (TAC) was assayed by a chemiluminescence method, based on luminol-Co(II)/EDTA-H_2O_2 system.

Results of the LC/MS/MS analyses (reported as mg standard/100 g dw) showed that catechin (0.543 ± 0.048 and 3.91 ± 0.018), chlorogenic acid (0.848 ± 0.054 and 3.01 ± 0.085) and gallic acid (0.152 ± 0.0051 and 0.417 ± 0.00204) are found in higher amounts than the other standards determined in the ethanolic extracts.

Values for TAC (reported as mg standard equivalents/100 g dw) varied between 385.4 ± 40.9 and 2115 ± 72.4 gallic acid equivalents and between 40.18 ± 2.64 and 304.5 ± 12.5 when expressed as quercetin equivalents.

The experimental results have shown that agrimony *herba* is an important source of polyphenolic antioxidant compounds.

PA6. EVOLUTION OF THE ANTIOXIDANT ACTIVITY OF SOME TYPES OF RED AND WHITE WINES

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Samples of commercially available Romanian wines were analyzed in order to determine total phenol content and the antioxidant activity. The content of total phenolics in the extracts was determined according to the gFolin-Ciocalteu method and calculated as gallic acid equivalents (mg GAE/100g). Antiradical activities of the extracts were evaluated by a micro assay using 1, 1¢-diphenyl-2-picrylhydrazyl spectrophotometric method.

Wine characteristics measurements were examined by multivariate data analysis, using principal component analysis (PCA). Total polyphenol content was correlated to the antioxidant activity of the studied wine samples. The values of the inhibition power of free radical, PI%, range between 1.68 for white wine and 0.95 for red wine ("Sânge de taur" bottled by SC Domeniile Viticole Tohani, Prahova, Romania).

PA7. STUDY OF PHENOLIC COMPOUNDS IN RED GRAPES AND OBTAINED WINES FROM MURFATLAR WINE CENTER

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The latest research revealed that phenolic compounds play an important role in the quality of red wine, particularly colour and astringency and also are responsible for the sanogenous effect on human health after a moderate consumption of wine.

This paper presents the ripening evolution of routine quality control parameters (sugars, acids, weight of 100 berries) and phenolic compounds (anthocyanins and polyphenols index) during 2013 year for the most representative red grape varieties (Cabernet Sauvignon, Merlot, Feteasca Neagra, Pinot Noir si Mamaia) authorized to obtain wines with denomination of origin controlled in Murfatlar wine center.

The findings reported here were useful to develop the optimum moment for harvest ensuring or enhancing the final quality of the wine. Also, the phenolic profile of obtained red wines was evaluated by reversed-phase high performance liquid chromatography.

PA8. NUTRITIONAL SUPPLEMENTS TYPE SYRUPS BASED ON MIXED EXTRACTS OF SOME INDIGENOUS FRUITS SPECIES WITH ANTIOXIDANT ACTIVITY

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With content rich in vitamins, minerals, polyphenols, carotenoids and many other compounds, extracts from *Rosa canina* L., *Morus nigra* L., *Cerasus avium* L. Moench. may be useful as an adjunct in the treatment and especially in preventing many diseases which arise from action of oxidative stress. The aim of this paper is to obtain selected syrups with increased antioxidant activity based on a mixture of fluid extracts from *Rosa canina* L., *Morus nigra* L., *Cerasus avium* L. Moench. *fruits.* Fluid extracts were obtained using different extraction methods (maceration, reflux) and solvents (alcoholum 40% and 70%). The obtained fluid extracts were mixed in different ratio and analysed for their physico-chemical properties, polyphenols assay (Folin–Ciocalteu, HPLC assay), vitamin C assay and antioxidative capacity by photochemiluminescence method (ACL, Analytik Jena AG procedure). The selected mixed fluid extracts with greatest content of polyphenols and antioxidant activity were used for syrups obtaining. The new syrups were analyzed for the physical-chemical properties (appearance, *p*H, relative density), polyphenols and vitamin C content and total antioxidative capacity. Preliminary results emphasize that syrups with highest antioxidant activity correlated with the polyphenols and vitamin C content would represent a possible new nutritional supplements used in associated oxidative stress dysfunctions.

PA9. CO-PROCESSED EXCIPIENTS USED IN NSAIDs ORALLY DISINTEGRATING TABLETS DEVELOPMENT

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Orally disintegrating tablets (ODTs) are dosage form which disintegrate in mouth within seconds without need of water. This type of quality in dosage form can be attained by addition of different varieties of excipients.

Pharmaburst™500 is a co-processed excipient system which allows rapid disintegration and low adhesion to punches. The aim of the present study was to develop and evaluate 25 mg sodium diclofenac ODT batches by direct compression method at different compression forces 10 and 20 kN (F1 –F2) and directly compressible excipients used in different ratio (Avicel PH 102, magnesium stearate and co-processed excipient Pharmaburst ™500 70 and 80% w/w).

The obtained batches were analysed for appearance, tablet thickness, uniformity of weight, hardness, friability, disintegration time, and non compendial methods (wetting time).

Co-processed Pharmaburst ™500 excipient 70% is used for sodium diclofenac ODT obtaining determined good results for quality control tests evaluation.

PA10. PHARMACEUTICAL FORMS TYPE CREAMS AND GELS BASED ON SOME VEGETAL FLUID EXTRACTS WITH ANTIOXIDANT ACTIVITY

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Particularly interest on herbs and plant extracts is due to their content of active principles with remarkable pharmacological properties. Different vegetal species contain natural antioxidants (polyphenols) used for their dermatological anti-inflammatory and healing activity, justified by their action on free radicals. The aim of this paper is to obtain selected gels and creams with increased antioxidant activity based on a mixture of fluid extracts from *Calendula officinalis* L., *Taraxacum officinale* L. and *Urtica dioica* L. Fluid extracts were obtained using different extraction methods (maceration, reflux), solvents (alcoholum 40% and 70%), parts of the vegetal product (radix, herba, leaves, whole plant). The obtained fluid extracts were mixed in different ratio and analysed for physico-chemical properties, polyphenols assay (Folin–Ciocalteu, HPLC assay) and antioxidative capacity by photochemiluminescence method (ACL, Analytik Jena AG procedure). The selected mixed fluid extracts with greatest content of polyphenols and antioxidant activity were used for gels and creams obtaining. The gels and creams were analyzed for the physical-chemical properties appearance, *p*H, penetration, spredability and total antioxidative capacity. Preliminary results emphasize that pharmaceutical forms type gels had highest antioxidant activity correlated with a good stability and increased polyphenols content and would represent a possible new dermatological anti-inflammatory and healing preparation.

PA11. INFLUENCE OF GEOGRAPHIC REGION ON NATURAL OCCURRING METABOLITES AS REVEALED BY NMR SPECTROSCOPY

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The metabolic profile of urine from a control group of voluntaries has been obtained by ^{1}H-NMR spectroscopy at 400 MHz. Data have been processed both as absolute (mmol/L) and relative (mmol/mol of creatinine) concentrations. The normal values have been compared with data from a group of type II diabetes mellitus (DM II) patients. Both groups belong to a population located in Romania (Eastern Europe). The average concentrations of various metabolites in urine for normal and DM II subjects are presented.

Our data are in good agreement with some previously reported data but they are not identical. Explanations for the variations are discussed in terms of lifestyle differences leading to nutrition and metabolism particularities. Thus, in clinical chemistry, a geographical origin discrimination of human population may be possible based on NMR spectroscopy in a similar (but not identical) way as the same NMR technique is used in food chemistry for authentication purposes.

PA12. FAST NMR DETECTION OF URINARY 2-OXOGLUTARIC ACID

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The paper describes the detection of 2-oxoglutaric acid by NMR spectroscopy in urine belonging to children with a specific inborn error of metabolism. The children's age is ranging from the day of birth up to 8 years old.

In all patients high urinary levels of 2-oxoglutaric acid (in the range 321-2090 mmol oxoglutaric acid /mol Creatinine) and lactate (in the range 311-3352 mmol lactate / mol Creatinine) were found.

Based on NMR spectra of body fluids reported here, and on the correlation with the medical diagnosis of the patients we conclude that the 2-oxoglutaric acid may be considered as an early marker for inborn errors of metabolism involving the citric acid cycle (Krebs cycle).

The experiments have been performed using a 400 MHz Bruker Avance III NMR spectrometer in 5 mm tubes using solutions made up of 90% sample and 10% deuterated water.

PA13. THE INFLUENCE OF SOME ENZYMATIC MIXTURES ON DOUGH RHEOLOGY AND BREAD QUALITY

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The enzymatic mixtures treatment of wheat flours is the most known alternative method for the improving of their functional properties and technological characteristics. The present paper shows the alveograph parameters of some dough samples obtained from a poor quality wheat flour (type 650), ameliorate with different enzymes (xylanase, lipase, amylase and hemicellulases), combinations of them and wet gluten 26% (15 mg/g flour) in order to increase the quality of the bread (the volume and the crumb structure). The rheological experiments have been carried out through baking samples. The effect of enzymatic mixtures and the gluten addition on the wheat flours are reflected in the alveograph characteristics: the increase of dough elasticity or tenacity (P; 65-100 mm) and a decrease dough extensibility (L; 90-130 mm); a decrease of extensibility index (swelling index, G; under 30 cm), an increase of the energy absorbed (deformation energy, W; 230-250x10-4 J) and the decrease of ratio P/L (0.5-0.8), respectively. The baking tests have shown an increase of the bread volume by 8% than the control samples, by 0.0525% adding of fungal amylase, bacterial amylase and xylanase mixture in wheat flours samples. The best results, especially concerning the increasing of bread volume, were obtained for the mixture with optimum level of xylanases and amylases content, but with well-balanced xylanase-hemicellulase content, which play a significant role in increasing shelf life of bread and reduce bread staling.

PA14. EVOLUTION OF TOTAL PHENOLIC CONTENT DURING STORAGE OF SOME ALCOHOLIC PLANTS EXTRACTS

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Considering the beneficial role which antioxidants plays for our bodies by increasing the immunity against infection, studies for identifying new sources of antioxidants are particularly an interest research area.

Based on literature data, we propose to determine the evolution of the total content of polyphenols during time for alcoholic extracts of some herbs (basil, coriander, mint, rosemary, sage, tarragon and thyme) in order to establish the variation of antioxidant capacity during storage.

Total antioxidant capacity was determined by Folin-Ciocalteau spectrophotometric method.

The evolution of total phenolic content for the studied extracts in five-month period indicated that the most stable extract is for rosemary plant, and the most sensitive to degradation is basil alcoholic extract

PA15. COMPARATIVE STUDIES OF ANTIOXIDANT ACTIVITY OF SOME AROMATIC PLANTS EXTRACTS

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Nowadays there is a growing concern to increase immunity and resistance to infection by means diet containing antioxidants.
Taking into account the human diet habit of using the traditional spices for food's flavor, we proposed to realize a comparative study of the antioxidant capacity of seven herbs extracts (basil, coriander, mint, rosemary, sage, tarragon and thyme).

The investigations included the measurement of two parameters: the total polyphenol content (TPC) through Folin-Ciocalteau method and antioxidant capacity of lipid soluble substances (ACL) using photochemiluminiscence method.

The obtained results indicated that the extracts of rosemary, followed by sage have the higher concentrations of polyphenols, respectively the best antioxidant capacity, while the tarragon extract has low content of polyphenols.

Section B: Analytical and Environmental Chemistry

OB1. EVALUATION OF TOXIC METAL LEVELS IN EDIBLE TISSUES OF THREE WILD CAPTURED FRESHWATER FISHES

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River ecosystems are vulnerable to heavy metal pollution. Fish samples are considered as one of the most indicative factors, in fresh water systems, for the estimation of trace metals pollution potential since they are the final chain of aquatic web.

The objective of the present study is to evaluate the concentration of some toxic elements (As, Hg, Pb, Cd and Ni) in edible part of three wild fresh water fish species (zander (*Sander lucioperca*), wels catfish (*Silurus glanis*) and European carp (*Cyprinus Carpio*)) caught from Bulgarian part of Danube river collected during 2010. The Danube River is the European Union's longest and the continent's second longest river that passes through or touches the borders of ten countries. It has a great importance in regard to biodiversity, economics and transportation.

The elements (As, Pb, Cd and Ni) were assayed using Perkin Elmer Zeeman 3030 electrothermal atomic absorption spectrophotometer with an HGA-600 atomizer. Determination of Hg was performed using Milestone Direct Mercury Analyzer DMA-80. The results were expressed as μg/g dry weight. The order of heavy metal accumulation in the edible part of zander is As>Hg>Pb> Ni> Cd while the other two fish species show a different metal accumulation Hg > As >Pb> Ni > Cd. In all heavy metals, the accumulation of mercuric and arsenic proportion was significantly high in all three fish types.

OB2. SENSORS BASED ON CARBONACEOUS MATERIALS FOR DETECTION OF BIOGENIC AMINES

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The present work describes the sensing properties of screen-printed electrodes (SPEs) modified with three different types of carbonaceous materials: graphite, graphene and carbon nanotubes. The electrochemical responses towards biogenic amines including tyramine, dopamine, histamine, and putrescine have been analyzed and compared. The electrochemical signals towards biogenic amines show redox processes related to the electrochemical activity of the amine under study.

It has been demonstrated that the electrodes based on graphene show the best performances in terms of kinetics and detection limit, whereas graphite-SPEs presented the smallest detection limit for all the biogenic amines under study. The detection limits have been in the range of 2.45–7.34 μM. The kinetic studies demonstrate diffusion-controlled processes at the electrode surface.

A sensors array has been constructed using the three types of electrodes. The multisensor system is able to discriminate among biogenic amines as a function of their chemical structure and reactivity as achieved by means of Principal Component Analysis and PLS-Discriminant Analysis. Biological, pharmaceutical and food samples have analyzed with sensors to evaluate its real feasibility in analysis and freshness monitoring.

Acknowledgments
This work was supported by a grant of the Romanian National Authority for Scientific Research, CNCS-UEFISCDI, project number PN-II-ID-PCE-2011-3-0255.

OB3. HEAVY METALS IN FISH FROM ROMANIAN MARKET

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The goal of this study was to analyze the content of heavy metals in fish, shellfish, molluscs cephalopods on the Romanian market. We have analyzed heavy metals traces in sixteen fish species. Analysys of heavy metal traces were conducted with mass spectrometer with inductively coupled plasma-ICP-MS, Agilent Technologies 7500 Series. Among the elements identified it was analyzed the content of Cd, Hg, Pb, metals with high toxicity to the human body, and the values obtained were interpreted in accordance with Commission Regulation (EC) No 1881/2006 concerning the maximum allowable quantity per kg wet product and Tolerated Weekly Intake Provisional (PTWI) established by the Joint Committee experts WHO / FAO.

OB4. STOCHASTIC MICROSENSORS AS SCREENING TOOLS FOR NEURON SPECIFIC ENOLASE

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Stochastic microsensors based on nanostructured materials from the classes of porphyrins and cyclodextrins, and carbon onions were used for new screening tools of whole blood samples for neuron specific enolase, a lung cancer biomarker. The neuron specific enolase was identified in whole blood sample based on its signature (t_{off} value). The best response was given by the microsensor based on the complex of Mn(III) with 5,10,15,20-tetraphenyl-21H,23H-porphyrin, that exibit a linear range between 476.75pg/mL and 7.628ng/ml, with the lowest determination limit of 51.74pg/mL. The proposed stochastic microsensors provides a fast, sensitive, reliable and lower cost assay for screening of neuron specific enolase from whole blood samples, without any pretreatement of whole blood samples.

OB5. MULTIMODE SENSORS FOR BPA ASSAY IN CHILDRENS' SALIVA

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Bisphenol A (BPA) chemically known as 2,2-bis(4-hydroxyphenyl)propane is a component of polycarbonate plastics, widely used in commercial products such as food cans, water bottles and pipes, printer ink or as dental binding material. BPA is an endocrine disrupting compound (EDC) which has brought concerns for doctors and researchers in the public health department. Its determination in samples like childrens' saliva cannot be performed with existing standard methods (e.g., ELISA) due to its very low concentration in this biological fluid.

Multimode sensors based on modified carbon matrices such as dopamine, fullerenes, graphene, and graphite were designed for the assay of bisphenol A in childrens' saliva. The proposed sensors are highly reliable, and are able to determine very small concentration of BPA directly from childrens' saliva.

OB6. PATTERN RECOGNITION OF HER-1 IN BIOLOGICAL FLUIDS USING STOCHASTIC SENSING

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Stochastic sensing was employed for pattern recognition of HER-1 in biological fluids. Nanostructured materials such as 5,10,15,20-tetraphenyl-21H,23H-porphyrin, maltodextrin and α-cyclodextrin were used to modify diamond paste for stochastic sensing of HER-1. Pattern recognition of HER-1 in biological fluids was performed in a linear concentration range between $5.60x10^{-11}$ and $9.72x10^{-7}$ mg mL^{-1}.

The lower limits of determination (10^{-12} mg mL^{-1} magnitude order) were recorded when maltodextrin and α-cyclodextrin were used for stochastic sensing. The pattern recognition test of HER-1 in biological fluids samples shown high reliability for both qualitative and quantitative assay.

OB7. PRELIMINARY APPLICATION OF NOVEL SYNTHESIZED CHIRAL HYDROXY AMIDES AS CATALYST IN ASYMMETRIC REDUCTION OF ACETOPHENONE

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In this study, different novel two chiral hydroxy amides and two chiral hydroxy diamides were synthesized from reaction of L-amino alcohols and L- amino acids with esters. They were then reacted with $NaBH_4$ in different ratios to form intermediate chiral complex structures used for reduction of acetophenone in 2- propanol. Enantiomeric excess (e.e %) and reduction yield values for each of them were determined. The best enantiomeric excess (76 % e.e) obtained from chiral hydroxy diamide (CHDA-1) / $NaBH_4$ in 1:3 mole ratio among four chiral hydroxy amides. Synthesized all chiral ligands were characterized with IR, ^{1}H NMR, ^{13}C NMR spectroscopic results and specific rotations.

PB1. FAT SOLUBLE VITAMINS AND FATTY ACID COMPOSITION OF WILD BLACK MUSSEL, RAPANA AND SHRIMP

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Many studies suggest that marine molluscs are one of the most important dietary sources of fat soluble vitamins (E, D3 and A) and essential fatty acids (FA). The most commercially important species from the Bulgarian Black Sea are the Black mussel, rapana and shrimp. There is scarce information in the scientific literature about fat soluble vitamins and FA composition of these Black Sea molluscs.

The aims of the present study are to determine and compare the fat soluble vitamins content as well as relative daily intake, FA composition and atherogenic index (IA) and thrombogenicity index (IT) in wild Black Sea mussel (*Mytilus galloprovincialis*), rapana (*Rapana venosa*) and shrimp (*Crangon crangon*). Fat soluble vitamins were analysed simultaneously using RP-HPLC system. The FA profile was analysed by GC-MS.

All of the analysed samples presented significant amounts of vitamin E, followed by vitamin A and D3. Black Sea molluscs are excellent sources of fat soluble vitamins, especially for vitamin D3 - one survey provides more than 100% of the RDI established in Bulgaria.

The FA composition of total lipids of molluscs species showed significant differences and the present study revealed that SFA content was significantly higher than MUFA ($p<0.001$) and PUFA ($p<0.001$) (SFA>PUFA>MUFA) in shrimp and mussel whereas rapana showed opposite trends (PUFA>SFA>MUFA). The omega6/omega3 and PUFA/SFA ratios of the analysed species were greater than the FAO/WHO recommendations.

PB2. EXAMINING THE IMPACT OF MEAT ON LIPID STATUS IN DIFFERENT AGES OF PEOPLE

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Meat intake has physiological significance in terms of fat content and the emphasis is on the use of meat with less fat and saturated fatty acids (SFA), a relatively high content of unsaturated (MUFA) and polyunsaturated fatty acids (PUFA). Research has been carried on lipid status in blood serum of 271 randomly selected people, 156 women and 115 men aged 25-75 years, with enzymatic spectrophotometric method ALCON- 300 ABBOT.

Total cholesterol in the control group of 55-65 years has the highest value of 5.65 mmol/L for men and 5.63 mmol/L for women, LDL cholesterol has max. value of 3.65 mmol/L, while in the age group of 65-75 years (men and women) have shown decreased levels of total cholesterol and LDL compared with other groups. HDL cholesterol has a higher concentration among women in the age group of 35-55 years and ranges from 1.55 -1.57 mmol/L. The determination of TG shows high variability and shows that no significant change and dependent on the described parameters.

Total cholesterol in subjects often use meat in the diet, the highest concentrations are in the age group of 55-65 years with a value of 5.61 mmol/L in men and 5.4 mmol/L for women, LDL is the maximum age group of 65-75, in men 3.48 mmol/L and for women is 3.35 mmol/L. HDL has the highest value among the young people of 20-35 years of 1.91 mmol/L, while TG calculated by coefficient of variation changes regardless of age, gender and cholesterol concentrations.

Total and LDL cholesterol in subjects who used meat occasionally shows a maximum in the age group of 65-75, and that among women with a value of 5.65 mmol/L and 3.65 mmol/L. Among women HDL has the highest value of 1.77 mmol/L in the group of 20-35 years and TG show high variability in both pola. Serumskata concentration of HDL and TG showed no effect depending on how subjects use meat diet.

PB3. HPLC/DAD ANALYSIS OF VITAMIN C AND ANTIOXIDANT CAPACITY DETERMINATION OF *VITIS VINIFERA* L. GRAPES DURING RIPENING

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A simple, fast and sensitive High–Performance Liquid Chromatography/Diode Array Detection (HPLC-DAD) method was developed for the determination of vitamin C (AA – ascorbic acid) from grapes (*Vitis vinifera* L.) samples from Murfatlar vineyard.

The LOD was 0.40µg/mL for proposed method. The advantages of the method are use of small amounts of sample and reagents, short analysis time and minimum steps for sample preparation. Total antioxidant activity was determined through photochemiluminiscence method as ACL (Antioxidant capacity of lipid soluble substances). Antioxidant activity of alcoholic extract from *Vitis vinifera* L. grapes was between 0.02 and 7.42 mmols equivalent TROLOX/100g product.

PB4. EVALUATION OF THE POLYPENOL CONTENT AND ANTIOXIDANT ACTIVITY OF WINE MACERATES (MEDICINAL WINES) WITH SAGE (*SALVIA OFFICINALIS* L. *LAMIACEAE*) AND SEA RUSH (*JUNCUS MARTITIMUS* LAM. *JUNCACEAE*) OBTAINED THROUGH TRADITIONAL TECHNOLOGY

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In order to estimate the polyphenol contents and the antioxidant activities of the medicinal wines (herbal wines) used in the folk medicine and obtained according to the traditional methods, two macerates of sage (*Salvia officinalis* L. *Lamiaceae*) dried leafs and sea rush (*Juncus maritimus* Lam. *Juncaceae*) dried rhisoma were prepared using natural red wine (10% alchool) as extraction phase. The amount of dried plants added into wine was 0.1% w/w for each sage and sea rush in the first extract (wine macerate 1) and 0.25% w/w for each sage and sea rush in the second one (wine macerate 2). The extraction conditions (darkness, 20° C, occasionally stirring) were similar in both products. During the extraction process, the polyphenolic content has been measured daily in each product. After 21 days, according to the traditional method, the two macerates were filtered and submitted to chemical analysis (polyphenol contents, monomeric anthocyanin contents, polymerised compounds percentage, E-resveratrol, Z-resveratrol, gallic acid, caffeic acid, chlorogenic acid, p-coumaric acid, cinnamic acid, vanillin, gallic acid, ferulic acid, 3-methylgallic acid, ellagic acid by HPLC). In both obtained extracts, in the raw wine used as extraction phase and in the hydro alcooholic sea rush and sage extracts (50%), the antioxidant activities using chemoluminiscence method were measured. Given to the raw materials (wine and dried plants hydro alcoholic extracts) the two macerates contain a higher polymerised compounds percentage, but also a higher amount of polyphenols. The antioxidant activities were higher in wine macerates than in the raw wine. The basis of this study was to demonstrate that wine behaves as a good selective extraction phase for some polyphenolic compounds.

PB5. FRAGMENTATIONS IN MASS SPECTROMETER AS A TOOL FOR PESTICIDES ANALYSES

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Pesticides are organic molecules used for plant protection. But to new generation of pesticides appears a large structure variety due to specific design. So that, the first generations of pesticides were generally thermal stable with a great half-time life in environment.

This kind of pesticides are very easy amenable to analyse by gas chromatography coupled with mass spectrometry.

During time the stringent needs of environment fate of pesticides led to another type of pesticides with a quick action and with a rapid degradation.

But these pesticides are not easy amenable to analyze by gas chromatography mass spectrometry due to nonvolatile and thermal unstable character.Today liquid chromatography with electrospray ionization mass spectrometry is one of the most used techniques for pesticides residues analyses. One of the greatest advantage of atmospheric pressure ionization interfaces is the possibility to use both positive and negativ ionization.

I used liquid chromatograph mass spectrometer for the analysis of pesticides. Main purpose is to obtain fragmentation of pesticides to elucidate the structures

Conclusions. By different way of ionizations we could obtain supplementary informations but
in ESI-MS only charge-induce mechanism of fragmentation we can observe due to low collision energies.

PB6. DYNAMICS OF WATER QUALITY SPECIFIC PARAMETERS IN LOWER DANUBE SECTOR IN 2011 AND 2012

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The analysis aims to determine the ecological status of the aquatic ecosystem in a sector of the Lower Danube in conditions of navigation improvement works. Specific parameters and water quality assessment results in 2011 and 2012 are presented: hydro morphological, chemical and physical parameters, as well the pollutants influencing biological indicators.

The ecological status was assessed by comparing the recorded values compared to the limits settled by the Ministry of Environment, order 161/2006. Field measurements, sampling of water and sediments and their analysis were performed. By performing correlations between physico chemical indicators and the status of abiotic factors, an integrated analysis matrix of the monitoring results and of ecological status evaluation was established.

Specific water quality parameters which were analyzed are in accordance with Water Framework Directive requirements, as suggested ICPDR for the entire Danube River Basin: organic pollution, nutrient and dangerous substances. The ecological status of aquatic ecosystem of the studied Danube sector is considered moderate.

PB7. APPLICATION OF NEW RELATIONSHIP TEMPERATURE DEPENDENCE OF DYNAMIC VISCOSITY IN THE STUDY OF THE RHEOLOGICAL OF SUNFLOWER OIL

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Sunflower oil is a non-volatile oil compressed from sunflower (Helianthus annuus) seeds. Sunflower oil contains predominantly trialkylesters (48–7%), oleic (14–40%), palmitic (4–9%) and stearitic (1–acids%). Depending on the fatty acid profiles, sunflower oil is classified as high linoleic (>=69% linoleic acid), high oleic (>=82% oleic acid) and mid oleic respectively.

The variation in the unsaturated fatty acids profile is strongly influenced by both genetics and climate. Sunflower oil also contains small quantities of lecithin, tocopherols, carotenoids and waxes. This vegetable oil is light in taste and appearance and has high vitamin E content. The refined oil is clear and slightly amber-coloured with a slightly fatty odour. Sunflower oil is liquid at room temperature and has the following characteristics: smoke point (refined): 232 °C, smoke point (unrefined): 227 °C, density (25 °C): 917 kg/m3, refractive index (25 °C): 1.473.

This study proposes two new correlations of logarithmic nature between sunflower oil viscosity and temperature. The dynamic viscosity was determined at two temperatures 40 oC and 100 oC, and for shear rates ranging from 3.3 to 120s-1.

The purpose of this study was to find a linear or polynomial dependence between temperature and natural logarithm of dynamic viscosity of sunflower oil using Andrade equation changes. Based on experimental data, equation constants were determined using regression method.

PB8. ANALYTICAL CHARACTERIZATION OF SOME APPLE JUICES

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Fruits and their preserves are rich sources of vitamins and phenolics and are negatively associated with lung cancer and coronary heart disease. Total antioxidant activity, levels of bio-active compound groups and the viscosity of some apple juices were measured.

The method applied for the determination of ascorbic acid concentration was with 2, 6-diclorophenolindophenol. Total phenols (TP) in apple juices were determined using the Folin-Ciocalteau method and antioxidant activity by the use of DPPH free radical method.

The viscosity of apple juices was investigated by a rotational viscometer, Brookfield viscometer (Brookfield Engineering Inc., Model RV-DV I Prime) with RV spindles.

Pasteurized apple juices obtained from different varieties of apples were characterized by varying content of the polyphenolic content. The differences in antioxidant activities between apple juices could be attributed to their different contents of polyphenols.

PB9. EVALUATION OF AMPEROMETRIC DOT MICROSENSORS FOR THE ANALYSIS OF FOLIC ACID IN URINE SAMPLE, PHARMACEUTICAL TABLETS AND FRUITS JUICE

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Folic acid is an essential water soluble vitamin which belongs to the B-vitamin group (B9). Sufficient dietary intake of FA during pregnancy prevents neural tube defects of the fetus (e.g. anencephaly or spina bifida). The protective effect of FA was also observed in the treatment of some diseases such as stroke, ischaemic heart disease or colorectal cancer. Deficiency of folic acid causes some types of anemia and increases the risk of cardiovascular diseases. The recommended daily intake of FA is 0.2 mg for adults and 0.4 mg for pregnant women (The European Food International Council). Foods rich in FA are especially yeast, green vegetables, oranges, nuts, liver and kidney.

In this study, nineteen amperometric dot microsensors based on graphite (G) modified with Fe^{III}porphyrin ($Fe^{III}P$), tetraphenyl-porphine (TPP), tetraphenyl-porphine cobalt (II) ($Co^{II}TPP$), Fe^{II}phthalocyanine ($Fe^{II}Pc$), Fe^{III}phthalocyanine ($Fe^{III}Pc$), tetraamino cobalt (II) phthalocyanine (CoTAPc), tetraamino zinc phthalocyanine (ZnTAPc), tetramino nickel phthalocyanine (NiTAPc), tetraamino manganese phthalocyanine (MnTAPc), tetranitro cobalt (II) phthalocyanine (CoTNPc), tetranitro zinc phthalocyanine (ZnTNPc), tetranitro nickel phthalocyanine (NiTNPc), tetranitro manganese phthalocyanine (MnTNPc) and graphene (GR) modified with $Fe^{III}P$, TPP, $Co^{II}TPP$, $Fe^{II}Pc$, $Fe^{III}Pc$, $Co^{III}Pc$ are evaluated and tested for the analysis of folic acid (FA) in urine sample, pharmaceutical tablets and fruits juice (e.g., orange, strawberry). Cyclic voltammetry (CV) was used to optimize the working conditions, e.g., pH, electrolyte for the proposed sensors. The optimum working pH was established to be 7.0 (phosphate buffer), in a 0.1 mol L^{-1} KCl supporting electrolyte. The linear concentration ranges for folic acid were between 10^{-6} and 10^{-3} mol L^{-1} for all dot microsensors except G-CoTAPc and G-MnTNPc wich had the linear concentration ranges between 10^{-6} and 10^{-4} mol L^{-1}.

Differential pulse voltammetry (DPV) was used for the reliable assay of folic acid in urine samples, pharmaceutical tablets and fruits juice.

PB10. PHYSICO CHEMICAL CHARACTERISATION OF SEABUCKTHORN EXTRACTS FOR COSMETIC USE

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Keeping a healthy skin and a good quality of life should remain the most important rule for an organic cosmetics manufacturer. After many years of study, making different combinations between plants, we managed to find some of the nature's mysteries that give and hold beauty, preventing oxidative stress that causes diseases and fastens organism ageing.
The purpose of the paper is to present original results of physico chemical analysis of different seabuckthorn (*Hippophae rhamnoides L.)* extracts and original cosmetic products containing these extracts.

Aqueous distilate from fruits and leafy branches, aqueous extract from seeds, fresh fruit juice and frozen fruit juice after 2 years of storage, ethanolic extracts of buds have been analysed using chemical (mineral and organic acidity, oxidability, calcium and magnezium) and physico chemical (pH, conductivity, oxidation-reduction potential- ORP) methods.

Interesant shapes of pH-ORP evolution have been observed, that could explain the confirmed benefit in the care and treatment of skin diseases.

Taking into account also the results of previous studies of other reserchers we consider that the ORP measurement of cosmetic mixtures could provide objective, cheap and reliable information about antioxidant activity of complex samples.

Section C: Physical Chemistry

OC1. ELECTROCHEMICAL STUDY OF SELENYL-AZULENES

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An electrochemical study of several selenyl-azulene compounds was performed by cyclic and differential pulse voltametry in order to establish the influence of donor and acceptor substituents on their electrochemical properties. The main characteristics of the oxidation and reduction processes for each compound as well as of the films that are polymerized on the electrode surface were established.

The oxidation potentials are quite similar in the disubstituted compounds having a substituent with –I effect, while an increase of the oxidation potentials occurs in those with –E effect. If the second substituent contains double bonds a decrease in the reduction potentials was observed. The reactivity of selenium azulene derivatives was compared with that of similar chalcogene compounds.

Acknowledgements
The authors are grateful to UEFISCDI - Exploratory Research Projects PN-II-ID-PCE-2011-3, project ID 15/2011.

PC1. THE INHIBITION EFFECTS OF METHIONINE ON MILD STEEL IN ACIDIC MEDIA

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The corrosion of metal surfaces causes huge financial damages to the industries annually, what has lead to an increase in the search for substances that can slow down or prevent corrosion rate. Green inhibitors which are biodegradable, without any heavy metals and other toxic compounds, are promoted. Amino acids are attractive as corrosion inhibitors because they are nontoxic. We have used methionine as corrosion inhibitor. Materials under investigation are two kind of low allow carbon steel marked as: Steel 39, Steel 44 usually applied to concrete as reinforcing bars, and manufacture in Elbasan. The inhibition effect of methionine on the corrosion behavior of low allow steel is investigated in sulfuric acid in presence of chloride ions, in form of NaCl (H_2SO_4 1M + Cl^- 10^{-3}M). Potentiodynamic polarization method is used for inhibitor efficiency testing. The pitting corrosion current shows that increasing concentration of the inhibitor causes a decrease in pitting current density, and inhibition efficiency increases with increasing concentration of the inhibitors.

PC2. STUDY OF PHYSICO-CHEMICAL PROPERTIES OF SUNFLOWER OIL

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Sunflower oil is a vegetable oil obtained from the seed of sunflower (HELIANTHUS ANNUUS L.). This vegetable oil represents an important source of fat in food when is used in frying, salad dressing, shortening of pasty, margerine and home cooking. In the literature, there are presented studies regarding physico-chemical properties of sunflower oil.

The major objective of this study was to determine the physico-chemical properties of samples of sunflower oil collected from different stages of the technological process for sunflower oil refining for food industry. The samples of oil were crude oil, washed oil, bleached oil and deodorized oil.

The estimation of the physico-chemical properties of sunflower oil is necessary for gasket plate heat exchangers design.

The density, viscosity, refractive index, saponification value, iodine value, acid value, peroxid value, ester value and free acidity for crude oil, washed oil, bleached oil and deodorized oil were experimentally determined.

Density, viscosity, refractive index were determined in the temperature range of 20 - 80 0C, with a 20 0C step increase. Density values varied between 0.9191 - 0.8782 g/cm3. Refractive index values ranged between 1.4732 - 1.4512. Dynamic viscosity varied between 66.1764 to 9.991 mPa·s. Kinematic viscosity values ranged between 71.9992 - 11.3790 mm2/s. Saponification, iodine and acid values were between 201.338 mg KOH/g to 209.776 mg KOH/g, 8.752 g I2/100 g to 85.916 g I2/100, and 0.366 mg KOH/g to 2.588 mg KOH/g, respectively.

Based on experimental data, density, viscosity and refractive index, were correlated with chemical properties of the vegetable oil like saponification value, iodine value and acid value. The accuracy of the proposed equations was compared with the accuracy of some models presented in the literature.

PC3. HYDROCOLLOIDS USED IN FOOD EMULSIONS

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A hydrocolloid is defined as a colloid system wherein the colloid particles are hydrophilic polymers dispersed in water. A hydrocolloid has colloid particles spread throughout water, and depending on the quantity of water available that can take place in different states, gel or sol (liquid). Hydrocolloids can be either irreversible (single-state) or reversible systems. Many hydrocolloids are derived from natural sources. For example, agar-agar and carrageenan are extracted from seaweed, gelatin is produced by hydrolysis of proteins of bovine and fish origins, and pectin is extracted from citrus peel and apple pomace. Other important hydrocolloids are xanthan gum, gum arabic, guar gum, locust bean gum, cellulose derivatives as carboxymethyl cellulose, alginate and starch. Starch has many uses as thickener, water binder, emulsion stabilizer and gelling agent.

The purpose of the present work was to compare the organoleptic (color, appearance, consistency, smell) and physico-chemical (type of emulsion, NaCl content, acidity index, total fat content, the saponification index, the control of pasteurization, water content, non-fat dry substance content) characteristics for market and homemade butters. The samples of homemade butters were prepared using different amounts of hydrocolloid (starch) and also were analyzed in terms of molecular dynamics and for the particle size the transmission electron microscopy (TEM) was used.

PC4. CORRELATIONS FOR REFRACTIVE INDEX OF VEGETABLE OILS

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Vegetable oils are raw materials of great interest for food, cosmetics and pharmaceutical industries, and also for biofuels production. Their characterization by the means of physical-chemical properties is of great importance.

The purpose of this study is to report experimental data on refractive index and density in the temperature range 298.15 - 378.15 K and acid value, iodine value and saponification value for four different vegetable oils: sunflower oil, corn oil, rapeseed oil and peanut oil. Sunflower oil was produced by Bunge Romania S.R.L. Company, Romania, corn oil by S.C. Man Ro S.R.L. Company, Romania, rapeseed oil by Group Auchan company, France, peanut oil by Group Auchan company, France. The refractive index was determined with an Attago 3T refractometer copled with a thermostatical bath. The density was measured with an Anton-Paar densitimeter, DMA 4500 type. The acid value, iodine value and saponification value were determined as presented elsewhere.

Empirical models between refractive index and physical and chemical properties of vegetable oils presented in the literature were tested:

Rudan-Tasic equations:

$$n_D = 1.4484 + 0.0002247 \cdot IV \quad (1)$$

$$n_D = 1.4446 + 0.000019 \cdot SV + 0.0042 \frac{AV}{SV} + 0.000226 \cdot IV \quad (2)$$

Wolff equation:

$$n_D = 1 + \rho(0.5557 - 0.00022AV + 0.000035IV) \quad (3)$$

where n_D represents the refractive index of the vegetable oil; IV – iodine value; SV – saponification value; AV – acid value; ρ – density.

An empirical equation was proposed to correlate the refractive index of the studied vegetable oils with other oil properties. The accuracy of the model evaluated by the means of absolute average deviation (AAD) was good, the model can be recommended for vegetable oils refractive index estimation.

PC5. STUDY OF THE INFLUENCE OF SOME FACTORS ON ALUMINUM ANODIZING PROCESS

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Anodizing is an electrochemical process that converts the metal surface into a decorative, durable, corrosion-resistant, anodic oxide finish. The anodic oxide structure originates from the aluminum substrate and is composed entirely of aluminum oxide. This aluminum oxide is not applied to the surface like a paint or a plating, it is fully integrated with the underlying aluminum substrate, so it cannot be chipped or peeled. It has a highly ordered, porous structure that allows for secondary processes such as coloring and sealing.

The purpose of this paper was to obtain a protective layer of Al_2O_3 by anodic oxidation of aluminum at different intervals of time and different voltages power. Using non destructive techniques, the thickness of the obtained plates, before and after anodizing, was measured. Penetrant testing increases the "seeability" of small surface discontinuities that the human eye might not be able to detect alone and was used to highlight the protective layer properties of the Al_2O_3 plates.

PC6. KINETIC STUDY FOR REMOVING Cr(VI) FROM WATER AND WASTEWATER USING METALLURGICAL COKE

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Hexavalent chromium is present in the effluents produced during the electroplating, leather tanning, cement, mining, dyeing and fertilizer and photography industries and causes severe environmental and public health problems. Cr(VI) is highly mobile and is considered acutely toxic and mutagenic for most organisms; in humans its main effects are on skin, liver, kidney and respiratory organs, resulting in a variety of diseases such as dermatitis, hepatic and renal tubular necrosis, bronchitis, perforation of the nasal septum and bronchogenic carcinoma.

The objectives of the present study were to characterize the adsorption behavior of metallurgical coke with respect to Cr (VI) and to explore the applicability of this material to purify actual chromium industrial wastewaters. The experiments showed that highest removal yield was 87.34% at solution pH 2.5, contact time 360 minutes, temperature 25^{o}C and initial chromium concentration of 31.2 mg/L.

Four simplified kinetic models including a pseudo-first-order equation, pseudo-second-order equation, Elovich and intraparticle diffusion equation were selected to follow the adsorption process. Kinetic parameters, rate constants, equilibrium sorption capacities and related correlation coefficients, for each kinetic model were calculated.

The pseudo-first order and pseudo-second order kinetic equations were used to model the adsorption kinetics, with the second order giving a better fit, as seen from the correlation coefficient (R^2) which ranged from 0.7654 to 0.9672 for pseudo first order and from 0.9950 to 1.000 for pseudo-second order model. It was shown that the adsorption of Cr (VI) ions could be better described by the pseudo-second order equation, suggesting that the adsorption process is presumable a chemisorption.

Section D: Chemical Engineering, Petroleum Technology and Management

PD1. COMSOL MULTIPHYSICS MODELLING AND ANALYSYS OF A HIGH TEMPERATURE PEM FUEL CELL

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Proton exchange membrane fuel cells (PEMFC) are highly efficient power generators, achieving up to 50-60% conversion efficiency and presenting high-energy density at low operating temperatures, quick start-up, zero emissions and system robustness.

In this study it was described a Comsol Multiphysics three dimensional simulation model for a high temperature PEMFC that can deal with both anode and cathode flow field for examining the micro flow channel with electrochemical reactions. The model was able to investigate the transport phenomena and electrical potential distribution for the various PEM fuel cell components including the gas channels, gas diffusion layers, catalyst layers and membrane.

PD2. ION-EXCHANGE KINETICS AND EQUILIBRIUM STUDIES OF WATER DEMINERALIZATION PROCESS USING MIXED BED RESIN PUROLITE MB400

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Demineralized water is completely or almost of dissolved minerals (between 1 – 10 mg/L of total dissolved salts) and it is quite important for the industrial processes (electro synthesis, steam, power, process, and cooling). Demineralization technology is the classical process for treatment of water using two basic types of resin – cation-exchange and anion-exchange resins. The mixed bed ion exchange resin can be used to remove virtually all the ionic impurities present in the feedwater.

Ion exchange processes are generally operated in fixed columns in practical applications. Knowledge of exchange dynamic phenomena at the solid - liquid interface is important for understanding the process. For a comprehensive representation it is necessary to account for ion exchange as well as chemical equilibria. The studies should investigate ion exchange kinetics and equilibrium in batch units.

The aim of this paper is to study and to model the removal of calcium chloride from water by Purolite MB400 ion exchange resin in batch mode and optimum operation conditions. This mixed bed resin is a high quality resin mixture for direct purification of water. The theoretical total combined capacity in the regenerated form is 0.55 eq/L. Batch kinetics and equilibrium experiments were conducted in a reactor immersed into a water bath continuously stirred and at constant temperature of 298 K. At fixed time intervals a sample of solution was withdrawn and analysed by conductometry and atomic adsorption spectroscopy methods.

The equilibrium distribution of calcium and chloride ions between resin and liquid phase was modelled using two-parameter adsorption isotherms models – the Langmuir and Freundlich. It was found that equilibrium data can be fitted by the both models. The uptake of calcium chloride by mixed bed Purolite MB400 resin follows first-order kinetics. The ion exchange process is controlled by chemical rate as the diffusion in the resin particles is not the limiting step for a temperature of 298 K.

PD3. MODELLING THE CHEMICAL AND PHYSICAL PROPERTIES OF OIL BLENDS

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Oil mixtures are used at present to increase the quality of finished petroleum products. They are considered to process both crude oils with very good features and less efficient crude oils together.

For transport, storage and processing it is needed to know the physical-chemical properties of the oil blends.

This article describes the evolution of additive properties (density, sulfur content) and non-additive properties (viscosity, pour point, distillation curve) of oil mixtures according to mixing ratio.

In this work, the author considers mixtures of two and then three crude oils.

Also it is presented here, a new learning algorithm for discrete-time neural network. The theoretical analysis of stability and convergence for the neural networks are given in this article. An application example is provided to illustrate the neuro- modeling approach. We believe that modelling of crude oil blending via neural networks is a very effective method.

PD4. HEAVY CRUDE OIL DEMULSIFYING THROUGH BLENDING WITH DILUENT

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In crude Roumanian Oil production fields, heavy oil is extracted by emulsioning (oil in water or water in oil).This emulsion is part of oil field depletion and its viscosity affect transporting and refinery processing costs. Failure to separate the oil and water mixture efficiently and effectively could result in problems such as overloading of surface separation equipment, increased cost of pumping wet crude, and corrosion problems.

Light hydrocarbon fraction is proposed as a diluent to be added in varied proportion to three emulsion samples collected from three different oil fields. The viscosity of three emulsions was considered to be reduced by adding 50, 25, and 15% vol light hydrocarbon fraction. The viscosity of mixtures and quantity of water separated were determined and it was deduced that the increase of diluent in emulsion blends leads to corresponding decrease in the value of viscosity.

The final basic sediment and water (BS&W) in the top dry oil was measured in all samples and the optimum value of diluent percentage was determined having in view the reduction of pumping cost.

PD5. RESEARCH ON THE ADDITION OF CELLULOSE DERIVATIVES IMPROVING THE OPERATION OF SPARK-IGNITION ENGINES

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As known, petroleum resurces are quantitatively limited and the price is increasing. It is therefore necessary to find new fuels for the operation of internal combustion as well as solutions for improving the properties of the existing ones.

To be competitive, a fuel must be renewable, possibly to be produced in sufficient quantities to reach a low price, to produce a sufficient quantity of energy by combustion for the required mechanical work in an internal combustion engine, the emissions resulting from combustion must be less polluting and its use in the operation of engines to include as few amendments as possible.

With a view to their combustion properties, alcohols are suitable for the operation of engines as a source of energy, with the understanding that they develop only 66 % of petrol power to concentrations of more than 90 % in blends with gasoline.

In this work the authors present the results obtained in the operation of spark-ignition engines by alcohols, as bioethanol and methanol in low concentrations, in the mixture with cellulose trinitrate.

PD6. TERNARY BLENDS WITH BIODIESEL

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Many studies on properties of binary biodiesel+diesel fuel blends presently sold as fuel for diesel engine, have been published in the literature. The study of ternary blends with biodiesel are of interest inorder to better understand biodiesel+diesel fuel blends behavior. A reduced number of works regarding properties of ternary blends with biodiesel were presented in the literature.

The purpose of this paper is to present experimental data on density of biodiesel+diesel fuel+benzene ternary systems. The density of the ternary systems with biodiesel was determined with an Anton-Paar densimeter DMA 4500 type.

Models used to estimate the density of binary biodiesel+diesel fuel mixtures were extended to ternary mixtures biodiesel+diesel fuel+benzene:

Kay's mixing rule:

$$\rho = v_1\rho_1 + v_2\rho_2 + v_3\rho_3 \quad (1)$$

density calculation as function of density and molar weight of pure components:

$$\rho = \frac{x_1M_1 + x_2M_2 + x_3M_3}{\frac{x_1M_1}{\rho_1} + \frac{x_2M_2}{\rho_2} + \frac{x_3M_3}{\rho_3}} \quad (2)$$

other density correlation with mixture composition:

$$\rho = av_1 + bv_2 + cv_3 + dv_1v_2 + ev_1v_3 + fv_2v_3 \quad (3)$$

density estimation at different temperatures:

$$\rho = aT + b \quad (4)$$

where ρ represents the density of the mixture; v_i and x_i – volume fraction and molar fraction of mixture components; M_i – molar weight of mixture

components; ρ_i – density of mixture components; T – temperature; a and b – correlation coefficients.

The accuracy of these models to predict the density of ternary mixtures with biodiesel, depending on mixture composition or temperature was evaluated by the means of absolute average deviation (AAD). The calculated absolute average deviations were low, demonstrating the suitability of these models to predict the density of ternary blends with biodiesel.

PD7. PROPERTY FEATURES BIOFUELS OBTAINED IN SPECIFIC ZONES

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The use of biofuls in transport, without excluding others possible alternative fuels for the car industry is one of means which could reduce dependency to energy import, it can influence the fuels market for transport and ensure the independence of the problem medium and long term energy. Biofuels replace the petroleum products (gasoline, diesel) and natural gas used in automotives.

Biodiesel is an environmentally friendly fuel that is produced from vegetable oils (soybean, canola, sunflower) by esterification reaction, which can be mixed with diesel fuel, resulting in a less polluting fuel. Biodiesel is a diesel equivalent, processed fuel from renewable biological sources, for all types of diesel engines.

Biodiesel is obtained from soybean seeds of colza, sunflower or palm tree.

Studies in Transylvania have shown it is possible to improve the production of biofuels based on rapeseed oil at both of agricultural production and commercial scale.

Biogas is the gaseous substance resulting from the anaerobic digestion process of different organic residues, without using oxygen in a container called "fermenter". The resulting gas consists of 45-70% methane proportion. Cogeneration plants using biogas for energy prevents the release of emissions into the atmosphere, which can not be achieved by burning fossil fuels.

Ethanol is an important renewable source.

Bioethanol derivatives is usually produced in the form of an aqueous solution containing between 8 and 12% weight of ethanol. It can be used as alternative fuel as a feedstock for the production of other chemicals (ethylene, acetaldehyde, acetone, etc.) or can be converted to hydrogen.

Carbon dioxide from the combustion of biofuels do not contribute to the "greenhouse effect". It comes from renewable vegetable oils and in the atmosphere is eliminated the same amount of carbon dioxide absorbed during the raw plant growes.

PD8. THE EFFECT OF SOME ADDITIVES ON THE ANTIKNOCK PROPERTIES OF GASOLINE

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The properties of the commercial gasoline are influenced by the origin of the crude oil, the refining processes and the presence of additives, which are added to improve the performance and to reduce the emissions. Methyl tert-butyl ether and ethanol are the oxygenates most commonly used. The MTBE market predominates in Europe; however, its use has become restricted due to its high solubility in water, as well as its toxic effect and the degradation products, which have become the object of environmental concern employed to increase the octane number of gasoline. The quality of gasoline is constantly based on its octane number, which indicates the antiknocking strength.

The goal of this research was to evaluate the effect produced by the addition of ethanol and MTBE on the octane number value for five types of gasoline with different chemical compositions. The addition of oxygenated additives has increased octane ratings, has improved combustion process and has reduced the carbon monoxide emissions and the levels of aromatic compounds.

PD9. PETROLEUM RECOVERY FROM SLIME BY SOLVENT EXTRACTION

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Large and increasing volumes of wastes proceed annually from extraction, transportation and processing of oil and this represents a hazard for the environment. The treatment of wastes has become one of the most important concerns of modern society to protect the environment. Slime is the most frequent petroleum wastes. This waste still contains a large proportion of valuable petroleum fractions that may be recovered to formulate new oil products if undesirable pollutants are separated by an appropriate recovery procedure.

Different waste management schemes result in various types of products or outputs i.e. recycled lubricating oil, energy in the form of fuel oil or oil to be reprocessed to the refinery. Solvent extraction technique is one of the cheapest and most efficient processes experienced in recycling of wastes.

Slime generated in the storage of crude petroleum, containing 20-30% petroleum product was treated with different solvent mixtures proportions (100% toluene; 80% toluene + 20% MEK; 60% toluene+40% MEK; 40% toluene + 60% MEK; 20% toluene + 80% MEK; 100% MEK), to feed ratios (from 1:1 to 6:1), at room temperature. The petroleum product was recovered from extracts by distillation at atmospheric pressure and vacuum distillation and the yield was determined in each case. The recovery yield varied between 70% -93%.

The results of the study have allowed to establish that the optimum mixture proportion (composition) is 20% toluene and 80% MEK for a solvent to slime mass ratio of 4:1, when the yield was 93%.

The petroleum recovered was characterised by standard methods for petroleum products. It resulted a heavy petroleum product with the properties of a vacuum distillation residue which can be used as a component in fuel for industrial burners.

Section E: Advanced Materials and Nanotechnologies

OE1. MESOSTRUCTURED SILICA-TYPE MATRIX FOR AMINOGLYCOSIDE DELIVERY SYSTEMS

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Drug-delivery systems (DDS) are hybrid materials consisting of a vehicle and an active pharmaceutical ingredient (API), designed to control the delivery profile of the biological active molecules and minimize their toxicity. Among inorganic carriers, mesostructured silica-type matrix exhibits high specific surface area and total pore volume, ordered pore array, tunable pore size, biocompatibility, and the possibility of surface properties modification by post-synthesis functionalization, features that recommend it for the design of DDS.

In this study, amikacin and kanamicin, which belong to aminoglycosides class of antibiotics, were used to prepare DDS. MCM-41, MCM-48 and SBA-15 silica and aluminosilicates were synthesized, characterized by various structural and morphological techniques and then employed as carriers. DDS were obtained by loading through adsorption from aqueous solutions of the drug into the carrier mesopores.

The prepared hybrid materials were investigated by small and wide angle X-ray diffraction, FTIR spectroscopy, differential scanning calorimetry and N_2 adsorption/desorption isotherms. The *in vitro* release profiles were carried out by immersing the hybrid sample in phosphate buffer solution (*p*H=7.4), at 37°C, under constant magnetic stirring and the delivery profile was determined by UV-Vis spectroscopy. We studied the influence of the textural features of the mesostructured support and its acidic nature determined by aluminium introduction in the silica matrix towards aminoglycoside adsorption and *in vitro* delivery.

OE2. MESOPOROUS BIOACTIVE $SrO\text{-}SiO_2$ GLASSES AS DRUG DELIVERY

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Mesoporous SiO_2 has a highly ordered structure, large surface area and pore volume – qualities that gives it an excellent drug release profile.

The aim of this study was to incorporate Sr^{2+} into mesoporous SiO_2 in order to develop a bioactive mesoporous material with an improved drug delivery profile.

A series of mesoporous $SrO\text{-}SiO_2$ species with different chemical compositions were prepared by a template-induced self-assembling method. As SiO_2 source, tetraethylortosilicate (TEOS) was used in the presence of Pluronic 123 template agent. The chemical and structural characterization of the obtained materials was realized by X-ray diffraction, scanning electron microscopy, transmission electron microscopy, thermal analysis, infra-red spectroscopy, specific surface measurements, pore size distribution and Raman and FTIR spectroscopy.

One described the effects of Sr cations on mesoporous structure and its suitable properties for drug delivery applications. The release profile of bioactive Sr^{2+} ions and a model drug – dexamethasone (DEX) can be controlled by altering the Sr content in mesoporous glass samples.

OE3. PREPARATION AND CHARACTERISATION OF MESOPOROUS NITROGEN-DOPED $SrTiO_3$

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Mesoporous-structured photocatalysts are highly desirable in photocatalysis since their large specific surface area and mesoporous channels greatly facilitate adsorption, diffusion and surface reaction of the reactants. The exceptional electro-optical properties and physicochemical stability of the perovskite $SrTiO_3$ (STO) give rise to its attractive performance in photocatalytic applications of solar power, including photocatalytic degradation of organic pollutants, water splitting and photoreduction of CO_2. Nonmetal-doping represents effective strategy to realize visible-light response, N-doped $SrTiO_3$ exhibing excellent photoreactivity and stability under visible-light irradiation.

Nitrogen (N)-doped $SrTiO_3$ ($SrTiO_{3-x}N_y$) photocatalysts were synthesized by a solvothermal method and also by a modified templete-induced and self-assembling method.

The microstructures and phase composition were characterised using X-ray diffraction (XRD), scanning electron microscopy (SEM), high resolution transmision electron microscopy (HRTEM) and UV-vis spectroscopy. The nitrogen adsorption–desorption isotherm was conducted on a surface area and pore size analyzer and the specific surface area was determined by BET method. The catalytic tests were conducted using a quartz immersion well photochemical reactor. The photochemical water splitting was carried out at 18^oC using CH_3OH as sacrificial hole scavengers. The compounds of interest (H_2 and O_2) were separated and measured quantitatively by using a GC packed with Haysept and molecular sieve 5A columns. The prepared SrTiO3-xNy photocatalyst showed also excellent photocatalytic activity for the decomposition of MO (methyl orange) under visible-light irradiation.

The results proved that the N doping amount had an important effect on the hotocatalytic activity of the catalysts.

OE4. PHOTOCATALYTIC BEHAVIOR OF DOPED $BiFeO_3$ NANOTUBES

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Most photocatalysts developed so far have wide band gaps, and therefore have low absorption of visible light, leading to their low photocatalytic activities. To use the solar energy more effectively, the development of efficient visible-light-active photocatalysts with a narrow, appropriate band gap (<3.0 eV) has been an urgent issue in photocatalysis research field. $BiFeO_3$ has been researched as a photocatalyst in visible light region because of its small band gap and good chemical stability during the photocatalytic process.

In this work $BiFeO_3$ 1D nanostructures were deposited on diffrent substrates (glass, silicon and ITO) by templates method and chemical solution deposition. The microstructures and phase composition were characterised using X-ray diffraction (XRD), scanning electron microscopy (SEM), high resolution transmision electron microscopy (HRTEM) , Raman and UV-vis spectroscopy. To demonstrated the photocatalytic activity of these structures as determined by degradation of methyl orange (MO), a typical azo dye, under UV and visible-light irradiation. The results show a greate effect on the degradation of the MO by means of the photocatalytic performances of BFO 1D nanostructures.

OE5. SYNTHESIS OF CeO_2- SiO_2 MESOPOROUS MATERIALS AND THEIR PROPERTIES

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The development of efficient methods to synthesize nanostructures with well-defined size and shape is one of the key trends in material chemistry because of their size/shape-dependent properties and potential applications.

Ceria plays multiple roles in various catalyst systems. A series of mesoporous CeO_2 - SiO_2 species with different chemical compositions were prepared by a template-induced self-assembling method. As SiO_2 source, tetraethylortosilicate (TEOS) was used in the presence of Pluronic 123 template agent. The chemical and structural characterization of the obtained materials was realized by X-ray diffraction, scanning electron microscopy, transmission electron microscopy, thermal analysis, specific surface measurements, pore size distribution and FTIR spectroscopy. There was obtained mesoporous structures with pore size about 3nm and the specific surface areas obtained were in range of 610 - 670m^2/g.

OE6. REDUCED ENTHALPY OF FORMATION FOR Mg/TiHx NANOCOMPOSITES PRODUCED BY SPARK DISCHARGE GENERATION

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Spark discharge generation was used to synthesize Mg-Ti nanocomposites with a much less negative enthalpy of formation of the hydride of -45±3 kJ/molH_2 compared to -75 kJ/molH_2 for bulk MgH_2. The entropy of the reaction is simultaneously reduced to 84±5 J/K molH_2. Interestingly, a linear relationship between enthalpy and entropy is found.

The hydrogenation leads to the formation of the intriguing cubic fluorite Mg-Ti-H "alloy" phase previously seen in thin films, which is less stable than the conventional rutile MgH_2 phase. However, this can only account for about 15% of the drastic change in enthalpy. Plausible mechanisms for the modified thermodynamics based on recent experimental and ab-initio results are discussed, including the effects of lattice strains, the presence of TiH_2/Mg interfaces and hydrogen vacancies.

PE1. SYNTHESIS AND ELECTRON TRANSPORT PROPERTIES OF SOME NEW 4,7-PHENANTHROLINE DERIVATIVES IN THIN FILMS

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Thanks to their remarkable features (energy band gap in the IR-Vis region, high mobilities of charge carriers, significant electroluminescence, photophysical characteristics, high processability and versatility), organic semiconducting materials are regarded as a viable alternative to inorganic semiconductors in molecular electronics - the new low cost flexible electronics [1-3]. We report here the synthesis of new 4,7-phenanthrolin-4-ium derivatives and the study of their electrical properties in thin films.

The compounds were obtained from the direct reaction of 4,7-phenanthroline with reactive halogenated derivatives.

Temperature dependences of electrical conductivity and thermoelectric power of the synthesized compounds are studied. Thin-film samples spin-coated from dimethylformamide solutions onto glass substrates were used, after they were submitted to a heat treatment within temperature range 295-530 K.

The crystalline structure and surface morphology of samples have been investigated by XRD and AFM (corroborated to optical microscopy) techniques, respectively. The studied polycrystalline compounds show typical semiconductor behaviour.

Some correlations between semiconducting parameters and molecular structure of the organic compounds have been discussed. The investigated compounds hold promise for thermistor applications.

PE2. INVESTIGATION ON Cu (II) ADSORPTION ON TRICALCIUM SILICATE, $3CaO \cdot SiO_2$

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Cement is the most adaptable binder currently available for the immobilization of heavy metals.

$3CaO \cdot SiO_2$, tricalcium silicate, is one of the main phases in ordinary Portland cement and many of its properties were related to $3CaO \cdot SiO_2$.

In the present work the stabilization of Cu (II) wastes by $3CaO \cdot SiO_2$ during its early hydration was studied.

Copper ions present in the added water for hydration, were doped inside $3CaO \cdot SiO_2$ during the hydration process.

The chemically combined water and $Ca(OH)_2$ contents were determined after 1, 3, 6 h and 1, 3 and 7 days of hydration. X-ray diffraction (XRD) and electron microscopy (SEM) examination was performed for some selected samples.

The results showed that the presence of Cu (II) ions retard the early hydration of $3CaO \cdot SiO_2$. This is due to the precipitation of the less soluble $Cu(OH)_2$ which retards the precipitation of $Ca(OH)_2$ as a result of the reduction in pH. Immobilization percentage of Cu (II) ions inside the $3CaO.SiO_2$ hydrated matrix was examined by the determination of the leached copper by using atomic absorption spectroscopy (ContrAA 700, Analytik Jena).

The effects of metal ion concentration, pH and contact time on binding ability was investigated by kinetic and equilibrium adsorption isotherm studies. The adsorption capacity for Cu(II) was found to be 6.356 mg/g. It is concluded that the composite adsorbent has considerable potential for the treatment of industrial wastewater containing heavy metals.

PE3. SOL-GEL SYNTHESIS AND STRUCTURAL CHARACTERISATION OF Fe-DOPED $LaMnO_3$ NANOPOWDERS

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Due to their electrical and magnetic properties, perovskite – type composite oxides are of both fundamental and technological importance. Perovskite are compounds with general formula ABO_3, where both A and B metal ions can be partially substituted, leading to a wide variety of compounds. These are often characterized by oxygen non-stoechiometry, which determines interesting catalytic properties for many reactions. If the B position is occupied by a first row transition metal ion these oxides are semiconductors possessing a relatively high electronic conductivity. Considerable interest has been shown in perovskite – type oxides, $LnMeO_3$ with lanthanide elements (Ln) and transition metal (Me), because these materials can be used in solid-oxide fuel (SOFCs) cells and catalysts and sensor materials for oxygen, humidity, alcohol and carbon monoxide. The functional properties of the $LnMeO_3$ powders are enhanced by the homogeneity and high surface area. $LaMnO_3$ is an insulating antiferromagnetic (AFM) material with orthorhombic perovskite structure.

Nano-sized perovskite – type oxides $La(Mn_xFe_{1-x})O_3$ (x=0.6) particles were successfully synthesized at a low temperature of 800^oC by a modified Pechini sol–gel process with starting materials of $La(NO_3)_3$, $Mn(Ac)_2{\cdot}4H_2O$ and $Fe(NO_3)_3{\cdot}9H_2O$ an ideal cation stoichiometry for $La(Mn_xFe_{1-x})O_3$ (x=0.6) perovskite. The method is based on condensation polymerization between ethylene glycol ($HOCH_2CH_2OH$) and citric acid $(HOH)(CO_2H)(CH_2CO_2H)_2$ in presence of soluble metal-citrate complexes.

The structural characterization of the precursors and derived synthesized oxide powders is done by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), thermal analysis (TG-DTG) and high-resolution electron microscopy (HRTEM) studies. Also the nano – crystals size distribution was studied and the main diameter of nanoparticles was about 11nm.

PE4. SYNTHESIS, STRUCTURAL AND IN VITRO BIOACTIVITY CHARACTERIZATION OF THE Zn-DOPED SOL-GEL DERIVED SiO_2-CaO -P_2O_5 GLASSES

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Bioactive glasses in the systems CaO-SiO_2-P_2O_5-ZnO were synthesized by sol-gel method using non-ionic block copolymer P123 as structure directing agent. The as prepared bioactive glass powders were immersed in a simulated body fluid (SBF) for periods of up to 28 days. XRD, FTIR and Raman Spectroscopy were used in order to confirm the formation of a hydroxyapatite (HA) layer on the bioactive glass powder. Microstructural characterization of the bioactive glass samples was investigated by scanning electron microscopy (SEM) technique. Pore size distribution and surface area of bioactive glass powders were also determined in order to characterize the textural properties of the samples. The influence of ZnO concentrations on the formation of HA layer on the glass powders was established.

PE5. NONDESTRUCTIVE EXAMINATION OF PRESSURE VESSELS

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The aim of this paper is to investigate carrying capacity of pressure vessels under hydrostatic pressure, based on the elastic-plastic theory. Pressure vessels are common in the chemical process industries.

Representative examples are examined and solutions are obtained for the cylindrical and spherical vessels using 5 types of steel.

Considering present manufacturing processes, they may be competitive for future manufacturing technologies, and contribute to a better understanding of the actual influence of shape of pressure vessels.

Only proper materials have to be used in the process and the producer survey the process with an implemented quality system. The material are filtered by a quality program in order to meet the requirements by the National I.S.C.I.R. Code.

PE6. DIMENSIONING PIPELINES FOR TRANSPORTING COMPRESSIBLE FLUIDS

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The purpose of this paper is to design the pipelines in three special flow conditions: incompressible when fluid density is constant, isothermal when fluid temperature is constant and adiabatic when there is no heat transfer between the fluid and its surroundings. Computational models are be applied for designing the pipelines for compressible flow.

When fluid density is constant, the dimensioning of the gas pipelines takes into consideration the pressure drop and Mach number. The isothermal flow equation is preferable for compressible fluids because it gives a conservative pressure drop. For adiabatic flow, specific heat ratio has significant effect on pressure drop.

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