

# ***Abstracts***

**for**

**The 8<sup>th</sup> Scientific Session of Undergraduate,  
Master and PhD Students, Iasi, Romania**

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## P01. Size distributions of water soluble aluminum and magnesium in atmospheric aerosols from Iasi, România

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Elemental composition of atmospheric aerosols is often predominated by various metal elements which are exerting toxic effects to human health even at very low concentrations.<sup>1</sup> Toxicity of an inhaled metal, the extent of dispersion via atmospheric transport and residence times in the atmosphere are highly influenced by particles size.<sup>2</sup> Moreover, metal elements can be used as tracers in identifying sources, so measuring metals is of great importance.<sup>3</sup>

In the present work, size distributions of water soluble aluminum and magnesium in atmospheric aerosols from Iasi, north-eastern Romania, are investigated. Atmospheric aerosols samples were collected during a one year measurement campaign at the Air Quality Monitoring Station (AMOS) of CERNESIM, "Alexandru Ioan Cuza" University of Iasi. Size resolved aerosol samples were collected over a time period of 36-hour using a 13 stages cascade Dekati Low-Pressure Impactor (DLPI) (0.0276-9.94  $\mu\text{m}$  size range and 29.85 L  $\text{min}^{-1}$  flow rate). Water soluble aluminum and magnesium fraction of the collected particles have been investigated with an Inductively Coupled Plasma Mass Spectrometer (ICP-MS) 7700X (Agilent Technologies, USA). The concentrations of water soluble magnesium, as derived from ICP-MS and ion chromatography (IC) data, showed significant statistical correlation (Pearson coefficient,  $r$ , higher than 0.98). This information is assigned as representing a major forward step within the validation process of the chemical composition analysis of the investigated aerosol particles. The magnesium mass concentrations resemble monomodal distribution with maximum in the fine mode during the winter and in the coarse mode during spring, summer and autumn. These observations would indicate that, except winter, magnesium originates from natural sources such as sea spray aerosols or soil dust. The size distribution of aluminum showed a dominant fine mode peaked at about 381 nm, suggesting that aluminum would be emitted from anthropogenic sources (i.e. diesel or gasoline powered vehicles) during the entire investigated period.

**Keywords:** atmospheric aerosols, size distribution, aluminum, magnesium.

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**P02. Gas-phase FT-IR kinetic study of the HO radicals reaction with phenol**Claudiu Roman<sup>a</sup>, Cecilia Arsene<sup>a,b</sup>, Iustinian Bejan<sup>b</sup>, Romeo-Iulian Olariu<sup>1,2\*</sup><sup>a</sup>"Alexandru Ioan Cuza" University of Iasi, Faculty of Chemistry, 11 Carol I, 700506 Iasi, Romania<sup>b</sup>"Alexandru Ioan Cuza" University of Iasi, Integrated Center of Environmental Science Studies in the North Eastern Region - CERNESIM, 11 Carol I, 700506 Iasi, Romania

Aromatic hydrocarbons emitted from combustion of fossil-fuels and solvent use<sup>1</sup> are important contributors to the formation of photo-oxidants and secondary organic aerosol (SOA) in urban area.<sup>2</sup> Reaction with HO radicals represents a major sink<sup>3</sup> of aromatic hydrocarbons in the troposphere during the day time. As part of a systematic study of the gas-phase atmospheric chemistry of hydroxylated aromatic hydrocarbons in the present work a kinetic study on the gas-phase reaction with OH radicals has been conducted. The measurements were performed in the (760±2) L ESC-Q-UAIC photoreactor at (298±2) K and 1000 mbar total pressure of air using relative kinetic technique. Tetrahydrofuran and propylene have been used as reference compounds in the present study. OH radicals were generated by photolysis of CH<sub>3</sub>ONO ( $\lambda_{\text{max}} = 365$  nm) in the presence of NO. Control experiments have shown that in the absence of oxidizing species phenol exhibits losses by wall adsorption only. The weighted average rate coefficient obtained in the present work shows good agreement with literature values within the experimental error limits.<sup>2</sup>

This result represents a major step forward within the validation of newly ESC-Q-UAIC simulation chamber for gas-phase kinetic and mechanistic investigations as well.

**Keywords:** Gas-phase kinetics, Phenol, OH radicals, FT-IR.

**Acknowledgements:** *The authors acknowledge the financial support provided by UEFISCDI within the PN-III-P2-2.1-PED-2016-0924 (DEV-TREC) Projects. European Union's Horizon 2020 research and innovation programme through the EUROCHAMP-2020 Infrastructure Activity under grant agreement No 730997 is also gratefully acknowledged. CERNESIM infrastructure is gratefully acknowledged.*

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### P03. New insights into brominated flame retardants structure: computational assessment of $\sigma$ -hole effect

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Brominated flame retardants include a diverse group of chemical classes, which are used or have been used, mostly embedded in target materials, with an array of commercial and industrial applications for fire prevention.<sup>1,2</sup> This has led to the widespread and substantial contamination of the environment, e.g. indoor air, dust.<sup>2</sup> However in the indoor environment increasing evidence of their presence, question their potential health risk to organisms exposed to these emerging classes of environmental contaminants. Understanding the chemical and physical properties of the most used compound of this family (decabromodiphenyl ether or BDE-209), can facilitate their analysis in order to control and further regulate this organobrominated compound. Therefore, by the use of theoretical methods the qualitative evaluation of the selected flame retardants interaction with a series of commonly used organic solvents for their analysis might be assessed.

This study aimed on evidencing of the presence of sigma-holes for selected polybrominated diphenyl ethers (PBDEs) and also for the most commonly used organic solvents during typical analytical protocols for their quantitative determination. By using a theoretical study assessment by DFT we evidenced the presence of numerous sigma-holes (an example is depicted in Fig.1). This can lead to halogen bonding:  $\sigma$  hole concept referred to the electron-deficient outer lobe of a half-filled  $p$  (or nearly  $p$ ) orbital involved in forming a covalent bond. If the electron deficiency is sufficient, there can result a region of positive electrostatic potential on the outermost portion of the halogen's surface, centered on the R-X (X= F, Cl, Br and I) axis.<sup>3,4</sup> However the positive region can interact attractively with negative sites on solvent molecules favoring an intermolecular connection. The most commonly reported PBDEs in environmental samples were tested and they were all shown to present sigma hole regions. These findings can lead to a better selection of solvents to be further used in order to properly assess the PBDEs presence in various environmental matrices.

**Keywords:** flame retardants, DFT, ESP

**Acknowledgement:** This work was supported by a grant of the Romanian National Authority for Scientific Research and Innovation, CNCS-UEFISCDI, project number PN-II-RU-TE-2014-4-1010.

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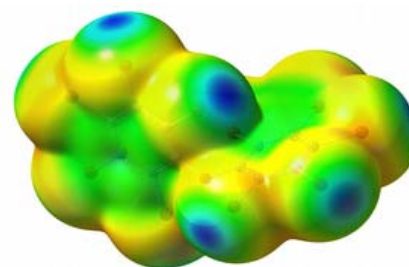


Figure 1. BDE-209 ESP map at M06/cc-pVTZ

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**P04. Synthesis of two fragments derivated from  $\beta$ -amiloidic peptide and mass spectrometry analysis of their complexes with various metal ions**

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Synthetic peptides have many practical applications and an important role in understanding and studying the properties of natural peptides.<sup>1</sup> For these reasons, there are always syntheses of new peptides and their structural analogs.<sup>2</sup> Recent research in this area focuses on the synthesis and characterization of reactions between the polypeptides and various compounds containing metal ions, representing a mutual problem in neurodegenerative diseases. The interaction between metal ions and peptides has been studied initially using spectroscopic or electrochemical methods such as circular spectroscopy (CD), NMR spectroscopy or cyclic voltammetry.<sup>3</sup> At present, mass spectrometry is a rapid method used more and more often in studies of proteins.

The main neuropathological feature of Alzheimer's disease is the extracellular deposits of  $\beta$ -amyloid peptides are associated with lipids, metal ions and other proteins. The development of neurodegenerative diseases focuses on abnormal accumulations of metals such as  $\text{Cu}^{2+}$ ,  $\text{Zn}^{2+}$ ,  $\text{Fe}^{3+}$ ,  $\text{Al}^{3+}$  at the neuronal level, leading to the production of toxic protein aggregates.<sup>4</sup>

Thus, two novel peptides modified with glycine and phenylalanine derived from the amyloid A $\beta$  (9-16) fragment were synthesized and characterized. Moreover, the peptides thus obtained have been subjected to interaction with various metal ions such as  $\text{Cu}^{2+}$ ,  $\text{Zn}^{2+}$  and  $\text{Ni}^{2+}$ . Both the structure of the manually synthesized peptides and their complexes with metal ions were confirmed by MALDI-ToF mass spectrometry.

**Keywords:** synthesis of peptides, A $\beta$ , metal ions, Alzheimer's disease, MALDI-ToF.

**Acknowledgements:** Authors acknowledge the PN-II-RU-TE-2014-4-0920 Project, for MS experiments.

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## **P05. Influence of textural properties of mesoporous silica on vitamin B<sub>2</sub>-based controlled release systems**

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The sol-gel synthesis of mesoporous silica was performed involving two different thermal treatments, namely: conventional (heating on an oil bath, stirring and refluxing) and sonochemical (heating and stirring using ultrasounds). These two treatments led to mesoporous silica nanoparticles, SBA-15 type, with different morphologies and sizes as Scanning Electron Microscopy revealed. Also, the ratio of the silicon source and the structuring agent was varied, obtaining 4 silica samples with different textural properties, that have been investigated by nitrogen sorption measurements at low temperatures. Because the ordinary sol-gel synthesis yields a rich mesoporous silica surface with hydroxyl groups, an additional surface functionalization was taken into account, with view of introducing amino-functional groups. This has been proposed to study how the textural properties and surface chemistry affect the sorption process of vitamin B<sub>2</sub> molecules, in view of a possible application of the synthesized materials as controlled release systems. Functionalization has been found to be a successful one, by anchoring APTES molecules inside mesoporous silica pores. Further, the adsorption tests have shown that the functionalization of the mesoporous silica surface increases the sorption capacity for vitamin B<sub>2</sub>, in relation to specific surface area and pore volume, such information being useful in controlled release systems preparation.<sup>1,2</sup>

**Keywords:** mesoporous silica (SBA-15), functionalization, controlled release systems, vitamin B<sub>2</sub>.

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## P06. Accumulation of selected tocopherols in *DATURA INOXIA* structural constituents

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Investigations on the accumulation of selected tocopherols, *i.e.*  $\alpha$ - and  $\gamma$ -tocopherols, in *Datura innoxia* plant structural constituents have been undertaken in the present work. Quantitative analysis of the interest secondary metabolites, known also as natural antioxidants, has been performed by using gas chromatography tandem mass spectrometry (GC-MS). Instrumental analyses have been undertaken only after appropriate preparative steps involving ultrasound assisted extraction as the most efficient method to enhance interest analyte concentration.<sup>1</sup> To our knowledge, these are the first attempts for the identification and quantification of the  $\alpha$ - and  $\gamma$ -tocopherols in extracts of *Datura innoxia* vegetative organs (leaves, stem, flowers, fruits and roots). From the obtained data it has been observed that the amount of  $\alpha$ -tocopherol, known also as vitamin E, in both methanol (MeOH) and butanol (BuOH) extracts showed a continuous accumulation trend in leaves, with highest concentrations at ripening and senescence. Interesting behavior of  $\alpha$ -tocopherol has been observed in plant corollas with the highest concentration during the initial in blossom period. In seeds, the trend observed for  $\alpha$ -tocopherol showed an almost steady concentration, while in capsules and loculs this natural antioxidant showed a very slight increase.

$\gamma$ -Tocopherol showed an interesting pattern especially in leaves, with an initial fast accumulation stage during leaf development, secondary stem elongation, vegetative part plants, in blossom and fruit development stages. This initial stage is followed by a slight cessation in  $\gamma$ -tocopherol concentration with an almost steady behavior up to senescence. While in corollas the behavior of  $\gamma$ -tocopherol was quite similar to that of  $\alpha$ -tocopherol, in seeds, the obtained data showed much higher dispersion.

$\alpha$ -Tocopherol abundances both in the MeOH and BuOH extracts of seeds and capsula were anti-correlated suggesting a possible export of this natural antioxidant from capsula/pods to seeds.

**Keywords:**  $\alpha$ - and  $\gamma$ -tocopherols, *Datura innoxia*, gas chromatography-mass spectrometry.

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

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## P07. Chitosan-disiloxane hydrogels. water retention and morphology

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Chitosan based biomaterials plays an important role in tissue engineering field due to their favorable properties such as biocompatibility, biodegradability and nontoxicity.<sup>1</sup> The presence of amine and hydroxyl groups along the chitosan's polymer chain provides excellent ligand properties and increases the ability to form ideal systems for skin regeneration.<sup>2</sup> To compensate the chitosan (CS) limitations, such as reduced mechanical strength and low solubility, this paper proposes the synthesis of N-succinyl-chitosan as a chemically modified derivative of the polymer by attaching the succinic anhydride (AS) to the free amino groups. A crosslinking process with 1,3-bis-(3-glycidoxypropyl)-tetramethyldisiloxane (DS) occurred in order to maintain the hydrodynamic stability of the system. The polymeric membranes were obtained by two methods (solvent casting and freeze drying) and exhibit swelling properties according to their composition and the preparation procedure. The surface structure and the morphology of gels with different CS/AS/DS ratios were determined by FTIR and SEM (Figure 1), respectively.

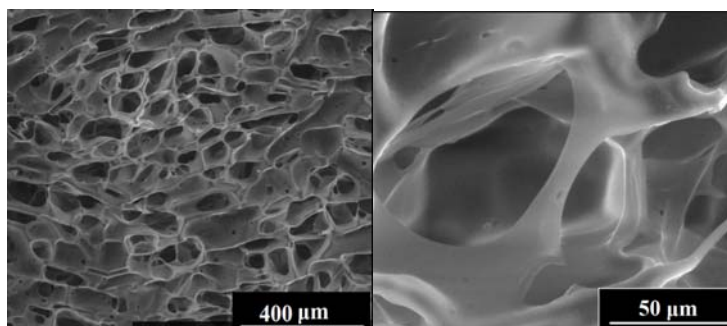


Figure 1. SEM images representing CS/AS/DS gels obtained by freeze drying.

**Keywords:** chitosan, chemical modification, N-succinyl-chitosan.

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## P08. NAP - neuroprotective peptide in alzheimer's disease: synthesis and characterization

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Alzheimer's disease (AD) is characterized neuropathologically by formation of highly insoluble amyloid  $\beta$  peptide deposits.<sup>1</sup> Evidence indicates that cognitive decline in ageing is the result of a growing vulnerability to an asymptomatic state of progressive neuroinflammation.<sup>2</sup> These plaques are co-localised with a broad variety of inflammation-related proteins such as proteic complement factors, acute-phase protein or pro-inflammatory cytokines.<sup>3</sup> Non-steroidal anti-inflammatory drugs (NSAIDs), such as aspirin, have been successful used in reducing the risk of developing AD.<sup>4</sup> Although it is not recommended for long-term use due to its side effects - the risk for bleeding complications.<sup>5</sup> Other drug candidate against A $\beta$  toxicity reported in the literature is the octapeptide NAPVSIPQ (NAP). Several studies have shown that NAP provides neuroprotection against the Alzheimer's disease neurotoxin at femtomolar concentrations.<sup>6</sup>

Thus, here we report novel synthesis of the acetyl salicylic acid-NAP mutant, a potent drug in reducing neuroinflammation and plaque formation. The Asp-NAPVSIPQ peptide was obtained using the well-known, F-moc solid phase peptide synthesis and the molecular mass was assessed by MALDI-ToF mass spectrometry and FT-IR spectroscopy.

**Keywords:** chemical synthesis, peptides, Alzheimer's disease, inflammation.

**Acknowledgements:** Authors acknowledge the PN-II-RU-TE-2014-4-0920 Project, for MS experiments.

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## P09. Investigations on the gas-phase ho radical initiated oxidation of 5-methyl-2-hexanone and 2-heptanone. A kinetic approach

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Ketones are emitted into the atmosphere from a variety of natural and anthropogenic sources. In the atmosphere these compounds represent one of the most abundant classes of oxygenated volatile organic compounds (VOCs). Photolysis and chemical oxidation are assigned as two important removal processes of ketones in the atmosphere.<sup>1</sup> Reaction with the hydroxyl radical (HO) is the predominant gas-phase removal process for the majority of the organics emitted into the troposphere.<sup>2</sup> The available kinetic data for the reaction of HO with saturated or alkylated ketones suggest that the reactions proceed by H-atom abstraction from the alkyl chain.<sup>3</sup>

The present work brings clear evidence about the possibilities of the 760 L ESC-Q-UAIC reaction chamber (Environmental Simulation Chamber made of Quartz, from the "Alexandru Ioan Cuza" University of Iasi) to be used for studying various atmospheric chemical processes. Measurements were performed at (298±2) K in synthetic air at atmospheric pressure. The relative rate technique has been used as a suitable tool for the estimation of the HO radical initiated oxidation rate constants for saturated ketones including 5-methyl-2-hexanone and 2-heptanone. Methylcyclohexane and diethyl ether were used as reference compounds. The HO radicals have been generated by using H<sub>2</sub>O<sub>2</sub> photolysis at λ=254 nm.

The variability of the rate coefficient values, such as those determined in the present work, provides a clear view about the reactivity of the investigated ketones. For the reaction of 5-methyl-2-hexanone with the HO radicals, a reaction rate coefficient value is reported for the first time using a relative rate method. The values reported in the present work are in good agreement with literature data.

For an HO radical concentration of 1.6×10<sup>6</sup> molecules·cm<sup>-3</sup>, often existent in the atmosphere, any of the investigated ketones have atmospheric lifetimes (τ) of fewer than 24 h, indicating that these molecules, once formed or emitted into the atmosphere, will rather have a regional influence. All data gathered from the present study can be useful for investigations of possible degradation mechanisms of gaseous ketones or for modeling studies.

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**P10. Synthesis and characterization of  $\text{La}_{0.67}\text{Sm}_{0.33}\text{Fe}_{1-x}\text{Co}_x\text{O}_3$  perovskites**Caterina Afloarei<sup>a\*</sup>, Georgiana Bulai<sup>b</sup>, Nicoleta Cornei<sup>a</sup><sup>a</sup> "Alexandru Ioan Cuza" University of Iasi, Faculty of Chemistry, 11 Carol I, 700506 Iasi, Romania<sup>b</sup> "Alexandru Ioan Cuza" University of Iasi, Faculty of Physics, 11 Carol I, 700506 Iasi, Romania

The present work studies the synthesis methods and structural, electrical and magnetic properties of  $\text{La}_{0.67}\text{Sm}_{0.33}\text{Fe}_{1-x}\text{Co}_x\text{O}_3$  perovskite-type oxides (LSFC). The LSFC compounds were prepared by sol-gel synthesis using anhydrous citric acid as complexing agent. Samples were pelleted, presintered at 750°C/6h and sintered at 1100°C/11h in air atmosphere.

The crystal and morphological structure of the samples sintered at 1100°C/11h were analyzed by means of powder X-ray diffraction (PXRD), FT-IR spectroscopy at 4000-250  $\text{cm}^{-1}$  and by scanning electron microscopy (SEM). The XR diffractograms showed almost pure samples (Figure 1), with orthorhombic Pnma space group structure. The cell parameters and phase cell element volume, respectively, decrease with the increase of cobalt content in the samples, variation explained on the basis of the smaller ionic radius of Co(III) (0.61 Å), compared to that of Fe(III) (0.78 Å), which matches literature data.<sup>1</sup>

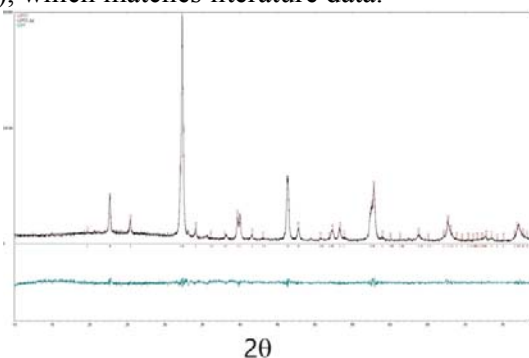


Figure 1. Observed (black), calculated (red) and differential (blue) diffractogram for  $x = 0.03$

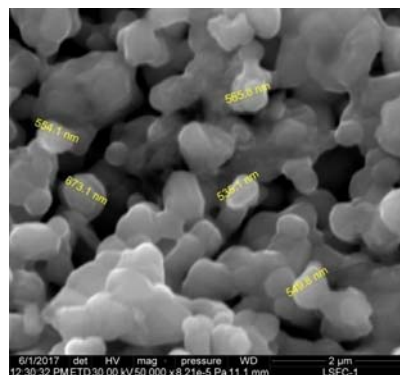


Figure 2. SEM microstructure at 2  $\mu\text{m}$  resolution for  $x = 0.03$

SEM analysis shows spherical particles (Fig. 2), the dimensions of which increase with the increase of cobalt content, while the inter-grain porosity decreases with the increase of cobalt content in the samples.

The variation of dielectric properties with frequency and the variation of magnetic properties with the magnetic field were also discussed. Samples with higher iron content display a higher coercive field.

**Keywords:** perovskite, sol-gel method, X-ray diffraction, electrical properties.

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