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DOI: 10.2478/achi-2018-0023

ACTA CHEMICA IASI, **26_2**, 369-394 (2018)

Abstracts

for

9th Scientific Session of Undergraduate, Masters and PhD Students, Iasi, Romania

june, 29, 2018

TABLE OF CONTENT

C-01. Meteorological parameters role on the formation and growth of new atmospheric particles in Iasi urban area ……. 373
Alina-Giorgiana Galon (Negru), Romeo Iulian Olariu, Cecilia Arsene
C-02. Synthesis and characterisation of cobalt(II), nickel(II) and cooper(II) complexes with thiosemicarbazide ……..… 374
Ana Maria Alexandru, Oleg Palamarciuc, Aurel Pui
C-03. Rate coefficients of the gas-phase ozonolysis of C5-C6 unsaturated aldehydes …… 375
Claudiu Roman, Cecilia Arsene, Marius Duncianu, Iustinian Gabriel Bejan, Alexandre Tomas, Véronique Riffault and Romeo-Iulian Olariu
C-04. Synthesis and study of Ni (II) and Co (II) coordinative compounds with active biological ligands ……... 376
Cristina Mihaela Idriceanu, Eugenia Melentiev, Svetlana Baca
C-05. Study of dielectric properties of nickel chromite against complexing / combustion agents used in synthesis …….. 377
Elena Daniela Chitoiu-Arsene, Alexandra Raluca Iordan, Adrian Iulian Borhan, Nicoleta Melniciuc-Puica, Georgiana Bulai, Aurelian Carlescu
C-06. Determination of absorption band shapes and conical intersections for barbituric acid 378
Gheorghe Paveliuc, Ionel Humelnicu, Dan Maftei, Robert Gora
C-07. Insights into innovative synthesis of mesoporous titania: effect of microwave annealing time on textural and structural properties ……..…….. 379
Elvira Mahu, Cristina Coromelci-Pastravanu, Maria Ignat, Petrisor Samoila Valeria Harabagiu 379
C-08. The theoretical study of vitamin C interactions …….. 380
Răzvan Ghiarasim, Ionel Humelnicu
C-09. Sinthesis and study of Cu(II) coordination compounds with ligands bazed on o-vanillin S-methylisothiosemicarbazone …….. 381
Mihaela Rotaru, Maria Cocu
C-10. Theoretical studies of several phenanthroline and benzimidazole derivatives ……. 382
Tudorel Chelariu, Ionel Humelnicu, Ionel Mangalagiu
C-11. The link between hyperconjugation and planarity - a DFT study of inorganic amines and isoelectronic compounds ……. 383
Florin Teleanu, Ionut-Tudor Moraru, Gabriela Nemes
C-12. Synthesis and crystal structure of a Copper(II) oxalate oxamide dioxime complexe: Toward the development of new anticancer drug …..……. 384
Patrick L. Djonwouo, Justin Nenwa, Michel M. Bélombé, E. Jeanneau, and Boniface P.T. Fokwa 384
P-01. Xerogels based on chitosan as delivery matrix for a potentially anticancer drug …… 385
Anda-Mihaela Olaru , Luminita Marin, Ramona Danac, Ionel Mangalagiu
P-02. The relationship between some heavy metal ion and the amyloid peptide fragments 386
Gabi Drochioiu
P-03. Nutrient pollution of some lakes in Neamt County, Romania ……... 387
Andana Maria Mihai, Gabi Drochioiu
P-04. Synthesis and anticance evaluation of new 7-(pyridin-2-yl)-indolizine derivatives …….. 388
Monica Cornelia Sardaru, Sinziana Diana Oniciuc, Catalina Ionela Ciobanu, Ionel Mangalagiu, Ramona Danac
P-05. Assessment of lake water chemistry using statistical analysis …… 389
Cornelia Amarandei, Alina Giorgiana Galon (Negru),
Simona-Maria Cucu-Man, Romeo-Iulian Olariu, Cecilia Arsene

P-06. Development of a new method for carbonyls analysis in the atmosphere by using solid phase derivatization coupled with GC/Ion Trap MS technique …… 390
Ana-Maria Rusu, Cecilia Arsene, Gabriel Iustinian Bejan, Romeo-Iulian Olariu
P-07. New hybrid quinoline derivatives with imidazole skeleton …… 391
Dumitrela Cucu, Dorina Amariucai-Mantu, Cătălina Ionela Ciobanu, Violeta Mangalagiu, Ionel Mangalagiu
P-08. Rate coefficient of the gas-phase OH radical initiated oxidation of 2,5-dimethylfuran at 298±2 K and atmospheric pressure ……. 392
Claudiu Roman, Cecilia Arsene, Romeo-Iulian Olariu, Iustinian Gabriel Bejan
P-09. Amphiphilic chitosan membranes for pain relief: preparation, characterization and in vitro lidocaine release ……..…… 393
Andra-Cristina Humelnicu, Valeria Harabagiu
P-10. Sintering as sample dissolution procedure for complex matrices prior analysis of REEs by ICP-MS .....…….. 394
Laurentiu-Valentin Soroaga, Cecilia Arsene, Romeo-Iulian Olariu

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C-01. Meteorological parameters role on the formation and growth of new atmospheric particles in Iasi urban area

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Fine and ultrafine atmospheric particles, known also as aerosols, are highly involved in climate changes on the global scale. Understanding the formation and growth processes of new atmospheric particles, determining aerosol number concentrations but also sources contributing to the generation of gaseous aerosol precursors and aerosols, is a very important task. The role of meteorological parameters on the formation and growth processes of new atmospheric particle in Iasi urban area, north-eastern Romania, is investigated in the present work. For particles in the 9.5-445 nm size range, a Scanning Mobility Particle Sizer (SMPS, TSI 3936) was used to obtain size dependent aerosol number concentrations. Data acquisition was performed with a 5 minutes time resolution. Measurements have been undertaken at the Air Quality Monitoring Station (AMOS) of CERNESIM, from the "Alexandru Ioan Cuza" University of Iasi, during the warm (12-17 May 2017) and the cold (06-17 December 2017) seasons. The meteorological parameters (temperature, relative humidity, solar radiation, wind speed, wind direction) were provided by Weather Hawk GSM-240 station of CERNESIM Center, installed at AMOS station.

Analysis of entire data-base and other derived parameters, i.e. growth of the measured "nuclei" mode concentrations, highlighted the existence within the investigated periods in Iasi urban area of a strong event (07 December 2017), 9 moderate events, 3 weak events and 4 non-new particle formation/unidentified events. For the investigated period the relative humidity was generally lower in those days with evident formation events compared to the non-event days. In addition, diurnal variability of investigated parameters showed that the solar radiation peak was usually associated with new particle formation events. The present work brings clear evidences on the solar radiation potential role in the initial step of atmospheric nucleation.

Keywords: ultrafine particules, size distribution, nucleation

Acknowledgements:
The authors acknowledge the financial support provided by UEFISCDI within the PN-III-P4-ID-PCE-2016-0299 (AI-FORECAST) Project. The authors acknowledge also PN-III-P2-2.1-PED-2016-0924, PN-III-P2-2.1-PED-2016-1621, PN-III-P4-ID-PCE-2016-0270 and PN-III-P4-ID-PCE-2016-0807 Projects.

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C-02. Synthesis and characterisation of cobalt(II), nickel(II) and cooper(II) complexes with thiosemicarbazide

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Thiosemicarbazide–based compounds have been extensively studied over the last couple of decades. Complexes of Ni(II), Zn(II) and Hg(II) with thiosemicarbazide exhibit antibacterial and antifungal activities.

The present study contains details about their synthesis and characterization by UV-VIS, FT-IR spectroscopy, ^{1}H Nuclear Magnetic Resonance (^{1}HNMR), thermal analysis (TGA) and X-ray diffraction. The obtained complexes have the formulas $[Co(C_8H_{10}N_4S)_2]Cl_2\cdot H_2O$; $[Ni(C_8H_{10}N_4S)_2]Cl_2\cdot 2H_2O$; $[Cu(C_8H_{10}N_4S)Cl_2]\cdot H_2O$.

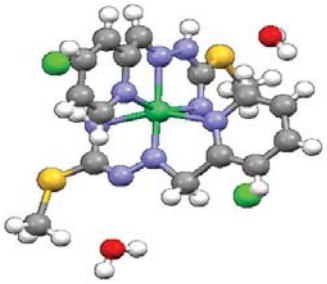

Figure 1. Structure of $[Ni(C_8H_{10}N_4S)_2]Cl_2\cdot 2H_2O$ complex.

Single-crystal X-ray diffraction studies revealed the molecular structure of the $[Ni(C_8H_{10}N_4S)_2]Cl_2\cdot 2H_2O$ complex represented in Figure 1. This complex shows an octahedral geometry, with molar ratio M/L=1/2. Outside of the coordination sphere, there are two chlorine atoms and two water molecules.

Keywords: complexes, thiosemicarbazide, antibacterial activity.

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C-03. Rate coefficients of the gas-phase ozonolysis of C5-C6 unsaturated aldehydes

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Unsaturated aldehydes are important biogenic volatile organic compounds (BVOC) and are believed to have a great influence on atmospheric chemistry through their impact on HO_x ($HO + HO_2$) cycle, photooxidants and Secondary Organic Aerosols (SOAs) formation especially from their highly oxygenated products of oxidation. Rate coefficients for the gas-phase reaction of three unsaturated aldehydes (4-pentenal, *trans*-2-pentenal and *trans*-2-hexenal) with ozone have been determined by using relative kinetic technique in the 760 l quartz glass reaction chamber ESC-Q-UAIC (Environmental Simulation Chamber made by Quartz from University "Alexandru Ioan Cuza" of Iasi).

Experiments were performed in synthetic air at a total pressure of 1000 ±50 mbar and temperature of 298±2 K. Ozone was generated by photolysis (at 180 nm) of a controlled oxygen flow. Two reference compounds (propene and methyl-vinyl-ketone) have been used in the present study.

The concentration–time behavior of unsaturated aldehydes and the reference organic compounds was followed for at least 15 min using FT-IR long path spectroscopy. Figure 1 shows the preliminary plots used in the estimation of the following rate constants (in units of 10^{-18} $cm^3molecule^{-1}s^{-1}$): $k_{1(4\text{-pentenal})} = 5.55 \pm 0.14$, $k_{2(trans\text{-2-pentenal})} = 1.34 \pm 0.07$ and $k_{3(trans\text{-2-hexenal})} = 1.74 \pm 0.13$. The obtained values are in good agreement with literature data and SAR estimations (Structure-Acivity-Relationship).

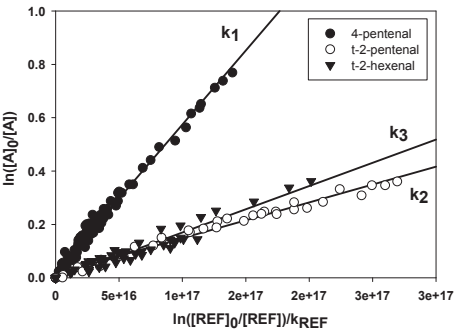

Figure 1: Kinetic plots for 4-pentenal, *trans*-2-pentenal and *trans*-2-hexenal

Keywords: unsaturated aldehydes, rate coefficient, ozone reaction.

Acknowledgements: The authors acknowledge for the financial support provided by UEFISCDI within the PN-III-P2-2.1-PED-2016-0924 (DEV-TREC), PN-III-P4-ID-PCE-2016-0270 (OLFA-ROA) and PN-III-P3-3.1-PM-RO-FR-2016-0047 (OzOA) 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.

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C-04. Synthesis and study of Ni (II) and Co (II) coordinative compounds with active biological ligands

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Chemistry of coordinative compounds is an important branch of fundamental research in inorganic chemistry and is one of the modern chemistry branches that can provide many components with programmed properties.

The synthesis of the new coordinative compounds of Ni (II) and Co (II) with the biological ligand activators: triethanolamine (H_3tea) and 2-hydroxy-5-methoxy-3-nitrobenzaldehyde (L). As a result, the optimal conditions for the synthesis of Ni (II) and Co (II) compounds with the named ligands were determined using Ni (II) isobutyrate and Co (II) pivalate and studied the structure of synthesized combinations (**Fig**. 1 and **Fig**. 2).

In order to determine the composition and structure of the coordinative combinations obtained, modern research methods were used, such as: elemental analysis, IR (infrared) spectroscopy and single-crystal X-ray diffraction.

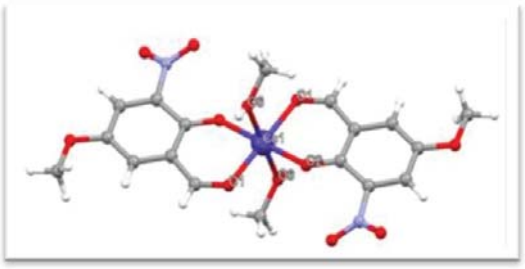

Figure 1. Molecular structure of $[Ni(H_3tea)_2](is)_2$.

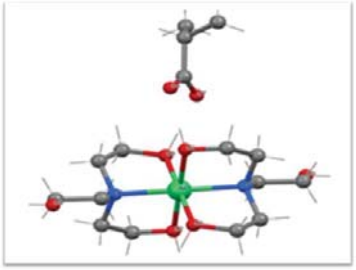

Figure 2. The molecular structure of $[Co(L)_2(MeOH)_2]$.

Keywords: coordinative compound, X-ray diffraction, IR spectroscopy

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C-05. Study of dielectric properties of nickel chromite against complexing / combustion agents used in synthesis

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Nickel chromite, $NiCr_2O_4$ (NCO) is a polymetallic oxide with AB_2O_4 spinel type structure. Ni^{2+} cations occupy the tetrahedral positions and Cr^{3+} occupy the octahedral positions of the unit cell. NCO is used in catalysis, photocatalysis, gas sensors elements, etc. The samples were synthesized through sol-gel auto-combustion method (**Fig**.1) by using starch (ST), cellulose (C), carboxymethylcellulose (CMC), ethylcellulose (E), fructose (F), galactose (GA), glucose (GL), manose (M), sorbitol (SO) and sucrose (SC) as complexing / combustion agents.

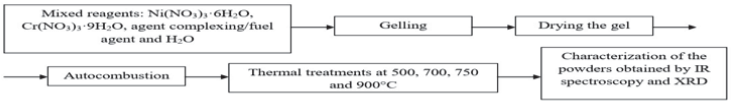

Figure 1: Synthesis protocol.

The X-ray diffraction of NCO powders thermally treated at 900 ^oC (**Fig**.2) show the influence of the complexing / combustion agents on the nickel chromite crystalline structure. Thus, when M, GA, GL, E, CMC, C and ST are used the NCO crystallized in the *Fd-3m* cubic system. The use of SC, SO and F leads to the samples crystallized in the $I4_1/amd$ tetragonal system. Also, the samples derived to the SC, C, CMC, E and F gels contain Cr_2O_3 as secondary phase which crystallizes in the rhombohedral system.

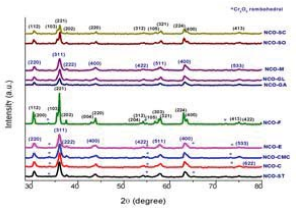

Fig. 2: X-ray diffraction patterns of samples sintered at 900°C.

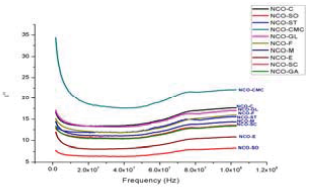

Fig. 3: The variation of the imaginary part of the dielectric constant according to the frequency for NCO treated at 900 °C.

Decreasing of the imaginary part of the dielectric constant with the frequency up to 30 MHz (**Fig**.3) can be caused by the polarization process, and then starts to increase. The most interesting decrease of the imaginary part caused by the polarization process can be seen in the case of NCO-CMC sample. Cr^{3+} plays an important role in the leakage conduction mechanism. The reduction of the chromium cation leads to relaxation processes

Keywords: chromite, auto-combustion, RXD, electric property.

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C-06. Determination of absorption band shapes and conical intersections for barbituric acid

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Barbituric acid, which has been known since 1863, is drawn in textbooks always as the *keto* tautomeric form. Indeed, this is the most stable form in the gas phase and in solution. Also in the solid state, the *keto* tautomer is observed in some metastabile phases. In contrast, it was observed presence of *enol* form in solid at ambient conditions. The preference for *enol* form in the solid state is explained by the formation of an additional strong hydrogen bond which lead to a more favorable lattice energy.

In general, the distribution of electronic spectra intensities sensitively depend on the details of ground - and excited - state potential energy surfaces (PESs), temperature, spin-orbit coupling, nonadiabatic effects and dipole moment transitions.

In the Franck-Condon (FC) approximation the electronic transition dipole moment coordinate dependence is neglected and the simulation of absorption spectra intensities is reduced to evaluation of the well-known FC factors that represent the overlap between the ground - and excited - state vibrational wave function. Unfortunately, the calculation of FC factors for general PESs is a complicated task, and thus it is usually done within the harmonic approximation. Different methods have been proposed for the evaluation of vibrational overlap integrals. For harmonic PESs vibrational eigenfunctions are expressed through dimensionless normal coordinates. The normal coordinates for ground - and excited - state surfaces are related by a linear transformation involving on original shift.

Many biological molecules, proteins and DNA contain chromophores that absorb light and undergo photophysical and photochemical processes. It has been shown that nonadiabatic events and conical intersections (CIs) govern these processes and play a fundamental role in the interaction of light with living matter. In this work we studied some aspects of the absorption bands of the barbituric acid molecule, the differences that occur between them when are treated by the harmonic oscillator approximation and a non-empirical model and determination of CIs for *keto* and *eno* tautomers. The *eno* tautomer forms spontaneously nucleotides in the aqueous solution.

Keywords: barbituric acid, nonadiabatic effects, chromophores, conical intersections.

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C-07. Insights into innovative synthesis of mesoporous titania: effect of microwave annealing time on textural and structural properties

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Mesoporous titania is one of the most investigated materials because of its multiple properties like biocompatibility, good chemical and thermal stability, good optical and electronic properties, and relatively low cost.

Mesoporous TiO_2 was prepared involving sonochemical method from titanium isopropoxide as titanium precursor, and pluronic F127 as structure directing agent. In order to remove the surfactant, the powdered sample has been subjected to the thermal treatment. The sample TiO_2 was calcined conventionaly at 723.15 K, for 4 hours. Also, in order to reduce synthesis time and energy consumption, TiO_2 samples were microwave annealed. The effect of the microwave treatment time on textural and structural properties of the newly obtained materials was investigated using different techniques: X-ray diffraction, N_2 sorption, UV-DR spectroscopy, and FTIR spectroscopy.

The newly synthetized TiO_2 particles with improved properties (e.g. specific surface area, crystallite size, band gap energy) may be used as photocatalysts for wastewater treatment.

Table 1. Textural properties of the TiO_2 synthesized samples.

Samples	S_{BET} cm3/g	Vtot. cm3/g	D.por. nm	D. crist. nm
TiO_2 conv.	157	0,129	3,5181	6,413
TiO_2 MW1	177	0,176	1,0936	0,872
TiO_2 MW2	185	0,17	1,0933	0,943
TiO_2 MW3	185	0,172	1,0823	1,03
TiO_2 MW4	206	0,202	1,0949	1,991
TiO_2 MW5	206	0,203	1,0553	1,842

Keywords: mesoporous titania, microwave annealing, sonochemical synthesis.

Acknowledgement: PN-III-P1-1.1-TE-2016-0805, within PNCDI III

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C-08. The theoretical study of vitamin C interactions

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The polar groups disposal from vitamin C (ascorbic acid) structure leads to a multitude of conformations corresponding to the stabilizing energies. Using *ab initio* and *DFT (Density Functional Theory)* methods were studied the interactions between the hydroxyl groups of the most stable conformer of vitamin C with polar solvents (water, inferior alcohols). Through this study it was observed the energy variation of the hydrogen bounds resulted from the investigated interactions. The geometries of all molecules were built using *Molden 5.0.6* program, and the obtained structures with the minimum energy was realized using *Gaussian 09* program using the *RHF (Restricted Hartree-Fock)* method with *6-31G(d,p)* basis set. The study of the molecular dynamics was realized using *VMD (Visual Molecular Dinamics)* and *Gromacs 2016* programs.

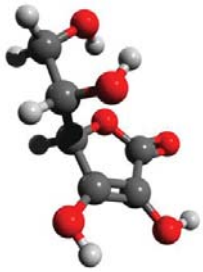

Figure 1. The most stable conformer of vitamin C.

Keywords: vitamin C, conformer, hydrogen bound, polar group.

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C-09. Sinthesis and study of Cu(II) coordination compounds with ligands bazed on *o*-vanillin S-methylisothiosemicarbazone

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Thiosemicarbazones are known for their ability to work as polydentate ligands and for their coordination to various metal ions, which are present in biological systems. Thus, there are obtained coordination complexes that have a much greater drug importance than free ligands. Among these coordinating agents, the derivatives of salicylic aldehyde thiosemicarbazones and their copper (II) coordination compounds represent much interest, because of their antibacterial properties.

New copper (II) complexes (CuL^1 and CuL^2) have been obtained by interaction of *o*-vanillin S-methylisotiosemicarbazone with salicylic aldehyde (H_2L^1) or *o*-vanillin (H_2L^2) and copper acetate (in 1:1:1 molar ratio) in methanol. These compounds have been characterized by elemental analysis, IR spectroscopy and X-ray diffraction method (for CuL^1).

The structural data of CuL^1 confirms the condensation of *o*-vanillin S-methylisothiosemicarbazone with salicylic aldehyde, which results in obtaining a tetradentat bideprotoneted asymmetrical ligand. The ligand coordinates to the metal forming one five membered CuN_3C and two six membered $CuOC_3N$ metallocycles, with the 6, 5, 6 sequence (**Fig. 1**)

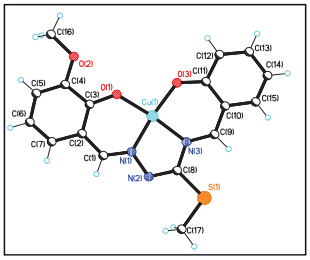

Figure 1. Structure of CuL^1 complex.

*Keywords***:** copper(II) complexes, S-methyisolthiosemicarbazone, *o*-vanillin

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C-10. Theoretical studies of several phenanthroline and benzimidazole derivatives

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The study present the results of theoretical investigation of spectral properties of two model compounds series: 2-[4-(1H-benzimidazol-2-yl)-pheyl]-1H-benzimidazole and 1,10-phenathroline derivatives using the Gaussian 09 suite programs with the time-dependent density functional theory (TD-DFT) and the b3lyp functional. The solvent effects on optical properties have been implemented through the PCM[23] model.

Keywords: TD-DFT, PCM, Vibrational spectra.

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C-11. The link between hyperconjugation and planarity - a DFT study of inorganic amines and isoelectronic compounds

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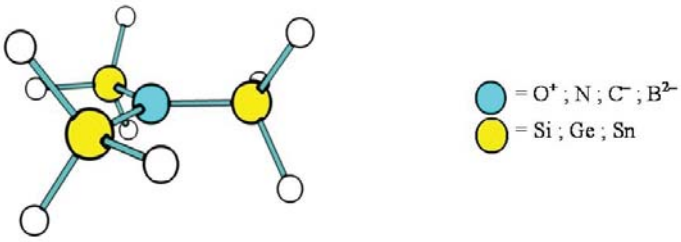
As far as 50 years ago, it was observed that the silicon derivatives of organic amines and ethers display much bigger angles than those predicted by the valence bond model. Also, the bond lengths are much smaller than the sum of covalent radii. The $p \rightarrow d$ interactions were initially proposed to account for abnormal structural features of molecules with 3r and 4th period elements, yet new interactions were proved to be more important.

This investigation focuses on the electronic interactions which are thought to be the main cause behind the planarity of inorganic amines. To make a consistent analysis, isoelectronic species (**Scheme** 1) were investigated at the DFT level of theory as correlation between geometrical parameters and electronic interactions emerged. Secondary interactions were evaluated quantitatively by using NBO techniques. To strengthen our hypothesis, we performed NBO DEL optimizations in the absence of hyperconjugative interactions. Furthermore, we investigated the case of boranes $(ER_3)_3B$ which serve as reference skeletons and also we studied the geometrical effects of adding one and two electrons.



Scheme 1.

*Keywords***:** DFT, NBO, hyperconjugation, planar geometry

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C-12. Synthesis and crystal structure of a Copper(II) oxalate oxamide dioxime complexe: Toward the development of new anticancer drug

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Motivated by the desire to create novel materials that could exhibit new properties and enable for new applications, the dimeric copper(II) complex $[Cu(C_2O_4)(H_2oxado)(H_2O)]_2$ (**1**), where H_2oxado is oxamide dioxime, has been synthesized in water and characterized by elemental and thermal analyses, IR spectroscopy, and single-crystal X-ray diffraction. Complex (**1**) is composed of two neutral $[Cu(C_2O_4)(H_2oxado)(H_2O)]$ entities (**Fig.** 1) connected by Cu–O bonds between oxalate oxygen atoms and copper(II) ions, thereby producing a centrosymmetric dimer, with the Cu(II) centers exhibiting a strongly distorted octahedral coordination. Neighboring dimers are hydrogen-bonded through O–H···O interactions leading overall to a layer structure (**Fig.** 2). In summary, the compound, $[Cu(C_2O_4)(H_2oxado)(H_2O)]_2$, is a novel dimeric layer-like copper(II) complex involving oxalate ions, oxamide dioxime and coordinated water molecules, with extensive hydrogen-bonding interactions stabilizing the 3-dimensional network. Its structural architecture is very similar to that of oxaliplatin. This compound presents potential anti-cancer properties.

With the synthesis of compound (**1**), the systematic synthesis of other members of this new family of materials becomes promising. A wide field of investigation is thus opened in the field of heteroleptic complexes of transition metals based on oxamide dioxime and oxalate ligands.

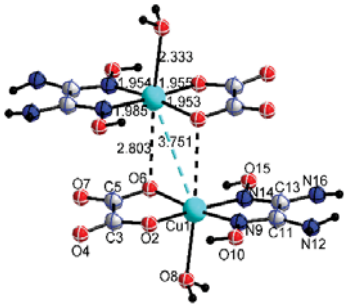

Figure 1. Ortep plot of complex **1.**

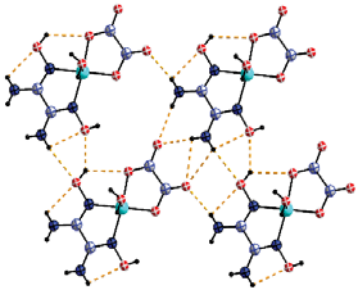

Figure 2. Hydrogen bonds (dashed lines) in compound **1.**

Keywords: Oxalate, Oxamide dioxime, Crystal structure, Cu(II) complex, Hydrogen bond

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P-01. Xerogels based on chitosan as delivery matrix for a potentially anticancer drug

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On the strength of a good compositional and morphological compatibility, the hydrogels are proper materials for controlled drug delivery, especially for local therapy. Their efficiency as drug matrix is increased by their intrinsic therapeutic action. In this view, the use of chitosan for such applications brings the advantage of biodegradability in the presence of the enzymes from tissues, which lead to non-toxic products.

In our previously work we found that the hydrogels based on chitosan and 5-nitrosalicylaldehyde show a good anticancer activity on HeLa cells and excellent *in vivo* biocompatibility on rats. On the other hand, our research revealed that *3,3'-((1,10-phenanthroline-2,9-dicarbonyl)bis(azanediyl))bis(1-methylpyridin-1-ium) trifluoromethane sulfonate* compound exhibits an excellent anticancer activity on several cell lines. Based on these studies, we found interesting to design new drug delivery systems based on these two components: the chitosan based hydrogel and phenanthroline based drug. The present study reports the preparation and properties of these new drug delivery systems. They were obtained by *in situ* hydrogelation and were characterized from structural and morphological points of view (**Fig**. 1). Their release kinetics has been investigated *in vitro* (**Fig**. 2).

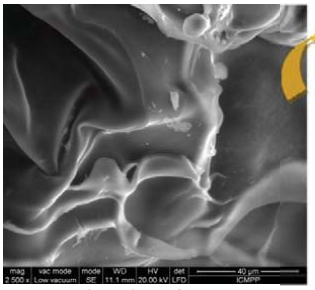

Figure 1. SEM imagine of A2F system.

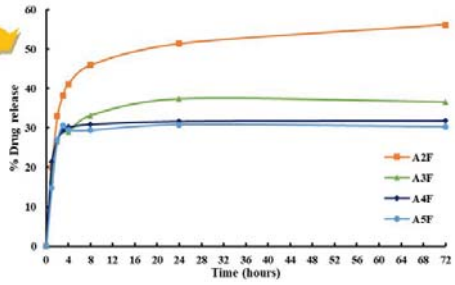

Figure 2. The drug release curves *in vitro*.

Keywords: chitosan based hydrogels, anticancer therapy, drug release.

Acknowledgement: This project has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement No 667387 WIDESPREAD 2-2014 SupraChem Lab.

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P-02. The relationship between some heavy metal ion and the amyloid peptide fragments

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Alzheimer's disease (AD) involves unusual conformational changes of amyloid-β peptides in the presence of metal ions, which result in peptide oligomerization and fibril formation and, finally, in the appearance of senile plaques and extensive neuronal loss. However, the formation of plaque-associated beta-amyloid peptide (Aβ) aggregation are less understood. Here, we report on the synthesis by SPPS according to Boc/Bzl strategy of some β-amyloid peptide fragments. Moreover, binding of metal ions to β-amyloid peptides was studied at two pH values. The results showed that Aβ(1-10) peptide binds only one Cu(II) ion at pH 7.4. The intensity of peak corresponding to metal-peptide complexes increases significantly with time and metal concentration. Aβ(1-16) peptide has bound one Cu(II) at 1:1 and 1:2 peptide-Cu ratio, and one and two Cu(II) at a peptide-Cu ratio of 1:10. Mass spectra showed metal-induced aggregation. During copper binding to N-terminal truncated β-amyloid peptides, no copper ion was found to bind to Aβ(31-40) at 1:1 or 1:2 peptide: Cu(II) ratios. There was found a close relationship between pH, metal concentration and the proportion of conformers of Aβ fragments. Indeed, copper ions bind strongly and specifically to β-amyloid(1-40) peptide and to its N- and C-terminal truncated versions. Our ESI-MS investigation showed that the C-terminal 31-40 sequence is not involved in copper binding. They also demonstrated that Zn(II) has lower affinity toward Aβ-peptides as compared to Cu(II). At 1:10 peptide-Zn(II), no peaks corresponding to the Aβ-peptides was detected by ESI-MS, where an aggregation process was suspected.

Keywords: Alzheimer, β-amyloid peptide, heavy metals, ESI-MS spectrometry

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P-03. Nutrient pollution of some lakes in Neamt County, Romania

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The complex limnological study on the natural lake ecosystem (Red lake) and the artificial ecosystems (Izvoru Muntelui and Bâtca Doamnei lakes) aimed at monitoring the total nitrogen concentration, total phosphorus, their dependence on oxygen concentration and the appreciation of eutrophication rate and rhythm in natural and anthropogenic impacts. Nutrient pollution and harmful algal blooms cause major environmental damage, though nitrogen and phosphorus are nutrients that are natural parts of aquatic ecosystems. However, nitrogen and phosphorus support the growth of algae and aquatic plants, which provide food and habitat for fish and smaller organisms that live in water. Too much nitrogen and phosphorus in water induce algae to grow faster than ecosystems can handle. Significant increases in algae harm water quality, food resources and habitats and decrease the oxygen that fish and other aquatic life need to survive. Large growths of algae are called algal blooms and they can severely reduce or eliminate oxygen in water causing the disease or even the death of the fish.

Based on analytical data obtained in each monitoring section, the surface water quality assessment has been done. The investigated indicators were: physical (temperature), chemical (pH, dissolved oxygen, total nitrogen, total phosphorus) and biological (numerical density, biomass and chlorophyll a). Total nitrogen and phosphorus as well as chlorophyll were spectrophotometrically determined. The dissolved oxygen was measured with a titrimetric method using sodium thiosulfate. The evolution of vegetal plankton in Red lake over time revealed a quantitative maximum of both analyzed indicators (numerical density and biomass) in October. Also, the chlorophyll indicator showed a peak in October. The lowest numerical densities and biomass were reported in March in the middle lake area, both for Batca Doamnei and Izvoru Muntelui lakes, as a result of increased values for total suspended matter, thus adversely affecting the development of phytoplankton. In brief the number of algal organisms and phytoplankton biomass were directly proportional to temperature and phosphorus concentration and inversely proportional to the dissolved oxygen and mineral nitrogen. Further research is needed to follow the eutrophication process of these lakes.

Keywords: limnology, monitorization, nitrogen, phosphorus, oxygen, biomass

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P-04. Synthesis and anticance evaluation of new 7-(pyridin-2-yl)-indolizine derivatives

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Cancer is a generic term for a large group of diseases that can affect any part of the body. Considerable efforts have been made in the last decades on the design and development of new anticancer drugs. Phenstatin and its derivatives are potential anticancer drug candidates according to their inhibitory properties on tubulin polymerization, cell growth and antivascular activity. Indolizine is an important structure in the design of new drugs, being known for a variety of biological activities, including anticancer, antibacterial, antifungal, anti-tuberculosis, anti-inflammatory.

Our work in this field was to synthesize several 7-(pyridin-2-yl)-indolizine as phenstatin analogues. The experiments are based on 3+2 cycloaddition reactions of the cycloimmonium ylides of 2,4'-bipyridin-1'-iu bromides to ethyl propiolate. The structures of the new compounds were proved by IR and NMR. All compounds were selected and tested by National Cancer Institute for their anticancer activity.

Keywords: cancer, Phenstatin, indolizine.

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P-05. Assessment of lake water chemistry using statistical analysis

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In the recent years, different statistical methods have been used to assess temporal and spatial variations in surface water quality and to identify potential sources of contamination. This study provides a description of a lake water chemistry using cluster and geostatistical analysis to identify the main sources of heavy metals and Piper diagram to define water type. The analysis involved 88 water samples collected from Podu Iloaiei Lake, Iasi, north-eastern Romania. Major ions (Cl^-, SO_4^{2-}, Na^+, K^+, Mg^{2+}, Ca^{2+}) and heavy metals (Cr, Cd, Co, Ni, Mn, Fe, Cu, Pb) were detected and quantified. Additionally, pH and electrical conductivity were determined. The Piper diagram revealed a mixed water type having no dominant group of ions, suggesting that water is exhibiting simple dissolution or mixing. Average milliequivalents percentage concentrations for groups of ions were 27.5% (Ca^{2+} + Mg^{2+}), 27.4% ($Na^+ + K^+$), 21.4% ($Cl^- + SO_4^{2-}$) and 23.7% ($HCO_3^- + CO_3^{2-}$). High contributions of Na^+ (47.2%) to total major cations, and of ($HCO_3^- + CO_3^{2-}$) (52.7%) to total major anions indicate that ion exchange processes can be involved in lake water chemistry. Pedologic contribution could be assigned by cluster analysis for Mg^{2+}, Ca^{2+}, Na^+, HCO_3^- and SO_4^{2-} while anthropogenic sources were merely attributed to heavy metals. Potential pH influence on Cd and Cr concentrations could be identified. Geostatistical analysis was applied for discrimination between point- and diffuse-sources of heavy metals contamination

Keywords: heavy metals, Piper diagram, cluster analysis, geostatistical analysis.

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

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P-06. Development of a new method for carbonyls analysis in the atmosphere by using solid phase derivatization coupled with GC/Ion Trap MS technique

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Volatile organic compounds, especially α-dicarbonyls, are both emitted directly in the atmosphere from biogenic or anthropogenic sources and formed *in situ* from the atmospheric oxidation of hydrocarbons arising from various sources. Methylglyoxal, an α-dicarbonyl extensively studied in the last recent years, seems to play an important role in the formation of Secondary Organic Aerosols (SOA). Derivatization methods are principal preparative techniques used for the analysis by gas chromatography or liquid chromatography of small volatile polar compounds.

The main objective of the present study was to develop a rapid and sensitive solid phase derivatization method for carbonyl compounds analysis in the gas phase by various chromatographic techniques. A new method based on solid phase derivatization has been developed in order to identify methylglyoxal formed in photo-oxidative gas-phase processes performed in an atmosphere simulation chamber. Derivatization technique consists on the reaction between the dicarbonyl compound with o-(2,3,4,5,6-pentafluorobenzyl)-hydroxylamine hydrochloride (PFBHA) retained into a C_{a8} solid phase. Separation and identification of the interest compound has been achieved on a HP-5 capillary column (30 m × 0.32 mm × 0.25 μm) by using gas chromatography tandem ion trap mass spectrometry with electron ionization.

The results obtained within the performed investigations help us to conclude that the developed method can be used to detect and quantify carbonyl products obtained by photo-oxidation of hydrocarbons in atmospheric simulation chambers or carbonyl compounds from ambient air samples.

Keywords: carbonyl compounds, methylglyoxal, derivatization, PFBHA, GC/Ion Trap MS.

Acknowledgements: The authors acknowledge the financial support provided by UEFISCDI within PN-III-P4-ID-PCE-20a6-0270 (OLFA-ROA) 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.

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P-07. New hybrid quinoline derivatives with imidazole skeleton

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The significance of quinoline heterocyclic nucleus in the field of medicinal chemistry research is worth mentioning. The wide range of its application has drawn an immense attention to the researchers to generate various quinoline derivatives, which may possess novel therapeutic efficacy.

Having in view the above consideration, our goal was to synthesize and characterize new compounds with the pyrrolo-benzimidazole structure having a quinolinic core. The strategy adopted for synthesis is straight and efficient, involving a four step setup procedure: *N*-acylation, *N*-alkylation, quaternization of nitrogen heterocycle and a [3+2] cycloaddition.

The structure of all new compounds was proved by spectral analysis (IR, H NMR, ^{3}C NMR, 2D-COSY, 2D-HMQC, 2D-HMBC).

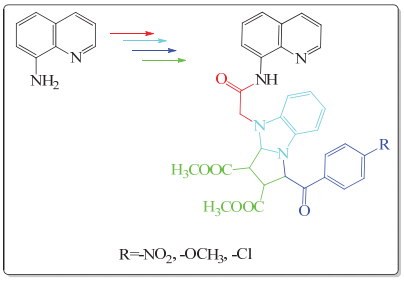

Figure a. Structure of new pyrrolo-benzimidazole compounds.

Keywords: quinoline nucleus, *N*-acylation, *N*-alkylation, dipolar cycloaddition

Acknowledgements: The authors thanks to the POSCCE-O 2.2.a, SMIS-CSNR a3984-90a, No. 257/28.09.20a0 Project, CERNESIM, for NMR measurements.

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P-08. Rate coefficient of the gas-phase OH radical initiated oxidation of 2,5-dimethylfuran at 298±2 K and atmospheric pressure

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Furans are directly emitted in the atmosphere from anthropogenic activities, fossil fuel combustion and biomass burning. These compounds have effect on the photooxidant budget and secondary organic aerosols (SOA) formation in the troposphere. Furans possess high atmospheric reactivity towards all important radical species.

Rate coefficient for the gas-phase OH initiated oxidation of 2,5-dimethylfuran (2,5-DMF) in synthetic air at 298±2 K and a000±5 mbar total pressure has been determined using the ESC-Q-UAIC chamber facility. Photolysis of methylnitrite at 365 nm was used for *in situ* OH radical formation. Fourier Transform Infrared Spectroscopy (FTIR) was used for monitoring the decay of the organic reactants. Relative kinetic technique has been employed in this study. Four reference compounds (furan, *E*-2-butene, isoprene and a,3,5-trimethylbenzene) have been used for the present kinetic investigations. The following average OH radical initiated reaction rate constant was obtained (in cm^3 $molecule^{-}$ s^{-}):

$k_{2,5\text{-}DMF+OH}$= (a.3a ± 0.a9) × a0^{-0}

Photolysis of 2,5-DMF has been corrected in this study. Control experiments for wall loss and photolysis were performed for all compounds involved in the kinetic study. Residence lifetime, reactivity trends and atmospheric implications will be discussed considering the obtained 2,5-DMF rate constant value. Although a comparison with the literature data is possible for one existing study only, however, the interpretation of the kinetic results with the value estimated from the Structure Activity Relationship method will be performed. These new results contribute to elucidate the gas phase chemical degradation mechanism of 2,5-dimethylfuran

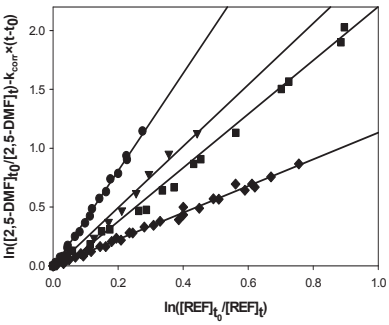

Figure 1: Plot of the kinetic data for the reaction of 2,5-DMF with OH radicals measured relative to isoprene (♦), *E*-2-butene (■), 1,3,5-trimethylbenzene(▼) and furan (●).

Keywords: furans, OH radical, gas-phase oxidation, ESC-Q-UAIC photoreactor

Acknowledgements: The financial support provided by UEFISCDI within the PN-III-P4-ID-PCE-20a6-0807 (IGAC-CYCLO), PN-III-P2-2.a-PED-20a6-a62a (CHARUSO) and PN-III-P2-2.a-PED-20a6-0924 (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

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P-09. Amphiphilic chitosan membranes for pain relief: preparation, characterization and *in vitro* lidocaine release

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Pain caused by skin injuries has a negative impact on he patient daily life. To reduce pain through a minimally invasive procedure, this work suggests the insertion of an analgesic ingredient into healing porous membranes. Lidocaine was chosen as a model compound due to its local anesthetic properties. Considering the anti-inflammatory, antifungal, haemostatic and mucoadhesive properties, chitosan was selected as drug delivery matrix. The presence of amine and hydroxyl groups in chitosan chemical structure allows the preparation of new biocompatible structures, ideal for drug release and tissue regeneration. Thus, succinic anhydride was introduced in the system mainly to increase the water solubility of chitosan, but also for the reduced toxicity and long-term retention in the body properties of the resulted N-succinyl chitosan materials. The hydrodynamic stability of the system was maintained by crosslinking with a,3-bis(3-glycidoxypropyl)-tetramethyldisiloxanes. Lidocaine was introduces *in situ* during the crosslinking process. Polymeric membranes were obtained by lyophilization. The structure and morphology of the membranes were determined by infrared spectroscopy (FTIR) and scanning electronic microscopy (SEM), respectively (**Fig.** a). Furthermore, absorption capacity, degradation degree in buffer solution and lidocaine release have been evaluated by *in vitro* experiments.

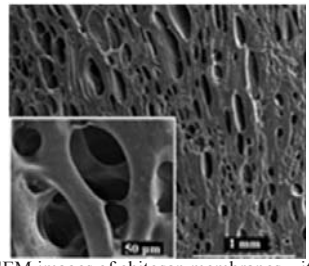

Figure a. SEM images of chitosan membranes with lidocaine.

Keywords: N-succinyl chitosan, lidocaine, analgesic effect

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P-a0. Sintering as sample dissolution procedure for complex matrices prior analysis of REEs by ICP-MS

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Rare Earth Elements (REEs) are embedded in most of modern technologies, especially in glass, catalysts, magnets and battery industries due to specific characteristics.

Inductively Coupled Plasma–Mass Spectrometry (ICP-MS) represents one of the most powerful technique used for REEs analysis. Samples to be analyzed by ICP-MS should always be in the liquid phase. Two main directions can be followed in order to transfer the analytes from the solid-state sample to the desired form. One implies samples digestion in the presence of strong concentrated acids, singular or in mixed forms, and the other suggests the use of a sintering agent and high temperature.

The present study was focused on sintering method with optimization of the sintering efficiency by adjusting the working temperature and process time. Fine powder of Na_2O_2 has been used as a sintering agent and HNO_3 3% in water solution was used for solubilization and dilution after completed sintering.

For less complex matrices temperatures in the 350 °C to 400 °C range proved to be suitable for complete dissolution of the solid samples. For more complex matrices, such as silicate-rich samples, temperature in the 460 °C to 480 °C range were determined as appropriate conditions to generate best results.

Time influence on the sintering process efficiency cannot be assigned at the present state due to furnace technical limitations. Sample cooling process is very slow. When operating at temperatures above 460 °C a gradient to 50 °C is obtained in a2 hours. Moreover, the temperature starts dropping only in 20 minutes after sintering program ends, regardless the last stage time assigned, i.e. 5, a0 or 20 minutes.

The procedure optimized in the present work has been successfully used to dissolute several samples prior to quantification of the REEs by ICP-MS. Effectiveness of the sintering process has been tested by using at least three different reference materials.

Keywords: Na_2O_2 sintering, Inductively Coupled Plasma - Mass Spectrometry, Rare Earth Elements

Acknowledgements: UEFISCDI within the European and International Cooperation - Horizon 2020, Project ENVIREE for the financial support.

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