

Abstracts

for

Faculty of Chemistry Conference

&

Mini-Hot-Conference:

„Recent Achievements in Organic and

Supramolecular Chemistry”

October 31 – November 02, 2013 Iasi, Romania

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Mini-Hot-Conference

„Recent Achievements in Organic and Supramolecular Chemistry”

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C 1. Photoswitchable Difurylethenes with Extended π -Systems for Applications in Single-Molecular Electronics

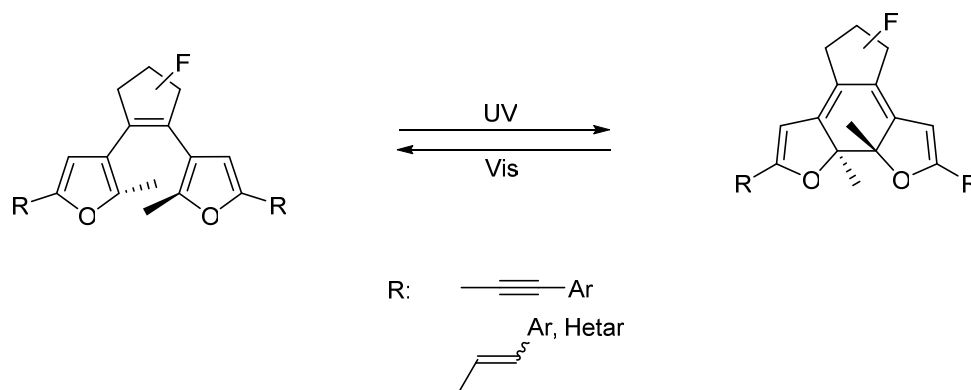
T. Huhn,¹ J. Wolf,¹ D. Sysoiev,¹ E. Scheer,² U. Groth¹

¹University of Konstanz, Department of Chemistry, D-78457 Konstanz, Germany

²University of Konstanz, Department of Physics, D-78457 Konstanz, Germany

Difurylperfluorocycloalkenes exhibit reversible photochromism with concomitant structural changes when irradiated with light of suitable wave length.¹ This cyclization-cycloreversion process changes the conjugation along the lateral direction of the molecule. Hence, those molecules have a great potential as switchable devices in the field of (single) molecular electronics,² for data storage and in materials sciences. Their application in single molecular electronics demands adjacently extended π -systems for bridging the gap between device and electrodes.

Here we will report on our endeavor of identifying suitable candidates serving as conjugated leads to "wire" difurylperfluorocycloalkenes. The difference between alkyne and alkene based wires and their influence on the switching behavior as well as the possibility to embed further functionalities are discussed.³



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C 2. Diamond D₅ allotropes

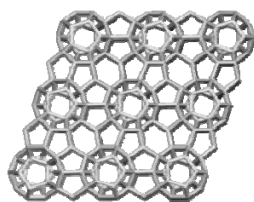
M. V. Diudea,^{1*} Cs. L. Nagy,² A. Bende²

¹Faculty of Chemistry and Chemical Engineering, “Babes-Bolyai” University, Arany Janos Str.,
400028 Cluj, Romania

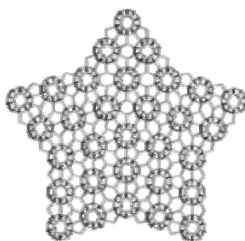
²Molecular and Biomolecular Physics Department, National Institute for R&D of Isotopic and Molecular
Technologies, Donath Street, No. 65–103, RO-400293, Cluj-Napoca, Romania

*E-mail address: diudea@chem.ubbcluj.ro

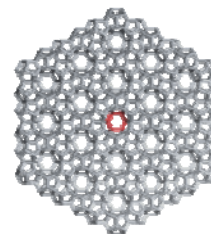
Carbon allotropes, designed as hyper-structures of the classical diamond and having a high percentage of sp^3 carbon atoms and pentagons, we generically call diamond D₅.¹ Five allotropes are discussed in this lecture: (i) a spongy net ($Fm-3m$ group); (ii) a dense hyper-diamond D₅, with an “anti”-diamantane structure (also known as *asmtn*, ZSM-39, or type II clathrate, of $Fd-3m$ group); (iii) the corresponding hyper-lonsdaleite L₅ (also known as *mgz-x-d*, of $P63/mmc$ group); (iv) a quasi-diamond which is a five-fold symmetry quasicrystal (of Pm group) with “sin”-diamantane structure and (v) a hyper-graphene, based on C₂₀ fullerene. The stability of the seed of D₅ and other substructures/intermediates/ fragments appearing in the construction/ destruction of D₅ net is evaluated on the ground of data computed at HF, DFT and DFTB levels of theory and by molecular dynamics simulation.



D₅Anti_333_860



D₅Sin_533_3305



D₅_6,3,1_882

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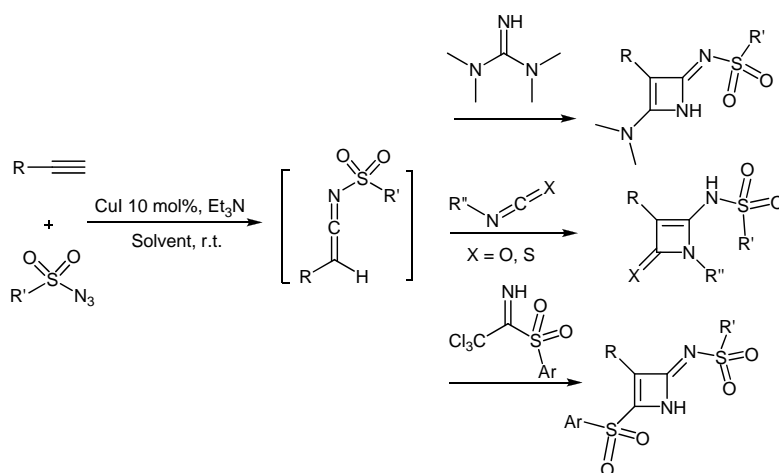
C 3. Sulfonoketenimides as key Intermediates for Tandem Synthesis of Organic Compounds

Issa Yavari

Department of Chemistry, TarbiatModares University, PO Box 14115-175, Tehran, Iran

E-mail address: yavarisa@modares.ac.ir

The sulfonoketenimide intermediates generated in the copper-catalyzed azide-alkyne cycloaddition reaction are trapped by various nucleophiles.¹ In this way, skeletons of various heterocycles and acyclic compounds were successfully synthesized.² Applying this strategy, we used amines, amidines, guanidines, and heterocumulenes to trap the *in situ* generated sulfonoketenimines and obtained highly functionalized four-to-six membered heterocycles and various open-chain heterodynes³ (Scheme).



Scheme

Various features of these transformations will be presented and discussed.

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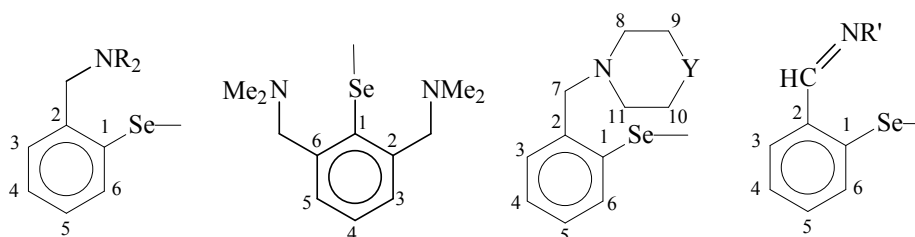
C 4. Structural diversity and chemical reactivity of organoselenium compounds

A. Silvestru

*Department of Chemistry, Babes-Bolyai University, Cluj-Napoca
E-mail address: ancas@chem.ubbcluj.ro*

Organoselenium compounds containing an intramolecular N→Se interaction have attracted an increased interest in the last two decades, mainly due to their stability as monomeric species and their applications in biology, asymmetric synthesis, catalysis or microelectronics. The presence of an organic group containing donor atoms capable for intramolecular coordination favoured also the isolation of monomeric metal chalcogenolates.

Our interests were focused on the synthesis and spectroscopic characterization of some organoselenium species of type R₂Se₂, RSeR', RSeX and RSeL, as well as compounds containing chalcogen – metal bonds (R = aromatic groups with pendant arms capable for intramolecular N→Se coordination, as depicted in Scheme 1, R' ≠ R, R' = organic group, X = halogen, L = dithioato ligand). The solution behavior of the reported compounds was investigated by means of multinuclear NMR spectroscopy [including ⁷⁷Se, ³¹P (where appropriate) and in some cases ¹⁵N]. VT NMR experiments were also performed in order to put in evidence the fluxional behavior concerning the intramolecular interaction in solution. Single-crystal X-ray diffraction studies revealed in most of the investigated compounds the presence of the intramolecular N→Se or N→M interaction.



Scheme 1

C 5. Self-assembled electron-rich receptors from molecular polygons to polyhedra

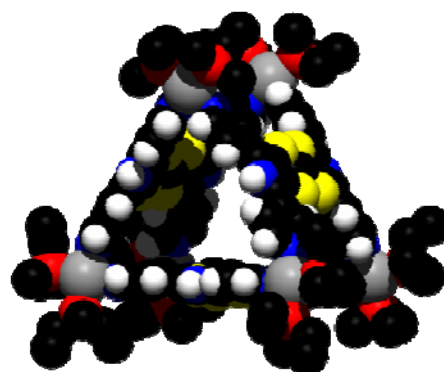
M. Sallé,* S. Goeb, V. Croué, S. Bivaud

Laboratoire MOLTECH-Anjou, Université d'Angers – CNRS 6200, 2 bd Lavoisier,
49045 Angers, France

*E-mail address: marc.salle@univ-angers.fr

Along the past decade, the metal-driven self-assembly methodology has allowed the preparation of a large number of molecular polygons (triangle, square,...) and polyhedra (cube, prism,...).¹

Nevertheless, very few of them are electro-active and present an electron-rich cavity. We have designed self-assembled discrete receptors based on the electron-donating tetrathiafulvalene unit (TTF).² In this presentation, the synthesis and the capability of this new class of receptors to bind electrode-deficient guests are described.



Keywords: metal-driven self-assembly, host-guest, TTF, redox

X-Ray Structure a TTF-based trigonal prism

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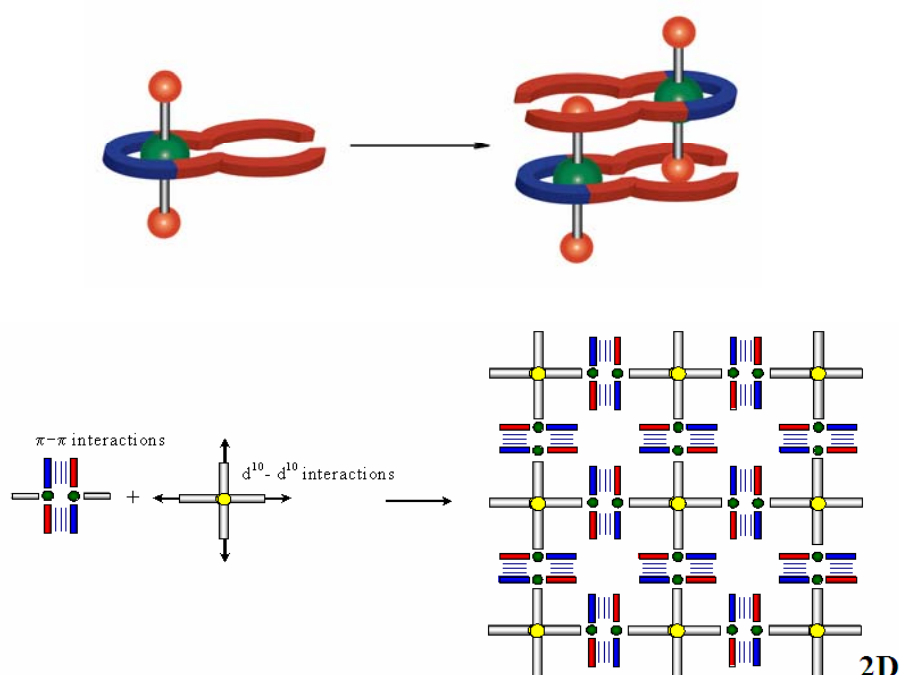
C 6. The interplay of non-covalent interactions in designing molecular crystals

Marius Andruh

Inorganic Chemistry Laboratory, Faculty of Chemistry, University of Bucharest,

Str. Dumbavaroşie nr. 23, Bucharest

Non-covalent interactions, together with coordination bonds, play a crucial role in stabilizing the solid-state architectures of inorganic molecular crystals containing metal ions. The present lecture focuses on several families of supramolecularmultimetallic systems which are assembled in solid-state by the convolution of various non-covalent interactions: (a) hydrogen bonds and p-p stackings; (b) p-p stacking and d^{10} - d^{10} (aurophilic or argentophilic) interactions; hydrogen bonds and d^{10} - d^{10} interactions. The leading roles are played by coordinative and hydrogen bonds, which are characterized by a strong directionality. On the other hand, it is shown that p-p stacking and metallophilic interactions can be manipulated in order to construct, in a rational way, interesting solid-state supramolecular architectures.



C 7. Design and Synthesis of Nitrogen-Containing Drimanic Compounds

Aculina Aricu

Institute of Chemistry, Academy of Sciences of the Republic of Moldova, Academiei str. 3,

MD- 2028, Chisinau, Republic of Moldova

E-mail: aricu_aculina@yahoo.com

Drimanes are useful natural compounds for synthesis of natural product hybrids for medicinal chemistry. The presence of nitrogen in the molecule is usually accompanied either by the appearance of a new activity or the intensification of original activity characteristic for the native drimanic sesquiterpenoids. This maintains alive the scientific interest in the synthesis of such compounds.

The presented data demonstrate that lately the vast series of known natural drimanes has been intensely supplemented by the nitrogen-containing metabolites of plant, microbial and animal origin. The unique structure of many so-called mixed metabolites, whose molecules include nitrogen, and their important biological properties make them attractive targets of the total synthesis. On the other hand, they can serve as plausible models for designing the molecules with useful functions.

Thus, the scientific interest remains opened to the exploration of new exciting facets of nitrogen-containing drimanic sesquiterpenoids.

The present communication put into discussion the recently elaborated methods for preparation of the nitrogen-containing drimanic compounds.

C 8. Bent Core Liquid Crystals

D. Scutaru^{*}, I. Carlescu

Department of Natural and Synthetic Polymers, "Gh. Asachi" Technical University of Iasi, Romania

**E-mail address: dscutaru@ch.tuiasi.ro*

Bent core liquid crystals represent a new class of non-conventional liquid crystals which explosively expanded in the last decade. Even the biaxial mesophase was predicted in the early 70^s, indubitable proofs of its existence appeared only in 2004. If compared with the conventional liquid crystals, the bent core class is expected to offer much faster responses to external stimuli.

The goal of our research deals with the synthesis, structural characterization and investigation of the liquid crystalline properties and thermal stabilities of some classes of bent core liquid crystals based on different disubstituted aromatic cores and containing azo-aromatic, ester or iminic linking groups. Mesomorphic properties were investigated by polarized optical microscopy and differential scanning calorimetry.

Structure–liquid crystalline properties relationships were established based on the correlation between structural parameters, determined by molecular mechanics and molecular dynamic simulations, and experimental data.

C 9. Helical (supra)molecular chirality in TTFs and derived materials

N. Avarvari

Laboratoire MOLTECH Anjou, UMR 6200 CNRS - Université d'Angers, UFR Sciences, Bât. K,
2 Bd. Lavoisier, 49045 Angers Cedex, France
E-mail address: narcis.avarvari@univ-angers.fr

Introduction of chirality into conducting systems is a topic of much current interest as it allows the preparation of multifunctional materials in which the chirality may modulate the structural disorder or expresses its influence through the electrical magneto-chiral anisotropy effect. The access to various chiral electroactive precursors for molecular conductors is therefore of paramount importance.¹ We have recently developed two new families of TTFs in which the chiral information is expressed in different ways. A first series is based on a C_3 symmetric core decorated with three TTF-amido-bipyridine fragments, which show self-assembling properties. One of the compounds provided for example an electroactive organogel and conducting nanowires.² Moreover, when substituted with chiral alkyl chains, these compounds show hierarchical chiral expression at nano- and meso-scale in solution and solid state.^{3,4} A second family of chiral TTFs we will discuss present helical chirality provided by helicene units fused with the TTF moiety.⁵

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C 10. Diversity oriented Generation of Quaternary Centers in Oxindoles

Fliur Macaev

Institute of Chemistry of the Academy of Sciences of Moldova,

str. Academiei 3, Chisinau, Moldova

E-mail address: flmacaev@cc.acad.md

Biologically active derivatives of oxindoles emerged recently as potent drug candidates. Thus, spirocyclooxindole exhibited nanomolar activity as an HIV-1 non-nucleoside reverse transcriptase inhibitor on both wild-type and drug resistant mutant viruses, showed promising antitumor activity and were also effective for treatment of obesity and diabetes. Stereochemistry of these compounds played a crucial role in their biological activity.

Currently, we have synthesized chemically and functionally diverse isatines scaffolds using this building block approach, and we are developing methodology for the synthesis of a plethora of diverse oxindoles scaffolds. Reactions of nucleophilic addition to atoms C1, C3, and nitrogen a typical to isatines due to its specific structure contained benzopyrrole ring with keto group, and amido group. Hemoselectivity of the reaction depends on nature and amount of reagent, nature of used solvent, and temperature: isatines can be considered as lactime or lactame. In the past, the main strategies for the construction of spirocyclopropyloxindole motif relied either on transition metal catalyzed cyclopropanation using diazooxindoles with a suitable alkene partner or addition of carbenoid species to unsaturated oxindoles. Both strategies produced various degrees of diastereoselectivity but so far were confined to racemic series. The major challenge in the synthesis of spirocyclopropyloxindole is to ensure a stringent control in the formation of the three contiguous stereocenters, which, in theory, can give rise up to 8 stereoisomers (4 diastereomeric pairs of enantiomers).

In our latest studies, we have discovered a formal [2+1] cycloaddition method for a highly enantio- and diastereoselective construction of spiro-cyclopropaneoxindoles featuring two quaternary centers. Magnetic ionic liquids were determined us to be useful as alternative simply catalysts in synthesis of chiral oxindoles. In addition, we have also developed several approaches for the incorporation of diverse substituent in oxindole scaffolds and their application in natural alkaloids, drugs and pro-drugs synthesis.

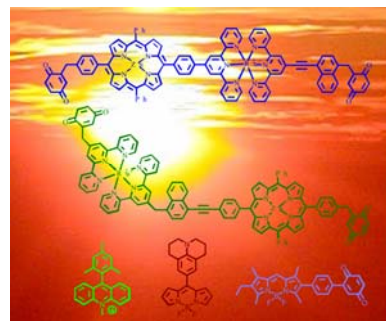
The features of such approach will be considered in this lecture.

C 11. Electron and Energy Transfer in Molecular Systems

Andrew C. Benniston

*Molecular Photonics Laboratory, School of Chemistry, Newcastle University,
Newcastle upon Tyne, NE1 7RU, UK
E-mail address: a.c.benniston@ncl.ac.uk*

Natural photosynthesis, the process whereby carbon dioxide is converted into carbohydrate and water is oxidised to molecular oxygen, has supplied the overwhelming majority of stored energy available on our planet. This stored energy, being mostly in the form of fossil fuels, had sufficed for billions of years and it is only very recently that the stocks of fuel have started to deplete at a rate faster than Nature can replenish. Indeed, our insatiable appetite for instant energy is set to expand at an unprecedented pace and our capability to generate carbon dioxide knows no bounds. The need to provide additional energy and to deal with the ensuing ecological problems associated with our current lifestyles pose tremendous challenges for the scientific community. The search for renewable energy supplies is now a major issue for all stable governments but it must be accompanied by new initiatives to reduce carbon dioxide levels and, in as much as it is possible, sequester CO₂ from the atmosphere. We already know that this is how natural photosynthesis works, but mimicking this on a grand scale is still at the development stage. Although there are many different facets to photosynthesis, two key parts are light capture and charge separation in which photons create redox equivalents to power the necessary reactions.



A popular approach by which to store the photonic energy has relied on the so called ‘cascade process’ in which charge is separated spatially by sequential electron transfer along an array of electron-affinic units. This method has been highly successful, but does rely on the synthesis of often complex superstructures that can be both time consuming and low yielding. Recently, it has been proposed that simple molecular dyads could do the same job if certain specific criteria are met. This talk will look into the specific strategies of using simple molecular dyads to store the photonic energy in the form of long-lived redox equivalents. The problems caused by competing charge recombination, triplet formation, exciplexes and side reactions from breakdown products will be mentioned in the context of Bodipy derivatives. The talk will also cover aspects of the ‘cascade’ approach and use of directional electron transfer to produce redox products. In addition, energy transfer in Bodipy derivatives both in solution and the crystalline state will be discussed in the framework of Förster theory where possible.

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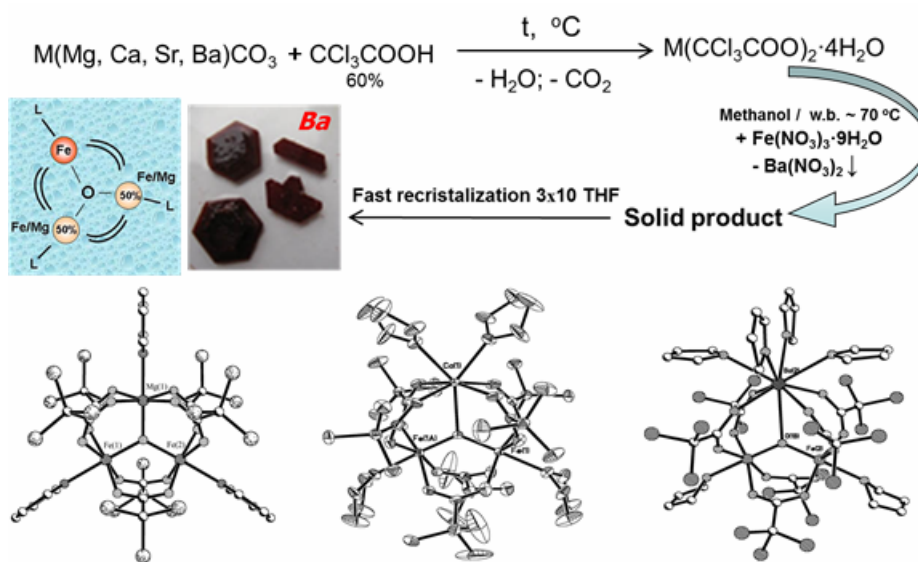
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C 12. Polynuclear metal coordination compounds: structure and properties

Constantin I. Turta

*Institute of Chemistry of the Academy of Sciences of Moldova, Academiei 3,
Chisinau-2028, Republic of Moldova*

Coordination compounds containing two or more metal atoms or ions in the intern coordination sphere are known as polynuclearmetal complexes. The two atoms may be held together through direct metal-metal bonds, through bridging ligands, or both. In our investigations we used as bridging ligands the mono- or polycarboxylate anions. This class of compounds has interesting geometrical structures (Figure), unusual magnetic (including single molecule magnets <SMM>), catalytic, biological active properties and precursors for nanomaterials.



Crystal structures of $[\text{Fe}_2\text{M}(\mu_3\text{-O})(\text{CCl}_3\text{COO})_6(\text{THF})_n]$,
where M=Mg(II), n=3 (left); M=Ca(II), n=4 (centre); M=Ba(II), n=6 (right).

Within this presentation it will be demonstrated some examples of all of these directions.

Acknowledgements: To SCRD of ASM, projects no. 11.817.08.22F.

C 13. Application of graph theory to genome sequencing

Ali Iranmanesh,* Nafiseh Jafarzadeh

*Department of Mathematics, Faculty of Mathematical Sciences
Tarbiat Modares University, P. O. Box: 14115-137, Teheran, Iran
E-mail address: iranmanesh@modares.ac.ir

Since Watson and Crick¹ proposed the helical structure of DNA, many problems about this structure have been posed. An important problem is how to read and recognize the primary structure of a DNA sequence. There are various methods for genome sequencing which use concepts of graph theory such as hybridization (SBH), fragment assembly and nanopore sequencing.

In this talk, at first we state a definition of DNA graph² and then discuss its properties and its role to determining the whole DNA structure and then will propose a new graph theoretical approach to genome sequencing by building DNA graphs.

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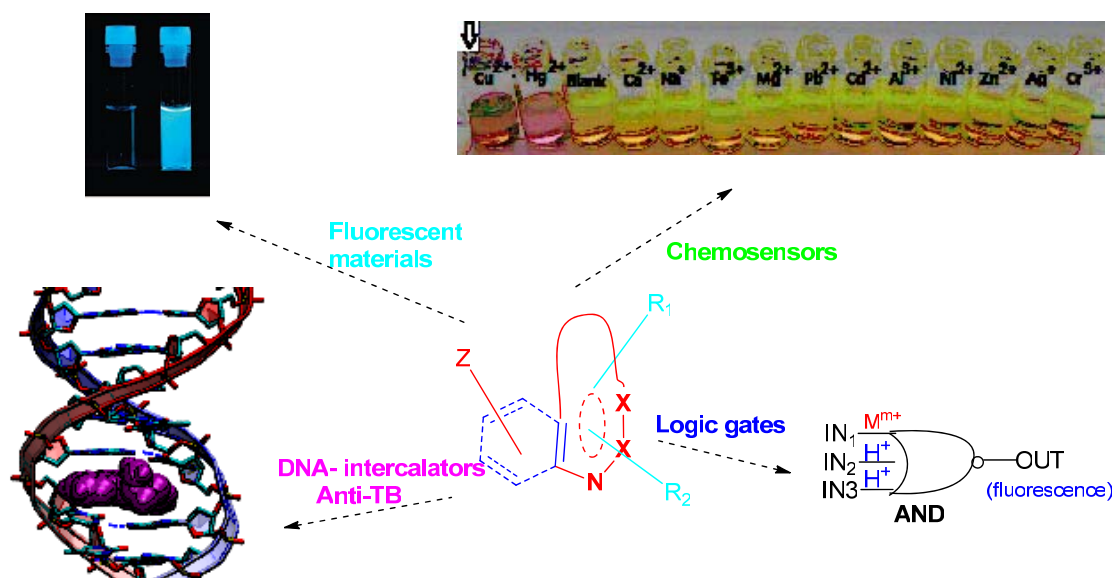
C 14. Azaheterocycles: an efficient way towards derivatives with multiple functions

Ionel I. Mangalagiu

*Department of Chemistry, "Al. I. Cuza" University of Iasi,
Bd. Carol I no. 11, 700506, Romania*

Azaheterocycles are fascinating compounds of invaluable potential for medicine, material science, agriculture, etc. Over the past decades advances in supramolecular chemistry have led to the development of miniaturized devices based on assemblies of single molecules that can execute functions on a "molecular level". Two of the most promising devices, widely discussed nowadays, are the fluorescent chemosensors and logic gates (or systems), the last one being the first step towards a "spearhead" in modern science, molecular computers.

Within this work we present some core results obtained by our group in the field of azaheterocycles derivatives as smart versatile building blocks for multiple tasks: new therapeutic agents, various sensor materials, logic gates, ionic liquids etc.



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CP. Comparative study of the acid hydrolysis of sucrose and cellobiose

Gheorghe Zgherea

*Department of Chemistry, Faculty of Sciences and Environment, Physics and Environment, „Dunarea de Jos”
University of Galati, 111, Domneasca Street, 800201 Galati, Romania*

Acid hydrolysis of the disaccharides are studied both for understanding the natural processes and to study compliance with the laws of chemistry. There are many studies dedicated to the acid hydrolysis of sucrose and cellobiose.^{1,4} They differ by the experimental conditions and the calculation modality of the concentration of each chemical species present in the reactant mixture.

For this comparative study, we considered that the most appropriate method for monitoring the reaction mixture is the value of its optical activity. The method was been used in several studies, with particular considerations.⁵ Thus, for the acid hydrolysis of sucrose, at any time, the concentration of sucrose is calculated by the simple relationship,

$$c_t = \alpha_t - \alpha_f$$

where α_f represents the optical activity of the mixture, when the total amount of sucrose has been consumed. In this paper, I consider that each sugar from the mixture has its own contribution to the value of the optical activity of the reactant mixture. Starting from that consideration, I have formulated an algorithm for calculating the molar concentration of each sugar from mixture. The most simple reactant mixture was used, the tube has a size of 200 mm, the catalytic agent is hydrochloric acid at a temperature of 20°C, without mechanical stirring; the initial concentration of disaccharide is very small, $c_0 = 0.2 \text{ g}/100 \text{ mL}$. Experimental determinations was made with a type AP-300 automatic polarimeter Atago, equipped with type HyperTerminal software installed on a Windows Vista computer. Experimental values are large populations, consisting of values measured after each interval of one minute. Physical quantities α_t were been converted, according to the algorithm proposed, in elaborated values c_t . They are used for studies the behavior of each disaccharide, such as: kinetic study, the calculation of the degree of hydrolysis and the study of the reaction mixture reached chemical equilibrium.

Each disaccharide is partially hydrolyzed, the degree of hydrolysis of sucrose is much greater than that of cellobiose, $\alpha_{\text{h zah}} \approx 90\%$, $\alpha_{\text{h cel}} \approx 25\%$. Each reactant mixture reaches a state of chemical equilibrium. As a result, there is no α_f value promoted in the literature. Each hydrolysis reaction takes place in steps of constant concentration. Acid hydrolysis of saccharose takes place with a very large number of steps of constant concentration, with lower amplitude. In contrast, in the case of acid hydrolysis of cellobiose, there are a very small number of levels of constant concentration, with higher amplitude. The experimental values obtained by sucrose hydrolysis study are very useful to calculate the kinetic parameters of the reaction; the reaction order value might calculate only by means of differential graphics.^{6,7}

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CO 1. The role of Mn^{2+} ion in the oscillating Briggs-Rauscher reaction

Gelu Bourceanu, Rodica Nitoi

Department of Chemistry, "Al.I.Cuza" University of Iasi, Romania

In this work we studied the role of Mn^{2+} ions in the mechanism and the production rate of I_2 and O_2 in the oscillating Briggs-Rauscher (BR) system $\{\text{IO}_3^-, \text{H}_2\text{O}_2, \text{H}^+, \text{Mn}^{2+}, \text{AM}\}$. Firstly it is analyzed the production rate of I_2 and O_2 in the sub-system $\{\text{IO}_3^-, \text{H}_2\text{O}_2, \text{H}^+, \text{Mn}^{2+}\}$, denoted BL+Mn. It is proved experimentally and by calculation that in this sub-system and implicitly in BR, an action of IO_3^- on Mn^{2+} takes place when the complex ion, $[\text{Mn}^{\text{II}} \text{IO}_3]^+$, is formed. This one reacts further with H_2O_2 leading to the appearance of the species $\text{Mn}^{\text{III}} (\text{OH})^{2+}$ and HO^\bullet , which initiate a set of radicalic reactions, with a fast production of the intermediate IO_2^\bullet and then of HIO_2 . The production of HO^\bullet radical was verified experimentally using a specific reagent, para-nitrozo-dimethyl-aniline, that captures HO^\bullet radicals.

CO 2. Chemicals in chemists' indoor dust. Case study for Department of Chemistry, "AL. I. Cuza" University of Iasi, Romania

Alin C. Dirtu,^{1,2} Adrian Covaci¹

¹Toxicological Center, Department of Pharmaceutical Sciences, University of Antwerp, Belgium

²Department of Chemistry, "Al. I. Cuza" University of Iasi, Romania

In order to evaluate the human exposure to organohalogenated chemicals (OHCs), multiple pathways are generally considered: food consumption, an important route for classical persistent organic pollutants (POPs), while more recently, indoor dust ingestion is acknowledged as an important route for exposure to flame retardants (FRs).¹

However, previous literature suggested that other chemicals, such as organochlorine pesticides (OCPs) are sometimes present in indoor dust at elevated levels.^{1,2} Therefore, in this study we have evaluated the levels and specific profiles of several organohalogenated contaminants, including: OCPs and polychlorinated biphenyls (PCBs) together with flame retardants (FRs), such as polybrominated diphenyl ethers (PBDEs), hexabromocyclododecanes (HBCDs), novel brominated FRs (NBFRs), and organophosphate FRs (OPFRs).

A number of 35 indoor dust samples were collected in 2010 from urban locations from Iasi, Eastern Romania. The dominant contaminants found in the samples were OPFRs (median sum OPFRs 7500 ng/g), but surprisingly, OCPs were also measured at high levels (median 1200 ng/g). Except for BDE 209 (median 250 ng/g), PBDEs were present in dust samples at relatively low levels (median sum PBDEs 6ng/g). PCBs were also measured at low levels (median sum PCBs 30ng/g), while NBFRs were only occasionally detected.

The results of the present study evidence the existence of a multitude of chemical formulations in indoor dust. FRs are usually associated to human exposure via ingestion of dust, but other chemicals, such as OCPs, are not commonly reported in such matrix. Although OCPs were found at comparable levels with OPFRs in Romanian dust, OCPs possess a higher risk to human health due to their considerably lower reference dose (RfD) values. Indeed, the OCP exposure calculated for various intake scenarios was only 2-fold lower than the corresponding RfD, while occasionally few samples showed OCPs exposure levels higher than their RfDs.

Therefore, the inclusion of OCPs as target chemicals in the indoor environment becomes important for countries where elevated levels in other environmental compartments have been previously shown.

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CO 3. Night chemistry of hydroxyl(methyl)benzenes: New directions in atmospheric chemistry at the A.I.Cuza University of Iasi

R. I. Olariu,¹ I. Barnes,² I. Bejan,^{1,2} C. Arsene,¹ D. Vione,³ B. Klotz,² K. H. Becker²

¹ *Department of Chemistry, "Al. I. Cuza" University of Iasi,
Carol I Bd. 11, 700506 Iasi, Romania*

²*Bergische Universität Wuppertal, FB C - Physikalische Chemie, Gaußstraße 20, D-42199 Wuppertal, Germany*

³*Dipartimento di Chimica, Università di Torino, Via Pietro Giuria 5, 10125 Torino, Italy*

Product analyses of the NO₃ radical-initiated oxidation of ortho-, meta- and para-cresols have been performed in two large-volume chamber systems QUAREC and EUPHORE. The reaction of O₃ with NO₂ was used for the in situ generation of NO₃ radicals in both QUAREC and EUPHORE chambers. The gas-phase reaction of all three cresol isomers with NO₃ yielded nitrocresols and HNO₃. Moreover, methyl-1,4-benzoquinone was detected and quantified from the reaction of NO₃ with ortho- and meta-cresol. The product formation yields determined in both chambers are compared with literature data. Based on all the identified products and yields, a gas-phase mechanism is proposed for the reactions of NO₃ with cresols. Atmospheric chemistry of these compounds is not fully understood. Thus, many additional studies will be necessarily for a better understanding. The newly reaction chamber and the state of art analytical instruments from CERNESIM centre at the A.I.Cuza University of Iasi will certainly bring new and important data relevant to the atmospheric chemistry of this compounds.

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CO 4. FESEM analysis for studying micro-nano-morphology features of LDH

Dragos Mardare,* Alexandru Buga, Gabriela Carja

¹“Gheorghe Asachi” Technical University of Iasi, Romania, Faculty of Chemical Engineering and Environmental Protection, Av. Prof. Dimitrie Mangeron, No.73, Iasi

* E-mail address: dragos.mardare@gmail.com

Layered double hydroxides (LDHs) are ordered layered compounds. Their application is related either to the capacity of changing interlamellar anionic species, by which they gained a wide usage area (from water purifying till control release drugs), either to their high specific surface, what made the LDH materials suitable as support for nanoparticles catalysts. The objective of our research was to study the micromorphology of some specific layered double hydroxides formulations such as MgLDH and ZnLDH as a function of the different physico-chemical parameters (e.g. synthesis method, raport between metal cations, synthesis temperature, rate of stirring, time of aging, and temperature of aging). The results point out that the micromorphologic features of the tested samples, such as the size of LDHs nanoparticles, their interconnection pattern and/or the interparticle sizes can be tailored as a function of optimized synthesis parameters.

Direct coprecipitation method and urea hydrolysis was used as synthesis methods. FESEM and XRD analyses were used like techniques for characterizing the structural and micromorphologic properties of the studied samples.

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CO 5. Investigation of ZnAl-layered double hydroxides for phenol photodegradation

C. M. Puscasu,^{1*} E. M. Seftel,² M. Mertens,³ P. Cool,² G. Carja¹

¹ Department of Chemical Engineering, Faculty of Chemical Engineering and Environmental Protection, Technical University "Gh. Asachi" of Iasi, Bd. D. Mangeron, 700554 Iasi, Romania

² Laboratory of Adsorption and Catalysis, Department of Chemistry, University of Antwerpen (CDE), Universiteitsplein 1, 2610 Wilrijk, Antwerpen, Belgium

³ VITO Flemish Institute for Technological Research, Boeretang 200, B-2400, Belgium

*E-mail address: magda.puscasu@yahoo.com

Phenol and phenolic compounds are major pollutants of aquatic environment. Phenol may occur in aquatic environment due to its widespread use in agricultural, petrochemical, textile, paint, plastic and pesticide chemical industries. Defined by a high carcinogenic and mutagenic potential, phenol poses a high risk to mammalian and aquatic life. Owing to its stability and solubility in water, its removal to a safety level (0.1 – 1.0 mg/L) is a difficult process. Consequently, a growing interest exists nowadays to develop new photocatalysts able to use the light energy for generating strongly oxidizing hydroxyl radicals ($\bullet\text{OH}$), which oxidize not only phenol but also a broad range of organic pollutants from wastewaters.

This work reports the synthesis and characterization of the nanostructured ZnAl-layered double hydroxides (LDHs) as novel nano-photocatalysts for phenol photodegradation under UV light.

The LDH layered matrix offers multiple advantages, such as manipulation of the brucite-like layer composition, but also the possibility to supply a good dispersion of the metal cations within the layers, which may act as charge separation centers enhancing the efficiency in subsequent applications.

These results open new opportunities in the development of nano-layered structures able to facilitate the photocatalytic degradation as "green" solution for removal of dangerous pollutants.

Acknowledgements: This work was supported by grant of the Romanian National Authority for Scientific Research, CNCS-UEFISCDI. Project number PN-II-ID-PCE-2012-4-0057 (contract number 75/2013). E. M. Seftel greatly acknowledges the Fund for Scientific Research – Flanders (FWO – Vlaanderen) for financial support.

CO 6. Oxidative dimerization of the salicylaldehyde thiosemicarbazone promoted by manganese ions: structure and magnetic studies

O. Palamarciuc,^{1,2*} M. Revenco,¹ R. Clerac,^{3,4} P. Bourosh,⁵ V. Cravtsov⁵

¹State University of Moldova, Mateevici 60, Chisinau, MD-2009, Moldova

²Department of Chemistry, "A.I.Cuza" University, Iasi, Romania

³CNRS, UPR 8641, Centre de Recherche Paul Pascal (CRPP), Equipe "Matériaux Moléculaires Magnétiques", 115 avenue du Dr. Albert Schweitzer, Pessac, F-33600, France

⁴Universite de Bordeaux, UPR 8641, Pessac, F-33600, France

⁵Institute of Applied Physics ASM, Academiei str., 5, Chisinau, MD2028, R. Moldova

*E-mail address: palamarciuc@usm.md

The coordination compounds of 3d elements containing as ligand thiosemicarbazide derivatives possess important biological, analytical and physical properties. The chemistry of manganese with this type of ligands is not much investigated. In this study we describe a new transformation of salicylaldehyde thiosemicarbazone (H₂L) promoted by manganese ions.

The state of salicylaldehyde thiosemicarbazone in solutions is depending on pH. The molecular form H₂L persists in acidic solution, the monodeprotonated form HL⁻ - in slowly alkaline solutions and the twice deprotonated form L²⁻ - in strongly alkalized solutions. The 3d elements prefer to form coordination compounds with the mono- or bis-deprotonated forms in neutral or alkaline media. The interaction of manganese(II) cations in neutral conditions gives rise to the formation of the complex Mn(HL)₂. If the reaction is realized in strongly alkalized solutions, the formation of a compound of composition Mn(L)·3H₂O was observed. The X-ray investigation of its structure demonstrated the formation of a binuclear complex of the composition [(MnL₂)(Mn(H₂O)₄)]·2H₂O (see figure 1 a). The investigation of the magnetic properties of the manganese(II) dimer shows a dominant antiferromagnetic interaction between paramagnetic centers.

The compound is not soluble in any solvent in inert atmosphere. In presence of the air oxygen, in the methanol solutions the oxidation of the central ions from Mn(II) to Mn(III), and an oxidative dimerisation of the coordinated salicylaldehyde thiosemicarbazone anion were detected. As a result, the formation of a new hexadentate bidentate ligand coordinated to two different manganese(III) ions has been observed. The manganese(III) units are assembled in polymer via μ₂-oxo bridges provided by methoxy groups coordinated to the metal ions. The coordination polyhedra of this complex is completed by methanol molecule coordinated in axial position. His general formula can be presented as [(Mn₂L)(CH₃O)₂(CH₃OH)₂]_n (see figure 1 b).

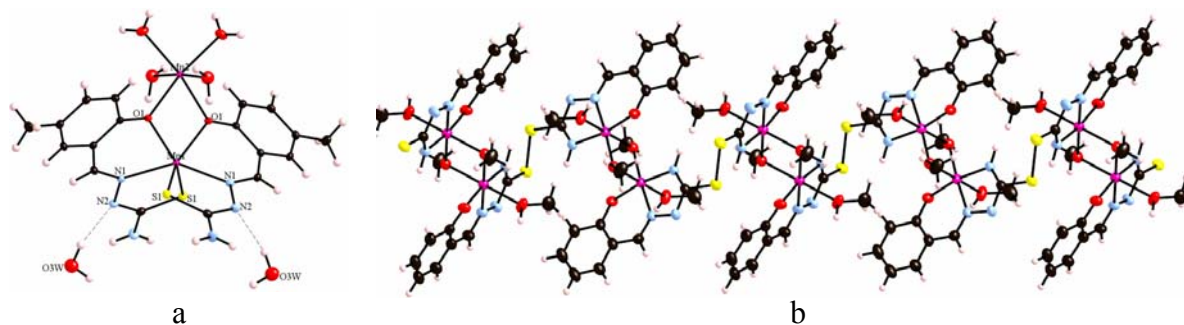


Figure 1: ORTEP representation of the manganese coordination compounds with salicylaldehyde thiosemicarbazone.

Low-temperature magnetochemical investigation of the polymer indicates a ferromagnetic interaction and a slow relaxation in ac susceptibility, confirming the SMM behavior of the complex.

CO 7. One step solution-combustion synthesis of $\text{La}_2\text{CoMnO}_6$ nanoparticles

Daniel Gherca,^{1*} Nicoleta Cornei,¹ Olivier Mentré,² Houria Kabbour,²
Sylvie Daviero-Minaud,² Nathalie Tancret,² Aurel Pui¹

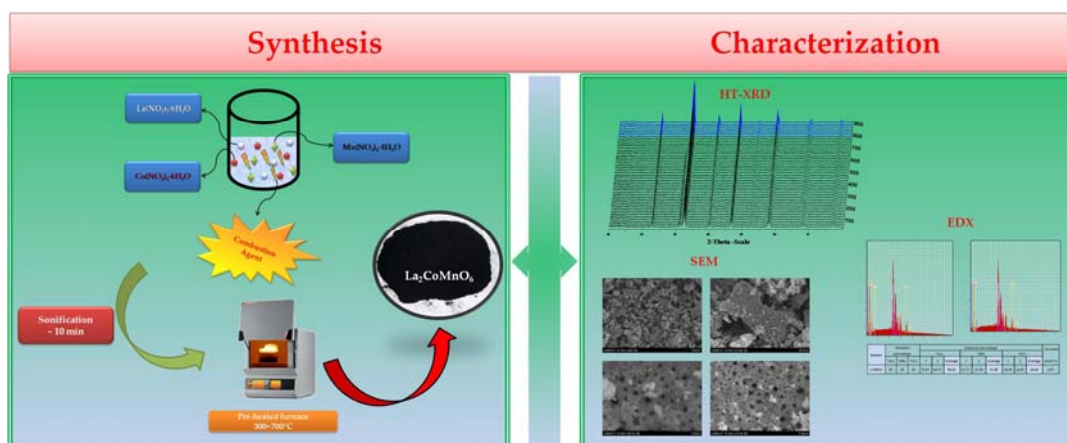
¹Department of Chemistry, "Al.I.Cuza" University, Iasi, Romania, Carol I Bd. 11, Iasi 700506, Romania

²Unité de Catalyse et de Chimie du Solide, Université Lille Nord de France, UCCS ENSCL/USTL F-59655
Villeneuve d'Ascq, CNRS UMR8181, France

*E-mail address: daniel.gherca@chem.uaic.ro

In the multifunctional magnetic materials field, the cobalt-based double perovskites systems, such as $\text{La}_2\text{CoMnO}_6$ (LCMO) are of great interest due to their functional properties like insulating behavior,¹ magnetodielectric effect² and colossal magnetoresistance.³ Several studies have shown that the physical properties of LCMO systems are related to the B cation site (Co/Mn) disorder, which depends on the cations stoichiometry and the synthesis conditions.⁴

In this study, we have prepared nanoparticles of the double perovskite $\text{La}_2\text{CoMnO}_6$ using an original one-step solution-combustion synthesis. The EDS spectra reveals the presence of La, Co, Mn and O elements and the SEM images showed a spongy aspect of the powder. In addition, the powder X-rays diffraction studies illustrate structural changes when increasing the synthesis temperature in the range 300-700°C. Finally, those characterizations were completed by physical properties studies trough magnetic measurements.



Scheme 1: Experimental process for one step solution-combustion synthesis of $\text{La}_2\text{CoMnO}_6$ nanoparticles.

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CO 8. Microwave Synthesis @ Anton Paar

Albert Istvan-GmbH

Few decades ago the application of microwaves in synthetic organic chemistry was just a curiosity more or less, but nowadays we are witnessing to an explosive growth in this field. This technology is used in both academic and industrial contexts. Especially in the pharmaceutical industry microwave assisted synthesis (MAOS) as laboratory practice become an accepted technology in just one decade. Today we can say that almost all pharmaceutical company and more and more academic laboratory actively using this technology for their research.

One of the barriers facing a synthetic chemist that contemplating to use microwave synthesis, apart from access to suitable equipment is to obtaining education and information on the fundamental principles and possible applications of this new technology.

This presentation is a short overview of the basics of the microwave assisted synthesis technology and an insight into the world of microwave synthesis at Anton Paar.

Starting with a short introduction to Anton Paar Company the presentation will lead through the basic principles of microwave heating the advantages of this technology and the range of equipment.

Complementary to this presentation participants will find a booklet in their conference folder with the title “A Chemist’s Guide to Microwave Synthesis” written by Dr. Jenifer M. Kremnsner and Dr. Alexander Stadler. In this small book you can read more details about the presented topics as well a comprehensive summary of application examples, a huge range of chemical reaction examples that already been successfully performed employing Anton Paar’s instrumentation.

Complementary to this presentation participants are invited to consult the booklet with the title “A Chemist’s Guide to Microwave Synthesis” written by Dr. Jenifer M. Kremnsner and Dr. Alexander Stadler. This small book shows more details about the presented topics and a comprehensive summary of application and a huge range of chemical reaction examples that already been successfully performed employing Anton Paar’s instrumentation as well.

SC 1. Flow reactor ozonolysis studies of selected dimethyl hexenes in the gas phase

Cecilia Arsene,¹ Romeo Iulian Olariu,¹ Marius Duncianu,² Veronique Riffault,² Alexandre Tomas²

¹Department of Chemistry, "Al. I. Cuza" University of Iasi, 11 Carol I, 700506 Iasi, Romania

²Universite Lille Nord de France, EMDouai, CE, F-59508, France

Alkene ozonolysis plays an important role in atmospheric chemistry. The process is assigned as a significant source of hydroxyl radicals in the atmosphere¹ or as a major route for carbonyls and carboxylic acids production.²

A kinetic and mechanistic investigation on alkene ozonolysis can be generally performed in environmental simulation chambers with large reaction times or, as it has been recently shown, in validated flow reactors at much shorter reaction times.³

In the present work, kinetic and product investigations were performed in a flow reactor on the ozonolysis of three selected dimethyl hexenes (trans-2,2-dimethyl-3-hexene (T22DM3H), trans-2,5-dimethyl-3-hexene (T25DM3H) and 2,3-dimethyl-3-hexene (23DM3H)). Absolute measurements of the rate coefficients have been performed by recording O₃ consumption in excess of organic compounds. Gas chromatography with flame ionization detector and thermal desorption system (GC-FID-TDS) was used in order to quantify alkenes concentrations.

For the investigated compounds the following ozonolysis rate coefficients are proposed (in cm³ molecule⁻¹ s⁻¹): $k_{T22DM3H} = (7.35 \pm 1.58) \times 10^{-17}$, $k_{T25DM3H} = (8.85 \pm 1.54) \times 10^{-17}$ and $k_{23DM3H} = (2.65 \pm 0.58) \times 10^{-16}$. The products of T22DM3H and 23DM3H ozonolysis have been investigated and branching ratios for the identified products have been determined.

Acknowledgements: C. Arsene and R. Olariu acknowledge the financial support provided by UEFISCDI within the PN-II-PCE-2011-3-0471 Project, Contract No. 200/05.10.2011.

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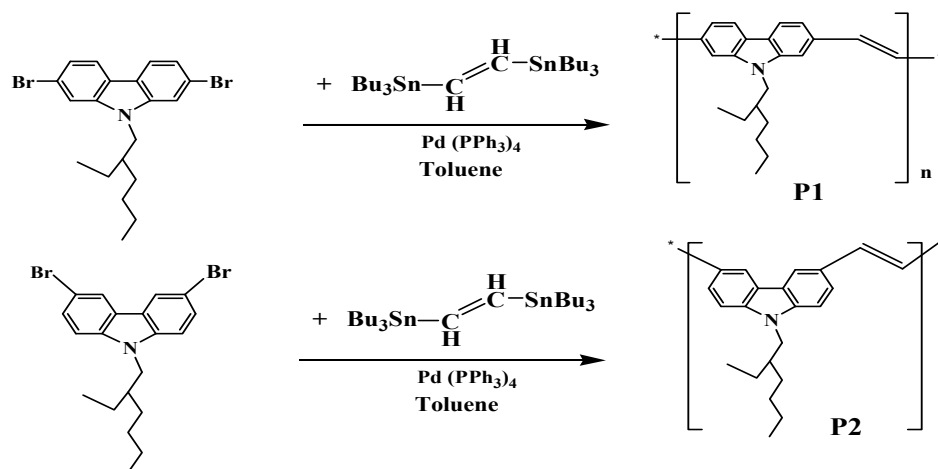
SC 2. Synthesis, spectral stability and photoluminescent properties of arylenevinylene polymers containing 2,7 - carbazolyldiyl and 3,6 – carbazolyldiyl moieties in the main chain

Ana-Maria Catargiu,* Loredana Vacareanu and Mircea Grigoras

“P. Poni” Institute of Macromolecular Chemistry, 41A Gr. Ghica Voda alley, Iasi-700487, Romania
E-mail address: anamaria.catargiu@icmpp.ro

Conjugated polymers are considered a very important class of electroactive and photoelectroactive materials by both academic and industrial laboratories. This development has been sustained by the clever utilization of a variety of synthetic tools as Stille, Kumada, Suzuki, Yamamoto coupling reactions, to prepare pure polymers with optimized physical properties. Polymers containing carbazole moieties in the main chain have attracted much attention due their unique properties such as photovoltaic cells, light emitting diodes, electrochromic materials, sensors and biosensors. Due to its structure, the carbazole molecule can be easily functionalized at (3,6), (2,7) or N-positions and then covalently bonded into polymeric systems, in the main chain as building blocks or as pendant units.

The aim of this study is to report the synthesis, the spectral stability and the photoluminescent properties of two polymers based on 2,7 or 3,6 - disubstituted carbazole units, connected by vinylene segments.



Scheme 1: The synthesis pathways for arylenevinylene polymers containing 2,7 - carbazolyldiyl and 3,6 – carbazolyldiyl moieties in the main chain.

Arylene vinylene polymers (P1 and P2) were synthesized by Stille coupling polymerization reactions. The structures of the polymers were confirmed by ^1H NMR and IR spectroscopy. The optical properties of the polymers were investigated by UV-Vis and fluorescence spectroscopies and the electrochemical behaviour of polymers was investigated by cyclic voltammetry.

Acknowledgements: The authors thank the Romanian National Authority for Scientific Research (UEFISCU) for financial support (Grant PN-II-ID-PCE-2011-3-0274 / Contract nr. 148/2011).

SC 3. Synthesis and characterization of poly(triphenylamine)-g-poly(ethyl methacrylate) using in tandem controlled radical polymerization and chemical oxidative polymerization

Oana Iuliana Negru, Mircea Grigoras

*Electroactive Polymers Department, "P. Poni" Institute of Macromolecular Chemistry, 41 Gr. Ghica Voda alley,
Iasi-700487, Romania
E-mail address: irimia.oana@icmpp.ro*

Synthesis of conjugated polymers has been extensively investigated in the last decades due to their scientific interest and wide range of applications. Among them, triphenylamine based polymers have good hole-transporting properties; high light-emitting efficiencies, photoconductivity, and photore-fractivity; and large two-photon absorption cross section and stabilization effect of high-spin polyradicals in organic magnets, which made them attractive materials for optoelectronic applications.¹⁻³ The aim of this communication is to present a new way to obtain processable polytriphenylamines having short saturated chains in every structural unit using in tandem controlled radical polymerization and chemical oxidative polycondensation. Thus, (4-diphenylamino) benzyl 2-bromo-2-methylpropanoate (ATRP initiator), it was used in the bulk ATRP polymerization of ethyl methacrylate to obtain oligomers with well-defined molecular weight, polydispersity, and chain-end functionality. The presence of triphenylamine moiety at one end of the macromonomer allowed the chemical oxidation of macromonomers to grafted polytriphenylamines having short polyethyl methacrylate grafts in every structural unit. An alternative way to obtain the same final grafted polytriphenylamines is based on synthesis of functionalised polytriphenylamine by chemical oxidative polymerization (interfacial and microemulsion techniques were studied) of (4-diphenylamino) benzyl 2-bromo-2-methylpropanoate followed by ATRP polymerization of ethyl methacrylate.

The graft polymer, poly(triphenylamine)-g-poly(ethyl methacrylate), was characterized *via* Fourier-transform infrared spectra (FTIR), ¹H and ¹³C-NMR and UV-Vis and fluorescence spectroscopy. The morphology was investigated using the atomic force microscope.

Acknowledgments: The authors thank the Romanian National Authority for Scientific Research (UEFISCDI) for the financial support (grant PN-II-ID-PCE-2011-3-0274, contract 148/2011).

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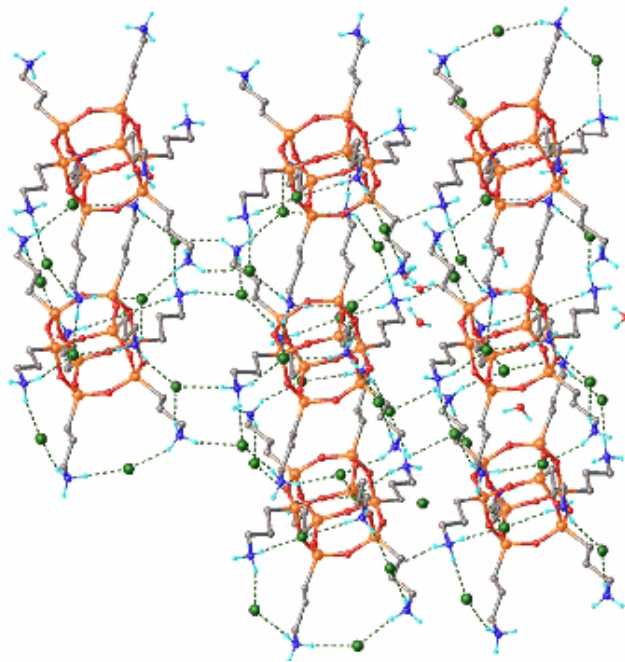
SC 4. New supramolecular polyhedral oligomeric silsesquioxanes: synthesis and structural characterization

Ana-Maria-Corina Dumitriu, Maria Cazacu, and Sergiu Shova

“Petru Poni” Institute of Macromolecular Chemistry, Aleea Gr. Ghica Voda 41A, 700487 Iasi, Romania

Completely condensed polyhedral oligosilsesquioxanes, (POSS) are constituted as a group of nanometer-scaled organosilicon compounds with well-defined and highly symmetrical structures, of the general formula $\text{Si}_n\text{O}_{3n/2}\text{R}_n$ or T_nR_n (where $n=4, 6, 8, 10, 12$, $\text{R}=\text{H}$, or any alkyl, alkylene, aryl, arylene, and their organofunctional derivatives). These compounds present organic-inorganic architectures, with inner inorganic frameworks consisting of silicon and oxygen atoms surrounded by easy-to-modify organic R substituents, in three dimensional arrangements.

The supramolecular structures were determined by X-ray single crystal diffraction, spectral (FTIR and NMR) methods, and elemental analysis. The thermal stability was evaluated by thermogravimetric analysis.



Depending on the functional group nature, the compounds are present either as singular or associated molecules, this behaviour being reflected in their thermal evolution. New functional organic-inorganic structures, with potential to be used in their present state or for further chemical modification, have been obtained.

Acknowledgements: This research was financially supported by European Regional Development Fund, Sectorial Operational Programme "Increase of Economic Competitiveness", Priority Axis 2 (SOP IEC-A2-O2.1.2-2009-2, ID 570, COD SMIS-CSNR: 12473, Contract 129/2010-POLISILMET).

SC 5. The synthesis particularities of some coordination compounds obtained using a series of new amide derivatives as ligands containing imidazole and benzimidazole

Irina Voda

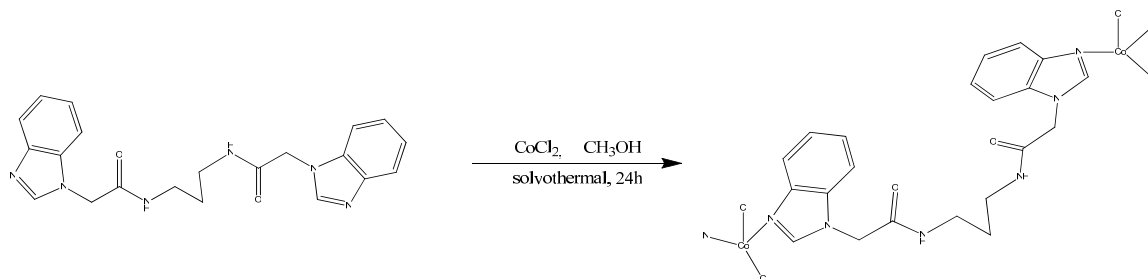
*Institute of Chemistry of the Academy of Sciences of Moldova, 3, Academiei str., MD-2028 Chisinau, Moldova
e-mail: iravoda@gmail.com*

Six newly synthesized amide derivatives: (N,N'-(ethane-1,2-diyl)bis(2-(1H-imidazol-1-yl)acetamide) **(1)**, N,N'-(propane-1,3-diyl)bis(2-(1H-imidazol-1-yl)acetamide) **(2)**, N,N'-(butane-1,4-diyl)bis(2-(1H-imidazol-1-yl)acetamide) **(3)**, N,N'-(ethane-1,2-diyl)bis(2-(1H-benzimidazol-1-yl)acetamide) **(4)**, N,N'-(propane-1,3-diyl)bis(2-(1H-benzimidazol-1-yl)acetamide) **(5)**, N,N'-(butane-1,4-diyl)bis(2-(1H-benzimidazol-1-yl)acetamide) **(6)** were used to obtain coordination compounds with some *3d* metals.

The experiments showed that a huge role in formation of the pure complexes play some important factors as:

- 1) the salts that were used in the synthesis (nitrates, chlorides, acetates, perchlorates);
- 2) the solvent (water, alcohols, DMF);
- 3) the reaction temperature.

The most efficient method of synthesis was demonstrated to be solvothermal one, using cobalt(II) chloride, methanol as solvent and a relatively low temperature (120°C). A 24 hours reaction gave clear blue crystals in a good yield of an one dimensional polymer with a „zig-zag” structure as shown in the following scheme:



Scheme 1: Scheme of synthesis of a coordination compound using cobalt (II) chloride and **(5)** in methanol.

When the water is used as solvent and the reaction temperature is higher than 120°C, the ligands appear to be unstable, the hydrolysis is taken place and only the resulting compounds are linked to the metal ions. The structures and compositions of the compounds were proved by physico-chemical methods (IR, XRD) and elemental analysis.

Acknowledgements: Present work was supported by PCAP FP7-PEOPLE-2009-IRSES, Nr. 246902 and Institutional Fundamental Project 11.817.08.22F.

SC 6. Synthesis, spectral characterization, and x-ray structure of a new coordination compound of cobalt(II) and *n,n'*-(butane-1,4-diyl)bis(2-(1*H*-benzimidazol-1-yl)acetamide)

Irina Voda,¹ Constantin Turta,¹ Gheorghita Zbancioc,² Costel Moldoveanu,² Mircea Odin Apostu,² Ionel I. Mangalagiu^{2*}

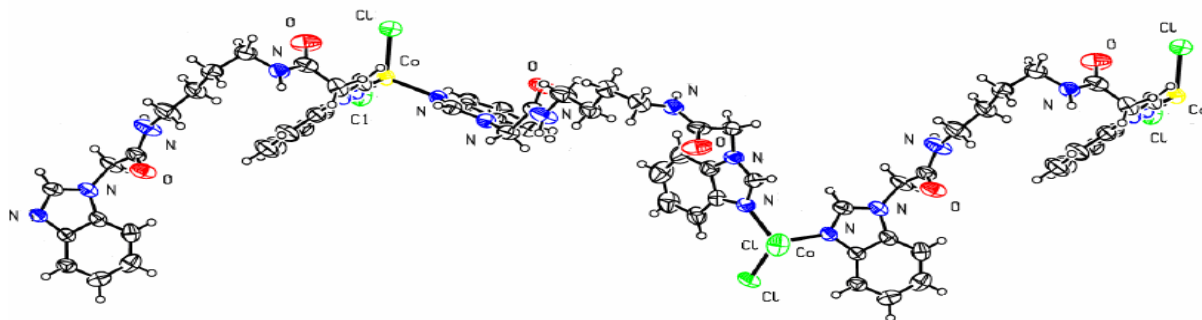
¹ Institute of Chemistry, Academy of Sciences of Moldova, 3, Academiei str., MD-2028 Chisinau, Moldova;

² Al. I. Cuza University, Organic Chemistry Dep., 11, Carol I Bd., 700506 Iasi, Romania

*E-mail address: ionelm@uaic.ro

Amides are important building blocks in both Nature and in macrocyclic chemistry.¹ Our aim was to synthesize coordination compounds of *3d* metals with some new amide derivatives that were so far prepared from imidazole/ benzimidazole and chloroacetamides (*N,N'*-(ethane-1,2-diyl)bis(2-chloroacetamide), *N,N'*-(propane-1,3-diyl)bis(2-chloroacetamide), *N,N'*-(butane-1,4-diyl)bis(2-chloroacetamide)) by an adaptation of reaction pathways known in the literature.²⁻³

The key role of obtaining crystalline compounds was found and we were able to prove the structure of the complexes not only by elemental and IR analysis, but also using X-ray diffraction. One can see from the figure below that every cobalt ion link together two units of *N,N'*-(butane-1,4-diyl)bis(2-(1*H*-benzimidazol-1-yl)acetamide) through nitrogen atoms from benzimidazole to give a continuous chain with spiral shape. There is no any coordination bond to amidic groups from this ligand.



The IR spectrum of the compound displayed bands at 3276 cm⁻¹ corresponding to $\nu(\text{N-H})$. Moderate intensity bands at 3109 cm⁻¹, and weak bands at 2960-2800 cm⁻¹ may be assigned to $\nu_{\text{asym,sym}}(\text{CH})$ of benzimidazole rings and CH₂ groups. The strong absorption band at 1654 cm⁻¹ is assigned to $\nu(\text{C=O})$ vibrations. The absorption bands in the range 1294-774 cm⁻¹ may be assigned to breathing vibrations, and C-H in/out of plane deformation of the benzimidazole rings. At 491 cm⁻¹ there is a band corresponding to $\nu(\text{Co-Cl})$.

Other attempts of obtaining coordination compounds are on the way.

Acknowledgements: Present work was supported by PCAP FP7-PEOPLE-2009-IRSES, Nr. 246902 and TE/0010 - 79/05.10.2011.

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SC 7. Synthesis and biological evaluation of new indolizine derivatives as antitumoral agents

Liliana Lucescu, Alina Ghinet, Dalila Belei, Elena Bicu

Department of Chemistry, "Al. I. Cuza" University of Iasi, Bd. Carol I, 11, 700506, Romania

Indolizine display a broad spectrum of potential pharmacological activities :anticancer, antibacterial, antifungal, anti-cholinergic and anti-histaminic, anti tubercular activity.¹

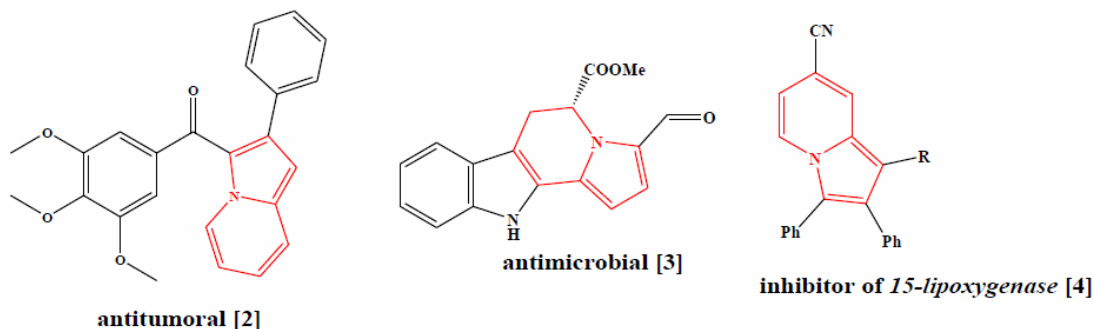


Figure 1: Indolizine derivatives with biological properties.

Phenstatin is a known inhibitor of tubulin polymerization. In the literature, there are many modulation described on the phenstatin skeleton.² In order to preserve the pharmacological properties and remove the side effects, we propose the synthesis of some new phenstatin analogues containing an indolizine unit. Therefore, we were interested in the replacement of the B ring of parent phenstatin by an indolizine core and the modification of substituents on ring A (Figure 2).

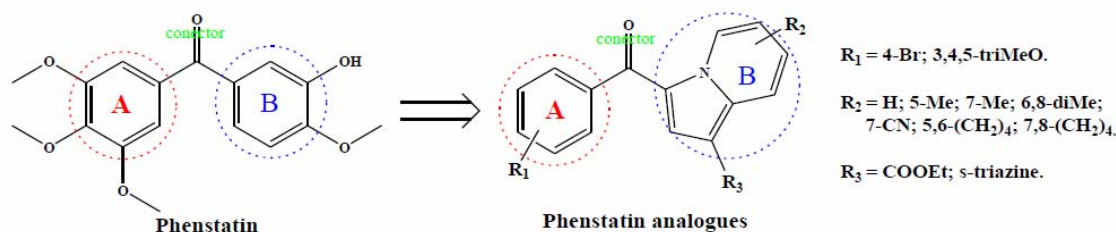


Figure 2: Design of some new phenstatin analogues.

All new synthesized compounds were characterized by IR, RMN and biologically evaluated on 60 tumor cells lines by National Cancer Institute (USA). The best results were registered on HOP-62 (lung cancer), SNB-75 (CNS cancer) and SK-OV-3 (ovarian cancer) cells lines.

Keywords: indolizine, phenstatin, atitumoral activity, tubuline.

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SC 8. New heterocyclic derivatives bearing amino acid units recognized by the protein farnesyltransferase

Gina-Mirabela Dumitriu,¹ Dalila Belei,¹ Alina Ghinet,^{1,2} Elena Bicu¹

¹Department of Chemistry, “Al. I. Cuza” University of Iasi, Bd. Carol I nr. 11, 700506 Iasi, Romania

²UCLille, EA 4481 (GRIIOT), Laboratoire de Pharmacochimie, HEI, 13 rue de Toul, F-59046 Lille, France

Farnesyltransferase (FTase) is a metalloenzyme which needs a zinc or a magnesium atom to be activated; it has a heterodimeric structure and is constituted by two sub-units: α and β . This metalloenzyme recognizes the CaaX unit from the C-terminal position of substrate proteins, where C is a cysteine residue, a is an aliphatic aminoacid, and X is a cysteine, a serine, a methionine, a glutamine, a valine or an alanine.^{1,2}

The inhibition of this enzyme blocks the farnesylation process; compounds with these properties are known as inhibitors of farnesyltransferase (InhFTase) and used in chemotherapy.³

New inhibitors of human FTase have been identified and described recently^{4,5,6} with IC_{50} values in the low micromolar range (Figure 1).

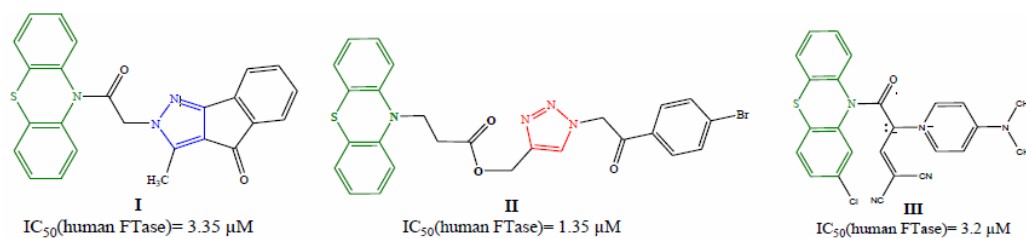


Figure 1: Inhibitors of human farnesyltransferase.

In order to continue our previous studies and identify new human FTase inhibitors, we synthesized, characterized and tested new series of nitrogen-heterocyclic derivatives bearing amino acid residues at the lateral chain (Figure 2).

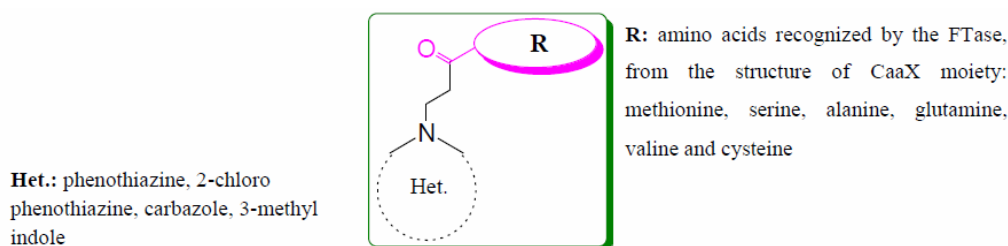


Figure 2: New heterocyclic derivatives with amino acids recognized by the FTase.

All synthesized compounds have been characterized (IR, ¹H and ¹³C-NMR). And the human FTase bioassays showed us promising results.

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SC 9. Synthesis and antiproliferative activity of new indolizine derivatives

Carmen Dumea, Dalila Belei, Alina Ghinet, Elena Bicu¹

Department of Chemistry, "Al. I. Cuza" University of Iasi, 11th Carol I Bvd., 700506 Iasi, Romania

The indolizine nucleus is often found in natural products, respectively in various derivatives with biological properties,¹⁻² their activities being closely associated to the nature of substituents from positions 1 and 3 of this heterocycle.

Usually, indolizine derivatives are obtained by [3+2] dipolar cycloaddition reactions between an 1,3-dipole and a dipolarophile (alkene or alkyne).³

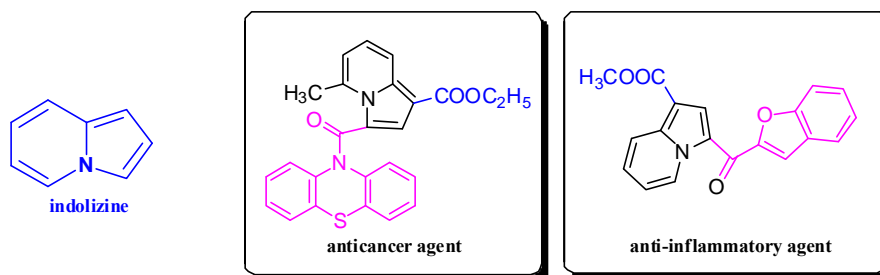
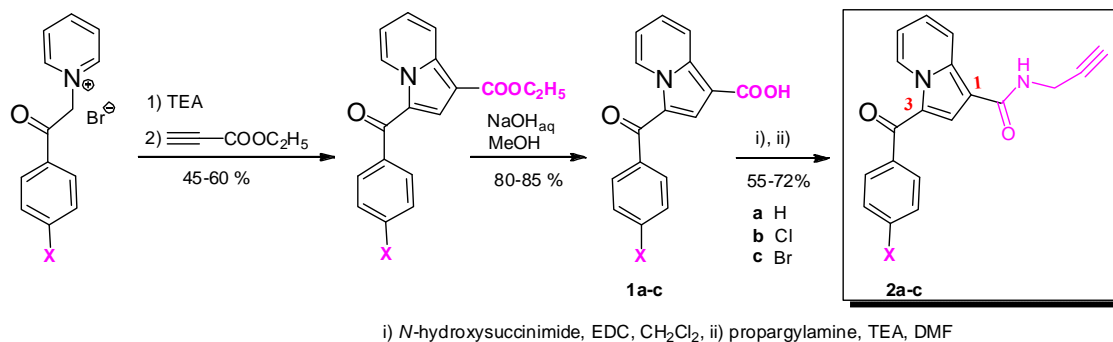


Figure 1

Starting from recent results reported in the indolizine class, the current study focuses on the synthesis, characterization and testing of new indolizine derivatives, analogues to phenstatin, presenting a propargyl moiety at the position 1 of the indolizine ring. The syntheses were performed in three steps (Scheme 1), propargyl derivatives **2a-c** were obtained in good yields.



Scheme 1

For biological evaluation of indolizine compounds **1a-c**, respectively **2a-c**, we considered their potential anti-tumor activity; the obtained results are promising.

Keywords: indolizine, propargyl derivatives, phenstatin.

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SC 10. Mass spectrometric based methods for rigorous characterization of antibody-antigen interaction

Claudia Andries,^{1,2} Laura Ion,^{1,2} Stefan Slamnoiu,² Michael Przybylski,²
Brindusa Alina Petre^{1,2}

¹*Department of Chemistry, “Al.I.Cuza” University of Iasi, 11 Carol I, Romania*

²*Laboratory of Analytical Chemistry and Biopolymer Structure, University of Konstanz, Germany*

It is well known that the nitration of tyrosine residues is an oxidative post-translational modification, which occurs both under physiological conditions and within pathophysiological processes associated with oxidative stress such as diabetes, chronic hepatitis, atherosclerosis, Alzheimer's and Parkinson diseases, asthma and lung disease. The identification of tyrosine nitration in proteins from biological samples is a challenging task for mass spectrometry because of the low levels of nitration in organism. Sputum samples from cystic fibrosis patients were analysed in order to identify nitrated proteins. Proteins from sputum were separated by 2D-Gel Electrophoresis, followed by the detection of nitrated proteins using immuno-analytical methods such as Western Blot, which employ specific anti 3-NT antibodies. In our case a false-positive identification of nitration was obtained; in fact, hydroxyl-tyrosine modifications were found. Because of this, the specificity of the 3NT-antibody was tested using synthetic model peptides with either nitro-tyrosine or hydroxy-tyrosine in their sequence. The peptides were synthesised by solid-phase peptide synthesis (SPPS), purified by RP-HPLC and characterized by ESI and MALDI Mass Spectrometry. The Surface Acoustic Wave (SAW) has been successfully applied for determination of binding affinities and specificities of the synthetic peptides with the modified tyrosine to monoclonal anti-3NT-antibodies. SAW technology in comparison with immuno-analytical techniques is more useful because of the direct and rapid determination of association/dissociation constants with small sample amounts.

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SC 11. Spectrophotometric methods applied in the investigation of corn meals and zeins

Sabina Bancila,¹ Brindusa Alina Petre,¹ Manuela Murariu,² Catalina Ciobanu,¹
Gabi Drochioiu^{1,2}

¹ Department of Chemistry, "Al. I. Cuza" University, 11 Carol I, Ro-700506 Iasi, Romania,

² Petru Poni" Institute of Macromolecular Chemistry, Romanian Academy, 41A Grigore Ghica Voda, Alee, Iasi-700487, Romania

Cereals are abundant and renewable resources, which are frequently processed into various food and industrial products. Some representative examples are the starch, sweeteners, corn oils, beverage and industrial alcohol, respectively the ethanol used as a fuel. Zein, a protein located in maize endosperm is a major co-product of the bio-fuel industry with different application in (i) biomedicine as drug-delivery compound, drug capsules that release in the body; (ii) industrial production of bioplastic, paper coating, and food products (chewing gum). Generally, zein contains around 21.4% glutamine, 19.3% leucine, 9.0% proline, 8.3% alanine, 6.8% phenylalanine, 6.2% isoleucine, 5.7% serine, and 5.1% tyrosine.^{1,2} However, it is deficient in tryptophan, lysine and methionine. In the dry-milling ethanol process, ethanol is used as a solvent to extract zein from dry-milled corn.³

In this paper, zein extraction from dry-ground whole corn as well as flour with different grain sizes was investigated. Hard grains deposit a greater number of protein bodies and a larger amount of prolamin (zein) than soft grains. A spectrophotometric method which quantifies the zein content of corn meals as well as of alcoholic extracts was implemented. Extraction studies of zeins have been performed over a temperature range from 25 to 60 °C using 70-95% aqueous ethanol. Moreover, the extraction was followed under both ultrasound and normal conditions.

Acknowledgements: Financial support of Romanian-American Foundation – ARTIE POC program (Qualifarin project).

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P 1. Synthesis and characterization of silver nanoparticles in the presence of pullulan and 6-carboxyl pullulan

Alina Spatareanu,¹ Liviu Sacarescu,¹ Cristina Rimbu,² Valeria Harabagiu,¹ Sergiu Coseri¹

¹“Petru Poni” Institute of Macromolecular Chemistry of Romanian Academy, 41 A, Gr. Ghica Voda Alley, 700487, Iasi, Romania

² University of Agricultural Sciences and Veterinary Medicine, Faculty of Veterinary Medicine - UASVM Iași, Aleea Mihail Sadoveanu nr.8, 700489, Iași, Romania

In the last decade, a large development in nanoscience and nanotechnology filed occurred due to the interest for the unique chemical and physical properties of the nanomaterials. Metal nanoparticles display special effectiveness¹ in different applications.²⁻⁴

In this work, pullulan has been oxidized in TEMPO-sodium hypochlorite-sodium bromide system, to convert primary OH groups to carboxylic groups. Afterwards, both raw and carboxylated pullulan have been used as mediators for the silver nanoparticles formation (AgNPs). The influence of the negatively charged groups on size, shape and morphology of the AgNPs was investigated. We have used energy-dispersive spectroscopy (EDX), X-ray diffraction (XRD), transmission electron microscopy (TEM), UV-VIS spectroscopy and FT-IR to characterize the formation of AgNPs obtained, see Figure 1.

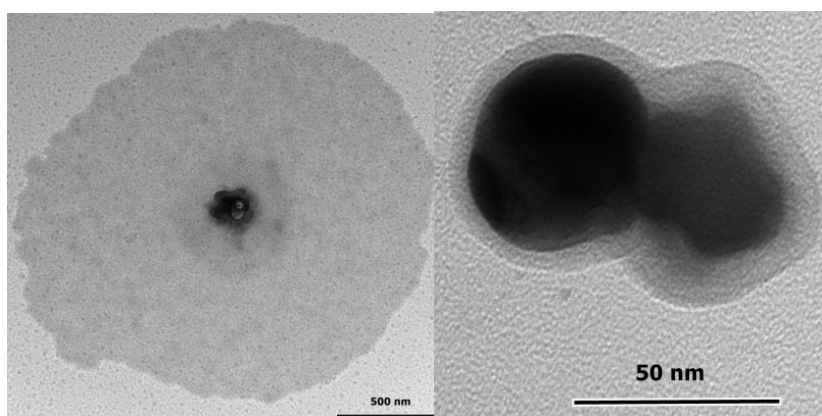


Figure 1: TEM micrograph of pullulan reduced AgNPs at different concentrations of AgNO₃.

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P 2. Synthesis and characterization of new imidazole/benzimidazole salts

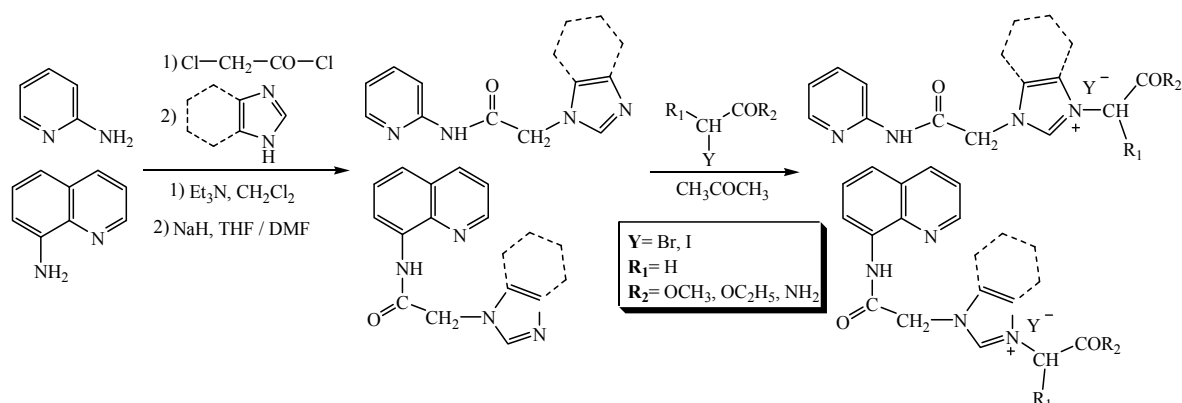
Dorina Mantu,^{*} Vasilichia Antoci, Costel Moldoveanu, Gheorghita Zbancioc, Ionel I. Mangalagiu

^{*}Department of Chemistry, "Al. I. Cuza" University of Iasi, 11 Carol 1st Bd., 700506, Iasi, Romania

^{*}E-mail address: dorinaiasi@yahoo.com

Imidazole and benzimidazole derivatives are well known compounds with a broad spectrum of biological activities, among them: antibacterial, anti-inflammatory, anticancer.¹⁻³ Also, pyridine and quinoline are intensively used as scaffolds for drug development.⁴ Moreover, imidazolium salts are potent room temperature ionic liquids.⁵

In the present work we rationalize the syntheses of new heterocyclic compounds having in their structure pyridine and quinoline moiety with imidazole/benzimidazole unit, looking also to the influence of structures to their biological properties. In order to synthesize the desired compounds, we obtained first the starting materials (acylated derivatives), which were subsequently treated with imidazole and benzimidazole, using sodium hydride as base. The corresponding salts were obtained by treatment with different halogenated derivatives with high reactivity.



The structure of all new compounds was proved by spectral analysis (IR, ¹H NMR, ¹³C NMR, 2D-COSY, 2D-HMQC, 2D-HMBC).

Acknowledgements: To CNCS Bucharest for financial support, project PN-II-DE-PCE-2011-3-0038, no. 268/05.10.2011.

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P 3. Synthesis and XRD structure elucidation of new fluorescent pyrrolo-imidazole

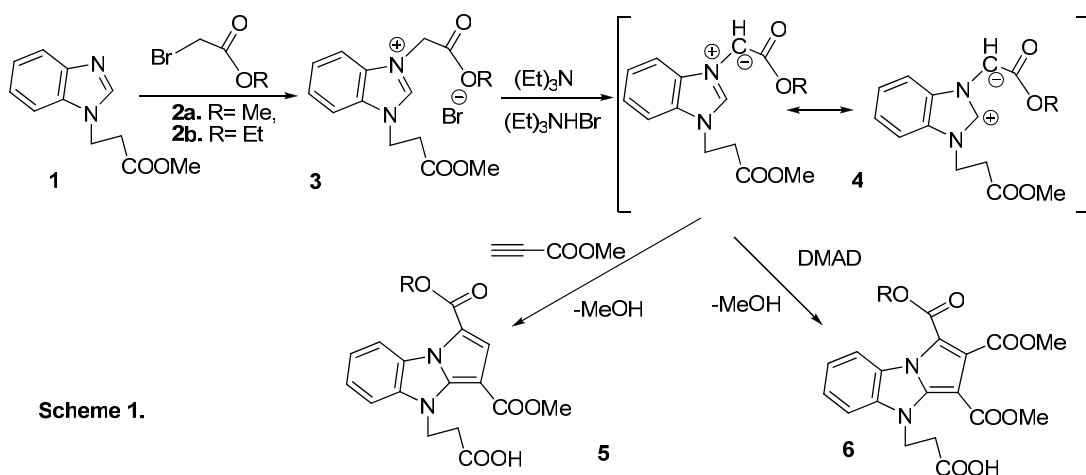
Gheorghita Zbancioc,* Costel Moldoveanu, Dan Maftai, Vasilichia Antoci, Ionel Mangalagiu

Department of Chemistry, "Al. I. Cuza" University of Iasi, Bd. Carol I no. 11, 700506, Romania

*E-mail address: zbanciocg@chem.uaic.ro

Synthesis of indolizines and azaindolizines has received increasing interest during the last years driven by a wide range of potential applications, from electroluminescent materials to macrocyclic fluorescent sensors.¹⁻³

To obtain ylides derived from benzo[d]imidazol **1**, we used the Kröhnke⁴ *salt method*. Thus, benzo[d]imidazolium salts **3** were prepared by treating methyl 3-(1H-benzo[d]imidazol-1-yl)propanoate **1** with alkylbromoacetate **2**. Then, for the obtaining of highly fluorescent pyrroloimidazole derivatives **5** and **6**, it was used a [3+2] dipolar cycloaddition of benzo[d]imidazolium ylides **4**, generated *in situ* from the corresponding cycloimmonium salts, to methyl propiolate or DMAD (Scheme 1).



Acknowledgements: To CNCS - UEFISCDI, grant PN-II-TE/ 0010 -79/05.10.2011 for financial support.

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P 4. Synthesis of new imidazolium salts with imidazol skeleton

C. Moldoveanu,* Ghe. Zbancioc, D. Mantu, P. M. Stiuleac, I. O. Silea, I. Mangalagiu

Department of Chemistry, "Al. I. Cuza University" of Iasi

*E-mail address: moldcos@chem.uaic.ro

Imidazole and its derivatives are well known biologically active and medicinally potent anticancer agents,¹ anti-HIV,² antibacterial and antifungal,^{3,4} or used in the treatment of cardiovascular diseases,⁵ etc. Moreover, imidazolium salts are potent room temperature ionic liquids of current great interest in industry.⁶

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

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

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

Acknowledgements: To CNCS-UEFISCDI, grant PN-II-TE/0010 -79/05.10.2011 for financial support.

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P 5. Synthesis of new pyrrolo[1,2-i][1,7] phenanthroline derivatives

M.C. Al-Matarneh,^{*} T. Daniloaia, R. Danac

Department of Chemistry, "Al. I. Cuza" University of Iași, 11 Carol I, 700506, Romania

*E-mail: almatarneh.cristina@yahoo.com

Synthesis of nitrogen heterocycles is an actual and challenging issue, due to their importance as classes of natural and unnatural compounds, many of them possessing interesting properties. 1,7-Phenanthroline is a less studied heterocycle, but few derivatives showed biological activities (antitumor, anti-asthma and anti-allergic activity), some monoquatarnary 1,7-phenanthroline salts showed antibacterial and antifungal properties¹ and a semiconductor behaviour²).

Therefore, we synthesized new cycloadducts having pyrrolo[1,2-i][1,7] phenanthroline structures by 1,3-dipolar cycloaddition of the symmetrical and unsymmetrical dipolarophiles to the *in situ* cycloimmonium ylides, generated from monoquatarnary 1,7-phenanthroline salts.

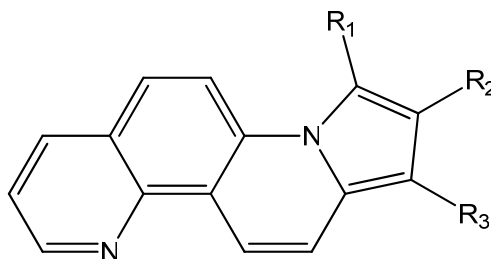


Figure 1: The general structure of pyrrolo-phenanthroline derivatives.

The cycloaddition reaction of unsymmetrical dipolarophile is regioselective according to the electronic and steric effects.

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P 6. New bis-imidazolium salts: synthesis and NMR characterization

Vasilichia Antoci,¹ Dorina Mantu,¹ Gheorghita Zbancioc,¹ Costel Modoveanu,¹ Alina Nicolescu,² Catalina Ciobanu,¹ Ionel I. Mangalagiu^{1*}

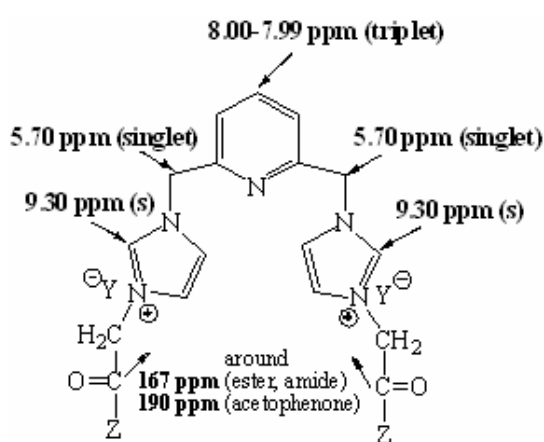
¹Department of Chemistry, "Al. I. Cuza" University of Iasi, 11 Carol I Bd., 700506, Romania

²"Petru Poni" Institute of Macromolecular Chemistry, Gr. Ghica Voda 41A, 700487, Iasi, Romania

*E-mail address: ionelm@uaic.ro

Literature describe that imidazolium salts are compounds with biological properties: antibacterial, anti-inflammatory, anticancer.^{1,2} Also, pyridine is intensively used as scaffold for drug development.³ Besides, imidazolium salts are some of the most frequently studied ionic liquids,⁴ due to their use as ligand precursors in the synthesis of metal-carbene complexes (excellent catalysts in many chemical reactions).^{5,6}

Having in view these considerations, our goal was to synthesize and characterize new pyridine bis-imidazolium salts. The syntheses were done in two steps: *N*-alkylation of imidazole with bis-bromomethyl pyridine, followed by quaternizations of pyridine bis-imidazole with different halogenated derivatives. The structures of new compounds were proved by NMR experiments (¹H NMR, ¹³C NMR, 2D-correlations). The NMR spectra have



been recorded on a Bruker Advance III 500 spectrometer, equipped with a 5 mm PABBO detection probe, operating at 500.1 and 125.7 MHz for ¹H and respectively ¹³C nuclei. In ¹H and ¹³C spectra, chemical shifts are reported in δ units (ppm) relative to the residual peak of solvent (ref: DMSO, ¹H: 2.50 ppm; ¹³C: 39.52 ppm).

Acknowledgements: To projects PN-II-DE-PCE-2011-3-0038, no.268/05.10.2011 and CERNESIM SMIS/CSNR 13984/901 No. 257/28.09.2010.

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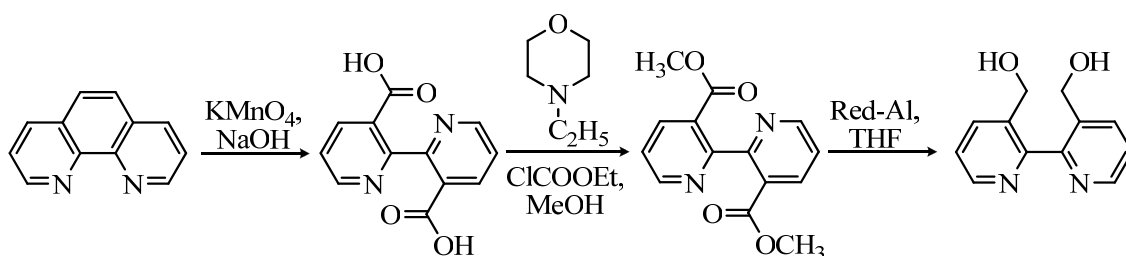
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P 7. Synthesis, spectral investigation and X-ray structure of 2,2'-bipyridyl-3,3'-dimethanol

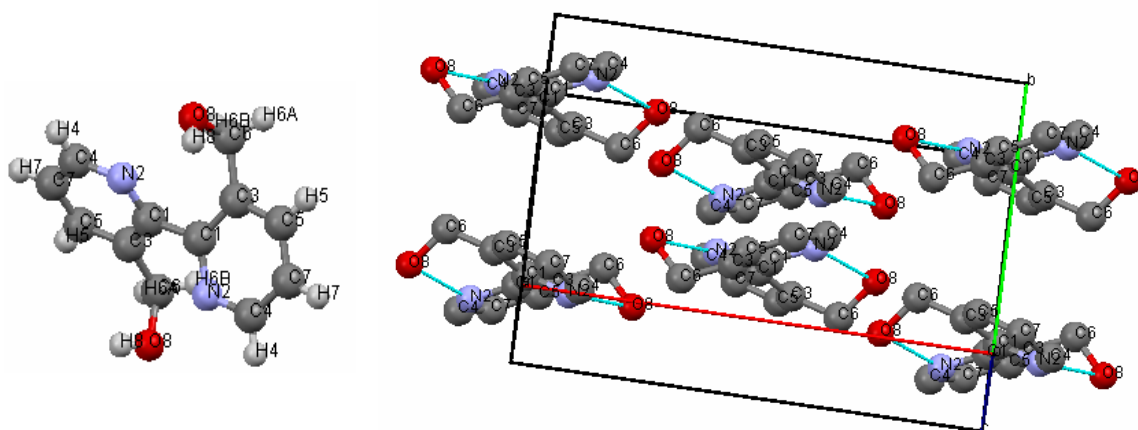
Gabriel Mengheres, Vasilichia Antoci, Ionel I. Mangalagiu

Department of Chemistry, "Al. I. Cuza" University of Iasi, Bd. Carol I no. 11, 700506, Romania

2,2'-Bipyridyls are azaheterocycles with important biological properties and with application in different fields (chemistry, biochemistry, pharmacy). The aim of this work was to synthesize 2,2'-bipyridyl-3,3'-dimethanol using a straight and efficient method starting from 1,10-phenanthroline. This compound can be used further as precursor for obtaining 3,3'-disubstituted derivatives.



The structure of these compounds were proven by spectral analysis $^1\text{H-NMR}$ and for the 2,2'-bipyridyl-3,3'-dimethanol the structure was also proven by X-ray diffraction.



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P 8. Sorption studies on anion exchange resins/gellan microparticles

Stefania Racovita, Silvia Vasiliu, Cristina Doina Vlad

Institute of Macromolecular Chemistry "Petru Poni", Aleea Gr.Ghica Voda, nr.41A, Iassy, Romania

The ion exchangers represent an important tool for the development of controlled or sustained release systems because of their excellent physico-chemical properties such as stability, inert nature, uniform size, and spherical shape, presence of functional groups and high capacity of drug loading. The anion exchange resins with macroporous structure have been prepared by suspension polymerization of styrene and divinylbenzene in the presence of toluene and gasoline as porogenic agents, followed by chloromethylation and amination reactions. The surface of porous microparticles obtained was covered after that with a natural polymer (gellan gum). For all type of microparticles the morphological characteristics such as apparent and specific densities, specific surface area, porosity and uptake of solvents have been determined. The knowledge of the factors that determine the interaction between the drug (Cefotaxime sodium salt) and macromolecular support is relevant in the design of pharmaceutical dosage forms. The adsorption isotherms can give the most important information about the distribution of the adsorbate molecules between both the liquid and solid phases when the adsorption process reaches an equilibrium state. Various isotherm equations such as Langmuir, Freundlich, Temkin, Dubinin–Radushkevich, Redlich-Peterson and Sips have been used in order to describe the adsorption equilibrium feature.

P 9. Substrate preference of serotonin receptors through in silico docking experiments

Roxana-Maria Amarandi,^{1*} Calin-Lucian Maniu,² Ramona Danac,¹ Aurel Pui¹

¹Department of Chemistry, “Al. I. Cuza” University of Iasi, Bulevardul Carol I nr. 11, 700506, Romania

²Faculty of Biology, “Al. I. Cuza” University of Iasi, Bulevardul Carol I nr. 20A, 700505, Romania

*E-mail address: amarandiroxana2006@yahoo.com

The serotonin type 2A receptor (5-HT_{2A}R) is a transmembrane G-protein coupled receptor involved in the etiology of several psychiatric disorders such as schizophrenia and depression, acting as the main molecular target for several drugs used as treatment for these debilitating conditions.¹ The difficulty in crystallizing membrane proteins such as the 5-HT_{2A}R makes the study of molecular interactions between the receptor and its ligands very troublesome. For this reason, most of the current research in the field of ligand design for the 5-HT_{2A}R relies on computational models of this receptor, generated based on crystal structures of closely related receptors, process known as homology modeling.²

In this study, a homology-based model of the 5-HT_{2A} receptor was generated with MODELLER² using the serotonin 5-HT_{2B} receptor structure (PDB ID: 4IB4) as template. The modeled structure was validated using PROCHECK³ and Ramachandran Plot⁴ and refined by energy minimization, with results indicating an overall good model. The binding site of the receptor was chosen based on available literature data, and several docking experiments were carried out using AutoDock.⁵ Results included the ionic interaction between all protonated amine ligands and an aspartic acid in position 3.32 (as defined by the Ballesteros-Weinstein nomenclature),⁶ the formation of a hydrogen bond with serine residues in positions 5.46 and 3.36, the latter only in the case of non-substituted tryptamines. Besides, hydrophobic contacts with aromatic amino acids phenylalanine and tryptophan were observed near the receptor binding site in the docking of ligands with bulky substitutes. Docking of the most selective agonist known so far for the 5-HT_{2A} receptor revealed an unexpected hydrogen bond between a tyrosine residue and the protonated amine in the ligand structure, which could be a molecular determinant of its high selectivity.

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P 11. Design of microparticulate systems with special architecture based on glycidyl methacrylate

Maria-Andreea Lungu,¹ Marcel Popa,¹ Florica Doroftei,² Gabriela Hitruc,²
Stefania Racovita,² Silvia Vasiliu²

¹ *Department of Natural and Synthetic Polymers, Faculty of Chemical Engineering and Environmental Protection "Gh. Asachi" Technical University of Iasi, Prof. Dr. Docent Dimitrie Mangeron Street, No. 73, 700050, Romania*

² *Institute of Macromolecular Chemistry "P. Poni", Aleea Gr.Ghica Voda, nr.41A, Iassy, Romania*

The evolution and fast development in the field of polymer science and engineering have a great impact on the discovery and creation of new advanced materials that could be used in medical and pharmaceutical fields for the elaboration of modern therapeutic strategies or in biotechnological field for enzyme immobilization. Glycidyl methacrylate is an attractive vinyl monomer because of its low toxicity, lower cost compared with other acrylic monomers, versatile properties due to the presence in its molecule of two functionalities such as, epoxy and acrylic groups, respectively. Porous microparticles based on glycidyl methacrylate, dimethacrylic monomers (mono-, di- and triethylene glycol dimethacrylate) and xanthan gum have been synthesized by aqueous suspension polymerization method in the presence of toluene as diluent. The idea of association a synthetic polymer with a natural one within the same structure can lead to the creation of a new class of materials that combines the physico-chemical properties of both starting components. The synthesized microparticles have been characterized by various techniques including FT-IR spectroscopy, TG analysis, SEM and AFM methods. In order to characterize the morphological structure of the microparticles, several parameters such as apparent and specific density, specific surface area, porosity, uptake of solvent have been determined as well.

The presence of xanthan in the structure of microparticles leads to the preparation of the microparticulate systems with special architecture that are characterized by the high content of epoxy groups, smaller sizes, high values of the specific surface areas and better sorption capacities compared to those based on glycidyl methacrylate and dimethacrylic monomers. Due to their properties these microparticles may be used in various applications, particularly for the retention, delivery and controlled release of various drugs as well as in biotechnological field as polymeric supports for enzyme immobilization.

P 12. Synthesis, characterization and potential application of ZnO/polymers nanocomposites in medical dentistry

G. Calin,¹ L. Olaru,² N. Olaru,² L. Dartu,¹ V. Burlui¹

¹ Faculty of Dental Medicine, "Apollonia" University, str. Music, nr. 2, 70051, Iasi Romania,

²"Petru Poni" Institute of Macromolecular Chemistry, Aleea Gr. Ghica Voda 41A, 700487, Iasi, Romania

Hybrid materials based on ZnO are largely studied because of their multifunctional capabilities. Nanostructured materials based on ZnO/polymers attracted attention in the recent years due to their multiple applications. This study presents the synthesis, characterization and potential applications of ZnO/polymer nanosystems in medical dentistry. The surface characteristics of the obtained material were analyzed by atomic force microscopy (AFM) and energy dispersive X-ray spectroscopy (EDS), while the structural features by X ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS). Scanning electron microscopy (SEM) was used in order to investigate the textural models and the presence of ZnO nanoparticles on the polymer substrate was revealed. Further studies will be performed in order to investigate the application of the synthesized materials as dental temporary restorations.

P 13. Dosage possibilities of antibiotics from wastewater produced as a result of dental treatment

Laura Dartu,¹ Carmen Zaharia,² Vasile Burlui¹

¹*Faculty of Medical Dentistry, "Apollonia" University, Iasi*

²*Faculty of Chemical Engineering and Environmental Protection, "Gh. Asachi" Technical University of Iasi*

The treatments used for the elimination of dental infections includes a series of medicines that can be administrated by using some specific doses of antibiotics such as tetracycline and metronidazole, individually or in combination. This study presents the analysis methods (e.g. spectrophotometry and advanced analysis such as HPLC and MS) of the two antibiotics used currently in dental treatments, presentation of the spectrophotometric methods more usable to apply in the physical-chemistry laboratories. Thus, it is outlined the facility of using the alkaline spectrophotometric method using NaOH (5N), in the case of dosing tetracycline, at a wavelength of 380 nm whereas for dosing metronidazole, the spectrophotometric method using methanol and HCl (1N) at a wavelength of 277 nm was used. The dosage methods are presented for an individual aqueous solution of medicine (tetracycline and metronidazole) while the calibration curves are shown for each case (individual or in combination). Also, it is specified the method sensibility, dosage range, precision and possible interfaces. This dosage methods, can be applied in further studies regarding the retention of these drugs in aqueous media under different conditions (diluted and concentrated form) in different final effluents (1:10, 1:100, 1:1000).

P 14. Symmetric banana-shaped liquid crystals with resorcinol as a central unit

Catalina-Ionica Ciobanu,¹ Irina Carlescu,² Dan Scutaru²

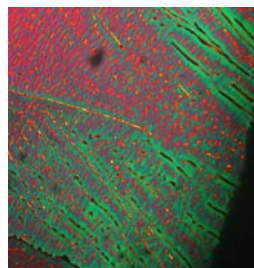
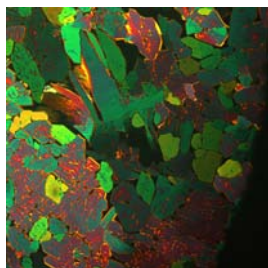
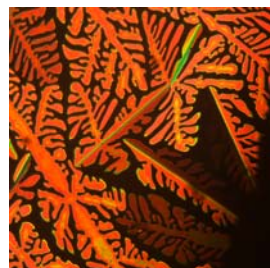
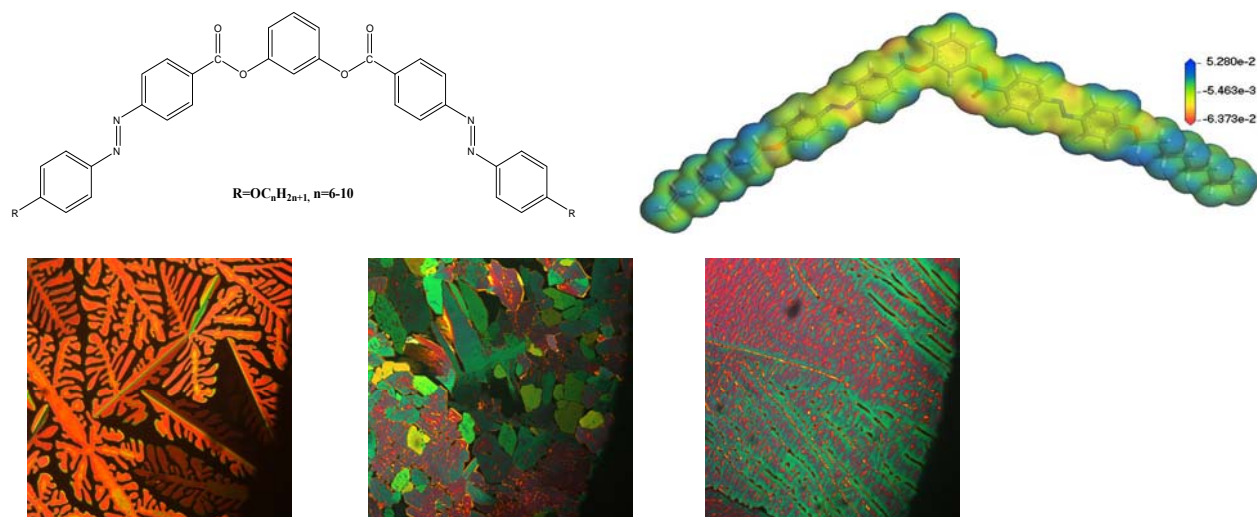
¹Department of Chemistry, „Al. I. Cuza” University of Iasi, 11 Carol I, 700506, Romania

² Faculty of Chemical Engineering and Environmental Protection, “Gh. Asachi” Technical University, 71A D. Mangeron Bd., 700050, Iasi, Romania

Banana-shaped liquid crystals are compounds synthesized for the first time in 1930 years by Vorlander and Apel, and more recently by Matsunaga and Miyamoto. They obtained the bent-core compounds based on 1,3-disubstituted phenylenes as a central unit.^{1,2} In last years, the bent-core molecules containing an azo linkage have been investigated for the possibility of photochromism and photoisomerization upon irradiations with UV and visible light.^{3,4} Most banana-shaped liquid crystals, reported up to now, correspond to five aromatic ring with a 1,3-phenylene central unit.⁵ These exhibited B type phases, smectic or nematic mesophases, but the B2 phase is most frequently observed.⁶

A new series of *bent-core* liquid crystals based on resorcinol central core have been synthesized and the mesomorphic properties were investigated. These newly compounds contain five benzene-rings connected through azo and esteric linkage and aliphatic chain at the end. Their structure was varied by changing the length of the terminal chains, considering that the appearance of liquid crystalline behaviour depends on the length of the flexible end chain.

Usual techniques like NMR, IR and UV-VIS spectroscopy were used for structural characterization. The liquid crystalline behaviour was confirmed by differential scanning calorimetry (DSC) and optical polarizing microscopy (POM) for three compounds from five synthesized. The thermogravimetric study showed that the banana derivatives have a good thermal stability, because the degradation of the compounds begins over the isotropization temperature.



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P 15. Synthesis and characterization of new vinyl acetate-based copolymers with urethane and urea groups

Mioara Murariu,* Emil C. Buruiana¹

¹Department of Photochemistry, Romanian Academy, "Petru Poni" Institute of Macromolecular Chemistry, 41 A Grigore Ghica Voda Alley, 700487 Iasi, Romania

*E-mail address: mioara.murariu@icmpp.ro

In last decade, an increased interest concerning the vinyl acetate-based copolymers with applicability in drug delivery,¹ natural biodegradable materials sources² a.s.o. was observed. In the present paper, two monomers, i.e., R-(+)- α -ethylbenzylacrylamide and N-methacryloyloxyethyl-N'- α -ethylbenzyl(urea), and their copolymers, i.e., poly[R-(+)- α -ethylbenzylacrylamide-co-vinyl acetate] and poly[N-methacryloyloxyethyl-N'- α -ethylbenzyl(urea)-co-vinyl acetate] were synthesized in different molar ratios, 46:54 and 28:72, respectively. These compounds were obtained through a radical polymerization reaction using azobis(cyclohexanecarbonitrile) as initiator. Within this study, the hydrolysis reaction of the synthesized copolymers, as well as their chemical modification with dansyl chloride were followed. The structure, purity and chemical composition of the synthesized compounds were supported through spectrophotometric analytic (¹H-NMR, FT-IR and UV/vis), thermal (DSC and TGA) and GPC methods, as well as fluorescence spectroscopy. The fluorescence studies in DMF solution were performed using different quenchers, i.e., camphorsulfonic acid, p-toluenesulfonic acid, HCl and divalent ions (Cu, Zn, Hg, Fe), these measurements evidencing the highest efficiency for Fe²⁺ and the lowest one for Zn²⁺. The fluorescence quenching was studied in acid medium through protonation of amine group from dansyl-based copolymers³, the synthesized compounds being thus useful as chemical sensors.

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P 16. Influence of organic and mineral fertilization on the content of polyphenols and tannins of forages from a permanent grassland in north-eastern Romania (Cosna)

Doina Tarcau,¹ Alina-Giorgiana Negru,² Vasile Vintu,¹ Costel Samuil,¹ Simona-Maria Cucu-Man²

¹Faculty of Agriculture, “Ion Ionescu de la Brad” University of Agricultural Sciences and Veterinary Medicine of Iasi, Aleea Mihail Sadoveanu 3, 700490, Iasi

²Department of Chemistry, “Al. I. Cuza” University of Iasi, Bd. Carol I 11, 700506, Romania

The optimal use of forages in ruminant nutrition requires the accurate determination of their quality. The polyphenolic compounds in forages may have beneficial or adverse effects on ruminants and may influence the quality of animal products, depending on their concentration and nature. In this study the influence of organic fertilization on the content of total polyphenols and tannins in forages obtained from permanent grassland of *Nardus stricta* L. and *Festuca rubra* L. was investigated. Two experiments were conducted, in north-eastern Romania (Coşna), which include: **1.** nine variants of organic fertilization; **2.** seven variants of mineral fertilization, both set-up in different graduations and applied annually or every two years.

The forage samples were collected in 2010, 2011 and 2012. The powdered samples were extracted with 30% methanol and total polyphenols and tannins content was spectrophotometrically determined by Folin-Ciocalteu method. Tannin content was calculated as a difference between total and non-tannin (non-casein-adsorbed) phenolic content. The content in polyphenols and tannins has been expressed as tannic acid.

Higher concentrations of total polyphenols and tannins were observed for variants where manure fertilization was applied compared with the control variant. For all variants of organic fertilization the total polyphenol and tannin content increased significantly in 2012 compared to 2010. The largest increase in tannin content was observed for fertilization variant with 20 t ha⁻¹ manure applied annually, from 5.2 mg g⁻¹ in 2010 to 13.9 mg g⁻¹ in 2012.

For variants of organic fertilizers applied every two years the tannins and polyphenols concentrations did not vary significantly over the three years. The use of mineral fertilizers decreased the concentration of tannins compared to the unfertilized control. Significant variation in the concentrations of total polyphenols and tannins was also observed between variants and years in forages harvested from mineral fertilized grassland.

Keywords: polyphenols, tannins, forages, organic fertilization, mineral fertilization.

P 17. Comparative study of field collected samples of aged silicon rubber composite coatings for high voltage insulators

I.V. Tudose,^{1,4} M. Sucheai,^{1,3,4} K. Siderakis,^{2,3} E. Thalassinakis,⁵ E. Koudoumas^{1,3}

¹Center of Materials Technology and Photonics School of Applied Technology, Technological Educational Institute of Crete, 71004 Heraklion, Greece

²Center of Energy and Photovoltaic Systems (CEPS), School of Applied Technology, Technological Educational Institute of Crete, 71004 Heraklion, Greece

³Electrical Engineering Department, Technological Educational Institute of Crete, Greece

⁴“Al.I.Cuza” University of Iasi, 11 Bulevard Carol I, 700506, Romania

Hellenic Electricity Distribution Network Operator S.A.

Pollution of high voltage insulators is a phenomenon with a considerable impact to the performance of transmission and distribution electrical networks. Salt spray, industrial pollutants, and even desert sand can lead to costly power interruptions due to arcing and flashover. The use of composite materials and especially Silicone Rubber proved to be an efficient improvement, capable of suppressing the problem and diminish the flashover probability. As a result ceramic insulators in transmission lines are replaced by insulators with composite housing, either HTV Silicone Rubber or LSR. In the case of high voltage substations however, the replacement of insulators is rather difficult, due to the complexity of the equipment and the corresponding financial cost. In this case the application of RTV Silicone Rubber is an equivalent alternative. The ceramic insulators are covered with a 0.5mm RTV SIR coating which provides the advantages of composite insulators on a ceramic substrate.

After installation the possible material lifetime, which is determined by the service conditions and the material formulation, is the primary concern. In Crete, a large scale application has taken place and coatings that exceed a service period of 10 years are still in operation. The present study focuses on the structural and morphological characterization of field collected composite insulators of various ages so that the degradation degree can be correlated with their service performance.

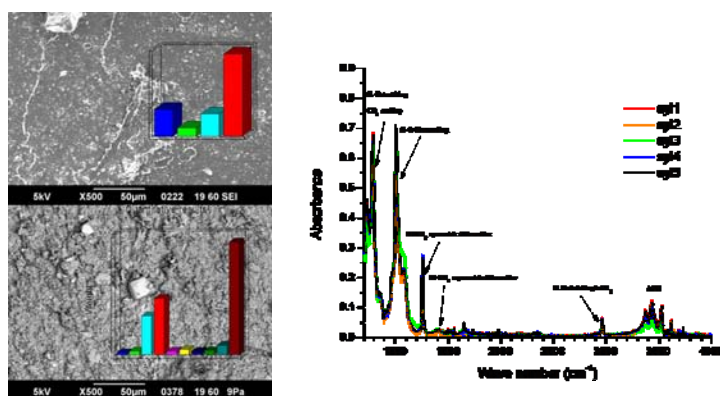


Figure 1: Reference sample comparison with a 10 years old field sample. Comparative FTIR spectra of various field collected samples.

Acknowledgments: This work was based on the project 11ΣYN-7-1503 which is implemented through the Operational Program “Competitiveness and Entrepreneurship”, Action “Cooperation 2011” and is co-financed by the European Union (European Regional Development Fund) and Greek national funds (National Strategic Reference Framework 2007 - 2013).

P 18. Precursor concentration effect on structure and morphology of ZnO for coatings on fabric substrates

M. Suchea,^{1,2} I.V. Tudose,^{1,2} N. Vrinceanu,^{1,3} B. Istrate,⁴ C. Munteanu,⁴ E. Koudoumas²

¹“A.I.Cuza” University of Iasi, 11 Bulevard Carol I, Iasi, 700506, Romania

²Center of Materials Technology and Laser, School of Applied Technology, Electrical Engineering Department, Technological Educational Institute of Crete, Heraklion, Greece

³“Lucian Blaga” University of Sibiu, Department of Textile Technologies, Sibiu, Romania

⁴“Gheorghe Asachi” Technical University of Iasi, Romania

*E-mail address: mirela.suceha@uaic.ro

ZnO is a versatile functional material that has a diverse group of growth morphologies. By controlling the growth kinetics, it is possible to change the growth behavior of ZnO structures. Growth of ZnO structures can be achieved in a cheaper way at low temperature using chemical growth techniques such as aqueous chemical growth, nonaqueous solution growth, sol gel and spray deposition. Up to date, there are quite few reports in the literature presenting state of art approaches of use of ZnO material onto textile substrates for several applications as antibacterial, deodorizing and UV protection, and none regarding any systematic approach of direct growth and optimization with respect the textile support. The successful exploitation of particles ZnO for use in various technological applications requires the development of techniques for controlling its photocatalytic activity. The present contribution presents a study of precursor concentration effect on structure and morphology of ZnO for coatings on fabric substrates. ZnO particles were obtained by direct growth onto the respective substrate by aqueous chemical growth using suitable precursors for each growth and characterized regarding their appearance, size and structure using microscopic techniques and X-ray diffraction.

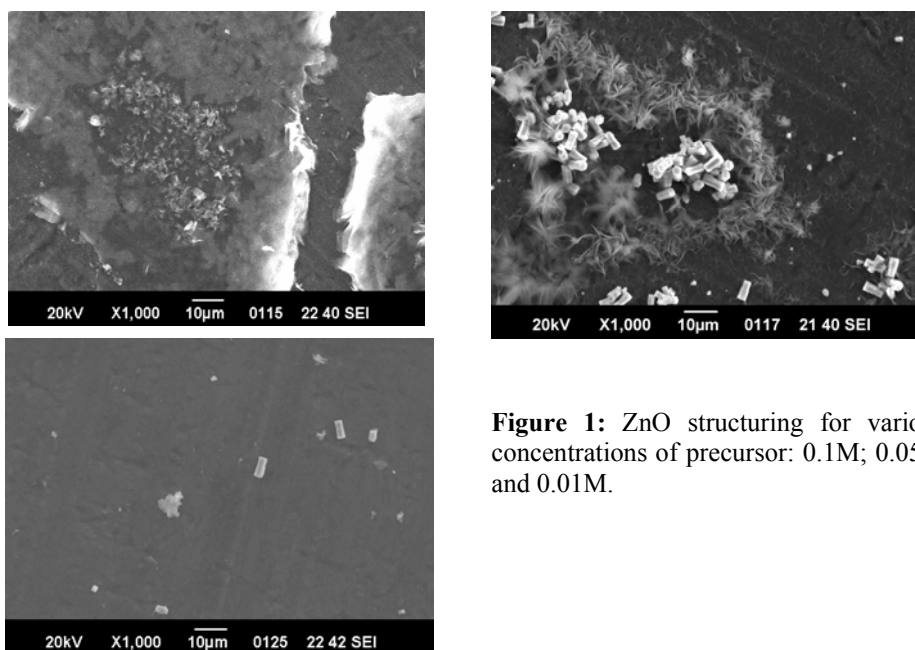


Figure 1: ZnO structuring for various concentrations of precursor: 0.1M; 0.05M and 0.01M.

Acknowledgments: This work was partially supported by a grant of the Romanian National Authority for Scientific Research, CNCS – UEFISCDI, project number PN-II-RU-TE-2012-3-0202.

P 19. Removal of organic azo dyes (Remazol Arancio 3R) from industrial effluents

Carmen Zaharia

*Department of Environmental Engineering and Management, Faculty of Chemical Engineering and Environmental Protection, "Gheorghe Asachi" Technical University of Iasi,
73 Prof.Dr.docent D.Mangeron Blvd, 700050
E-mail address: czah@ch.tuiasi.ro*

This paper presents some data from comparative physico-chemical treatment processes studies applied for removal of Remazol Arancio 3R (Orange 16) from industrial effluents (i.e. textile effluents). These treatments have leaned mostly on color retention performance, suspended solids and organic matter expressed by chemical oxygen demand (COD) removal. The influence of different operating parameters (e.g. pH, added chemicals/materials content, temperature, agitation regime, working regime) have been also summarized for each treatment (i.e. coagulation-flocculation, advanced oxidation such as Fenton oxidation, adsorption on different commercial well-known or non-conventional adsorbents, etc.). The obtained results suggest that these physico-chemical treatments could be used for reducing the environmental impact of effluent discharging in different aqueous receptors and to comply with the limits imposed by environmental legislation as well.

P 20. Quality Control Study of Siret River from Pascani Town Area and Estimation of Its Pollution Level

Carmen Zaharia^{1*} and Iuliana Radu²

¹ *Department of Environmental Engineering and Management, Faculty of Chemical Engineering and Environmental Protection, "Gh. Asachi" Technical University of Iasi,*

73 Prof.Dr.docent D.Mangeron Blvd, 700050-Iasi, Romania

² *Geodesy and Environmental Engineering, Faculty of Hydrotechnics, "Gh. Asachi" Technical University of Iasi,*

53 Prof.Dr.docent D.Mangeron Blvd, 700050-Iasi, Romania

**E-mail address: czah@ch.tuiasi.ro*

The study presents some experimental results regarding quality indicators (general, specific and toxic physical-chemical indicators) analyzed during spring season (April-May, 2013), in two control sections of Siret River from Pascani town area (i.e. entrance Lunca-Pascani and upstream of Pascani bridge).

The real pollution state of Siret River from Pascani town area has been also estimated by the global pollution index, and corresponds to values between 3.296-3.356. These values may indicate "an aquatic environment modified by economic activities with generation of stress effect against life forms".

P 21. Eco-friendly synthesis of new nitrogen heterocycles compounds using ultrasound irradiation

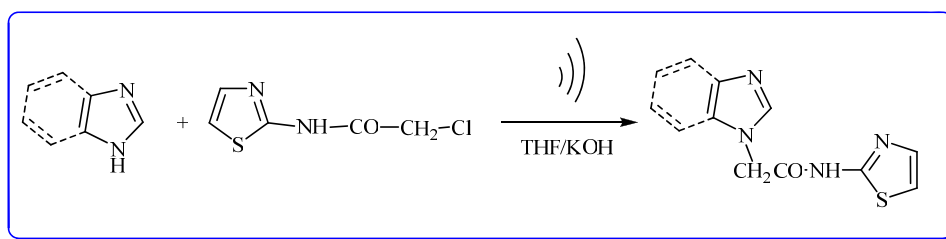
Eliza-Lorena Ene (Plesnicute), Vasilichia Antoci, Dorina Mantu, Ionel I. Mangalagiu*

Department of Chemistry, "Al. I. Cuza" University of Iasi, 11 Carol I Bd., 700506, Romania,

*E-mail address: ionelm@uaic.ro

Nitrogen heterocycles are invaluable compounds demonstrating fascinating potential applications for medicine, opto-electronics, agriculture, etc.,¹ being a top and widely discussed research field in modern science. "Sonochemistry", the chemical applications of ultrasound, has become an exciting new field of research during the past decade, since it offers a versatile and facile pathway in a large variety of syntheses.²⁻⁴

In the present work we have synthesized new nitrogen heterocycles compounds using ultrasound irradiation. Ultrasound assisted reactions were carried out using two different reactors: Sonics (Sonics VCX-130, USA), with a nominal power of 130 W and Bandelin (Sonopuls GM 3200), with a nominal power of 200 W. Both ultrasound reactors have the same frequency: 20 kHz. The structure of new nitrogen heterocycles compounds was proved by spectral analysis: IR, ¹H NMR, ¹³C NMR, and 2D-experiments (COSY, HMQC, HMBC). The NMR spectra have been recorded on a Bruker Advance III 500 spectrometer.



Scheme: Synthesis of new nitrogen heterocycles

Acknowledgements: Financial support was provided by the project PN-II-DE-PCE-2011-3-0038, no.268/05.10.2011. The POSCCE-O 2.2.1, SMIS-CSNR 13984-901, no. 257/28.09.2010 Project, CERNESIM, is gratefully acknowledged for the infrastructure (Bruker Advance III 500 spectrometer) used in this work.

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P 22. Highly monodispersed hydrophobic CoFe_2O_4 nanoparticles by non-aqueous pathway

Radu-George Ciocarlan,^{*} Daniel Gherca, Aurel Pui

¹Department of Chemistry, “Al. I. Cuza” University of Iasi, Bulevardul Carol I nr11, 700506, Romania

Hydrophobic CoFe_2O_4 nanoparticles have been synthesized through co-precipitation route using a non-aqueous solution. The method developed to prepare the nanoparticles was facile, reproducible and low-cost.

These hydrophobic nanoparticles present different physical properties compared with another nanoparticles obtained in aqueous solution. In water, because of the hydrophobic properties, CoFe_2O_4 nanoparticles are located on the top of the solution.

The nanoparticles CoFe_2O_4 were characterized by X-ray diffraction (XRD), transmission electron microscopy (TEM), infrared spectroscopy (FT-IR).

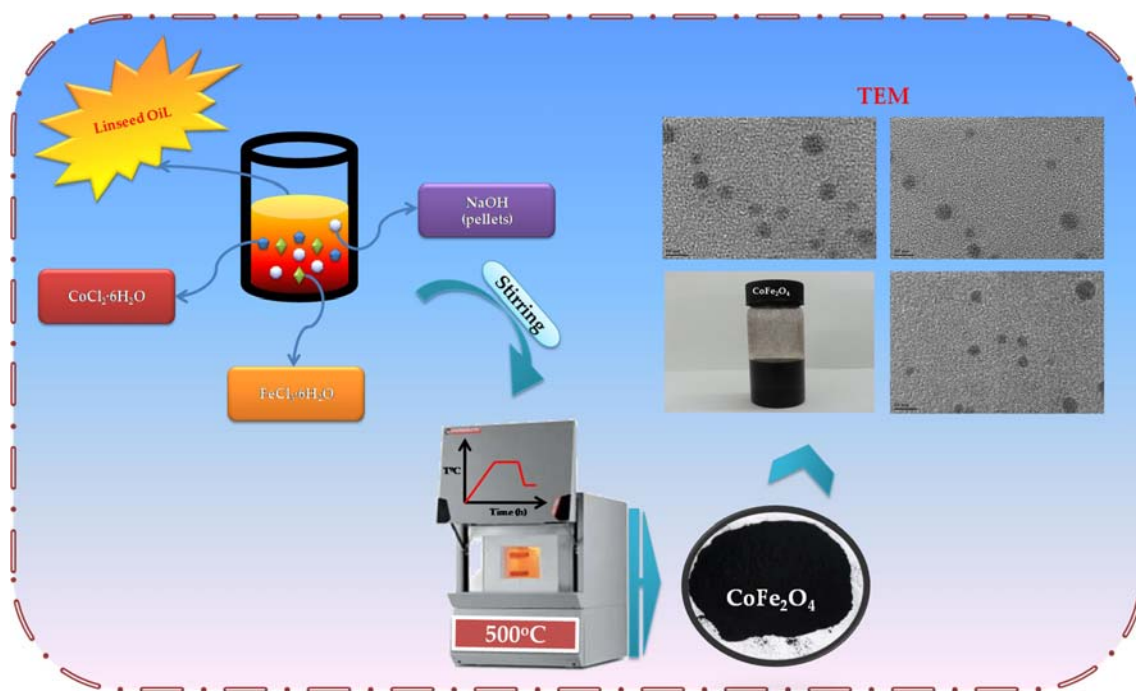


Figure 1: Schematic representation of non-aqueous synthesis of hydrophobic CoFe_2O_4 nanoparticles.

P 23. Vibronic structure and intramolecular charge transfer character of the lowest singlet excited state in indolizine and azaindolizines: insights from theory

Dan Maftai,^{1*} Dumitru Claudiu Sergentu,² Ionel Humelnicu,¹ Ionel Mangalagiu¹

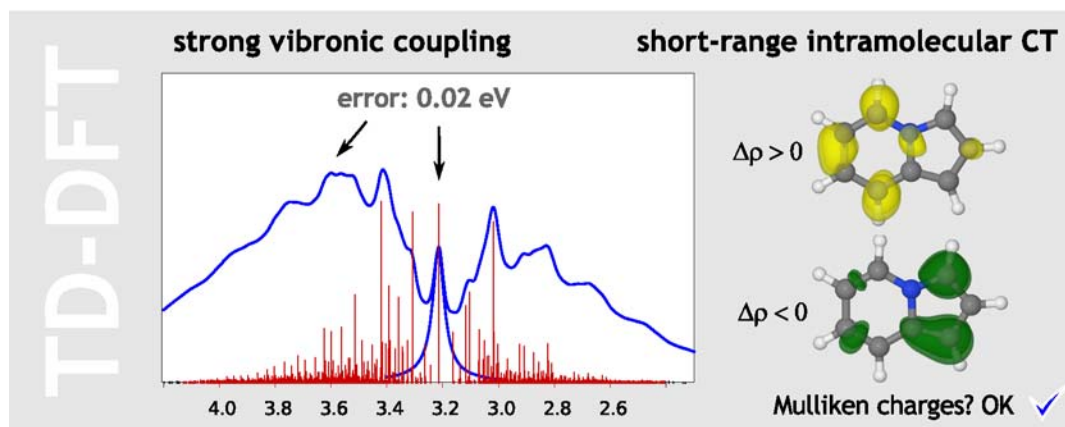
¹Department of Chemistry, "Al. I. Cuza" University of Iasi, Romania

²Department of Theoretical Chemistry, University of Groningen, Nijenborgh 4, 9747AG Groningen, The Netherlands,

*E-mail address: dan.maftai@chem.uaic.ro

Optical (near-UV) absorption and fluorescence spectra of indolizine and its aza-derivatives (azaindolizines) are computed at the time-dependent density functional theory (TD-DFT) level in both gas phase and nonpolar solvent (accounted using PCM). Experimental data (where available) and theoretical reference values computed at CASPT2//CASSCF level are used in a preliminary step to assess the performances of three widely-used density functional (DF) approximations (B3LYP, PBE0 global hybrids and the long-range corrected CAM-B3LYP) in reproducing the first three singlet excitation energies.

We show that both *ab initio* and density functional approaches employed in the vertical approximation, while catching the overall trend observed in the spectra of indolizines, overrate the first excitation energy. Upon modeling the vibrational-resolved band-shape of the first absorption band, B3LYP/CAM-B3LYP underestimate or overestimate excitation energies while the parameter-free PBE0 DF foresee the band origin and the position of absorption maxima for indolizine (1-azaindolizine) in only 0.02 eV (0.05 eV) discrepancy from experiment. In a further step, we rely on the unprecedented accuracy achieved in TD-DFT computations to account the intramolecular charge-transfer (CT) character of the first excited state. Red (blue) spectral shifts of the first absorption band in azaindolizines with respect to the parent indolizine relates not only to the acceptor (donor) role of the second nitrogen atom in the former, but also to a reorganization of CT density within each of the two fused rings.



P 24. Computational (PCM TD-DFT) study of the first electronic transitions in *cis* and *trans* isomers of azobenzene and of some derivatives

Dragos Lucian Isac,* Dan Maftai, Ionel Humelnicu

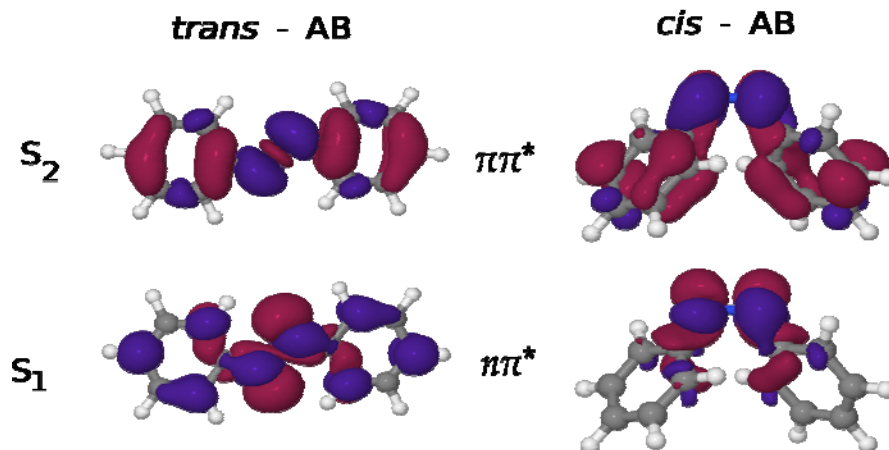
Department of Chemistry, "Al. I. Cuza" University of Iasi, Romania

*E-mail address: dragos.isac@chem.uaic.ro

Photophysics and photochemistry of azobenzene (AB), featuring a photoinduced *trans*-to-*cis* isomerization that reverts thermally to the most stable (*trans*) isomer, has received significant interest during the last decade provided the potential use for energy storage at molecular level. While most of the aspects involved in the photoisomerization process have been elucidated, and *ab initio* tools gave valuable insights on the reaction path, previous works have not approached the influence of substituents. Since highly-accurate wavefunction-based methods are prohibitive for large molecules, we focus in this respect on time-dependent density functional theory (TD-DFT) methods.

The two lowest singlet excited states ($n\pi^*$ and $\pi\pi^*$) of *cis*- and *trans*-AB and of some recently synthesized derivatives are investigated at TD-DFT level using the parameter-free PBE0 density functional, in conjunction with a moderately balanced basis set. Transition energies are computed both in vacuum and in condensed phase (DMF solvent) where bulk solvent effects are included using the implicit Polarizable Continuum Model (PCM).

Preliminary results show that the chosen theory level provides a satisfactory description of the two lowest excited states, in quantitative agreement with *ab initio* results in the case of AB, and at affordable computational costs even for large derivatives.



P 25. New octahydropyrrolo[2,1,5-cd]indolizin-6-one derivatives

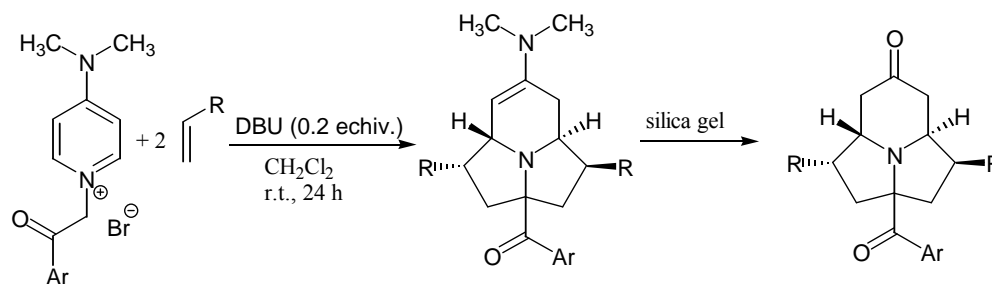
Simona Stefanovici,¹ Lucian M. Birsa,¹ Peter G. Jones,² Elena Bicu,¹ Dalila Belei¹

¹Department of Chemistry, "Al. I. Cuza" University of Iasi, 11th Carol I Bvd., 700506, Romania

²Institute of Inorganic and Analytical Chemistry, Technical University of Braunschweig, Hagenring 30, 38106 Braunschweig, Germany

The 1,3-dipolar cycloaddition reactions between pyridinium ylides and an array of acetylenic and olefinic dipolarophiles represent an interesting way to synthesize indolizine derivatives.¹ Depending on the nature of the reagents involved and/or the experimental conditions used, aromatization or isomerization often occurs during the cycloaddition reactions, initial reaction products being rarely isolated.²

Recent researches concerning 1,3-dipolar cycloaddition reactions between *p*-dimethylamino-pyridinium ylides and asymmetrically substituted activated olefins (Scheme 1), emphasize the direct and selective conversion to octahydropyrrolo[2,1,5-*cd*]indolizin-6-one derivatives.³



Scheme 1

The aim of the study was to evaluate the 1,3-dipolar cycloaddition reactions between *p*-dimethylaminopyridinium ylides **1** and **2** and dimethyl fumarate/dimethyl maleate (Figure 1).

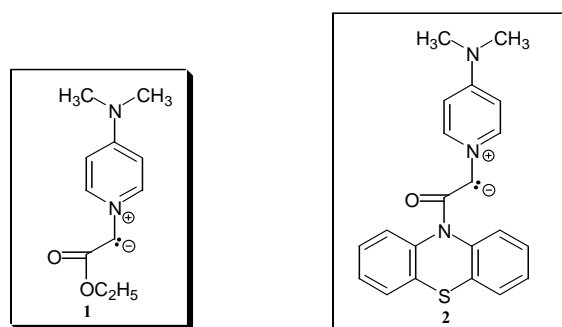


Figure 1

Keywords: cycloaddition, dimethylaminopyridinium ylides, dimethyl fumarate

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P 26. Synthesis of novel N-mustard compounds with support of 2-mercapto-benzoxazole derivatives with potential antitumoral activity

Mariana Cantemir,¹ Radita Aparaschivei,¹ Corina Cheptea,² Mihaela Holban,³ Dana Ortansa Dorohoi,⁴ Valeriu Sunel¹

¹*Department of Chemistry, “Al.I.Cuza” University of Iasi,*

²*Faculty of Medical Bioengineering, “Gr.T.Popa” University of Medicine and Pharmacy of Iasi*

³*Faculty of Dental Medicine, University “Apollonia” of Iasi*

⁴*Faculty of Physics, “Al.I.Cuza” University of Iasi*

In order to obtain novel antitumoral substances, N-mustards derivatives were synthesized by grafting a di-(β -chloroethyl)-amine group through ethyl, ester and acetyl bridges to the 2-mercapto-benzoxazole molecule. The main aim is to obtain a possible cleavage of the molecule within the organism, followed by a release of the alkyl fragment to the targeted cancerous cell. The chemical structure of the novel compounds was confirmed by spectroscopy (FT-IR, ¹H-NMR) and elemental analysis. The synthesized N-mustard compounds were tested for their toxicity (by determining the lethal dose DL₅₀) and their cytostatic action on experimental tumor.

P 27. Effect of some new imidazole derivatives on the peroxidase activity of wheat seeds (*triticum aestivum*) during germination

Ioan-Marian Risca,^{1*} Costel Moldoveanu,² Liviu Fartais,¹ Violeta Vasilache¹

¹ *Faculty of Silviculture, "Ștefan cel Mare" University, 13 Universitatii Street, RO-720229, Suceava, Romania*

² *Department of Chemistry, "Al. I. Cuza" University, 11 Carol I Avenue, RO-700506, Iasi, Romania*

^{*}*E-mail address: risca@usv.ro*

The biological activity of a new group of diazaheterocyclic salts – synthesized by addition of acrylonitrile to N-1 of imidazole, followed by the quaternization of 1-(2-cyanoethyl) imidazole derivatives with high-reacting halogen derivatives (halogen esters and halogen amides) – against wheat germination were investigated.

For all those compounds the hypocotyl's length and the peroxidase activity of the germinated wheat seeds, under various concentrations of imidazole derivatives, were measured. The results showed that the level of peroxidase activity is correlated with the length of wheat hypocotyls, as a function of concentration and structure of each investigated compound. The investigated compounds exhibited a general stimulating activity on the hypocotyls growth, especially at lower concentrations.

Keywords: imidazoles; N-alkylation; wheat; hypocotyls elongation; peroxidase.

P 28. Natural polymers based submicronic particles for the release of hydrophilic active principles

Mihaela Holban,¹ Elena Folescu,¹ Valeriu Sunel²

¹Faculty of Dental Medicine, “Apollonia” University of Iasi

²Department of Chemistry “A.I.Cuza” University of Iasi

Micro and nanoparticulated systems show promise as drug carriers, due to their enhanced capacity to release drugs in a controlled manner,^{1,2} to improve the stability of the loaded active substances and their biocompatibility or biodegradability (when synthesized from materials with such characteristics).

The aim of the paper was the preparation and characterization chitosan and gelatin based submicronic particles, prepared by double crosslinking (ionic and covalent) of polymers in an O/W/O double emulsion (Figure 1).

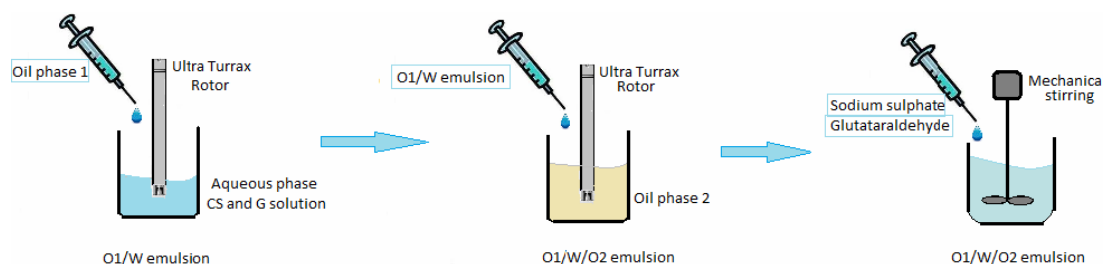


Figure 1: Microcapsule preparation step.

There have been prepared chitosan and gelatin based particles (Figure 2), with rather large polydispersity (0.2-10 μm).

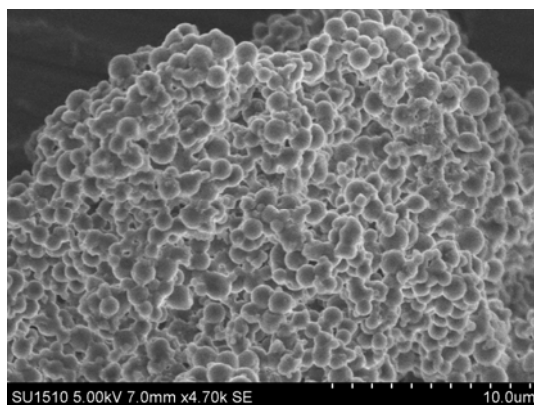


Figure2: Scanning electron microscopy images of polymer microcapsules.

The varying ionic crosslinker/polymer molar ratio influenced particle size, morphology, swelling degree and their capacity to release hydrophilic model molecules.

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P 29. Structural, spectral and magnetic properties of Co(II), Rh(III) and Cd(II) complexes with 2-(1H-1,2,4-triazol-3-yl) pyridine.

Petronela Gospei (Horlescu)¹, Daniel Sutiman¹, Carmen Mita², Peptu Cristian³, Cornel Stan¹

¹Faculty of Chemical Engineering and Environmental Protection, "Gheorghe Asachi" Technical University of Iasi, 73 D. Mangeron Bd., 700050, Romania

²Department of Chemistry, "Al. I. Cuza" University of Iasi, 11 Carol I Bd., 700506, Romania

³"Petru Poni" Institute of Macromolecular Chemistry, 41A Grigore Ghica Voda Aley, 700487 Iasi, Romania

Co(II), Cd(II) and Rh(III) complexes containing 2-(1H-1,2,4-triazol-3-yl)pyridine (Htzip) have been synthesized and characterized. The neutral mononuclear $[M(\text{tzip})_n]$ complexes have been prepared from Htzip, $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$, $\text{CdCl}_2 \cdot \text{H}_2\text{O}$ and $\text{RhCl}_3 \cdot 3\text{H}_2\text{O}$ in the ratio 2:1 and 3:1, respectively, in H_2O –EtOH. All the chemicals were of reagent grade and were used as received. The isolated crystalline complexes have been characterized by elemental and thermal analysis, magnetic and molar conductivity measurements, X-ray crystallography, IR and UV-Vis spectroscopy. The experiments indicate that Htzip acts as bidentate anionic ligand, $[\text{Co}(\text{tzip})_2] \cdot 1.5\text{H}_2\text{O}$ and $[\text{Cd}(\text{tzip})_2]$ are in the tetragonal coordination, whereas six coordinate octahedral $[\text{Rh}(\text{tzip})_3] \cdot \text{H}_2\text{O}$ complex undergoes a weak tetragonal distortion.

Keywords: Co(II), Cd(II), Rh(III) complexes, 2-(1H-1,2,4-triazol-3-yl) pyridine, spectral and magnetic properties

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P 30. Synthesis and characterization of some new bent core liquid crystalline compounds based on 2,7-dihydroxynaphthalene

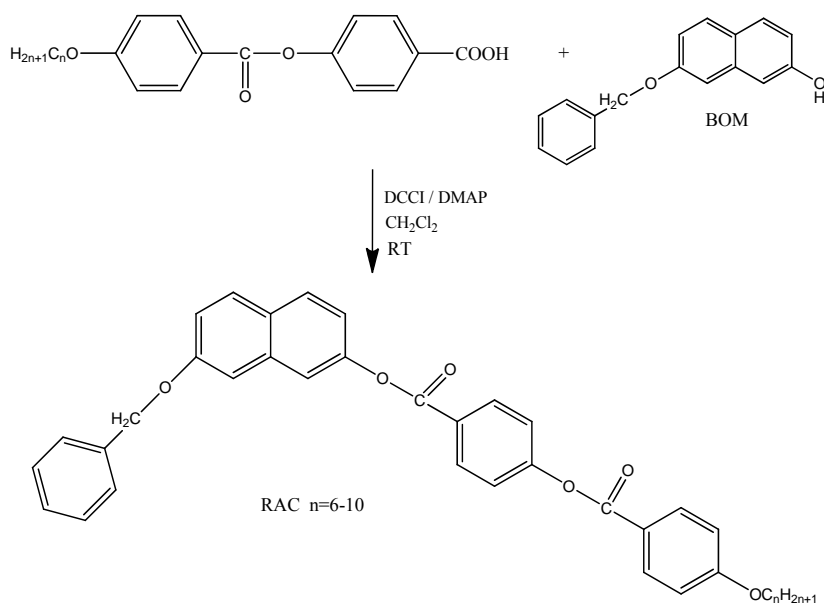
Aurel Simion, Irina Carlescu, Dan Scutaru*

Department of Natural and Synthetic Polymers, Gheorghe Asachi Technical University of Iași, Romania

*E-mail address: dscutaru@ch.tuiasi.ro

The field of liquid crystals is a current research direction, which has direct implication in numerous top technologies. Ever since the beginning of the extensive research on the bent-core liquid crystals (also named banana-shaped, boumerang or biaxial) numerous such compounds have been synthesized and their mesomorphic properties have been investigated.

The paper presents the synthesis and spectral characterization of some asymmetric bent-core compounds based on 2,7-dihydroxynaphthalene as central core. The synthesis involved a two steps esterification of the hydroxyl groups of the core molecule with benzoyl chloride and a mesogenic unit based on several 4-alkyloxy-benzoic acid moieties (Scheme 1). The structure of the final products was confirmed by common spectral techniques. The liquid crystalline properties have been investigated by POM and DSC analysis. All the synthesized products presented monotropic liquid crystalline properties, mainly with nematic textures.



Scheme 1: Synthesis of the final bent core compounds.

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P 31. Optimization Study for the Photocatalytic Degradation of Rhodamine 6G Dye Using Doped Titania

Doina Lutic,¹ Cristina Coromelci-Pastravanu, Igor Cretescu²

¹ Department of Chemistry, "Al. I. Cuza" University of Iasi

² Department of Chemical Engineering and Environmental Protection, "Gh. Asachi" University of Iasi

*E-mail address: doilub@yahoo.com

The treatment of wastewaters containing dyes using the heterogeneous photocatalytic processes has been widely approached in the research during the recent years, due to its efficiency and green-procedure character. The photoactive behavior of semi-conducting TiO₂ captured a high interest in different applications connected to materials science, due to its excellent chemical stability, low toxicity and band gap value of 3.2 eV,¹ allowing to absorb both UV and visible light.

In our work, mesoporous titania was synthesized by the hydrolysis-condensation method, using titanium tetra-isopropoxide as precursor and cetyl-trimethyl-ammonium bromide (CTAB) as surfactant. The mesoporous TiO₂ was doped with wolfram oxide and/or platinum. The mesoporous structure of TiO₂, with rather uniform pores and high specific BET surfaces of 200 – 290 m²/g was preserved after the doping procedure.

The photocatalytic potential of several samples containing, respectively, 2% WO₃, 5%WO₃ and 2%WO₃ + 1% Pt (mass ratios) on commercial P-25 titania and on our mesoporous TiO₂ samples were tested in the degradation of aqueous solutions of Rhodamine 6G (R6G) dye. The dye degradation was monitored by photocolourimetry and by TOC (Total Organic Carbon) measurements.

The experimental matrix of 2ⁿ-experiments type foresaw a parametric optimization study, allowing us to determine the best values of several factors (pH value, catalyst dose, initial dye concentration) on the dye degradation process.

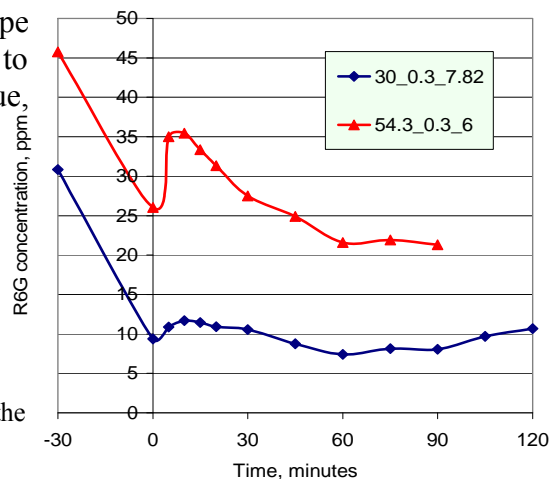
Some interesting and unexpected results were obtained on the mesoporous solids, concerning the dye strong adsorption during the equilibrium time, followed by its photoreaction.

Acknowledgements

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P 32. Studies regarding fabrication of ZnO functionalization cotton fibers through electroless method

Nicoleta Preda¹, Monica Enculescu¹, Irina Zgura¹, Marcela Socol¹, Elena Matei¹, Violeta Vasilache,^{2*} Ionut Enculescu¹

¹National Institute of Materials Physics, Magurele-Bucharest, P.O. Box MG-7, R-77125, Romania

² Faculty of Food Engineering, “Stefan cel Mare” University, 13 Universitatii Street, RO-720229, Suceava, Romania

*E-mail address: violetav@fia.usv.ro

During the last decade, nanotechnologies were successfully applied in textile industry. Treatment and coverage of textile fibers and/or fabrics with nanostructures conduce to improvement of some characteristics, like strength, mechanical resistance, self-cleaning and antibacterial properties. Textile fibers offer an excellent substrate for adhesion of different substances in nanostructure form. Zinc oxide is one of these substances because it exhibits a high occurrence and a low cost. It is used also in optoelectronic devices, because it presents a direct band gap of 3.37 eV, a large exciton binding energy of 60 meV and a high transmittance of visible light. Due to the antibacterial activity, zinc oxide is an inorganic biocompatible substance and as consequence could be also used for biomedical applications.

The aim of the study was to investigate properties of cotton fabrics coated with arrays of ZnO hexagonal prisms, using an electroless (cathalitic/autocathalitic) deposition process. It was used a typical three step method, similar to methods used for electroless deposition of metals on insulating substrates.

The three steps were pre-activation, activation and deposition. An aqueous solution containing zinc nitrate as source of zinc ions and dimethylamineborane as reducing agent were used to grow the nano-dimensional ZnO particles. Further, cotton fabrics coated with ZnO were characterized to emphasize the structure by X-ray diffraction (XRD) and to point the morphology by scanning electron microscopy (SEM). The XRD studies highlighted that ZnO particles present a hexagonal wurtzite crystalline structure. The SEM observations proved that cotton fibers are homogeneously covered by hexagonal prisms which have uniform base size of approximately 500 nm and heights of 1 μm .

The described technique is highly reproducible, easy scalable and cheap, allowing a wide range of applications.

Keywords: ZnO hexagonal prisms; cotton fabrics; electroless deposition; UV-blocking.

P 33. Contributions to the Thermal Degradation Mechanism under Nitrogen Atmosphere of PTFE by TG-FTIR Analysis. Influence of the Particle Size

L. Odochian,* C. Moldoveanu, D. Maftai

¹*Department of Chemistry, "Al. I. Cuza" University of Iasi*
**E-mail address: lodochian@yahoo.com*

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

The goal of this work was to find the best degradation conditions having in view the monomer (C₂F₄) recovery from polymer residues due to the highly cost both of the polymer obtaining and especially to the monomer synthesis.^{1,2}

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

The TG-FTIR analysis of the gaseous products evolved by thermal degradation of the samples under nitrogen atmosphere was applied for the first time with the different particle size PTFE leading to results regarding the obtaining of the monomer (C₂F₄) from residue resulted on PTFE mechanical processing, in view of its recovering.

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

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**P 34. Scaling up Microwave Synthesis –
Moving common technology beyond the R&D laboratory scale**

Alexander Stadler

“Anton Paar GmbH”

Within 25 years microwave synthesis has matured and stepped into several fields of applications other than pure microwave-assisted organic synthesis (MAOS). In recent years besides classic pharmaceutical research especially material science (e.g. preparation of nanomaterials) and polymer synthesis have taken advantage of the benefits of microwave heating. Improved features and enhanced specifications of modern microwave instruments together with special accessory have significantly broadened the scope of microwave synthesis making it an attractive tool for several chemical disciplines.

Not only small-scale R&D but also the scale-up of microwave-mediated chemical transformations is of considerable industrial interest. Herein an appropriately designed 1L batch-type microwave benchtop reactor is introduced for the multigram synthesis of relevant building blocks and key intermediates.

P 35. Recent Developments Towards Microwave-Assisted Method Development and Optimization

Alexander Stadler

“Anton Paar GmbH”

New accessory for efficient microwave-assisted method development and optimization is introduced allowing efficient handling of small-scale applications and first grade laboratory scale-up at elevated pressure and enhanced temperature.

Precise reaction control and extended operation limits allow for developing new reaction pathways in microwave synthesis, thus broadening the scope of chemical research.

The concept of a modular equipment family is outlined, which enables applying optimized protocols on any applicable scale in the instrument without reoptimization. This increases the efficiency of microwave-mediated synthesis even further, speeding up the entire process of academic and industrial research.

P 36. Hydrodynamics of fluidized bed consisting of adsorbent particles

Gabriela Muntianu,¹ Vasilica Alisa Arus¹, Nicoleta Platon¹, Ana Maria Rosu¹, Denisa Ileana Nistor¹, Gheorghita Jinescu²

¹Chemical and Food Engineering Department, “Vasile Alecsandri” University of Bacau, 157, Calea Marasesti Str., 600115, Bacau, Romania

²Politehnica University of Bucharest, Chemical Engineering Department, 313, Splaiul Independentei Str., 060042, Bucharest, Romania

A hydrodynamic study was carried out to establish the optimal operating hydrodynamic parameters in fluidized bed for the adsorbent particles (sodium clay particles and pillared clay particles). The particles of the adsorbent material possess surface properties and selective adsorption.¹ The intensification technique of the adsorption process aims to realize a uniform contact between the fluidization agent and the granular layer.^{2,3} In order to determine the influence of the adsorbent particles on the structure of the fluidized bed, the conditions in which the incipient fluidization appears were determined: nature of the adsorbent particles, diameter and density, fixed bed height and gas velocity. Using fluidized bed as an intensification technique in the adsorption of gaseous pollutants presents a series of advantages given by these hydrodynamic parameters.^{4,5}

The minimum fluidization velocity, the minimum pressure drop and bed porosity were determined experimentally. The experimental determination of hydrodynamic conditions assures a high surface contact between the adsorbent particles and fluidization agent. The aim of this paper is to study the intensification of the adsorption process of pollutants on clays which correspond to class B and D depending on the diameter of particles according to Geldrat's dimensional dynamic classification.⁶ Correlation relations were established in order to approximate the minimal error for the experimental results. The purpose is to obtain the optimum hydrodynamic conditions for sodium clay particles and pillared clay particles used in adsorption process under influence of magnetic field.

Keywords: adsorbent particle, fixed bed, fluidized bed, minimum fluidization velocity, pressure drop

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P 37. Hydrotalcites with different molar ratios Mg/Al - preparation and characterization

Vasilica Alisa Arus, Ileana Denisa Nistor, Neculai Doru Miron, Rosu Ana-Maria, Platon Nicoleta, Muntianu Gabriela

“Vasile Alecsandri” University of Bacau, Calea Marasesti 156, Bacau, 600115, Romania

Anionic clays are natural or synthetic combinations of hydroxides with lamellar structure, having between layers spaces containing exchangeable anions and water molecules.¹ Because hydrotalcites possess excellent properties (low or no toxicity, good biocompatibility, the possibility of controlled release) present a continuous interest in the discovery of new applications.²

This work presents the preparation and characterization methods of the hydrotalcites from structure point of view. Anionic clays are characterized by a lamellar structure like that of brucite, $Mg(OH)_2$ (Figure 1).^{3,4}



Figure 1: Structure of layered double hydroxide [4].

The objectives of this experimental study were: the preparation of anionic clays by co-precipitation method using different molar ratios Mg/Al; the characterization of prepared anionic clays; the influence of molar ratios Mg/Al on the properties of anionic clays. The anionic clays with different molar ratios Mg/Al (1/1, 2/1, 3/1, 4/1, 5/1) were prepared by co-precipitation method at low supersaturation at constant pH.⁵

The anionic clays obtained were studied by following physical and chemical characterization techniques: SEM analysis and granulometric analysis.

The experimental results revealed the influence of operating parameters values on the properties of materials prepared. SEM analysis confirm that the anionic clay with molar ratio Mg/Al = 5/1 has the specific structure by hydrotalcite. Volume size distribution was the representative granulometric distribution, which had the highest level of confidence regardless of the type of sample.

Keywords: hydrotalcites, co-precipitation, electron microscopy SEM, granulometric analysis

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P 38. Hosoya-Diudea polynomial in supramolecular structures

M. V. Diudea,^{1*} M. P. Vlad²

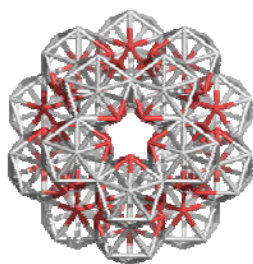
¹Faculty of Chemistry and Chemical Engineering, “Babes-Bolyai” University, Arany Janos Str., 400028 Cluj, Romania

²Faculty of Economic Sciences, “Dimitrie Cantemir” University, Bucharest, No 56 Teodor Mihali Str., 400591, Romania

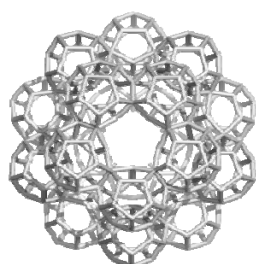
*E-mail address: diudea@chem.ubbcluj.ro

Hosoya polynomial¹ counts finite sequences of distances in a graph G; more exactly, it counts the number of points/atoms lying at a given distance in G. The polynomial coefficients are calculable by means of layer/shell matrices. Shell matrix operator (invented by Diudea and implemented in TOPOCLUJ software program) enables the transformation of any square matrix in the corresponding layer/shell matrix, thus generalizing the local property counted according to its distribution by the distance in the graph. This represents the “Hosoya-Diudea” generalized counting polynomial.^{2,3}

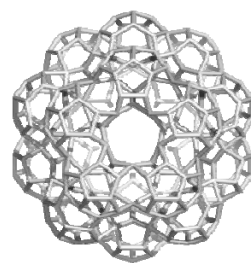
Carbon allotropes, designed as hyper-structures of the Dodecahedron (see the below figure) are described in terms of Hosoya-Diudea polynomials. They represent yet hypothetical nanostructures.



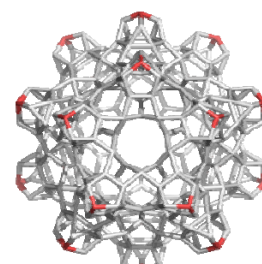
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DoXDiad_{20_340}

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