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Abstracts

for

14th Scientific Session of Undergraduate, Masters and PhD Students, Iasi, Romania

June 23, 2023

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C1. Tuning the properties of materials through crystal growth

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An important part of the materials used in the everyday life are in polycrystalline form and most of them have been extracted from the earth's crust or synthesized using different synthesis methods.

Using the approach of a chemist, we are looking into how to enhance some of the properties (electric, magnetic, and structural) of the materials found in everyday life devices. To this extent, our work focuses on understanding if the properties of interest have their origin in the crystallographic structure of the solid and/or how much they are influenced by microstructural parameters. It is well known, for some time, that nano-particles, the bi-dimensional materials or even thin layers have different properties than the bulk material due to new interesting phenomena originating in their 1D, 2D nano-scale size or resulting from the interaction with the substrate. It is thus crucial to achieve a better understanding of the source of the properties of a "perfect" material, i.e. the single crystal. The availability of a material in the form of a single crystal will give us access to the intrinsic properties of the compound, un-altered by the interaction with the substrate, grain boundaries, etc. Once the origin of the properties of a material has been elucidated, a chemist could envisage applying chemical pressure through doping with a similar sized ion as a mean to change inter-atomic distances and tune the desired property.

The present study involves the synthesis, characterization and improvement of a series of compounds that are potential candidates for environmental barriers. Most of the environmental barriers used in different application are polycrystalline samples that are very well compacted. A high number of crystalline materials have anisotropic properties, originating in their crystallographic structure, thus it is important to study the properties of the single crystal form of these materials [1]. This will allow the enhancement of the properties that are significant in environmental barrier applications: thermal insulation, chemical resistance, as well as hardness and the compactness through the thermal expansion coefficient. It is well known that the rare earth silicates are a good candidate for such applications that require high temperature, however through studies of their single crystals we can improve the properties and extend their applicability [2].

Keywords: solid-state chemistry, crystal growth, material optimization

References:

[1] Rey-García, F., Bao-Varela C., Costa F.M., Laser Floating Zone: General Overview Focusing on the Oxyorthosilicates Growth, I*ntechOpen* [Online] (2019)
[2] Huang, P., Zou, B., Zhang, Y., Niu, X., Wang, Y., *Inorg. Chem. Commun*., 135, 109129 (2022)

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C2. Synthesis and characterization of Cu(II) coordinative compounds with 1,2,3-triazole derivative

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1,2,3-triazole based ligands are widely exploited in therapeutic chemistry, with numerous biological activities, the most important are the anticancer ones [1]. Likewise, metal complexes [2] show interest in this field, therefor the use of coordination compounds with 1,2,3-triazole based ligand could give expected results.

The 1,2,3-triazole 1,4-disubstituted derivative, ethyl 1-(2-phenyl-2-oxoethyl)-1H-1,2,3-triazole-4-carboxylate (L), was synthesized by click chemistry.

Subsequently, 2 complexes based on Cu(II) were synthesized starting from its salt ($CuCl_2 \cdot 2H_2O$) in the presence of MeOH or EtOH by stirring at 40 °C, in the reaction with L in ratio Cu(II):L = 1:2.

All the compounds were characterized by IR, UV-VIS spectrometry, conductometric, thermogravimetric and magnetic methods. The ligand was supplementary analyzed by NMR spectrometry. The kinetics of the substitution reaction of coordinated ligand with cysteine was also studied.

The cytotoxicity of L, and CuL_2 complexes was tested by the MTT method and the cell morphology by evaluating the impact of the complexes and L at 6.25, 12.5, 25 and 50 μM after 24 and 48 h on the normal cell line V79-4 (pulmonary fibroblasts, derived from the Chinese hamster *Cricetulus griseus*) and the tumor cell line MCF-7 (human mammary adenocarcinoma). DMSO 0.1% was used to solubilize the compounds. The results regarding IC_{50} after 48 h for MCF-7 were 55.13 for L, 21.73 for CuL_2 in MeOH and 54.43 for CuL_2 in EtOH.

Keywords: 1,2,3-triazole, anticancer, coordinative compounds.

References:

[1] Bozorov, K., Jiangyu, Z., Haji, A.A., *Bioorg. Med. Chem.*, 27, 3511-3531 (2019)
[2] Gou, Y., Huang, G.J., Li, J., Yang, F., Liang, H., *Coord. Chem. Rev.*, 441, 231975 (2021)

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C3. FT-IR kinetic studies of the gas-phase reaction of the OH radical with a series of nitrotoluene compounds

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Nitroaromatic hydrocarbons (NAHs) are widely present in urban air and are important constituents of biomass burning emissions. These compounds, including nitrotoluenes (NTs), have toxic effects on human health and can potentially impact air quality and Earth climate [1]. While the primary emissions of NAHs in the atmosphere are mainly associated with anthropogenic activities, NAHs are formed in both the gas and aerosol phase, through the oxidation of aromatic compounds [2].

The direct photolysis of 2-nitrotoluene, investigated under atmospheric conditions, potentially leads to the production of HONO, important precursor of OH radicals in the atmosphere, following a mechanism similar to the one proposed for 2-nitrophenol [3]. However, the gas-phase chemistry of NTs is not well characterized, with only one available kinetic study on the reaction between 3-nitrotoluene and OH radicals [4].

The ESC-Q-UAIC quartz-glass atmospheric simulation chamber was employed to investigate the gas-phase reactivity of the 2-, 3- and 4-nitrotoluene with the OH radicals. The chamber has a volume of 760 L and is equipped with a long-path FT-IR measurement technique. OH radicals were generated in the reactor through the photolysis of methyl nitrite or isopropyl nitrite in the presence of NO_x or through the ozonolysis of tetramethylethene. Dimethyl ether, cyclohexane and ethyl acetate were used as reference compounds for the relative rate kinetic method. The kinetic process was monitored over a period of 15-20 minutes, with IR spectra collected every minute at a resolution of 1 cm^{-1}. Wall loss and photolysis of the reactants were used to correct the kinetic results.

The atmospheric implications of these kinetic and photolysis processes, along with their impact and their potential effects on a regional scale will be assessed.

Keywords: nitroaromatics, gas-phase kinetic, OH radical, ESC-Q-UAIC chamber

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References:

[1] Cai, D., Wang, X., George, C., Cheng, T., Herrmann, H., Li, X., Chen, J., *J. Geophys. Res.: Atmos.,* 127, e2021JD036167 (2022)

[2] Calvert, J., Atkinson, R., Becker, K.H., Kamens, R., Seinfeld, J., Wallington, T., Yarwood, G., The Mechanisms of Atmospheric Oxidation of the Aromatic Hydrocarbons, Oxford University Press, 2002

[3] Bejan, I.; Abd El Aal, Y.; Barnes, I.; Benter, T.; Bohn, B.; Wiesen, P.; Kleffmann, J., *Phys. Chem. Chem. Phys*., 8, 2028 (2006)

[4] Atkinson, R., Aschmann, S., Arey, J., Carter, W., *Int. J. Chem. Kinet.*, 21, 801 (1989)

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C4. Strategies to optimize bioavailability and bioactivity of phytocompounds

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The metabolic processes that take place in plant organisms result in a wide variety of phytocompounds. Among them, polyphenols (PF) and volatile terpenes (TPVL) are the most studied for potential therapeutic uses [1]. Although both PF and TPVL showed a wide spectrum of biological actions (such as antioxidant, antimicrobial, anti-inflammatory, chemopreventive, etc.) when studied *in vitro* or *in vivo* on animal models, their clinical use is limited by their stability and pharmacokinetic issues [2,3]. Current studies focus on including these bioactive substances in various delivery systems to protect them while still preserving or even enhancing their bioactivity and bioavailability. Hydrogels (HG) are of increased interest due to the fact that they allow control over composition, presentation, and release pattern [4,5].

This paper aims to present the most common strategies for preparing hybrid HG/PF or HG/TPVL systems, as well as the synergy between the HGs and the phytocompounds in terms of physicochemical and biological properties.

Keywords: hydrogels, polyphenols, volatile terpenes

References:

[1] Hăncianu, M.; Gîrd, C.E.; Stănescu, U., Farmacognozie. Produse vegetale cu substante bioactive, Ed.; Polirom, 2020

[2] Turek, C., Stintzing, F.C., *Compr. Rev. Food Sci. Food Saf.*, 12, 40–53 (2013)

[3] Deng, J., Yang, H., Capanoglu, E., Cao, H., Xiao, J., In Polyphenols: Properties, Recovery, and Applications, Elsevier, 295–323, 2018

[4] Micale, N., Citarella, A., Molonia, M.S., Speciale, A., Cimino, F., Saija, A., Cristani, M., *Molecules*, 25 (2020)

[5] Dinu, M.V., Gradinaru, A.C., Lazar, M.M., Dinu, I.A., Raschip, I.E., Ciocarlan, N., Aprotosoaie, A.C., *Int. J. Biol. Macromol.*, 184, 898–908 (2021)

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C5. Grafted pullulan derivatives for reducing the content of some pesticides from simulated wastewater

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Grafted polymers are widely used in the particle separation processes for wastewater purification, as they combine the advantages of both synthetic and natural polymers [1]. In this context, the goal of the present study was the application of a series of soluble grafted pullulan derivatives for removal of some pesticide formulations from model wastewater. The pullulan derivatives are cationic polyelectrolytes, with various content and length of grafted poly[(3-acrylamidopropyl)-trimethylammonium chloride] chains onto the pullulan (P-*g*-pAPTAC). The commercial pesticides are either fungicides (Bordeaux Mixture – *BM*) or insecticides (Decis – *Dc*: active ingredient Deltamethrin, Confidor Oil – *CO*: active ingredient Imidacloprid, Confidor Energy – *CE*: active ingredients Deltamethrin and Imidacloprid and Novadim Progress – *NP*: active ingredient Dimethoate). The removal efficiency has been assessed by UV–Vis spectroscopy measurements as a function of some parameters, namely polymer dose, grafted chains content and length, pesticides concentration. The P-*g*-pAPTAC samples showed good removal efficacy at dose_{op}, more than 94% for *BM*, between 84–90% for *DC*, *CO*, *CE* and around 93% for NP. The maximum percentage removal decreased with the pesticides (*DC*, *CO*, *CE*, *NP*) concentration declining; no effect of *BM* concentration in suspension on its removal efficiency process has been noted. The removal mechanisms of pesticides (charge neutralization, bridging, etc.) have been established by zeta potential and particle size distribution measurements.

Keywords: pullulan-based flocculant, pesticides, flocculation mechanism

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References:

[1] Lapointe, M., Barbeau, B., *Sep. Purif. Technol.*, 231, 115893 (2020)

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P1. The determination of enzymatic activity of α-glucosidase following the interaction with $MgFe_2O_4$@HaP@APTES nanocomposite

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This study aimed to test the enzymatic activity of α-glucosidase following the interaction with the nanocomposite of magnesium ferrite with hydroxyapatite amino-functionalized - $MgFe_2O_4$@HaP@APTES. The enzymatic activity of α-glucosidase was determined based on the reaction of cleavage of glycosidic bonds in the substrate 4-Nitrophenyl α-D-Glucopyranoside (pNPG) [1]. After the reaction, the substrate is completely converted to p-nitrophenol, which can be spectrophotometrically determined at 405 nm. In this regard, the enzymatic activity of both simple α-glucosidase and the $MgFe_2O_4$@HaP @APTES@α-glucosidase nanocomposite was studied. An average absorbance value of 0.39 ± 0.03 (N=3, SEM at 95% confidence level) at 405 nm was obtained for the enzyme alone in the enzyme activity assay, and for the immobilized enzyme an average absorbance of 0.2367 ± 0.07 was determined (N= 3, SEM-the standard error of the mean, at a confidence level of 95%) [2,3].

Keywords: α-glucosidase, nanocomposite, absorbance

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References:

[1] Wubshet, S.G., Brighente, I.M.C., Moaddel, R., Staerk, D., *J. Nat. Prod.*, 78(11), 2657-2665 (2015)

[2] Shen, Y., Wang, M., Zhou J., Chen, Y., Wu, M., Yang, Z., Yang, C., Xia, G., Tam, JP, Zhou, C., Yang, H., and Jia, H., *Int. J. Biol. Macromol*, 165, 1361-1372 (2020)

[3] Cheng, G., Xing, J., Pi, Z., Liu, S., Liu, Z., Song, F., *Chin. Chem. Lett.*, 30(3), 656-659 (2019)

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P2. Oxidation of pyrite with molecular oxygen

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Pyrite (FeS_2), the most important mineral sulfide, forms in sedimentary areas such as marshes and marine or fluvial deposits. The process of FeS_2 formation involves anoxic aqueous environments with appropriate sulfur and iron concentrations. In contact with oxygen in the air and water, pyrite oxidizes forming sulfuric acid (H_2SO_4). The process is favored by high oxygen concentrations, being also accelerated by increasing temperature and a high pH [1]. The low pH and the presence of oxygen favor secondary reactions of oxidative dissolution of other mineral sulfides leading to the release of some toxic species, such as Cu, Cd, Hg, Mn, Sb or As ions [2].

Taking into consideration the special implications of the oxidation of pyrite with dissolved oxygen ($O_{2(aq)}$), we have carried out a series of experimental studies and quantum calculations, in order to clarify the interaction mechanism between pyrite and oxygen. Experimentally, pyrite oxidation was studied by electrochemical methods (potentiodynamic polarization, electrochemical impedance spectroscopy and cyclic voltammetry) and FTIR spectroscopy.

The obtained results showed that the oxidation of the mineral produces trivalent iron (Fe^{3+}) and sulfate (SO_4^{2-}). Although the quantum calculations showed that the proton adsorption process is spontaneous, the experimental results showed that the pH variation has no significant influence on the electron transfer rate from FeS_2 to oxygen (pyrite oxidation rate). The reaction order of pyrite oxidation with respect to $[H^+]$ is 0.1.

These results help to better understand the oxidation of pyrite with $O_{2(aq)}$, which is essential for evaluating the impact of the reaction on the environment and for developing appropriate management strategies for the acid waters formed.

Keywords: pyrite, oxidation, pH

References:

[1] Williamson, M.A., Rimstidt, J.D, *Geochim. Cosmochim. Acta*, 58, 5443-5454 (1994).

[2] Janzen, M.P., Nicholson, R.V., Scharer, J.M., *Geochim. Cosmochim. Acta*, 64, 1511-1522 (2000)

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P3. Gas-phase kinetic study of 3-hydroxybenzaldehyde with OH radicals under simulated atmospheric conditions

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Harmful volatile organic compounds (VOCs) are emitted in the atmosphere in large quantities from anthropogenic sources. Aromatic hydrocarbons (AHs) are an important class of VOCs present in the atmosphere, which contribute significantly to the chemistry of urban air [1]. The AHs degradation is mainly initiated by reaction with the hydroxyl radical (OH) leading to oxygenated volatile organic compounds (OVOCs). However, OVOCs with AH structure can also reach the atmosphere as constituents of biomass burnings and wildfire events, more frequent in the last decade as a consequence of global warming and climate change [2].

In this study, the kinetic rate coefficient for the reaction of 3-hydroxybenzaldehyde with the OH radical is determined for the first time under simulated atmospheric conditions. The ESC-Q-UAIC reaction chamber, a cylindrical quartz-made reactor with a volume of 760 L connected to a long path FT-IR technique, was used for the present kinetic experiments. An external White type multiple reflection optical system helps to achieve a total pathlength of (492±1) m inside the chamber.

The OH radical was produced through the isopropyl nitrite photolysis at λ_{max}=365nm. Propene and cyclohexane were used as reference compounds in the present investigations. The wall loss was measured to correct for secondary decay processes.

The reactivity of 3-hydroxybenzaldehyde towards OH radicals will be compared with other aromatic compounds and with Structure Activity Relationship (SAR) estimated values. The associated atmospheric lifetime will be assessed together with potential improvement to current understanding of the degradation mechanism and atmospheric oxidation chemistry of aromatic compounds.

Keywords: 3-hydroxybenzaldehyde, gas-phase kinetic, OH radical, ESCQUAIC simulation chamber

Acknowledgement: The study was carried out with the financial support provided by the project PN-III-P2-2.1-PED2021-4119 (SOA-REACTOR) from UEFISCDI. Also, recognition is given to the RECENT AIR project under the MySMIS grant agreement no. 127324

References:

[1] Calvert, J.G., Atkinson, R., Becker, K.H., Kamens, R.M., Seinfeld, J.H., Wallington, T.J., Yarwood, G.. The Mechanisms of Atmospheric Oxidation of Aromatic Hydrocarbons, Oxford University Press, London, 2002
[2] Akherati et al., *Environ. Sci. Technol.*, 54(14), 8568 (2020)

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P4. Composite biomaterials based on titanium dioxide. synthesis, properties and applications

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Biomaterials are biocompatible materials used in the biological world to analyse, treat and support living organisms. They can be obtained naturally or synthesized in the laboratory. Among the synthesized materials, TiO_2, is one of the most well-known semiconductor materials used in the biological world. Nowadays, TiO_2, it is widely used in cosmetics, paints, ceramics, photocatalysis, solar cells, food dyes, drug delivery and photodynamic therapy due to its stability, sensitivity, selectivity, biocompatibility and non-toxic nature to living beings [1,2]. The development of new materials based on TiO_2 is necessary to achieve improved properties and applications.

For increasing applicability and efficiency of TiO_2 some studies reported that the addition of silver enhances, on the hand, the photocatalytic efficiency of TiO_2 and, on the other hand silver has a broad spectrum of antibacterial activity, being active against gram-negative and gram-positive bacteria. The optimization of photocatalytic activity of TiO_2 can be realized by preparation of TiO_2-ZnO composites.

In order to enhance the properties of TiO_2, the purpose of this work was to study the synthesis condition, structural and morphological characterization of TiO_2 and the composites materials with silver and zinc oxide respectively.

The composites materials were obtained by using coprecipitation method. The structure and morphology of the synthesized materials was performed by X-ray diffraction, FTIR spectroscopy and SEM analysis. The XRD analysis confirms the formation of the composite materials. For the TiO_2/ZnO composite the particles of this sample are spherical in flower form in agreement with the literature data [2]. The particles in the form of a flower have high porosity and thus they become efficient in absorbing UV rays, respectively in photocatalysis.

Keywords: coprecipitation method, titanum oxide, composites, biomaterials

Acknowledgement: Mr. Prof. A. Pui that provided the facility to perform FTIR analyzes and *Integrated Centre for Environmental Science Studies in the North-East Development Region – CERNESIM* for SEM analyses

References:

[1] Zhang, X., Lv, Y., Shan, F., Wu, Y., Lu, X., Peng, Z., Liu, B., Yang, L., Dong, Z., *Appl. Surf. Sci.,* 531, 147399 (2020)
[2] Kighut, K., Gopalan, A.I., Lee, D.E., Saianand, G., Hou, Y.L., *J. Environ. Chem. Eng.,*106417 (2021)

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P5. Cinnamic acid derivatives

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Widespread in nature, cinnamic acid (2*E*-3-phenylpropenoic acid, Fig. 1) is an *α,β*-unsaturated carboxylic acid, containing a double bond in the *trans* configuration and is found mainly in cinnamon oil and shea butter [1]. Our researches were aimed at synthesizing ester derivatives of cinnamic acid, with a propargylic residue, in two stages, using benzoic aldehyde as starting material.

Stage I: Attainment of the cinnamic acid by the Perkin condensation between benzoic aldehyde and acetic anhydride in the presence of anhydrous K_2CO_3 at a temperature of 170˚C (Fig. 1).

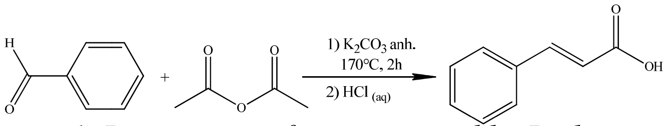

Figure 1. Preparation of cinnamic acid by Perkin

Stage II: Esterification of cinnamic acid with propargyl alcohol in the presence of the condensing agents CDI and EDC·HCl:

Method	Reactants	Molar ratio	Solvent	Time
1	CDI : Propargylic alcohol	1.1:1.2	Tetrahydrofuran	24 h
2	CDI : DMAP : Propargylic alcohol[2]	1.1:0.1:1.1	Dichloromethane	24 h
3	EDC·HCl : DMAP : TEA : Propargylic alcohol[3]	1.5:1:2:1	Dichloromethane	24 h

The compound of interest (propargyl cinnamate, Fig. 2) was obtained by working method 3, then purified and physically and spectrally characterized.

Esterification by working method 3, of ferulic acid (2*E*-3-(4-hydroxy-3-methoxyphenyl)propenoic acid, Fig. 3), did not lead to the desired propargylic ester

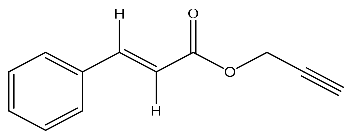

Figure 2. Propargyl cinnamate.

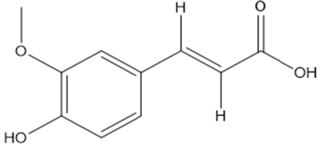

Figure 3. Ferulic acid.

Keywords: cinnamic acid, propargylic ester, propargyl cinnamate, condensing agent

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References:

[1] Ruwizhi, N., Aderibigbe, B.A., *Int. J. Mol. Sci.*, 21(16), 5712 (2020)
[2] Vale, J.A., Rodrigues, M.P., Lima, M.A., Santiago, S.S., Lima, G.D.A., Almeida, A.A., Oliveira, L.L., Bressan, G.C., Teixeira, R.R., Machado-Neves, M., *Biomed. Pharmacother.*, 148, 112689 (2022).
[3] Pradhan, T., Mohapatra, D.K., *Adv. Synth. Cat.*, 361(15), 305-3611 (2019)

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P6. *1,3*-dipolar cycloadditions of dimethyl fumarate

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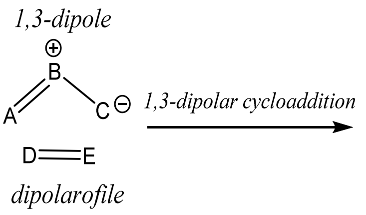
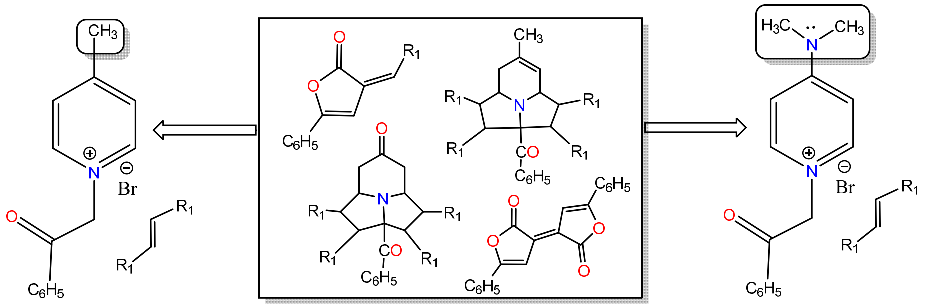


1,3-dipolar cycloadditions are commonly used in organic synthesis to obtain heterocyclic skeletons with various medical and technical applications [1]. The study aimed to investigate the chemical behavior of dimethyl fumarate in the presence of *1,3*-dipoles generated *in situ* from 4-substituted pyridinium salts.

By alkylation of 4-methylpyridine and *N,N*-dimethylaminopyridine with *ω*-bromoacetophenone, the pyridinium salts (1) and (2) were obtained as substrates generating *N*-ylides in a basic medium. Dimethyl fumarate acts as a good dipolarophile in these reactions and also serves as a reactant in Michael-type additions [2].

After separating the products resulting from the cycloaddition reactions, the lactonization capacity of certain intermediate products was observed, and derivates of octahydro- and decahydro-pyrrolo[2,1,5-*cd*]indolizine-6-one type obtained through a double *1,3*-dipolar cycloaddition were identified [3,4].



(1) (2)

Keywords: *1,3*-dipolar cycloaddition; lactonization; dimethyl fumarate, pirroloindolizine

Acknoledgements: The authors are grateful to the project POSCCE-O 2.2.1, SMIS-CSNR 13984-901, No. 257/28.09.2010, CERNESIM for the NMR spectra.

References:

[1] Angyal, A., Demjén, A., Wölfling, J., Puskás, G., Kanizsai, I., *J. Org. Chem.*, 85, 3587 (2020)
[2] Fang, Y., He, L., Pan, W., Yang, Y., *Tetrahedron*, 75, 3770 (2019)
[3] Belei, D., Abuhaie, C., Bicu, E., Jones, P. G., Hopf, H., Birsa, M. L., *Synlett*, 23, 545 (2012)
[4] Hopf, H., Jones, P. G., Nicolescu, A., Bicu, E., Birsa, M. L., Belei, D., *Chem. Eur. J.*, 20, 5565 (2014)

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P7. C-alkylation reactions of 4-substituted 1-(benzoylmethyl)-1,2,3-triazoles

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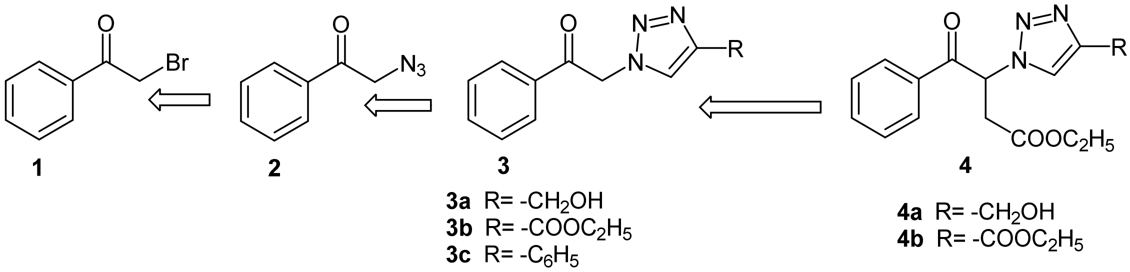
Due to its presence in numerous molecules with pronounced biological activity, the 1,2,3-triazole fragment is an important candidate in medicinal chemistry [1]. The solubility of this *aza*heterocycle in a polar biological medium, its high chemical stability, and its ability to mimic other groups, make the presence of the 1,2,3-triazole moiety in different molecular architectures of wide interest [2].

To identify new biologically active compounds, the reactions of *C*-alkylation were performed for 1,2,3-triazoles (**3a-c**), in the presence of sodium hydride or potassium carbonate as the base and ethyl bromoacetate as the alkylating agent. The 1,2,3-triazoles used in this study were synthesized in two steps from ω-bromoacetophenone in 85-90% yields. (Scheme1)



Scheme 1: Transformation of ω-bromoacetophenone to 1,2,3-triazole-1,4-disubstituted derivatives.

Research has led to the conclusion that the methylene bridge of **3(a-b)** triazoles can be alkylated and a suitable reaction mechanism has been proposed. In the case of triazoles **3c**, elimination products have been identified. All synthesized compounds were purified and characterized physically and spectrally (IR, ^{1}H-NMR, ^{13}C-NMR, MS). The structure of derivative **4b** was also confirmed by single-crystal XRD.

Keywords: 1,2,3-triazole; *C*-alkylation; ethyl bromoacetate

Acknowledgments: The authors are grateful to:The project POSCCE-O 2.2.1, SMIS-CSNR 13984-901, No. 257/28.09.2010, CERNESIM for the NMR spectra and Ms. Brindusa-Alina Petre for the MALDI-TOF Mass Spectrometry analyses performed in the Proteomics Laboratory, TRANSCEND-IRO Iasi Center

References:

[1] Forezi, S. M., Lima, L., Amaral, C. G. S., , Ferreira, A. A. P., Souza, P. G., Cunha, M. C., Fernando, C. S., Ferreira, A. C., *Chem. Rec.,* 21(10), 2782-2807 (2021)

[2] Nemallapudi, B. R., Guda, D. R., Ummadi, N., Avula, B., Zyryanov, G. V., Reddy, C. S., Gundala, S., *Polycycl. Aromat. Compd.,* 42(6), 3874-3892 (2022)

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P8. 4-arylcumarin derivatives

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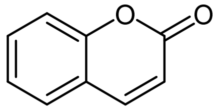
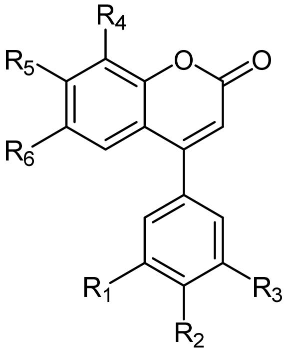
Coumarin (2H-1-benzopyran-2-one) (1) contains an α-pyronic oxygen heterocycle fused with a benzene nucleus and is the basic skeleton of a large class of phenolic derivatives. Due to its pleasant smell, similar to vanilla, coumarin is used in perfumery and cosmetics [1]. Coumarin frame organic compounds are found in plants, with over 1300 coumarin derivatives identified from natural sources [2].

Small molar mass, simple structure, high solubility in organic solvents and high bioavailability make coumarin derivatives usable in research and development of pharmaceutical compounds [3]. Heart diseases, central nervous system disorders, the aging process, and the development of cancer can be caused by excess free radicals. 4-arylcoumarins (2) are reported to have significantly stronger free radical trapping properties than traditional antioxidants, namely vitamin C or vitamin E [4].

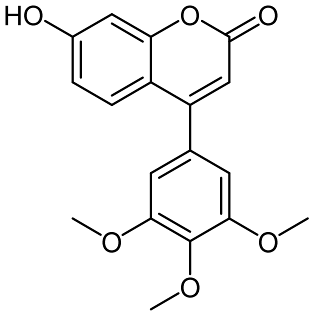
Knowing the biomedical potential of 4-arylcoumarins, the most efficient route was pursued to convert 3,4,5-trimethoxyacetophenone into coumarin derivative (3), by converting it to *b*-ketone ester and then condensation with resorcine in the presence of sulfuric acid. The structure of the obtained compounds was spectrally confirmed (IR, ^{1}H-NMR, ^{13}C-NMR).



Coumarin
(1)



4-arylcoumarins
(2)



Compound of interest
(3)

Keywords: coumarin; 4-arylcoumarins; 3,4,5-trimethoxyacetophenone; *b*-ketone ester

Acknowledgements: The authors thank the project POSCCE-O 2.2.1, SMIS-CSNR 13984-901, No. 257/28.09.2010, CERNESIM for recording MRI spectra

References:

[1] Kaur, N., Grewal, P., Poonia, K., *Synth. Commun.*, 51(16), 2423–2444 (2021)
[2] Jumal, J., Sakinah, N., *Malays. J. Med. Health Sci.,* 7(1), 62–68 (2021)
[3] Annunziata, F., Pinna, C., Dallavalle, S., Tamborini, L., Pinto, A., *Int. J. Molec. Sci.*, 21(13), 4618 (2020)
[4] Zhang, K., Ding, W., Sun, J., Zhang, B. Lu, F., Lai, R., Zou, Y., Yedid, G., *Biochimie*, 107, 203-210 (2014)

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P9. Synthesis and characterization of new 1,2,3-triazole derivatives

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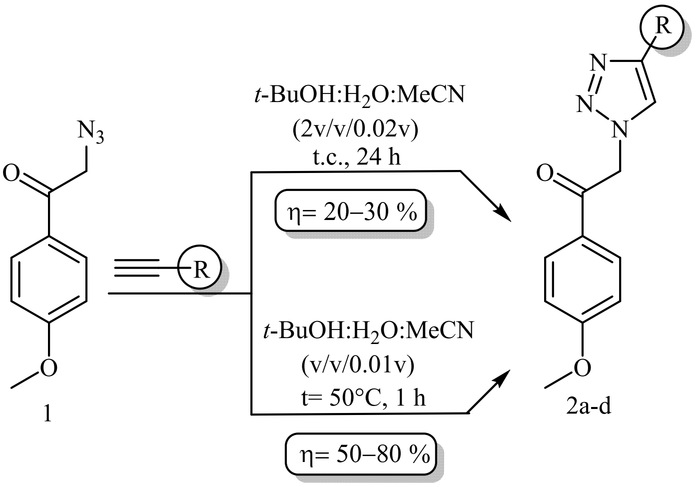
Triazoles are a class of chemical compounds known for their diversity and usefulness in chemistry and medicine [1,2]. Their structure allows obtaining of a wide range of derivatives [3]. The most widely used method of synthesis of 1,2,3-triazole derivatives is the "*Click Chemistry"* reaction between azides and marginal alkynes in Cu (I) catalysis [4]. Using a series of four marginal alkynes and 2-azido-1-(4-methoxyphenyl)ethanone (1), the 1,2,3-triazolic derivative *(*2a) known in the literature and three new derivatives (2b-d) were obtained by the click method. In order to increase the azide transformation yield, changes were made in the synthesis mode, thus establishing the optimal path to obtain the desired triazole derivatives. All synthesized compounds were purified and characterized physically and spectrally (IR, ^{1}H-NMR, ^{13}C-NMR).



Triazol 2	R
a	$-COOC_2H_5$
b	$-C_6H_4CH_3$(p)
c	$-CH_2CH_2CH_3$
d	$-CH_2CH_2CH_2CH_3$

Keywords: azides; 1,2,3-triazoles; Click Chemistry

Acknowledgements: The authors are grateful to the project POSCCE-O 2.2.1, SMIS-CSNR 13984-901, No. 257/28.09.2010, CERNESIM for the NMR spectra.

References:

[1] Agalave, S.G., Maujan, S.R., Pore, V.S., *Chem. Asian J.*, 6, 2696-2718 (2011)
[2] Zhou, X.Z., Liu, T., Wu, G., Kang, D., Fu, Z., Wang, Z., De Clercq, E., Pannecouque, C., Zhan, P., Liu, X., *Org. Biomolec. Chem.*, 17(12), 3202-3217 (2019)
[3] Giofrè, S.V., Tiecco, M., Ferlazzo, A., Romeo, R., Ciancaleoni, G., Germani, R., Iannazzo, D., *Eur. J. Org. Chem.*, 2021(34), 4777-4789 (2021)
[4] Meldal, M., Diness, F., *Cell Press Rev.*, 2, 569-584 (2020)

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P10. Effect of Zn^{2+} treatment on the growth of *Phaseolus vulgaris* and *Pisum sativum* seedlings

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The salinity of the plant growth environment and the mineral composition of water soil, respectively, influences the physiological activity of plants [1].

In this study we showed that the presence of an exogenous factor, Zn^{2+}_{aq} in the soil solution ($ZnCl_2$, 10 mg/L, 25 mg/L and 50 mg/L) significantly influenced the seeds germination and shoots growth rate of the bean (*Phaseolus vulgaris)* and peas (*Pisum sativum)*, especially at treated bean plants compared to control samples. After watering with 5 mL of 25 and 50 mg $ZnCl_2$/L solution at 3-day intervals during 15 days a significant decrease of the bean leafing speeds was observed. In the peas case, the administration of an additional amount of zinc had the opposite effect to that recorded for bean. The zinc cations were improved cell functions and plant morphology during low and medium salt stress [2]. Also, the photosynthetic system responded differently, the higher concentration of zinc increased the amount of chlorophyll pigments and carotenoids in the peas leaves.

Keywords: *Phaseolus vulgaris*, *Pisum sativum,* zinc, stress, plant growth

References:

[1] Barrs, H.D., Weatherley, P.E., *Aus. J. Biol. Sci.,* 15, 413-428 (1962)

[2] Rojsanga, P., Sithisarn, P., Buranaphalin, S., *J. Pharm. Sci.*2, 41, 41-47 (2014)

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