

Materials Science and Applied Chemistry 2022

PROGRAMME AND ABSTRACT BOOK

Riga, Latvia
21 October, 2022



October 21, 2022

Program

Plenary Session (Room 272)

9:30-9:40 Opening ceremony Prof. M. Turks, Dean of Faculty of Materials Science and Applied Chemistry, RTU

9:40-10:00 **Prof. Māris Turks**, RTU FMSAC ITOC,
ITOC-i(y)nes

10:00-10:20 **Assoc.prof. Kaspars Traskovskis**, RTU FMSAC IAC,
Development of organic materials for photonics

10:20-10:40 **Prof. Dagnija Loča** RTU FMSAC IGCE,
Biomaterials for bone engineering and local delivery of therapeutic agents

10:40-11:00 **Raivis Eglītis**, RTU FMSAC IMSE,
Photochromic titanium dioxide: past, present and future

11:00-11:20 **Doc. Pāvels Onufrijevs**, RTU FMSAC ITP,
Nano- and femtosecond laser technology for GeSn epilayers: potential for IR devices

11:20-11:40 **Prof. Remo Merijs-Meri**, RTU FMSAC IPM,
Polymers, their composites and nanocomposites: from laboratory to practical application

11:40-12:00 **Baiba Lukaševiča** RTU FMSAC IDT,
The evolving role of design

Lunch 12:00-13:00

Poster Session (second-floor passage)

13:00-14:00

Oral Presentation Sessions

14:00-15:10

General Materials Science (Room 271)

14:00-14:10	Ramona Dūrena	Amphoteric aqueous Zn-MnO ₂ rechargeable battery with 2.4 V open-circuit potential
14:10-14:20	Agija Stanke	The promotional effect of potassium on iron-based silica-supported catalyst for the hydrogenation of carbon oxides
14:20-14:30	Līga Britala	Inert coatings for cycle life extension of cathodes for Li-Ion batteries
14:30-14:40	Mārtiņš Randers	Hydrosodalite synthesis from illite clay by alkali-thermal treatment
14:40-14:50	Dārta Ūbele-Kalniņa	Improving surface wettability on hydroxyapatite coatings by electrical polarization
14:50-15:00	Agnese Stunda-Zujeva	Comparison of antioxidant activity in various spirulina containing products
15:00-15:10	Kristīne Irtiševa	Development of peat binder biocomposites and their physical properties

Polymer Materials and Composite Materials (Room 272)

14:00-14:10	Anda Barkāne	Modified cellulose nanocrystals for UV-assisted additive manufacturing resin reinforcement
14:10-14:20	Madara Žiganova	Structural and thermal properties of poly(3-hydroxybutyrate) and poly(3-hydroxybutyrate- <i>co</i> -3-hydroxyvalerate)
14:20-14:30	Ritvars Bērziņš	Modification of cellulose-type fibers with naturally renewable cardanol and incorporation into recycled polypropylene
14:30-14:40	Mārtiņš Nābels-Šneiders	Preparation of biopolymer cellulose laminates
14:40-14:50	Kristaps Zvirgzds	Use of agricultural production residues in the production of board materials
14:50-15:00	Zanda Iesalniece	Rapeseed straw fiber reinforced recycled polypropylene/polyethylene composites
15:00-15:10	Osvalds Verners	A comparison of contact electrification mechanisms of selected polymers, surface functionalization molecules, and ionized water

Chemistry of Organic Compounds (Room 445)

14:00-14:10	Rūdolfs Beļauņieks	Use of propargyl silanes for the selective synthesis of trisubstituted alkenes via 1,2-silyl migration
14:10-14:20	Aleksejs Burcevs	Synthetic pathways to purines as molecular systems for a photo-catalysis
14:20-14:30	Anastasija Gaile	Investigation of quinone hydrazones/thiosemicarbazones as potential bifunctional ligands for metal ion complexation
14:30-14:40	Ralfs Pomilovskis	Polymer developments from tall oil fatty acids using Michael addition
14:40-14:50	Laimdota Vilcēna	Betulin integration method into solutions for needleless electrospinning
14:50-15:00	Armands Maļeckis	Synthesis and fluorescent properties of novel benzanthrone α -aminophosphonates
15:00-15:10	Vladislavs Kroškins	Rh catalyzed C-H amination of pentacyclic triterpenoids

Development of organic materials for photonics

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Linear two-coordinate metalloorganic complexes composed of coinage metals (Cu, Ag, Au), electron accepting carbene and electron donating amide ligands have recently emerged as a promising emitter class for organic light emitting diode (OLED) applications.¹ These compounds combine excellent photoluminescence quantum yield values with low excited state lifetimes, even below 1 μ s.

Here structural modifications of carbene-metal-amides (CMAs) are explored by introduction of novel thiazoline and imidazole-based carbene ligands (Figure 1). CMAs based on thiazoline ligands (**1**) exhibit dual emission from monomer and excimer excited states allowing single-emissive-layer white electroluminescence.² This provides means to production of simple design, low-cost white OLED devices.

In the case of imidazole carbenes (**2**) the presence of auxiliary electron acceptors enables through-space charge transfer process, substantially decreasing the singlet-triplet energy gap thus lowering thermal activation barrier for thermally activated delayed emission (TADF) process.³ Carbene fragment in these compounds acts a simple connecting structural fragment and is not directly involved in the emissive process.

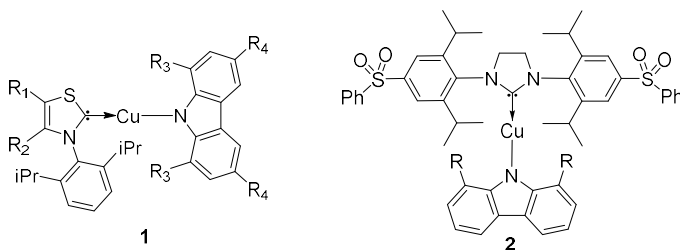


Figure 1. Chemical structures of the investigated CMA complexes.

Acknowledgements

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References

1. Di, D.; Romanov, A. S.; Yang, L.; Richter, J. M.; Rivett, J. P. H.; Jones, S.; Thomas, T. H.; Abdi Jalebi, M.; Friend, R. H.; Linnolahti, M.; Bochmann, M.; Credgington, D. *Science* **2017**, *356*, 159.
2. Ruduss, A.; Turovska, B.; Belyakov, S.; Stucere, K. A.; Vembris, A.; Baryshnikov, G.; Ågren, H.; Lu, J.-C.; Lin, W.-H.; Chang, C.-H.; Traskovskis K. *ACS Appl. Mater. Interfaces* **2022**, *14*, 15478.
3. Ruduss, A.; Turovska, B.; Belyakov, S.; Stucere, K. A.; Vembris, A.; Traskovskis, K. *Inorg. Chem.* **2022**, *61*, 2174.

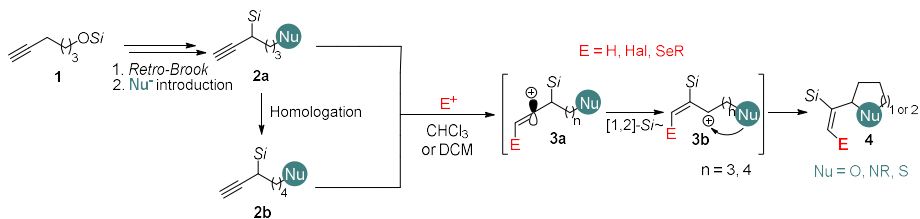
Heterocyclization of Terminally Functionalized C6-Chain Containing Propargyl Silanes via 1,2-Silyl Shift

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Electrophilic activation of propargyl silanes has been known to induce the 1,2-silyl shift, generating allylic cations, stabilized by the β -silicon effect. In the absence of reactive nucleophiles silyl dienes as reaction products are obtained. Intramolecular Friedel–Crafts reactions in aryl-substituted propargylic systems, when activated by Brønsted acids, give access to silyl indenes.^{1,2}

Herein we investigate the 1,2-silyl shift in propargyl silanes containing an intramolecular nucleophile **2a–b**, derived from the silylated hex-5-yn-1-ol **1**, and subsequent cyclization as a novel synthetic approach towards 2-(1-trialkylsilyl)vinyl-substituted heterocycles **4**. This transformation could be induced by addition of various electrophiles (H^+ , Hal^+ , RSe^+), providing diverse substitution for the C=C bond in the final products. The versatility of this approach has been demonstrated by synthesis various tetrahydrofuran, tetrahydro-2H-pyran, pyrrolidine and thiolane derivatives.



Scheme 1. General scheme for heterocyclization of propargyl silanes **2a–b**

References

1. Beļāunieks, R.; Puriņš, M.; Turks, M. *Synthesis*. **2020**, 52, 2147.
2. Puriņš, M.; Mishnev, A.; Turks, M. *J. Org. Chem.* **2019**, 84, 3595.

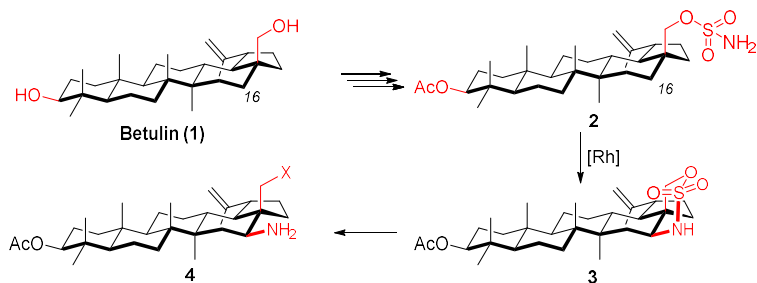
Rh catalyzed C-H amination of pentacyclic triterpenoids

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Betulin, erythrodiol and uvaol are pentacyclic triterpenoid natural products that are observed as secondary metabolites in many plants. These triterpenoids and their semi-synthetic analogs exhibit several important pharmacological properties such as antitumor, anti-inflammatory, antiparasitic, and anti-viral activities.¹ The aim of this work is to develop synthetical approach towards unexplored introduction of amino functionality at triterpenoid C(16).



Scheme 1. C-H amination of betulin

For this purpose, precursors **2** bearing sulfamate ester moiety were obtained, and converted to oxathiazinanes **3** via Du Bois γ -C-H bond amination.² Key intermediates **3** are further converted into variously functionalized compounds **4** through the ring opening reactions ($X=N_3, OSO_3H$, etc.)

Acknowledgements

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References

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