Chemistry: Shaping the FUTURE

6th EuCheMS Chemistry Congress

Congress Program





SEVILLE Spain

11th–15th September 2016

Organized by

ANQUE
ASOCIACIÓN NACIONAL DE QUÍMICOS DE ESPAÑA

EuCheMS
EUROPEAN CHEMICAL SCIENCES

6th EuCheMS MAIN CONGRESS PARTNER

JUNTA DE ANDALUCIA

invest in Andalucía SPAIN

Platinum Sponsors

CEPSA

ACS Chemistry for Life

Gold Sponsors

REPSOL

Silver Sponsors

ChemPubSoc Europe

DOW

Bronze Sponsors

MERCK

POSTER DISCUSSIONS

Topic E1- Materials Chemistry . *Poster Area - Module A*

Poster **Abstract 116**
Turning Quinones into Cyanoarenes: Developing a reaction from sketch to application
Florian Glöcklhofer ***(AT),*** Markus Lunzer, Berthold Stöger, Johannes Fröhlich.

Poster **Abstract 135**
Discovering new materials through computational methods
Lucas Viani ***(ES).***

Poster **Abstract 238**
Electrodeposition of Niobium and Aluminium from chloroaluminate melts onto Gold
Nataša Vukicevic ***(RS),*** Vesna Cvetkovic, Jovan Jovicevic.

Poster **Abstract 239**
Al-Pd alloy formation by aluminium underpotential deposition onto palladium from chloroaluminate melt
Vesna Cvetkovic ***(RS),*** Niko Jovicevic, Nataša Vukicevic, Jovan Jovicevic.

Poster **Abstract 292**
Porous inverse vulcanised polymers for mercury capture
Tom Hasell ***(AF)***.

Poster **Abstract 312**
High pressure CO2, CH4 and N2 adsorption on metalloporphyrin-based Solid Coordination Frameworks (SCFs)
Arkaitz Fidalgo-Marijuan ***(ES),*** Gotzone Barandika, Begoña Bazán, Miren Karmele Urtiaga, Maria Isabel Arriortua.

Poster **Abstract 318**
Synthesis, Characterization and Conductivity in Fluorite Nd5-xLnxMo3O16 (Ln = Tb, Dy, Ho) and in Lacunar Apatite Pb8-xCaxK2(VO4)6
Lyudmyla Ardanova (Stackpool) ***(US),*** Evgenii Getman, Alexey Ignatov, Konstantin Chebyshev, Lyudmila Pasechnik, Alisa Zhegailo, Nelya Selikova.

Poster **Abstract 328**
A new class of highly efficient supramolecular rotors based on halogen bonding
Luca Catalano ***(IT),*** Salvador Pérez-Estrada, Giancarlo Terraneo, Tullio Pilati, Giuseppe Resnati, Pierangelo Metrangolo, Miguel A. Garcia-Garibay.

Poster **Abstract 335**
ZnO synthesis from Zn-C and alkaline spent batteries by alkaline leaching: properties and applications
Irene García-Díaz ***(ES),*** Olga Rodríguez Largo, Teresa Cebriano, Ana López Fernández, Germán Escalante, Paloma Fernández, Félix A. López.

Poster **Abstract 375**
Hydrophilic Nd3+ Sensitized Upconverting Core-Shell Nanoparticles for Biomedical Applications
Anne Nsubuga ***(DE),*** Julia Hesse, Massimo Sgarzi, Holger Stephan.

Poster **Abstract 405**
Chemical microcharacterisation of high entropy alloys acting as binder phase in Ti(C,N)-based cermets
Alma G. de la Obra ***(ES),*** M. A. Avilés, M. J. Sayagués, F. J. Gotor.

Turning Quinones into Cyanoarenes: Developing a reaction from sketch to application

Florian Glöcklhofer (1), Markus Lunzer (1), Berthold Stöger (2), Johannes Fröhlich (1)
(1) Institute of Applied Synthetic Chemistry, TU Wien, (2) Institute of Chemical Technologies and Analytics, TU Wien
Getreidemarkt 9/163 Vienna Austria
Email: florian.gloecklhofer@tuwien.ac.at
Presenting author: Florian Glöcklhofer

Type: Poster
Theme: E. Materials, Devices and Nanochemistry
Topic: E1. Materials Chemistry
Keywords: Arenes, Cyanides, Fused-ring systems, Quinones, Functional Materials

SUMMARY:

Small modifications to a well-known reaction can lead to something completely new. That is what we realized after drawing the first sketch of a reaction turning quinones into cyanoarenes (Scheme 1). Considering the (commercial) availability of quinones in a wide range of different substitution patterns and the positive effect of the cyano groups on the material properties (such as improved light emission and stability), this reaction and the resulting materials are extraordinary interesting for a range of applications; especially for organic field-effect transistors and organic light-emitting diodes.

Scheme 1. Sketch of a reaction turning quinones into cyanoarenes; modifying the well-known reaction from quinones to alkynyl-substituted arenes.

However, it has been a bumpy road from the initial sketch to the materials for applications. Finding suitable reagents and solvents was challenging; particularly for the reductive aromatization in the second reaction step. In situ IR spectroscopy helped to overcome these challenges and finally led to a protocol to carry out both steps in a one-pot reaction. [1] This protocol has been optimized for the preparation of halogenated cyanoarenes and other poorly soluble cyanated acenes, including 6,13-dicyanopentacene for organic field-effect transistors (Scheme 2, top). [2]

Scheme 2. Examples showcasing the general applicability of the novel reaction.

The scope of the optimized reaction was further investigated from a general perspective (Scheme 2, bottom) by turning an ortho-quinone instead of para-quinones into the corresponding cyanoarene. Furthermore, the alkynyl-substituted 9,10-dicyanoanthracene and its precursor proved to be surprisingly stable towards the reaction conditions.
Our recent investigations focused on increasing the yield for the synthesis of 6,13-dicyanopentacene, but we also managed the first quadruple cyanation: the synthesis of 5,7,12,14-tetracyanopentacene. In

the field of organic light-emitting diodes, promising results were obtained by Suzuki coupling brominated dicyanoanthracenes and sterically hindering substituents.

The development of the novel reaction will be presented from the initial ideas to the recent investigations. The importance for the field of material chemistry will be emphasized by characterization results; most importantly, the data obtained from X-ray diffraction measurements, which accompanied the development of the reaction from the most simple reaction intermediate [3] to the quadruple cyanated 5,7,12,14-tetracyanopentacene.

[1] F. Glöcklhofer, M. Lunzer, J. Fröhlich, *Synlett* **2015**, *26*, 950-952.
[2] F. Glöcklhofer, M. Lunzer, B. Stöger, J. Fröhlich, *Chem. - Eur. J.* **2016**, *22*, 5173-5180.
[3] F. Glöcklhofer, J. Fröhlich, B. Stöger, M. Weil, *Acta Crystallogr. Sect. E* **2014**, *70*, 77-79.

Attachement 1

Attachement 2