



CROATIAN CRYSTALLOGRAPHIC ASSOCIATION
FACULTY OF CHEMISTRY AND CHEMICAL TECHNOLOGY,
UNIVERSITY OF LJUBLJANA

The Twenty-Sixth Croatian-Slovenian Crystallographic Meeting – CSCM26

Poreč, Croatia, June 13 - 17, 2018

Programme book

The Twenty-Sixth Croatian-Slovenian Crystallographic Meeting
will be held in the HOTEL VALAMAR DIAMANT, POREČ, CROATIA,
from Wednesday to Sunday, June 13 - 17, 2018.

The opening of the Meeting will take place on Thursday at 9:00.

Honorary Chairs

Stanko Popović, Zagreb
Ivan Leban, Ljubljana

Chairs of the Meeting

Dubravka Matković-Čalogović, Zagreb
Anton Meden, Ljubljana

Chair of the Scientific and Organizing Committee

Željko Skoko, Zagreb

Scientific and Organizing Committee Members

Mario Cetina, Zagreb
Amalija Golobič, Ljubljana
Marijana Jurić, Zagreb
Teodoro Klaser, Zagreb
Matic Lozinšek, Ljubljana
Andrej Pevec, Ljubljana
Marta Počkaj, Ljubljana
Michele Zema, Pavia

The Meeting is organized jointly by the *Croatian Crystallographic Association* and the *Faculty of Chemistry and Chemical Technology, University of Ljubljana*



Wednesday, June 13, 2018

- 18⁰⁰-19⁰⁰ Registration
19⁰⁰ Welcome drink

Thursday, June 14, 2018

- 8³⁰-9⁰⁰ Registration of participants
9⁰⁰-9¹⁰ Opening of the Meeting Ž. SKOKO, D. MATKOVIĆ-ČALOGOVIĆ, A. MEDEN

SHORT ORAL CONTRIBUTIONS

CHAIRS: K. MOLČANOV, I. TUREL

- 9¹⁰-9²⁵ Anton Meden, Jernej Stare, Dušan Hadži
X-ray Powder Diffraction and Quantum Calculations Used to Determine the Structure of Pentadecafluorooctanoic Acid Hydrate
- 9²⁵-9⁴⁵ Vladimir Stilinović, Dominik Cinčić
Coexistence of halogen and hydrogen bonds in crystal structures – competition, cooperation and antagonism
- 9⁴⁵-10⁰⁰ Martin Adam, Holger Ott, Tobias Stuerzer, Michael Mrosek, Michael Ruf, Bruce C. Noll, Matthew Benning, Juergen Graf
Best Data Quality from D8 QUEST and D8 VENTURE
- 10⁰⁰-10²⁰ Stanko Popović
Quantitative Phase Analysis by XRD – Simple Routes – New Perspectives / Applications
- 10²⁰-10³⁰ Franc Požgan, Miha Drev, Uroš Grošelj, Franc Perdih, Jurij Svete, Bogdan Štefane
Atropisomerism in hexapyridylbenzenes

10³⁰-11⁰⁰

Coffee break

PLENARY LECTURE

CHAIR: M. CETINA

- 11⁰⁰-12⁰⁰ **Andrzej Katrusiak**
High-pressure effects in hydrogen-bonded crystals

SHORT ORAL CONTRIBUTIONS

CHAIRS: D. MATKOVIĆ-ČALOGOVIĆ, A. MEDEN

- 12⁰⁰-12¹⁵ Teodoro Klaser, Jasminka Popović, Panče Naumov, Michele Zema, José Fernandes, Željko Skoko
Is the thermosalient effect without phase transition possible?
- 12¹⁵-12²⁵ José A. Fernandes, Teodoro Klaser, Željko Skoko
Thermosalient Behavior on the Dehydration of Scopolamine Bromide Hydrate
- 12²⁵-12³⁵ Krištof Kranjc and Franc Perdih
Preparation and Characterization of Cycloadducts with 3,9-Dioxatricyclo[5.2.2.0^{2,6}]undec-10-ene-4,8-dione Skeleton
- 12³⁵-12⁴⁵ Tino Šeba, Vladimir Stilinović
Iodoform – a forgotten halogen bond donor
- 12⁴⁵-12⁵⁵ Miha Drev, Uroš Grošelj, Franc Perdih, Jurij Svete, Bogdan Štefane, Franc Požgan
Molecular Structure of Heteroleptic Ruthenium(II) Complex Containing a Bidentate Bispyridyl-pyrimidyl Ligand
- 12⁵⁵-13¹⁰ Marcus J. Winter
Advances in X-ray crystallography

13¹⁰-16⁰⁰

Lunch break

SHORT ORAL CONTRIBUTIONS
CHAIRS K. KRANJC, Z. ŠTEFANIĆ

- 16⁰⁰-16¹⁵ Gligor Jovanovski, Panče Naumov, Branko Kaitner, Durga Prasad Karothu, Ilma Jahović
Structural Evidence for Molecular Saccharin Embedded in Ionic Saccharinates of Rubidium and Cesium
- 16¹⁵-16³⁵ Albert Guskov
Transport of glutamate in archaea and eukaryotes
- 16³⁵-16⁵⁰ Patrick Shaw Stewart
New strategies to improve productivity - rMMS microseeding for crystallization and DLS for cryoEM
- 16⁵⁰-17⁰⁰ Ivana Kekez, Mario Kekez, Mario Stojanović, Jasmina Rokov-Plavec, Dubravka Matković-Čalogović
Revealing the structure of the first plant aminoacyl-tRNA synthetase at 2.3 Å

 17⁰⁰-17³⁰

Coffee break

PLENARY LECTURE
CHAIR: S. POPOVIĆ

- 17³⁰-18³⁰ **Paolo Scardi**
SRXRD of metal nanocrystals: learning from mistakes

SHORT ORAL CONTRIBUTIONS
CHAIRS: A. TONEJC, F. POŽGAN

- 18³⁰-18⁴⁰ Petra Stanić, Katarina Lisac, Vinko Nemec, Dominik Cinčić
Halogen-bonded cocrystals of an imine derived from N-aminomorpholine and 4-nitrobenzaldehyde: a playground for halogen bonding
- 18⁴⁰-19⁰⁰ Krešimir Molčanov, Biserka Kojić-Prodić, Vladimir Stilinović, Zhongyu Mou, Miklos Kertesz, Bruno Landeros-Rivera, Jesús Hernández-Trujillo
Two-electron multicentric covalent bonding: how many centres?
- 19⁰⁰-19¹⁰ Luka Šmital, Mladen Borovina, Ivan Kodrin, Marijana Đaković
Computational study of hydrogen bond in systems of selected acetylacetonato complexes of Cu^{II} – theory vs. Experiment
- 19¹⁰-19²⁰ Wilfried Gille
Isotropic, linear particle growth and the parallel body set problem in SAS
- 19²⁰-19³⁰ Nikola Jakupec, Vladimir Stilinović
Halogen Bonding in Halogenopyridinium Hexacyanoferrates

Friday, June 15, 2018

SHORT ORAL CONTRIBUTIONS
CHAIRS: B. MODEC, I. KEKEZ

- 8³⁰-8⁴⁰ Marin Liović, Nikola Bedeković, Vladimir Stilinović, Dominik Cinčić
Cocrystallization of halogenide salts of organic bases with 1,4-diiodotetrafluorobenzene
- 8⁴⁰-8⁵⁰ Mladen Borovina, Ivan Kodrin, Marijana Đaković
Can MEPs obtained from DFT calculations be used to a priori determine the effectiveness of the employed supramolecular strategies?
- 8⁵⁰-9⁰⁵ Tomislav Piteša, Vladimir Stilinović, Ivan Ljubić, Vinko Nemec, Dominik Cinčić
Structural and DFT study of pyridine and imine nitrogen atoms as halogen bond acceptors: interplay of halogen bonds in the solid state
- 9⁰⁵-9¹⁵ Matjaž Kristl, Amalija Golobič, Nejc Babič, Brina Dojer
Synthesis and structure of a new iron(II) coordination compound with isonicotinamide
- 9¹⁵-9³⁰ Alen Bjelopetrović, Stipe Lukin, Ivan Halasz, Krunoslav Užarević, Ivica Đilović, Dajana Barišić, Ana Budimir, Marina Juribašić Kulcsár, Manda Ćurić

X-Ray Analysis of Intermediates and Products involved in Solid-State C–H Bond Activation by Pd(II) Chloride Precursors

9³⁰–9⁴⁰ Very short break

KEYNOTE LECTURE

CHAIR: G. GIESTER

9⁴⁰–10⁴⁰

Lutz Nasdala

Structural radiation damage in minerals: What can we learn?

10⁴⁰–11⁰⁰

Coffee break

PLENARY LECTURE

CHAIR: Ž. SKOKO

11⁰⁰–12⁰⁰

Serena C. Tarantino

Crystals' warm-up, stretching and ... workout!

SHORT ORAL CONTRIBUTIONS

CHAIRS M. JURIĆ, M. LOZINŠEK

12⁰⁰–12¹⁰

Božena Lovrić, Mladen Borovina, Marijana Đaković
Supramolecular synthesis of Co^{II} and Ni^{II} complexes with acetylacetonate derivatives and pyridyl oximes

12¹⁰–12²⁵

Barbara Modec, Petra Stare, Janez Košmrlj
A solved mystery? A novel zinc(II) ammine complex

12²⁵–12³⁵

Aleksandar Meštrić, Ivana Pavličić, Sandra Čičić, Nenad Judaš
Combined mechanochemical and solution synthesis of copper(II) carboxylates

12³⁵–12⁴⁵

Iztok Turel, Katja Traven, Branko Stanovnik, Julia Koziskova, Jozef Kožíšek
Organometallic ruthenium(II) complexes with selected N,N-donor ligands – interesting systems where also concomitant polymorphism was observed

12⁴⁵–12⁵⁵

Andrej Pevec, Anja Sedminek, Janez Košmrlj
Thiosemicarbazides and Thiosemicarbazones as Ligands in Ni(II) Coordination Compounds

12⁵⁵–13⁰⁵

Mario Cetina, Lucija Ptiček, Livio Racané
Intermolecular interactions in two cyclic amidino-derivatives built three-dimensional network

Afternoon - Excursion

Saturday, June 16, 2018

SHORT ORAL CONTRIBUTIONS

CHAIRS A. PEVEC, V. STILINOVIĆ

8³⁰–8⁴⁰

N. Penić, M. Borovina, D. Pajić, M. Đaković
Supramolecular architectures of copper(II) halide complexes with amine and lactame derivatives of pyrazine and pyrimidine

8⁴⁰–8⁵⁰

G. Dražić, G. Štefanić, T. Jurkin, **M. Gotić**
Impact of cadmium and phosphate ions on the hematite nanorings formation

8⁵⁰–9⁰⁰

Sara Cepić, Katarina Lisac, Dominik Cinčić
One-pot mechanochemical synthesis of a metal-based halogen bonded cocrystal with the CoCl₂L₂ building block

9⁰⁰–9¹⁰

Toni Grgurić, Nikola Bregović, Vladimir Stilinović
The study of pyridine adducts of VO(acac)₂ in the solid state and solution

9¹⁰–9²⁰

Darko Vušak, Dubravka Matković-Čalogović, Biserka Prugovečki

- Supramolecular diversity in copper(II) complexes with L-homoserine/L-serine with heterocyclic bases*
- 9²⁰-9³⁰ Nikola Bedeković, Marta Klepić, Vladimir Stilinović, Dominik Cinčić
Influence of the intramolecular hydrogen bonding on structures and stability of adducts of copper and zinc b-diketonates with N-donor ligands
- 9³⁰-9⁴⁰ Alen Bjelopetrović, Stipe Lukin, Ivan Halasz, Krunoslav Užarević, Ivica Đilović, Dajana Barišić, Ana Budimir, Marina Juribašić Kulcsár, Manda Ćurić
X-Ray Identification and Characterization of Azobenzene Palladacycles Obtained by Solid-State C–H Bond Activation
- 9⁴⁰-9⁵⁰ Kristina Smokrović, Ivica Đilović, Dubravka Matković-Čalogović
Structural characterization of 3D coordination polymers of copper(II) and short, uncharged side chain amino-acids with a 4,4'-bipyridine linker
- 9⁵⁰-10⁰⁵ Lidija Kanižaj, Krešimir Molčanov, Marijana Jurić
Chloride- and oxalate-bridged heterometallic [Cu^{II}Cr^{III}] compounds with 2,2':6',2''-terpyridine – the influence of the starting copper(II) salt
- 10⁰⁵-10¹⁵ Mateja Pisačić, Marijana Đaković
Understanding the role of weak interactions in responsiveness of molecular crystals to external mechanical stimuli
- 10¹⁵-10²⁵ Robert Katava, Gordana Pavlović
Dioxovanadium(V) complexes with 2-benzothiazolyhidrazones as potential antitumor agents

 10²⁵ - 11⁰⁰

Coffee break

PLENARY LECTURE
CHAIR: A. MEDEN

- 11⁰⁰-12⁰⁰ **Nataša Zabukovec Logar**
Crystallography in Microporous Materials Research...

SHORT ORAL CONTRIBUTIONS
CHAIRS: A. M. TONEJC, E. GORESHNIK

- 12⁰⁰-12¹⁵ A. Stricker, J. Wiesmann, J. Graf, C. Michaelsen
Upgrading Home-Lab X-ray Diffractometers with Incoatec's Unique Microfocus Source
- 12¹⁵-12³⁰ Bogdan Kotur, Volodymyr Levytskyy, Volodymyr Babizhetskyy
Crystal chemistry of metal-rich R–T–C carbides
- 12³⁰-12⁴⁵ Evgeny Goreschnik, Lev Akselrud, Zoran Mazej
Incommensurately modulated crystal structures of [XeF₅][As_xSb_{1-x}F₆] (x ~0.3 and ~0.5)
- 12⁴⁵-13⁰⁰ Matic Lozinšek, Katarina Starkl Renar, Jernej Iskra
Structural Investigations of Organic Geminal Dihydroperoxides

 13¹⁰ - 16⁰⁰

Lunch break

SHORT ORAL CONTRIBUTIONS
CHAIRS: M. KRISTL, J. POPOVIĆ

- 16⁰⁰-16¹⁰ Marijana Jurić, Lidija Kanižaj, Jasminka Popović, Lidija Androš Dubraja
Preparation of the Ba₂CrNbO₆ and NiNb₂O₆ Oxides by Thermal Decomposition of the Mixture of Oxalate Precursors
- 16¹⁰-16²⁰ M. M. Radanović, Lj. S. Vojinović-Ješić, M. V. Rodić, V. M. Leovac
Crystallographic study of cadmium(II) complexes with 2-acetylpyridine-aminoguanidine and bromide as coligand
- 16²⁰-16³⁰ Nikola Tasić, Jovana Ćirković, Aleksandra Dapčević, Lidija Ćirković, Vesna Ribić, Milan Žunić, Goran Branković, Zorica Branković
Ag/TiO₂ nanoparticle composites and their photocatalytic performance
- 16³⁰-16⁴⁰ Andreas Ertl, Gerald Giester, Ekkehart Tillmanns

Tetrahedrally-coordinated boron in Fe-bearing dravite from a metamorphic schist from Brandrücken, Weinebene, Koralpe, Styria, Austria

16⁴⁰-16⁵⁰ Tamara Đorđević, Ljiljana Karanović, Zvonko Jagličić
A new copper(II) arsenate, Na₂Cu₃(AsO₃OH)₄·4H₂O containing discrete [Cu₃O₁₂]¹⁸⁻ units: synthesis, crystal structure and magnetic properties

16⁵⁰-17⁰⁰ Iovana Ćirković, Danijela Luković Golić, Aleksandar Radojković, Aleksandra Dapčević, Nikola Tasić, Mirta Čizmić, Goran Branković, Zorica Branković
BiFeO₃-based nanoparticles obtained by different synthetic routes and their structural, optical and photocatalytic properties

 17⁰⁰-17³⁰

 Coffee break

PLENARY LECTURE
CHAIR: J. POPOVIĆ

17³⁰-18³⁰ Zoran Štefanić, Marija Luić
Purine nucleoside phosphorylases: understanding enzyme mechanism and allosteric pathways

SHORT ORAL CONTRIBUTIONS
CHAIRS Ž. SKOKO, G. ŠTEFANIĆ

18³⁰-18⁴⁰ Valentina Martinez, Nikola Bedeković, Vladimir Stilinović, Dominik Cinčić
Halogen-bonded complexes of perhalogenated hydrocarbons and benzoyl-4-pyridoylmethane

18⁴⁰-18⁵⁰ Karla Kelemen, Krunoslav Užarević, Ivica Đilović
Proof-of-concept: flexible receptor in complexes with malonic acid

18⁵⁰-19⁰⁰ Silvia-Maria Franov, Vinko Nemec, Dominik Cinčić
Cooperativity of halogen bonds in cocrystals of 4-halogenoanilines and 1,4-diidodotetrafluorobenzene

19⁰⁰-19¹⁰ Sara Marijan, Vinko Nemec, Vladimir Stilinović, Dominik Cinčić
Halogen bonded cocrystals of N-bromophthalimide with 2-chloro- and 2-bromopyridine

19¹⁰-19²⁵ Alen Bjelopetrović, Stipe Lukin, Ivan Halasz, Krunoslav Užarević, Ivica Đilović, Dajana Barišić, Ana Budimir, Marina Juribašić Kulcsár, Manda Ćurić
X-Ray Analysis of Intermediates and Products involved in Solid-State C–H Bond Activation by Pd(II) Chloride Precursors

19²⁵-19³⁵ Babu A. Manjasetty
Indo-Italian Macromolecular Crystallography (MX) Beamline XRD2 at Elettra Synchrotron Light Source

19³⁵-19⁴⁵ Award ceremony for:
 (1) IUCr award for best short oral presentation for young scientists
 (2) Bruker award for best short oral presentation for young scientists
 (3) Bruker award for best short oral presentation

19⁴⁵-19⁵⁰ Closing remarks A. MEDEN, D. MATKOVIĆ-ČALOGVIĆ

 20⁰⁰

 Meeting dinner

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