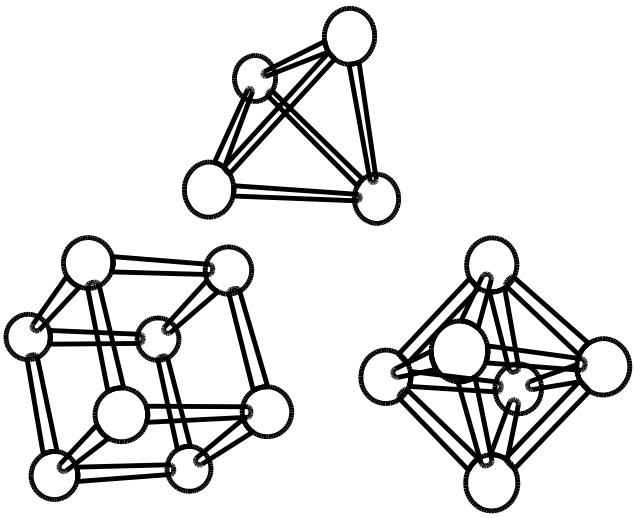
SLOVENIAN CRYSTALLOGRAPHIC SOCIETY
CROATIAN CRYSTALLOGRAPHIC ASSOCIATION

DEVETINDVAJSETO SLOVENSKO-HRVAŠKO KRISTALOGRAFSKO SREČANJE

TWENTY-NINTH SLOVENIAN - CROATIAN CRYSTALLOGRAPHIC MEETING

14 - 18 June, 2023
Hotel Vesna
Topolšica, Slovenia



PROGRAMME

Topolšica, SLOVENIA
June, 2023

WEDNESDAY, June 14, 2023

18^{00} – 19^{00} **REGISTRATION OF PARTICIPANTS**

19^{00} **WELCOME RECEPTION**

THURSDAY, June 15, 2023

9^{00} **OPENING REMARKS** Chairpersons: A. Meden
M. Đaković

MORNING SESSION

9^{15} **PLENARY LECTURE** Chairperson: A. Meden

ANTON KOKALJ
DFT modeling of materials and crystal structures using periodic-boundary conditions

10^{15} **COFFEE BREAK**

ORAL PRESENTATIONS Chairpersons: M. Počkaj
M. Cetina

10^{45} **Nikola Bedeković, Luka Fotović, Vladimir Stilinović, Dominik Cinčić**
Robustness of pyridine hydrogen-bonded homosinthon in halogen-bonded systems

11^{00} **Klemen Motaln, Matic Lozinšek**
The elusive crystal structure of $XeOF_2$

11^{10} **Lidija Posavec, Dominik Cinčić**
Structures, stoichiometric diversity and solvates of halogen bonded cocrystals with Werner complex as acceptor

11^{20} **Mirela Dragomir, Qianli Ma, Bruce D. Gaulin**
The role of crystal symmetry on the superconducting properties of Nd-LSCO

11^{35} **Lea Čolakić, Lidija Posavec, Dominik Cinčić**
Picky halogen bonding in isocyanate-based Werner complexes

11^{45} **Suzanna C. Ward, Ilaria Gimondi**
Insights from over a million structures

12^{05} **LUNCH BREAK**

AFTERNOON SESSION

14^{00} **CCDC WORKSHOP** Chairperson: F. Perdih

16^{00} **COFFEE BREAK**

ORAL PRESENTATIONS Chairpersons: F. Perdih
M. Borovina

16^{30} **Petra Stanić, Krešimir Molčanov**
Crystal structures and charge density studies of *pancake bonded* radicals in organic salts

16^{50} **Antonio Magnabosco, Vinko Nemec, Vladimir Stilinović, Dominik Cinčić**
Cocrystallization of the adamanzane with perfluorinated halogen bond donors

17^{00} **Erik Uran, Luka Fotović, Kristian Radan, Vladimir Stilinović, Matic Lozinšek**
Salts, adducts and cocrystals formed in reactions of SO_2 with organic amines

17^{15} **Ana Lozančić, Krešimir Molčanov, Sanja Burazer, Marijana Jurić**
Structural diversity of homo- and heterometallic compounds prepared using $[M^{III}(C_2O_4)_3]^{3-}$ (M^{III} = Cr, Fe) building blocks with alkyl-ammonium cations

17^{25} **Filip Kučas, Vinko Nemec, Lidija Posavec, Dominik Cinčić**
Novel 4-iodotetrafluorophenoxy azobenzene ethers as halogen bond donors in synthesis of cocrystals with bipyridyl derivatives

17^{35} **BREAK**

17^{55} **Uroš Rapuš, Zala Stopar, Iztok Turel, Jakob Kljun**
When result of the crystal structure is not what you expected

18^{05} **Marta Počkaj**
Complexes of nickel(II) and cobalt(II) bromide with 2-pyridinemethanol

18^{15} **Ana Siljanovska, Miha Virant, Matic Lozinšek, Janez Cerkovnik**
Bulky NHC ligand and its metal complexes through the lens of single-crystal X-ray diffraction

18^{30} **Boris Gomaz, Zoran Štefanić**
Understanding allostery in oligomeric enzymes through big data visualization

18^{50} **Ivica Cvrtila, Krešimir Molčanov, Ivan Halasz**
Chiral crystallization of hippuric acid from carvone

19^{05} **Neven Strukan**
Sponsor's presentation

19^{25}-19^{35} **Soufiane Zerraf, M.E. Belghiti, Said Belaaouad**
Synthesis, crystal structure and computational studies of newly 2-ethylanilinium phosphite ($C_8H_{12}N^+ \cdot H_2PO_3^-$)

FRIDAY, June 16, 2023

MORNING SESSION

8^{30} **PLENARY LECTURE** Chairperson: I. Leban

KRISTINA DJINOVIĆ CARUGO
Order from disorder: towards molecular architecture of the muscle Z-disk assembly by integrative structural biology

9^{30} **COFFEE BREAK**

ORAL PRESENTATIONS Chairpersons: J. Kljun
N. Baus Topić

10^{00} **Slavko Žižek**
Presentation of SCAN and JEOL company, with emphasis on ED XRF spectrometer

10^{20} **Simona Gričar, Matija Uršič, Jakob Kljun, Boris Šket, Iztok Turel**
Structural characterization of selected ruthenium complexes with *O,O*-ligands

10^{30} **Miha Virant, Janez Košmrlj, Biprajit Sarkar, Matic Lozinšek**
Crystal structures of arylated triazoles and their metal-NHC complexes

10^{45} **Izabela Đurasović, Goran Dražić, Goran Štefanić, Marijan Marciuš, Mile Ivanda, Marijan Gotić**
Influence of Pt/SnO_2 synthesis procedures on the catalytic reduction of 4-nitrophenol to 4-aminophenol

11^{00} **Nina Podjed, Barbara Modec**
Amidine from piperidine and acetonitrile in the form of amidinium salts with zinc(II) coordination anions

11^{10} **Matic Belak Vivod, Graham King, Zvonko Jagličić, Mirela Dragomir**
Synthesis, structural and magnetic characterisation of an unknown phase, $Ag^{I}_{2}Ag^{II}F_4$

11^{20} **Bogdan Kotur, Volodymyr Babizhetskyy, Chong Zheng**
New zirconium palladium gallide $Zr_{12}Pd_{40}Ga_{31}$

11^{30} **Urban Novak**
Enhancing polymorph differentiation with Bruker FM wide range FIR-MIR spectroscopy

11^{45} **LUNCH BREAK**

13^{00}
Conference trip to the Coal mining museum in Velenje.

SATURDAY, June 17, 2023

MORNING SESSION

8^{30} **PLENARY LECTURE** Chairperson: M. Lozinšek

SIMON PARSONS
High pressure phase transitions in molecular crystals

9^{30} **COFFEE BREAK**

ORAL PRESENTATIONS

Chairpersons: K. Radan
K. Molčanov

10^{00} **Mišel Hozjan, Franc Perdih**
Vanadium(IV) complexes with dipicolinic acid and its derivatives

10^{10} **Saša Petriček**
Cobalt and zinc complexes with pyrazine-2-carboxylic acid

10^{20} **Marijana Đaković**
Mechanically flexible crystalline coordination polymers – what do we know about the crystals' mechanically induced adaptability?

10^{35} **Nea Baus Topić, Dominik Cinčić**
Perhalogenated hydroxyl aryl imines as halogen bond donors in cocrystals with nitrogen-containing acceptors

10^{45} **Lewis Clough, Simon Parsons, Matic Lozinšek, Kristian Radan, Nico Giordano**
The high pressure behaviour of $Nd(XeF_2)_3(TaF_6)_3$

11^{55} **Vesna Zalar Serjun, Marija Đurić, Mateja Štefančič, Romana Cerc Korošec, Anton Meden**
Characterisation and pozzolanic activity of ashes from different incineration processes

11^{10} **Žan Zakošek, Marta Počkaj, Gerald Giester**
Nickel complexes with 4-pyridinemethanol ligand

11^{20} **Olha Sanko, Erik Uran, Matic Lozinšek**
A new polymorph of vanadium trifluoride oxide, VOF_3

11^{30} BREAK

11^{40} **Leonarda Vugrin, Ivan Halasz, Hervé Geneste**
Solid-state potassium encapsulation with 18-crown-6 ether

11^{50} **Valentina Milašinović, Luka Rejc, Janez Košmrlj, Matic Lozinšek**
X-ray charge density analysis of pyridine and pyrimidine-based fluorescent molecular probes

12^{00} **Marko Dunatov, Andreas Puškarić, Lidija Androš Dubraja**
Structural transformations of (L-tartrato)oxovanadium(V) complex salt with ferroelectric switching and thermistor properties

12^{10} **Mladen Borovina, Mateja Pisačić, Marijana Đaković**
Crystallography on the verge – solving crystal structures of bent crystals

12^{25} **Jakob Kljun, Tina P. Andrejević, Biljana Đ. Glišić, Iztok Turel**
Structures of antimicrobial copper and silver complexes of pyridine-3,4-dicarboxylates

12^{35} **Monika Šoltić, Nikola Baran, Goran Dražić, Goran Štefanić, Marijan Marciuš, Mile Ivanda, Marijan Gotić**
Synthesis and gas sensing properties of platinum nanoparticles dispersed on α-Fe_2O_3 and Fe_3O_4 supports

12^{45}-13^{05} **Felix Hennersdorf**
Rigaku advances in X-ray and electron crystallography

LUNCH BREAK

AFTERNOON SESSION

15^{00} **PLENARY LECTURE** Chairperson: M. Đaković

DOMINIK CINČIĆ
Crystal engineering of organic and metal-organic multicomponent halogen-bonded solids

16^{00} **COFFEE BREAK**

ORAL PRESENTATIONS Chairpersons: M. Dragomir
I. Cvrtila

16^{30} **Krešimir Molčanov, Lidija Molčanov, Luka Pavić, Marijana Jurić**
Charge transport and conductivity through π-hole interaction

16^{50} **Kristian Radan, Matic Lozinšek**
The crystal structure of nickel difluoride tetrahydrate

17^{00} **Goran Štefanić, Ivan Marić, Monika Šoltić, Goran Dražić, Matthijs Van Spronsen, Georg Held, Tanja Jurkin, Mile Ivanda, Klemen Bohinc, Marijan Gotić**
X-ray powder diffraction analysis of Pt/MnO_2 nanorods used as a catalyst for the reduction of 4-nitrophenol to 4-aminophenol

17^{10} **Hans-Georg Stammler**
In situ crystallisation made easy

17^{25} **Matic Lozinšek, Anže Zupanc, Erik Uran, Miha Virant, Marjan Jereb**
Intermolecular interactions in crystal structures of *N*-iodo sulfoximines

17^{35} **BREAK**

17^{55} **Evgeny Goreshnik, Svitlana Petrusenko**
Supramolecular crystal structure of Hdabco based mixed-cation metal-free salts

18^{10} **Mario Cetina, Andrea Bistrović, Silvana Raić Malić**
Conformation and self-assembling of purine and pseudopurine derivatives containing triazole ring

18^{20} **Luka Setnikar, Franc Perdih**
Zinc(ii) complexes with indole-3-propionic acid: structural elucidation and luminiscence properties

18^{30} **Vladimir Stilinović, Luka Fotović, Nikola Bedeković, Josip Požar**
Structural and thermodynamic study of a series of cocrystals comprised of liquid coformers

18^{45} **Anton Meden**
My first experience with electron diffractometers

18^{55} **CLOSING REMARKS**

Chairpersons: M. Đaković
A. Meden

20^{00} **CONFERENCE DINNER**

SUNDAY, June 18, 2023

9^{00} **EVALUATION AND FAREWELL COFFEE**