



## Wednesday, September 7, 2022

- 16<sup>30</sup>-18<sup>30</sup> Registration of participants  
18<sup>30</sup> Welcome drink

## Thursday, September 8, 2022

- 8<sup>00</sup>-8<sup>30</sup> Registration of participants  
8<sup>30</sup>-8<sup>40</sup> Opening of the Meeting M. Đaković, D. Matković-Čalogović, A. Meden

## SHORT ORAL CONTRIBUTIONS

CHAIRS: D. MATKOVIĆ-ČALOGOVIĆ, Z. ŠTEFANIĆ

- 8<sup>40</sup>-8<sup>50</sup> Anton Meden  
*Is thinking a good idea? Example of structure solution from powder diffraction data*
- 8<sup>50</sup>-9<sup>05</sup> Ivana Brekalo, David E. Deliz, Leonard J. Barbour, Michael D. Ward, Tomislav Friščić, K. Travis Holman  
*The single crystal-to-single crystal transformations and porosity of guanidinium 1,4-benzenedisulfonate*
- 9<sup>05</sup>-9<sup>15</sup> Ivana Kekez, Sara Matić, Sanja Tomić, Dubravka Matković-Čalogović  
*Binding of peptide mimicking the ETGE loop of dipeptidyl peptidase III to the Kelch domain of Keap1*
- 9<sup>15</sup>-9<sup>30</sup> Mirela Dragomir, Adam W. Phelan, Lucas Presley, Patrick J. Clancy, John E. Greedan, *Revisiting the Structure and Magnetism of the Quasi-One-Dimensional La<sub>3</sub>MoO<sub>7</sub>: A Single Crystal Study*
- 9<sup>30</sup>-9<sup>45</sup> Vladimir Stilinović, Luka Fotović, Nikola Bedeković  
*Halogen bonding in an isostructural series of N-(4-halogenobenzyl)-3-halogenopyridinium halogenides*
- 9<sup>45</sup>-10<sup>00</sup> Matic Lozinšek, Dominique Cahard, Andrej Emanuel Cotman  
*Mechanically flexible crystals of homochiral β-CF<sub>3</sub>, β-SCF<sub>3</sub>, and β-OCF<sub>3</sub> benzylic alcohols*

10<sup>00</sup>-10<sup>30</sup>

Coffee break

## PLENARY LECTURE

CHAIR: M. ĐAKOVIĆ

- 10<sup>30</sup>-11<sup>30</sup> Alessia Bacchi  
*Smart materials for the release of liquid ingredients*

## SHORT ORAL CONTRIBUTIONS

CHAIRS: V. STILINOVIC, A. MEDEN

- 11<sup>30</sup>-11<sup>45</sup> Jasminka Popović, Željko Skoko, Juraj Ovčar, Luca Grisanti, Martina Vrankić, Ivor Lončarić, Aleksandra Djurišić  
*Mixed halides – a way to stabilize Ruddlesden-Popper structures*
- 11<sup>45</sup>-12<sup>00</sup> Yizhi Xu, Joseph M. Marrett, Hatem M. Titi, James P. Darby, Andrew J. Morris, Tomislav Friščić, Mihails Arhangelskis  
*Experimentally-validated ab initio crystal structure prediction of novel metal-organic framework materials*
- 12<sup>00</sup>-12<sup>15</sup> Teodoro Klaser, Jasminka Popović, Ana Šantić, Luka Pavić, Željko Skoko  
*Some relevant results from electrical analysis of thermosalient crystals of 1,2,4,5-tetrabromobenzene and 1,2,4,5-tetraclorobenzene*



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12 <sup>15</sup> -12 <sup>30</sup>	<u>A. El Hachmi</u> , B. Manoun, M. Sajieddine, Y. Tamraoui, S. El Ouahbi <i>Structural and optical properties of perovskites: Sr<sub>3</sub>Fe<sub>2+x</sub>Mo<sub>1-x</sub>O<sub>9-3x/2</sub> (0.3 ≤ x ≤ 1)</i>
12 <sup>30</sup> -13 <sup>40</sup>	<u>Vladyslav Levruk</u> , Małgorzata Rybczyńska, Karol Krzymiński <i>Unique structural features of new acridan aryl esters – promising indicators in luminescence analysis</i>
12 <sup>40</sup> -13 <sup>00</sup>	Vernon Smith, Mirko Giansella <i>Structure determination on challenging samples – how modern X-ray instrumentation can help</i>

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13<sup>10</sup>-15<sup>00</sup>

Lunch break

**WORKSHOP****CHAIRS:** A. BELOPETROVIĆ, L. PAVIĆ15<sup>00</sup>-17<sup>00</sup> CCDC Workshop17<sup>00</sup>-17<sup>30</sup>

Coffee break

**PLENARY LECTURE****CHAIR:** I. BREKALO

17 <sup>30</sup> -18 <sup>30</sup>	<u>Dominik Cinčić</u> <i>Crystal engineering of organic and metal-organic multicomponent halogen bonded solids</i>
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**SHORT ORAL CONTRIBUTIONS****CHAIRS** I. KEKEZ, M. DRAGOMIR

18 <sup>30</sup> -18 <sup>40</sup>	<u>Valentina Martinez</u> , Bahar Karadeniz, Nikola Biliškov, Ivor Lončarić, Alexey A. Popov, Krunoslav Užarević <i>Mechanochemical strategy for controllable encapsulation of Buckminsterfullerene for preparation of fulleritic ZIF materials</i>
18 <sup>40</sup> -18 <sup>50</sup>	<u>Katarina Ležaić</u> , Mia Jurković, Darko Vušak, Biserka Prugovečki <i>A new copper(II) metal-organic frameworks constructed from N-alkyl glycinate and 3,3'-bipyridine: synthesis, structure and thermal behavior</i>
18 <sup>50</sup> -19 <sup>00</sup>	<u>Nea Baus Topić</u> , Dominik Cinčić <i>Perhalogenated amines as bifunctional donor molecules in cocrystals with nitrogen-containing acceptors</i>
19 <sup>00</sup> -19 <sup>10</sup>	<u>Mia Jurković</u> , Katarina Ležaić, Darko Vušak, Biserka Prugovečki <i>Syntheses and structures of copper(II) coordination polymers with N-methylglycinate and 4,4'-bipyridine</i>
19 <sup>10</sup> -19 <sup>20</sup>	<u>Soufiane Zerraf</u> , Malika Tridane, Said Belaaouad <i>Structural and vibrational study of single crystal (C<sub>6</sub>H<sub>9</sub>N<sub>2</sub>)<sub>2</sub>H<sub>2</sub>P<sub>2</sub>O<sub>7</sub></i>
19 <sup>20</sup> -19 <sup>30</sup>	<u>Thomas Kendall</u> <i>Problem solving with co-crystals: Screening and single crystal</i>



Friday, September 9, 2022

## SHORT ORAL CONTRIBUTIONS

CHAIRS: D. Vušak, K. Kranjc

- 8<sup>30</sup>-8<sup>45</sup> M. Kušter, Z. Samardžija, A. Meden, B. Markoli, M. Vončina, P. Boulet, E. Gaudry, J.-M. Dubois, S. Šturm  
*TEM studies of a Newly Discovered Ternary Phase in the Al-Cr-Sc system*
- 8<sup>45</sup>-8<sup>55</sup> Matjaž Kristl, Ivana Goričan, Brina Dojer, Amalija Golobič  
*Crystal structures of three 2,6-diaminopyridine compounds*
- 8<sup>55</sup>-9<sup>05</sup> Lidija Posavec, Dominik Cinčić  
*Building ternary halogen bonded cocrystals with Werner coordination compound and perhalogenated benzenes*
- 9<sup>05</sup>-9<sup>15</sup> Filip Kučas, Vinko Nemeć, Dominik Cinčić  
*Methylated isatin derivatives as halogen bond acceptors in multicomponent crystals*
- 9<sup>15</sup>-9<sup>30</sup> Lavanya Kumar, Katarina Leko, Vinko Nemeć, Nikola Bregović, Dominik Cinčić, Mihails Arhangelskis  
*Inspiring mechanochemical interconversions of halogen-bonded cocrystals by periodic DFT calculations*
- 9<sup>30</sup>-9<sup>45</sup> Valentina Milašinović, Vedran Vuković, Anna Krawczuk<sup>3</sup> Krešimir Molčanov, Christoph Hennig, Michael Bodensteiner  
*A novel  $\pi$ -hole interaction between an iodide anion and a quinoid ring involving an  $n \rightarrow \pi^*$  charge transfer*
- 9<sup>45</sup>-10<sup>00</sup> Khai-Nghi Truong  
*Rigaku Advances in X-ray and Electron Crystallography*

10<sup>00</sup>-10<sup>30</sup> Coffee break

## PLENARY LECTURE

CHAIR: J. Popović

- 10<sup>30</sup>-11<sup>30</sup> Anna Moliterni  
*Crystallography, a powerful lens for Materials Science*

## SHORT ORAL CONTRIBUTIONS

CHAIRS: O. Mišura, S. Petriček

- 11<sup>30</sup>-11<sup>40</sup> Krištof Kranjc, Amadej Juranovič, Marijan Kočevar, Franc Perdih  
*Cycloaddition of vinyl-moiety-containing dienophiles on 2H-pyran-2-one derivatives: A surprising diversity of possible products*
- 11<sup>40</sup>-11<sup>50</sup> Dominik Fendre, Bor Lucijan Turek, Marijan Kočevar, Franc Perdih, Krištof Kranjc  
*Synthesis of linked double 2H-pyran-2-one derivative: A possible precursor to double Diels–Alder cycloadducts and various macrocycles*
- 11<sup>50</sup>-12<sup>00</sup> Bor Kolar Bačnik, Luka Jamšek, Franc Perdih, Krištof Kranjc  
*Use of derivatization with hydrazine to determine the correct stereostructure of maleic anhydride-double cycloadducts with substituted 2H-pyran-2-ones*
- 12<sup>00</sup>-12<sup>15</sup> Darko Vušak, Silvija Štriga, Biserka Prugovečki  
*Crystallization and structural transformations of ternary copper(II) coordination compounds with 1,10-phenanthroline and glycine*
- 12<sup>15</sup>-12<sup>25</sup> Boris Gomaz, Zoran Štefanić  
*Oligomeric symmetry of purine nucleoside phosphorylases*



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- 12<sup>25</sup>-12<sup>35</sup> Bogdan Kotur, Volodymyr Babizhetskyy, Chong Zheng  
*New ternary scandium cobalt silicide Sc<sub>38</sub>Co<sub>144</sub>Si<sub>97</sub>: crystal and electronic structures*
- 12<sup>35</sup>-12<sup>45</sup> Antonio Magnabosco, Vinko Nemeć, Dominik Cinčić  
*Cocrystallization of the Schiff base derived from ethylenediamine and pyridine-2-carbaldehyde with perfluorinated halogen bond donors*
- 12<sup>45</sup>-12<sup>55</sup> Mario Cetina, Silvija Maračić, Jasmina Lapić, Senka Djaković, Silvana Raić-Malić  
*Conformation and supramolecular architecture of novel 1,1'-disubstituted ferrocene–quinoline hybrids*
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Afternoon - Excursion

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Saturday, September 11, 2022

## SHORT ORAL CONTRIBUTIONS

CHAIRS: T. KLASER, M. CETINA

- 8<sup>30</sup>-8<sup>45</sup> Krunoslav Užarević, Dijana Žilić, Senada Muratović, Valentina Martinez, Bahar Karadeniz, Teodoro Klaser, Željko Skoko, Damir Pajić, Ivana Brekalo  
*The magnetism of solvatomorphic copper(II)-intermediates in the synthesis of mixed-metal MOF-74 materials*
- 8<sup>45</sup>-8<sup>55</sup> Ana Lozančić, Krešimir Molčanov, Sanja Renka, Sanja Burazer, Marijana Jurić  
*High proton conductivity in 2D oxalate [Mn<sup>II</sup>Cr<sup>III</sup>] polymer with alkyl ammonium cations and its oxide-related usage*
- 8<sup>55</sup>-9<sup>05</sup> Alen Bjelopetrović, Marina Juribašić Kulcsár, Manda Ćurić  
*Mechanosynthesis of Pd(II) photosensitizers under solvent-free conditions in a ball mill*
- 9<sup>05</sup>-9<sup>15</sup> Klemen Motaln, Kristian Radan, Matic Lozinšek  
*Structures of the XeF<sub>2</sub>-MnF<sub>4</sub> adducts*
- 9<sup>15</sup>-9<sup>25</sup> Nina Podjed, Barbara Modec  
*An interesting case of polymorphism involving acetamide*
- 9<sup>25</sup>-9<sup>35</sup> Marin Liović, Nikola Bedeković, Vladimir Stilinović, Dominik Cinčić  
*Crystal structures of 2,4,6-collidinium and 3,5-lutidinium halogenides' cocrystals with 1,4-diiodotetrafluorobenzene*
- 9<sup>35</sup>-9<sup>45</sup> Lidija Molčanov, Dario Barišić, Pavla Šenjug, Damir Pajić, Krešimir Molčanov, Marijana Jurić  
*Anion-directed synthesis of oxalate-based [CuM] (M = Cr or Fe) complexes containing a tridentate ligand: Structural and magnetic properties*
- 9<sup>45</sup>-10<sup>00</sup> Zoran Štefanić, Aleksandra Maršavelski, Boris Gomaz  
*Search for Allostery in Purine Nucleoside Phosphorylases via Database of Molecular Interactions*

10<sup>00</sup>-10<sup>30</sup>

Coffee break

## PLENARY LECTURE

CHAIR: K. MOLČANOV

- 10<sup>30</sup>-11<sup>30</sup> Mariana Klementová  
*Structure determination of nanomaterials from electron diffraction data*

## SHORT ORAL CONTRIBUTIONS

CHAIRS: K. UŽAREVIĆ, K. MOTALN

- 11<sup>30</sup>-11<sup>40</sup> Vinko Nemec, Dominik Cinčić  
*A bromine-containing imine and its copper(II) and nickel(II) coordination compounds in cocrystals with perhalogenated aromates*
- 11<sup>40</sup>-11<sup>50</sup> Patryk Nowak, Artur Sikorski  
*Review of the CSD crystallographic database for selected structures containing acridine and benzoic acid derivatives*
- 11<sup>50</sup>-12<sup>00</sup> Saša Petriček  
*Pyridin-2-one in a manganese(II) complex, cocrystals and an ionic liquid*
- 12<sup>00</sup>-12<sup>10</sup> Nikola Jakupc, Vladimir Stilinović, Krešimir Molčanov  
*Charge density study of a halogen bonded salt of 2-chloropyridine and hexacyanocobaltate(III) acid*



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12 <sup>10</sup> -12 <sup>20</sup>	<u>Marko Dunatov</u> , Andreas Puškarić, Zoran Štefanić, Lidija Androš Dubraja <i>Reversible single-crystal-to-single-crystal transformations in the pleochroic complex salt of the bis(oxalato)chromium(III) anion</i>
12 <sup>20</sup> -12 <sup>30</sup>	<u>Amalija Golobič</u> , Srečo D. Škapin <i>Structural characterization of LaNbTiO<sub>6</sub>-La<sub>4</sub>Ti<sub>9</sub>O<sub>24</sub> based solid solution</i>
12 <sup>30</sup> -12 <sup>40</sup>	<u>Simona Gričar</u> , Matija Uršič, Jakob Kljun, Iztok Turel <i>Structure of ruthenium(II) diketonato complexes designed as potential anticancer agents</i>
12 <sup>40</sup> -12 <sup>50</sup>	<u>Erik Uran</u> , Mirela Dragomir, Kristian Radan, Matic Lozinšek <i>Exploring the XeF<sub>2</sub>-TaF<sub>5</sub> system with mechanochemistry</i>
12 <sup>50</sup> -13 <sup>00</sup>	<u>Miha Virant</u> , Kristian Radan, Matic Lozinšek <i>Metal(II) salts of [MoOF<sub>5</sub>]<sup>-</sup> and [Mo<sub>2</sub>O<sub>2</sub>F<sub>9</sub>]<sup>-</sup> and their HF complexes</i>

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13<sup>00</sup>-15<sup>00</sup>

Lunch break

**SHORT ORAL CONTRIBUTIONS****CHAIRS:** V. NEMEC, S. GRIČAR

15 <sup>00</sup> -15 <sup>10</sup>	<u>Ozana Mišura</u> , Marijana Đaković <i>Variability of mechanical responsiveness of crystals of copper(II) halides with a family of pyridine-based ligands</i>
15 <sup>10</sup> -15 <sup>20</sup>	<u>Anja Pečkaj</u> , <u>Marta Počkaj</u> <i>Reactions between Co(NO<sub>3</sub>)<sub>2</sub>·6H<sub>2</sub>O and 2-(hydroxymethyl)pyridine</i>
15 <sup>20</sup> -15 <sup>30</sup>	<u>Kristian Radan</u> , Juan Forero Saboya, Alexandre Ponrouch, Matic Lozinšek <i>Novel BF<sub>3</sub> adducts of organic carbonates: Syntheses and crystal structures</i>
15 <sup>30</sup> -15 <sup>40</sup>	<u>Uroš Rapuš</u> , Mihaela Rebernik, Jakob Kljun, Iztok Turel <i>p-Cymene ruthenium pyrithionato complexes with triphenylphosphine and triphenylarsine</i>
15 <sup>40</sup> -15 <sup>50</sup>	<u>Małgorzata Rybczyńska</u> , Artur Sikorski <i>Structural characterization of multicomponent crystals formed from nimesulide and quaternary ammonium compounds</i>
15 <sup>50</sup> -16 <sup>00</sup>	<u>Lia Šibav</u> , Denis Arčon, Zvonko Jagličić, Graham King, Mirela Dragomir <i>Doping effects on the structural and magnetic properties of SrCu<sub>2</sub>(BO<sub>3</sub>)<sub>2</sub></i>
16 <sup>00</sup> -16 <sup>10</sup>	<u>Sara Cerovski</u> , Ruđer Sušanj, Vinko Nemec, Dominik Cinčić <i>Competition of different halogen bond acceptors in oxazole derivatives for halogen bonding with perhalogenated benzenes</i>
16 <sup>10</sup> -16 <sup>20</sup>	<u>Viktoria Drushliak</u> and Marek Szafrański <i>Modification of crystal structure and optical absorption edge in compressed perovskite-like CsPb<sub>2</sub>Br<sub>5</sub></i>
16 <sup>20</sup> -16 <sup>30</sup>	<u>Petra Stanić</u> , Krešimir Molčanov <i>π-stacking and multicentric bonding of TMPD (Wurster's blue) in charge-transfer complexes with different quinones</i>

16<sup>30</sup>-17<sup>00</sup>

Coffee break

**PLENARY LECTURE****CHAIR:** A. GOLOBIČ

17 <sup>00</sup> -18 <sup>00</sup>	<u>Jakob Kljun</u> <i>Development of bioactive metal compounds: structural insights into design and molecular modes of action</i>
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**SHORT ORAL CONTRIBUTIONS****CHAIRS:** L. MOLČANOV, M. POČKAI

- 18<sup>00</sup>-18<sup>10</sup> Matic Belak Vivod, Matic Lozinšek, Mirela Dragomir  
*Single-crystal growth and structure determination of BaAgF<sub>4</sub> and (BaF)<sub>2</sub>AgF<sub>4</sub>*
- 18<sup>10</sup>-18<sup>20</sup> Petar Šrbac, Valentina Milašinović, Krešimir Molčanov  
*Salts of 1,1,2,3,3-pentacyanopropenide carbanion with aromatic cations*
- 18<sup>20</sup>-18<sup>30</sup> Ruđer Sušanj, Vinko Nemeć, Nikola Bedeković and Dominik Cinčić  
*Halogen bond motifs in cocrystals of Schiff bases that contain a morpholine or piperazine moiety*
- 18<sup>30</sup>-18<sup>40</sup> Mišel Hozjan, Franc Perdih  
*Sodium salt with zinc dipicolinato anionic complex*
- 18<sup>40</sup>-18<sup>50</sup> Leon Poljanić, Nea Baus Topić, Nikola Bedeković, Vladimir Stilinović, Dominik Cinčić  
*Cocrystallization of perhalogenated halogen bond donors with imines derived from 2-nitrobenzaldehyde and 4-haloanilines*
- 18<sup>50</sup>-19<sup>00</sup> Valentina Milašinović, Krešimir Molčanov, Petar Šrbac  
*Multicentre bonding in dimers of tetracyanoethylene (TCNE) radical anions*
- 19<sup>00</sup>-19<sup>10</sup> Marijana Đaković  
*Crystals' adaptability to external mechanical stimuli: Structural causes and consequences*
- 19<sup>10</sup> Closing remarks A. Meden, D. Matković-Čalogović

20<sup>00</sup>

Meeting dinner