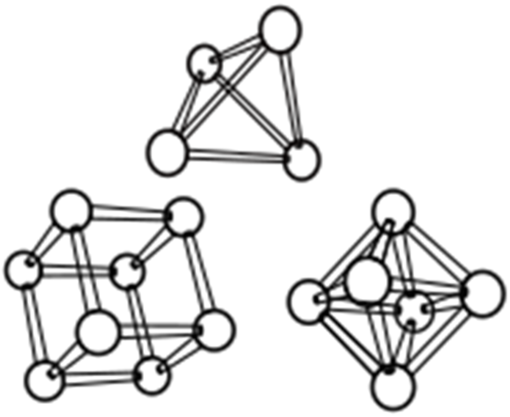
**Croatian Crystallographic Association**

**Slovenian Crystallographic Society**

# Thirty-Second Croatian–Slovenian Crystallographic Meeting

Book of Abstracts



Vodice, Croatia
17–21 June 2026

# Scientific and Organising Committee

The Thirty-Second Croatian–Slovenian Crystallographic Meeting is organised jointly by the *Croatian Crystallographic Association, Faculty of Chemistry and Chemical Technology*, and the University of Ljubljana, under the auspices of the Department of Mathematical, Physical, and Chemical Sciences of the *Croatian Academy of Sciences and Arts*.

## Honorary Chairs

Dubravka Matković-Čalogović, Zagreb

Ivan Leban, Ljubljana

## Chairs of the Meeting

Marijana Đaković, Zagreb

Anton Meden, Ljubljana

## Chair of the Scientific and Organising Committee

Željko Skoko, Zagreb (chair)

## Members of the Scientific and Organising Committee

Andrea Čobić, Zagreb

Lea Čolakić, Zagreb

Gerald Giester, Vienna

Amalija Golobič, Ljubljana

Teodoro Klaser, Zagreb

Jakob Kljun, Ljubljana

Matic Lozinšek, Ljubljana

Valentina Milašinović, Zagreb

Luka Pavić, Zagreb

Nina Podjed, Ljubljana

# PROGRAMME

# PROGRAMME

## WEDNESDAY, June 17, 2026

**18:30 – 19:00 REGISTRATION OF PARTICIPANTS**
**19:00 – 19:30 WELCOME RECEPTION**

## THURSDAY, June 18, 2026

**08:00 – 08:45 REGISTRATION OF PARTICIPANTS**
**08:45 – 09:00 OPENING CEREMONY**

*Chairpersons: A. Meden, M. Đaković*

**09:00 – 10:00 PLENARY LECTURE**
**Marta Počkaj**
*Exploring 3D electron diffraction: first experiences and lessons learned*

*Chairperson: A. Meden*

**10:00 – 10:30 COFFEE BREAK**

**10:30 – 11:40 SHORT PRESENTATIONS**
*Block A — Structural methods and crystal-structure determination*

*Chairpersons: M. Razum, M. Dragomir*

10:30 – 10:40 **Anton Meden**
*Crystal structure of $Bi_4Ti_3O_{12}$ nanowires determined by 3D electron diffraction*
10:40 – 10:45 **Andreas Ertl**
*Correlations between site-occupations and temperature in synthetic tourmaline: caused by the crystal structure?*
10:45 – 10:50 **Andreas Ertl**
*Development of a new geothermometer using zoned tourmaline*
10:50 – 11:00 **Goran Štefanić**
*X-ray diffraction analysis of platinum-modified hematite nanowires*
11:00 – 11:10 **Nina Podjed Rihtaršič**
*Copper(II) complexes with deprotonated furosemide: X-ray evidence of novel coordination modes*
11:10 – 11:20 **Matjaž Kristl**
*Crystal structures of copper(II) complexes with halogenated pyridines*
11:20 – 11:30 **Matic Lozinšek**
*Coordination of $XeF_2$ to the $BrF_2^+$ Cation*
11:30 – 11:40 **Emilia Buchsteiner**
*Variable temperature diffraction and polymorph screening with the XtaLAB Synergy-ED*

**11:40 – 12:00 BREAK**

**12:00 – 13:20 SHORT PRESENTATIONS**
*Block B — Crystal dynamics, functional materials and coordination chemistry*

*Chairpersons: M. Lozinšek, S. Burazer*

12:00 – 12:15 **Željko Skoko**
*Tailoring thermosalient phase transitions by molecular alloying*
12:15 – 12:25 **Mateja Pisačić**
*Heat it, push it, watch it move: structural origins of crystal dynamics*
12:25 – 12:35 **Božena Tokić**
*Dynamic responses of cadmium(II) coordination polymer crystal to mechanical and thermal stimuli*
12:35 – 12:45 **Katarina Lucija Lakota**

*Ruthenium(II) complexes with novel pyrithione ligands*

12:45 – 12:55 **Marta Razum**
*Tuning polaronic pathways in vanadate-phosphate glasses by mixed transition metal oxide substitution*

12:55 – 13:05 **Uroš Rapuš**
*Organoruthenium(II) complexes with pyrithione and ligands containing group V. donor atoms*

13:05 – 13:20 **Dora Balen**
*Linking synthesis to crystal structure in* $LaCoO_3$*: a detailed crystallographic investigation*

**13:20 – 15:00 LUNCH BREAK**

**15:00 – 16:00 PLENARY LECTURE**
**Jan Dohnálek**
*How Far Do We Understand Protein–Nucleic Acids Interactions? Nucleases at Atomic Resolution*
*Chairperson: D. Matković-Čalogović*

**16:00 – 16:30 COFFEE BREAK**

**16:30 – 18:30 CCDC WORKSHOP**
**Matthew Lightfoot**
*From Crystal Structures to Solid Forms – Exploring CSD Tools for Interactions, Morphology and Particle Properties*

## FRIDAY, June 19, 2026

**08:00 – 09:00 REGISTRATION OF PARTICIPANTS**

**09:00 – 10:00 PLENARY LECTURE**
**Sarah Guerin**
*Accelerating organic molecular crystals as sustainable piezoelectric energy harvesters*
*Chairperson: M. Đaković*

**10:00 – 10:30 COFFEE BREAK**

**10:30 – 11:45 SHORT PRESENTATIONS**
*Block C — Halogen bonding, crystal engineering and applied crystallography*
*Chairpersons: J. Jakoš, T. Klaser*

10:30 – 10:45 **Dominik Cinčić**
*Metal-organic halogen-bonded cocrystals based on the robust I···SCN synthon*

10:45 – 10:55 **Vinko Nemec**
*Halogen-bonded cocrystals of* $M(NCS)_2(3\text{-}Xpy)_4$ *coordination compounds (M = Co, Ni, Fe, Mn; X = Cl, Br, I)*

10:55 – 11:05 **Mladen Borovina**
*Comparison of chloride and isothiocyanate ligands (X) as halogen bond acceptors in cocrystals based on* $[Co(X)_2(2\text{-acetylpyridine})_2]$ *complexes*

11:05 – 11:15 **Lidija Posavec**
*Tetrakis(4-pyridyl)porphyrin as a building block in halogen-bonded cocrystals*

11:15 – 11:30 **Sanja Burazer**
*Operando XRD study of practical battery configurations with the DANOISE Cell*

11:30 – 11:45 **Mirela Dragomir**
*Mechanochemistry as a Route to Novel Silver(II) Compounds*

**11:45 – 12:00 BREAK**

**12:00 – 13:15 SHORT PRESENTATIONS**

*Block D — Coordination chemistry and solid-state structural chemistry: complexes, MOFs and intermetallic compounds*

*Chairpersons: M. Kristl, I. Đilović*

12:00 – 12:10 **Nikola Jakupec**
*Investigation of an O···π 'lamp motif' in 2,3-dichloro-5,6-dicyanobenzoquinone modified in highly acidic media*

12:10 – 12:20 **Jakob Kljun**
*Synthesis and structure of new chelating mercaptopyrimidines*

12:20 – 12:30 **Jure Jakoš**
*Modifying and coordinating caerulomycin A*

12:30 – 12:40 **Sabi William Konsago**
*Caerulomycin K inspired chelating pyridine oximes*

12:40 – 12:55 **Marin Liović**
*Drug solubility modification: indomethacin salts/cocrystals with isonicotinamide and imidazole*

12:55 – 13:05 **Bohdan Kotur**
*Crystal structure of the ternary gallide* $Zr_{10}Ru_5Ga$

13:05 – 13:15 **Darko Vušak**
*Expanding the Structural Diversity of 3,3'-Bipyridine to Dual-Ligand Metal–Organic Frameworks*

**13:15 – 15:00 LUNCH BREAK**

**15:00 – 19:00 CONFERENCE TRIP**

**19:30 CONFERENCE DINNER**

## SATURDAY, June 20, 2026

**09:00 – 10:00 PLENARY LECTURE**

**Emil S. Božin**
*Femtosecond access to hidden nanoscale non-equilibrium states in quantum materials*

*Chairperson: Ž. Skoko*

**10:00 – 10:30 COFFEE BREAK**

**10:30 – 11:40 SHORT PRESENTATIONS**

*Block E — Coordination chemistry: transition-metal complexes I*

*Chairpersons: L. Čolakić, E. Goreshnik*

10:30 – 10:50 **Krešimir Molčanov**
*Salts of tetracyanoquinodimethane (TCNQ) radical anion with low partial charges of −1/3 and −2/5*

10:50 – 11:05 **Yurii Slyvka**
*Allyl-substituted pyridines as powerful tools for the construction of novel copper π,σ-coordination compounds*

11:05 – 11:15 **Andrii Hultiaiev**
*The novel DABCO-chlorocuprate(I) coordination compounds*

11:15 – 11:25 **Ivica Đilović**
*The first structure of a discrete cis-bis(L-prolinato)copper(II) in co-crystals with urea and water. The influence of crystallization conditions on the occurrence of urea cocrystals*

11:25 – 11:40 **Igor Picek**
*Supramolecular Pyridinium Oxime–Ferrocyanide Complexes: Structurally Driven Chromic Response*

**11:40 – 12:00 BREAK**

**12:00 – 12:55 SHORT PRESENTATIONS**

*Block F — Macromolecular crystallography, bioactive compounds and supramolecular chemistry*

*Chairpersons: M. Potočnik, L. Pavić*

12:00 – 12:15 **Mirjana Radanović**
*Comparative structural analysis of a series of halogenated thiocarbohydrazone derivatives*

12:15 – 12:35 **Ivana Kekez**
*Engineering metagenomic esterases: from ancestral reconstruction to crystal structure*

12:35– 12:45 **Khalida Khalil**
*Supramolecular macrocycles for water purification: structural and computational studies of inclusion complexes*

12:45– 12:55 **Rehana Bano**
*Crystal structure and intermolecular interaction analysis of imidazolium-based molecular salts*

**12:55 – 15:00 LUNCH BREAK**

**15:00 – 16:00 PLENARY LECTURE**

**Vladimir Stilinović**
*Halogen bond – a not so non-covalent interaction*

*Chairperson: K. Molčanov*

**16:00 – 16:30 COFFEE BREAK**

**16:30 – 17:45 SHORT PRESENTATIONS**

*Block G — Structural analysis of materials: modulation, mechanochemistry and characterization*

*Chairpersons: I. Kekez, S. W. Konsago*

16:30 – 16:40 **Clivia Hejny**
*From mystery to modulation: the structural story of* $Rb_2[Si_2O_5]$

16:40 – 16:50 **Aleksandra Šaponjić**
*Production of durable mullite-based ceramics from diatomite*

16:50 – 17:00 **Martina Potočnik**
*Thermal behaviour of virgin and recycled polyethylene terephthalate analysed by differential scanning calorimetry*

17:00 – 17:10 **Fouad Alloun**
*Crystal structure and magnetic properties of the novel langbeinite-type phosphate* $Ba_2FeCo(PO_4)_3$

17:10 – 17:25 **Lea Čolakić**
*Discovery of the intermediate crystalline phase in the mechanochemical synthesis of silver sulfadiazinate*

17:25 – 17:45 **Teodoro Klaser**
*Surface patch characterization and crystal orientation effects on the photoelectric properties of gold-coated surfaces*

**17:45 – 18:00 BREAK**

**18:00 – 18:50 SHORT PRESENTATIONS**

*Block H — Applied crystallography: inorganic materials and the solid state*

*Chairpersons: J. Kljun, I. Picek*

18:00 – 18:15 **Luka Pavić**
*From structure to transport: phosphate glasses containing transition metal-oxides*

18:15 – 18:30 **Sara Marijan**

*Catalytic behavior and dielectric properties of V-P-O-based glasses*

18:30 – 18:40 **Vesna Zalar Serjun**
*Valorisation of industrial combustion by-products as alternative binders for low-carbon construction*

18:40 – 18:50 **Evgeny Goreshnik**
*New hydrazinium salts with bifluoride anion*

18:50 – 19:00 **Nives Kitanovski**
*From discrete complexes to coordination polymers in cobalt coordination chemistry*

**19:00 CLOSING REMARKS**

*Chairpersons: A. Meden, M. Đaković*

## SUNDAY, June 21, 2026

**09:00 – 10:30 EVALUATION AND FAREWELL COFFEE**
**10:30 DEPARTURE**

**The Thirty-Second Croatian–Slovenian Crystallographic Meeting**

is financially supported by

## GOLD SPONSOR

Rigaku

## SPONSORS

RENACON

Official agent of

Malvern Panalytical

aparatura
ANALYTICAL EQUIPMENT AND SYSTEMS

ThermoFisher
SCIENTIFIC

ITRLAB
JUST FOCUS

Anton Paar

Selvita

## PARTNERS

European Crystallographic Association

CCDC
advancing structural science

# PLENARY LECTURES

# EXPLORING 3D ELECTRON DIFFRACTION: FIRST EXPERIENCES AND LESSONS LEARNED

Marta Počkaj[1]

[1] Faculty of Chemistry and Chemical Technology, University of Ljubljana, Večna pot 113, SI-1000 Ljubljana, Slovenia; *E-mail:* marta.pockaj@fkkt.uni-lj.si

The electron diffraction (ED) started to evolve only a few years after X-ray diffraction, in 1920s. However, the stronger interaction between electrons and the sample compared to the interaction between X-rays and sample has long hindered the development and widespread use of electron diffraction for crystal structure determination of materials. [1] At the intersection of electron microscopy and crystallography, both quite demanding methods, a lot of time must have passed for ED to become accessible to a wider scientific audience. The first part of the talk will cover a short historical overview of the development of ED.

With the progress in science and technology, in last years the number of crystal structures determined from ED data has risen dramatically. [2] This number is expected to increase even more due to the 3D electron diffractometers, dedicated for 3D ED, which came to the market in last years. In our institution, XtaLAB Synergy-ED diffractometer has been installed last year. In the second part of the talk, we will shortly revise its features, the requirements of the sample, its preparation, data collection and structure solution/refinement workflow.

The last part of the presentation will focus on results, i.e. crystal structures of various materials determined by ED, spanning from simple organic commercial samples through complex reaction mixtures obtained in the process of recycling of precious metals to completely inorganic materials.

## References:

[1] Zou, X., Hovmöller, S & Oleynikov, P. (2011) Electron Crystallography. IUCr Texts on Crystallography 16, Oxford University Press.
[2] Groom, C.R., Bruno, I.J., Lightfoot, M.P. & Ward, S.C. (2016). *Acta Crystallogr*. B72, 171-179.

### Acknowledgement

We acknowledge the financial support of the Slovenian Research and Innovation Agency (ARIS, program grant P1-0175), and also the support of the Centre for Research Infrastructure at the University of Ljubljana, Faculty of Chemistry and Chemical Technology, which is part of the Network of Research and Infrastructural Centers UL (MRIC UL) and is financially supported by ARIS; Infrastructure program No. I0-0022.

# HOW FAR DO WE UNDERSTAND PROTEIN-NUCLEIC ACIDS INTERACTIONS? NUCLEASES AT ATOMIC RESOLUTION

Jan Dohnálek,[1] Kristýna Adámková,[1] Mária Trundová,[1] Blanka Husťáková,[1] Jarmila Dušková,[1] Lars H. Østergaard,[2] Petr Kolenko,[1,3], Lukáš Gajdoš,[4] Tereza Skálová,[1] and Tomáš Kovaľ[1]

[1] Institute of Biotechnology, Czech Academy of Sciences, Průmyslová 595, 25250 Vestec, Czech Republic; *E-mail:* dohnalek@ibt.cas.cz
[2] Novonesis A/S, Biologiens Vej 2, DK-2800 Kgs Lyngby, Denmark
[3] Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, Břehová 7, 115 19 Prague 1, Czech Republic
[4] Life Sciences Group, Institut Laue-Langevin, 71 Avenue des Martyrs, 38000, Grenoble, France

Protein-nucleic acids interactions are essential for many biological processes. Even though numerous structural studies provided answers to the basic questions about these interactions, very high resolution or even atomic resolution data with the focus on the atomic details of interactions are missing. At the same time these types of interactions have never been studied by neutron diffraction.

S1-P1 nucleases are coded for by fungi, trypanosomatids, plants and some pathogenic bacteria [1]. These 25-40 kDa enzymes are typically zinc-dependent. The active site relies on the metal cluster and the nucleobase-binding site 1 stabilizing the –1 nucleotide with respect to the cleaved O3’-P3’ bond. The enzymes are universal with respect to the cleaved substrate, which enables their application in biotechnologies.

Our studies of S1-P1 nucleases from plants, fungus, and two bacterium species [2-5], including crystal structures, mutagenesis, numerous product/ligand complexes helped us better understand the structure-function questions, such as active site remodelling, sensitivity to metal replacement, and key mobility elements in the active site. Recently, we have identified a “supernuclease” SmNuc1 from an opportunistic pathogen *Stenotrophomonas maltophilia* capable of previously unseen rates for this enzyme class and explained its main properties in a crystallographic study [6]. S1 nuclease from *Aspergillus oryzae* and SmNuc1 show outstanding crystallization properties and enable subatomic resolution X-ray studies and also neutron diffraction analysis. They open up the possibility to study details of protein-nucleic acid interactions, including the key protonation patterns.

## References:

[1] Koval, T., Dohnalek, J. *Biotechnol. Adv.* (2017) Epub 2017 Dec 14, 10.1016/j.biotechadv.2017.12.007.
[2] Kovaľ, T., Østergaard, L.H., Lehmbeck, J. *et al. PLOS One* 11, (2016), e0168832.
[3] Trundová, M., Kovaľ, T., Owens, R.J. *et al. Int J Biol Macromol* **114**, (2018), 776.
[4] Adámková, K., Koval', T., Østergaard, L.H. *et al. Acta Crystallogr D***78,** (2022), 1194.
[5] Husťáková, B., Trundová, M., Adámková, K. et al. *FEBS Lett* **597**, (2023), 2103.
[6] Adámková, K., Trundová, M., Kovaľ, T., Husťáková, B., *et al. FEBS J.*, **292**, (2025), 129.

## Acknowledgement

This work was supported by the Czech Science Foundation (25-17546S), and by the Czech Academy of Sciences (86652036). CIISB, Instruct-CZ Centre of Instruct-ERIC EU consortium, funded by MEYS CR infrastructure project LM2023042 and European Regional Development Fund-Project No. CZ.02.01.01/00/23_015/0008175 is acknowledged for providing access to all facilities at CMS in BIOCEV for this project.

# ACCELERATING ORGANIC MOLECULAR CRYSTALS AS SUSTAINABLE PIEZOELECTRIC ENERGY HARVESTERS

Sarah Guerin[1,2]

[1] Department of Chemical Sciences, Bernal Institute, University of Limerick, Ireland; *E-mail*: sarah.guerin@ul.ie
[2] SSPC, the Research Ireland Centre for Pharmaceuticals, Bernal Institute, University of Limerick, Ireland

Billions of piezoelectric sensors are produced every year, improving the efficiency of many current and emerging technologies. By interconverting electrical and mechanical energy they enable medical device, infrastructure, automotive and aerospace industries, but with a huge environmental cost. Amino acids are the most basic biological components, and they are cheap and (relatively!) simple to crystallize, with significant piezoelectricity in single crystal and polycrystalline forms. However, this response is highly anisotropic, and precise, orientated control over crystallisation is required to maximize the piezoelectric output of a crystalline amino acid device for development into a cohesive ceramic-type element. Our research is taking on the challenge of developing biomolecular crystals as organic, low-cost, high-performance sensors and energy harvesters, to out-perform and phase-out inorganic device components with dramatically reduced environmental impact. In this talk I will discuss our methodologies for the design, growth, and engineering of these novel piezoelectric materials under three pillars:

- An ambitious computational workflow to enable the design of super-piezoelectric crystalline assemblies by combining high-throughput quantum mechanical calculations with machine learning algorithms;
- A new method of growing polycrystalline biomolecules, allowing for easy, efficient creation of macroscopic piezoelectric structures;
- Establishing effective coating and electroding procedures to characterise fully insulated and contacted biomolecular device components.

This interdisciplinary approach has led to the understanding, design, and discovery of a large number of amino acid-based systems, which due to their low permittivity produce large voltages under an applied force.

**References:**

[1] Guerin, S., Stapleton, A., Chovan, D., Mouras, R., Gleeson, M., McKeown, C., ... & Thompson, D. (2018). *Nat Mat*, *17*(2), 180-186.
[2] Vishnoi, S., Kumari, G., Guest, R., Cazade, P. A., & Guerin, S. (2025). *Ang Chem*, *137*(18), e202501232.
[3] Hari, K., Ryan, T., Bhattacharya, S., & Guerin, S. (2024). *Phys Rev Lett*, *133*(13), 137001.
[4] Bhattacharya, S., Zubair, M., Moffat, J., Ryan, T., Hari, K., & Guerin, S. (2026). *J Mat Chem A*.

**Acknowledgement**

Research funded by the European Union under the ERC Starting Grant Number. 101039636, and Research Ireland under grant numbers 21/PATH-S/9737 and 12/RC/2275_P2. Calculations are run via the Irish Centre for High-End Computing (ICHEC).

# FEMTOSECOND ACCESS TO HIDDEN NANOSCALE NON-EQUILIBRIUM STATES IN QUANTUM MATERIALS

Emil S. Bozin[1]

[1]Center for Solid State Physics and New Materials, Institute of Physics Belgrade, Serbia: *E-mail:* bozin@ipb.ac.rs

Understanding the evolution of quantum materials far from equilibrium demands experimental probes capable of capturing both ultrafast dynamics and local structural correlations beyond crystallographic symmetry. Ultrafast X-ray pair distribution function (uf-PDF) analysis, enabled by femtosecond X-ray free-electron lasers (XFELs), provides direct access to transient local atomic arrangements on femtosecond–picosecond timescales, revealing hidden states inaccessible to conventional diffraction (Fig. 1) [1]. Recent advances demonstrate that high-quality total scattering and PDFs can be obtained from a single ~30 fs XFEL pulse over an extended Q-range, enabling quantitative structural analysis of crystalline, nanocrystalline, amorphous, liquid, and solution-phase systems alike [2]. This capability establishes a powerful framework for resolving hierarchical lattice responses and emergent orders in correlated materials, including lattice instabilities and intertwined electronic phases [3]. Beyond quantum materials, ultrafast PDF provides a broadly applicable platform for tracking structural dynamics in catalysis, energy materials, shock-compressed liquids, nanoparticle formation, and molecular conformational changes, offering a universal approach to time-resolved total scattering across disciplines.

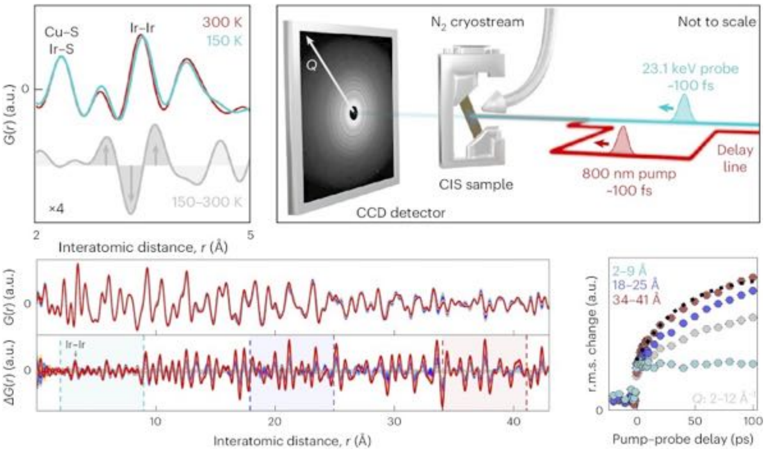


Figure 1. Resolving length-scale-dependent transient disorder through an uf-phase transition.

**References:**
[1] Griffiths, J. et al (2024). *Nature Materials* 23, 1041.
[2] Sapnik A. F. et al (2025). *IUCrJ* 12, 531.
[3] Bozin E. S. et al, (2023). *Nature Communications* 14, 7055.

**Acknowledgement**
Work at BNL was supported by the U.S. DOE Office of Science, Basic Energy Sciences (Field Work Proposal DE-SC0012704), and at IPB by the EU Horizon Europe program (Grant 101185375).

# HALOGEN BOND – A NOT SO NON-COVALENT INTERACTION

Vladimir Stilinović[1]

[1] Department of Chemistry, Faculty of Science, University of Zagreb; *E-mail:* vstilinovic@chem.pmf.hr

Halogen bond (XB), an attractive supramolecular interaction between a halogen atom acting as a Lewis acid and a Lewis base, has over the recent decades risen as one of the main intermolecular interactions in supramolecular chemistry and crystal engineering, and has also been found to play a significant role in several biological systems. In spite of its ubiquitous use in supramolecular chemistry today, the nature of halogen bond still remains a somewhat contentious question. The earliest description of halogen bond as a charge-transfer by Mulliken, has at the end of last century been replaced by the concept of halogen bond as a primarily electrostatic interaction between an electron-depleted region of a halogen atom (a σ-hole), corresponding to a positive electrostatic potential, and an electron-rich (negative) region of an acceptor. This elegant and simple model depicts halogen-bond as a quintessentially non-covalent interaction between molecules. More recently however there has been growing body of evidence indicating that a $n \rightarrow \sigma^*$ charge transfer component also has a considerable contribution, particularly for strong halogen bonds. Indeed, the triiodide ion ($I_3^-$), a classical textbook example of a hypervalent molecule exhibiting a (covalent) 3-center 4-electron (3c–4e) bond, can also be viewed as a halogen bonded complex of an iodine molecule as a donor and iodide as an acceptor – a halogen-bonded equivalent of hydrogen difluoride ($HF_2^-$) anion! The line separating covalent and non-covalent halogen bonds seems therefore to be somewhat less than clear.

In this talk we shall give an overview of some of our previous work which has been aimed towards maping the ‘border area’ between the ‘non-covalent’ and the ‘covalent’ halogen bond. Through a series of examples of crystallographic, computational and solution studies, we shall attempt to find the general trends, similarities and differences between halogen bonded systems involving *classical* ‘non-covalent’ halogen bonds with various types of C–X donors (with bond energies generally in the range 20–40 kJ mol$^{-1}$); halogen bonding involving donors with more polarised halogens (such as *N*-haloimides) which form some of the strongest halogen bonds between neutral molecules (40–60 kJ mol$^{-1}$), and finally halogen bonds in bipyridylhalonium cations (40–180 kJ mol$^{-1}$) which are generally considered to be ‘covalent’.

# SHORT ORAL PRESENTATIONS

# CRYSTAL STRUCTURE OF $Bi_4Ti_3O_{12}$ NANOWIRES DETERMINED BY 3D ELECTRON DIFFRACTION

Anton Meden[1] and Darko Makovec[2]

[1] Faculty of Chemistry and Chemical Technology, University of Ljubljana, Večna pot 113, SI-1000 Ljubljana; *E-mail*: tone.meden@fkkt.uni-lj.si
[2] Jožef Stefan Institute, Jamova 39, SI 1000 Ljubljana, Slovenia

The physical properties of bismuth titanate ($Bi_4Ti_3O_{12}$) may enable its use as a ferroelectric or piezoelectric material in various devices.

Two morphologically and structurally distinct phases of this material were prepared hydrothermally by varying the concentration of NaOH during the hydrothermal treatment ofthe corresponding hydroxides (Fig. 1). The nanoplatelets had the well-known structure of an Aurivillius phase, while the nanowires exhibited a new structure. High-resolution STEM imaging enabled determination of the unit cell and possible cationic structure of the novel nanowire phase, although the complete crystal structure, including oxygen positions, remained unknown [1].

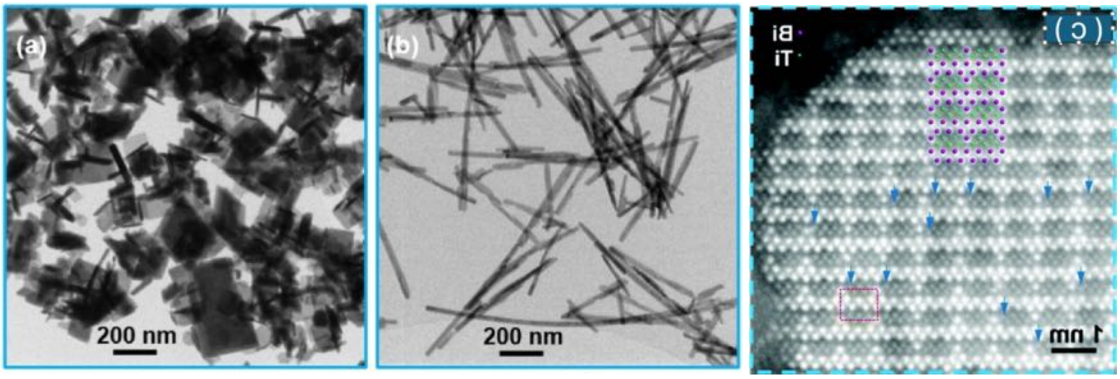


Fig. 1: STEM image of $Bi_4Ti_3O_{12}$ nanoplatelets (a), nanowires (b), and a projection of the cationic structure on the HR STEM image (c).

Using 3D electron diffraction, single-crystal data were collected on several nanowires, despite their extremely small width and thickness, allowing determination of the crystal structure, including the oxygen positions. However, interpretation of these positions raised some unexpected questions about charge balance. Additional information was therefore sought using thermal analysis and FTIR to clarify these issues.

The outcomes of these analyses and the status of the nanowires crystal structure elucidation will be reported at the conference.

## References:

[1] Makovec, D., Kosi Križaj, N., Meden, A., Dražić, G., Uršič Nemevšek, H., Kostanjšek, R., Šala, M. and Gyergyek, S. (2022). *Nanoscale* 14, 3537.

**Acknowledgement**

Financial support of ARIS through research program P1-0175 is gratefully acknowledged.

# CORRELATIONS BETWEEN SITE-OCCUPATIONS AND TEMPERATURE IN SYNTHETIC TOURMALINE: CAUSED BY THE CRYSTAL STRUCTURE?

Andreas Ertl [1,2]

[1] Mineralogisch-Petrographische Abt., Naturhistorisches Museum, Burgring 7, 1010 Wien, Austria; *E-mail*: andreas.ertl@a1.net
[2] Institut für Mineralogie und Kristallographie, Universität Wien, Geocenter, 1090 Wien, Austria

Minerals from the tourmaline supergroup have the formula $XY_3Z_3(BO_3)_3[T_6O_{18}]V_3W$, where the *X* site is usually occupied by Na or Ca, the *Y* site by Al, Fe, Mg, Li, Cu or Ti, the *Z* site by Al, Mg or Fe, the *T* site by Si, Al or B, the *V* site by OH or O, and the *W* site by OH, F or O. An excellent correlation between the total charge of the *X*-site cations and the fluorine content in Mg-free tourmaline was first reported by [1]. Similar correlations were now identified in tourmaline crystals synthesized at 650 °C and 0.15 GPa [2]. The following linear correlations (Fig. 1) were observed: $y = 1.013x + 0.411$ ($r^2 = 0.98$; 5 data points), $y = 1.002x + 0.453$ ($r^2 = 0.98$; 5 data points) and $y = 1.006x + 0.503$ ($r^2 = 0.99$; 4 data points). While the slope is 1.007(5), the *y*-intercept varies significantly (0.41, 0.45, 0.50). As the syntheses conditions were always 650 °C, it can be concluded that the slope corresponds to the temperature, while the *y*-intercept may reflect variations in the composition of the starting material. A more or less closed system was also present in small miarolitic pockets, found within a relatively small distance in a pegmatite [3]. Similar correlations with comparable slopes, but with significantly different *y*-intercept values, were observed in two strongly zoned tourmaline crystals. The *X*-site charge seems to represent the dominant crystallographic control determining how F partitions into tourmaline, a relationship that appears to be temperature-dependent.

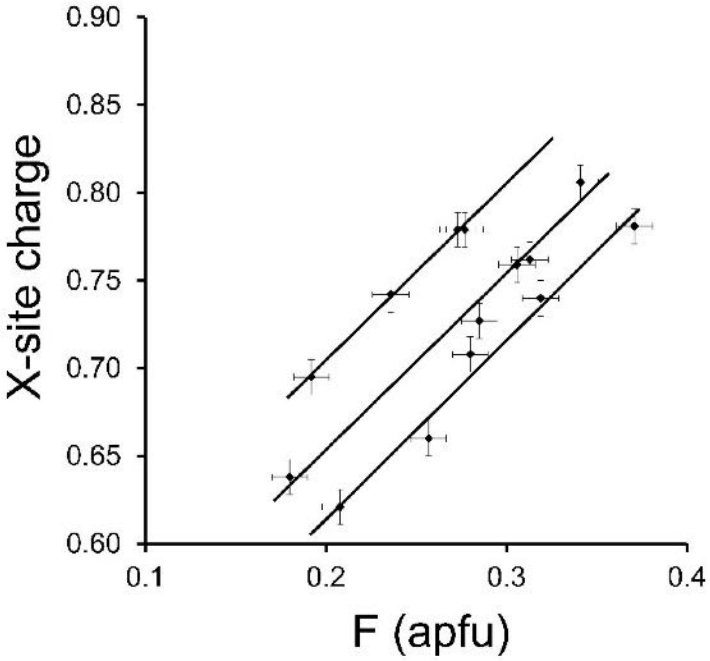


**Fig. 1**. Correlation between *X*-site charge and fluorine.

**References:**
[1] Ertl, A., Rossman, G.R., Hughes, J.M., et al. (2010). *Am. Mineral.*, 95, 24–40.
[2] Ertl, A., Vereschagin, O.S., Giester, G., et al. (2015). *Can. Mineral.* 53, 209–220.
[3] Ertl, A., Pezzotta, F., Hughes, J.M., et al. (2025). *Geol. Carp.* 76, 301–309.

**Acknowledgement**
This study was funded in whole by the Austrian Science Fund (FWF) project P 35585.

# DEVELOPMENT OF A NEW GEOTHERMOMETER USING ZONED TOURMALINE

Andreas Ertl [1,2]

[1] Mineralogisch-Petrographische Abt., Naturhistorisches Museum, Burgring 7, 1010 Wien, Austria; *E-mail*: andreas.ertl@a1.net
[2] Institut für Mineralogie und Kristallographie, Universität Wien, Geocenter, 1090 Wien, Austria

A dependence of the alkali/alkaline-earth cation *X*-site occupancy to the formation conditions during tourmaline crystallization was already suggested by [1]. Over the last 15 years, several excellent linear correlations between *X*-site charge and F content have been observed in zoned tourmalines from various pegmatites, such as that reported by [2]. These correlations are independent of the $Li^{1+}$, $Fe^{2+}$, $Mn^{2+}$, $Al^{3+}$ content of the different zones, if these zones are crystallized at the same temperature in a (more or less) closed system. Studies on synthetic tourmalines also provided evidence that the slope of such a correlation depends on the temperature during the crystallization. However, first attempts were not very accurate, as tourmalines with strongly varying Mg contents were also used to calibrate such a thermometer. Earlier attempts to develop tourmaline-based geothermobarometers concluded that such models cannot be realized without accounting for inter-site partitioning and non-ideal interactions [3]. Since the proposed geothermometer is based on charges, the inter-site partitioning of $Mg^{2+}$ between the *Y* and *Z* sites appears to be problematic, as it results in the *Z* site no longer being exclusively occupied by trivalent cations. Hence, Mg-rich samples were not used for calibration. The geothermometer was calibrated by using 10 different data sets ($r^2 = 0.80$) with excellent linear correlations (mean $r^2 = 0.9$). Based on the resulting correlation (Fig. 1) the temperature can be estimated as follows: T [°C] = $(k + 1.144)/0.0034$, where $k$ is the slope of a linear correlation between the *X*-site charge and the F content of zoned tourmaline.

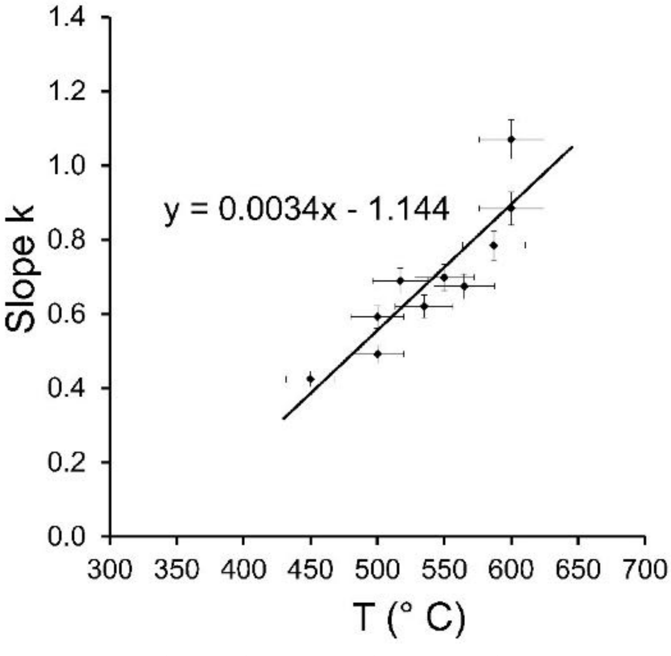


**Fig. 1**. Correlation between slope *k* and temperature.

**References:**

[1] *Henry, D.J. & Dutrow, B.L. (1996). Rev. Mineral. Geochem*. 33, 503–557.
[2] Ertl, A., Rossman, G.R., Hughes, J.M., et al. (2010). *Am. Mineral.* 95, 24–40.
[3] Hinsberg, V.J. & Schumacher, J.C. (2009). *Am. Mineral*. 94, 761–770.

**Acknowledgement**

This study was funded in whole by the Austrian Science Fund (FWF) project P 35585.

# X-RAY DIFFRACTION ANALYSIS OF PLATINUM-MODIFIED HEMATITE NANOWIRES

Goran Štefanić[1], Monika Šoltić[1], Nikola Baran[1], Goran Dražić[2], Marijan Marcijuš[3], Mile Ivanda[1], Marijan Gotić[1]

[1] Laboratory for Molecular Physics and Synthesis of New Materials, Division of Materials Physics, Ruđer Bošković Institute, Bijenička cesta 54, 10 000 Zagreb, Croatia; *E-mail*: stefanic@irb.hr
[2] Department of Materials Chemistry, National Institute of Chemistry, Hajdrihova 19, SI-1001 Ljubljana, Slovenia
[3] Laboratory for the synthesis of new materials, Division of Materials Chemistry, Ruđer Bošković Institute, 10000 Zagreb, Croatia

Hematite ($\alpha$-$Fe_2O_3$) nanowires decorated with 0, 1, and 5 mol% platinum for hydrogen gas sensing applications were prepared via a wet-chemical co-precipitation route, using ethanol or water as the dispersing solvent, while selected samples were subjected to post-deposition annealing. The structural and microstructural properties of the resulting materials were characterized by X-ray powder diffraction (XRPD) using two complementary analytical approaches. Phase analysis and precise unit-cell parameter determination were carried out by Rietveld refinement using the program MAUD. Hematite was confirmed as the dominant phase in all samples. Metallic platinum reflections were detected only in the 5 mol% annealed sample, while the invariance of the hematite unit-cell parameters across the entire platinum-loading range ($a \approx 0.5038$–$0.5040$ nm, $c \approx 1.3761$–$1.3765$ nm) demonstrates that platinum does not incorporate into the α-Fe2O3 crystal lattice but remains on the nanowire surface as finely dispersed nanoparticles. Anisotropic size–strain analysis was performed using the Popa line-broadening model with crystallographic symmetry rules (trigonal Laue class), as implemented in MAUD, and cross-validated by individual pseudo-Voigt profile fitting using XFIT. The symmetry-constrained Popa model was preferred over an unconstrained anisotropic approach, which showed strongly correlated parameters and risk of overparameterisation. Volume-averaged coherent domain sizes (Dv) of 21–41 nm and upper-limit microstrain values (e) of 1.1 –$2.2 \times 10^{-3}$ were obtained for four selected reflections — (104), (110), (006) and (113) — probing distinct crystallographic directions. The results reveal a pronounced anisotropy of both Dv and e in the reference sample, consistent with preferential nanowire elongation along [110]. Platinum loading progressively increases microstrain and reduces domain coherence, most clearly along the c-axis direction. Water-based platinum dispersion introduces marginally greater lattice disorder than ethanol-based deposition at 1 mol% Pt. Post-deposition annealing produces a moderate, direction-selective redistribution of microstrain without significant change in domain size or unit-cell parameters, consistent with thermally driven restructuring of the Pt–hematite interface.

# COPPER(II) COMPLEXES WITH DEPROTONATED FUROSEMIDE: X-RAY EVIDENCE OF NOVEL COORDINATION MODES

Nina Podjed Rihtaršič[1], Barbara Modec[1]

[1]Faculty of Chemistry and Chemical Technology, University of Ljubljana, Večna pot 113, SI-1000 Ljubljana, Slovenia; *E-mail:* nina.podjed@fkkt.uni-lj.si

Furosemide, a widely used sulfonamide-based diuretic, has recently attracted attention in its deprotonated form as a versatile ligand in coordination chemistry [1]. In our earlier work, zinc(II) complexes containing the furosemide anion demonstrated moderate antibacterial activity against *Staphylococcus epidermidis* [2]. Based on these findings, we investigated the coordination behavior of furosemide toward copper(II) ions. Several new copper(II) compounds were prepared, and their solid-state structures were determined by single-crystal X-ray diffraction analysis. Monodentate coordination of furosemide anion through a single carboxylate oxygen has been described previously [3]. In contrast, our study revealed two novel coordination modes (Fig. 1). One involves a $\mu^{2}$-$\eta^{1}$:$\eta^{1}$ bidentate bridging coordination of the carboxylate group, generating dinuclear paddle-wheel copper(II) complexes. The second is an unusual bridging mode ($\mu^{3}$-$\eta^{1}$:$\eta^{1}$:$\eta^{1}$) that links three copper(II) ions into a one-dimensional coordination polymer. In this motif, the ligand binds not only through carboxylate oxygens but also *via* the sulfonamide oxygen atom [4].

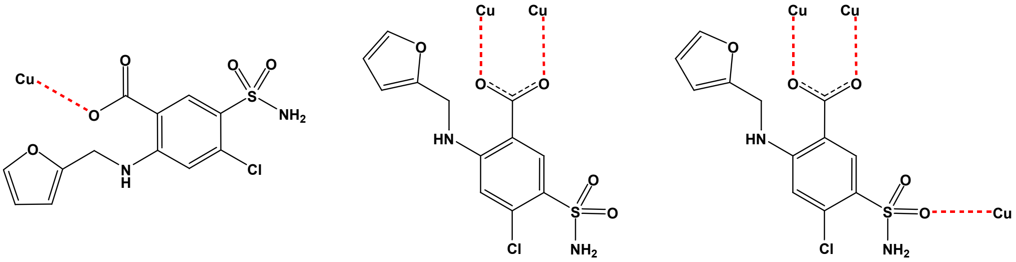


**Figure 1**. Coordination modes of furosemide anion, observed in our study [4].

**References:**
[1] Groom, C.R., Bruno, I.J., Lightfoot, M.P. & Ward, S.C. (2016) *Acta Crystallogr.*, Sect. B 72, 171–179.
[2] Podjed, N., Uranjek, Z., Cerc Korošec, R., Hrast Rambaher, M., Golob, M. & Modec, B. (2025) *New J. Chem.* 49, 9113–9122.
[3] Bontchev, P., Kadum, H., Gochev, G., Evtimova, B., Macicek, J. & Nachev, C. (1992) *Polyhedron* 11, 1973–1980.
[4] Podjed Rihtaršič, N. & Modec, B. (2026) *Inorg. Chem. Commun.* 184, 115916.

**Acknowledgement**
The financial support from the Slovenian Research and Innovation Agency (Research Core Funding grant P1-0134) is gratefully acknowledged. The authors acknowledge the support of the Centre for Research Infrastructure at the University of Ljubljana, Faculty of Chemistry and Chemical Technology, which is part of the Network of Research and Infrastructural Centres UL (MRIC UL) and is financially supported by the Slovenian Research and Innovation Agency (Infrastructure program no. I0-0022). The authors would also like to thank Maša Pirnat for checking the reproducibility of the syntheses.

# CRYSTAL STRUCTURES OF COPPER(II) COMPLEXES WITH HALOGENATED PYRIDINES

Matjaž Kristl[1], Brina Dojer[2], Ana Koleša[1], Amalija Golobič[3]

[1] University of Maribor, Faculty of Chemistry and Chemical Engineering, Smetanova 17, 2000 Maribor, Slovenia; *E-mail:* matjaz.kristl@um.si

[2] University of Maribor, Faculty of Natural Sciences and Mathematics, Koroška cesta 160, 2000 Maribor, Slovenia

[3]University of Ljubljana, Faculty of Chemistry and Chemical Technology, Večna pot 113, 1000 Ljubljana, Slovenia

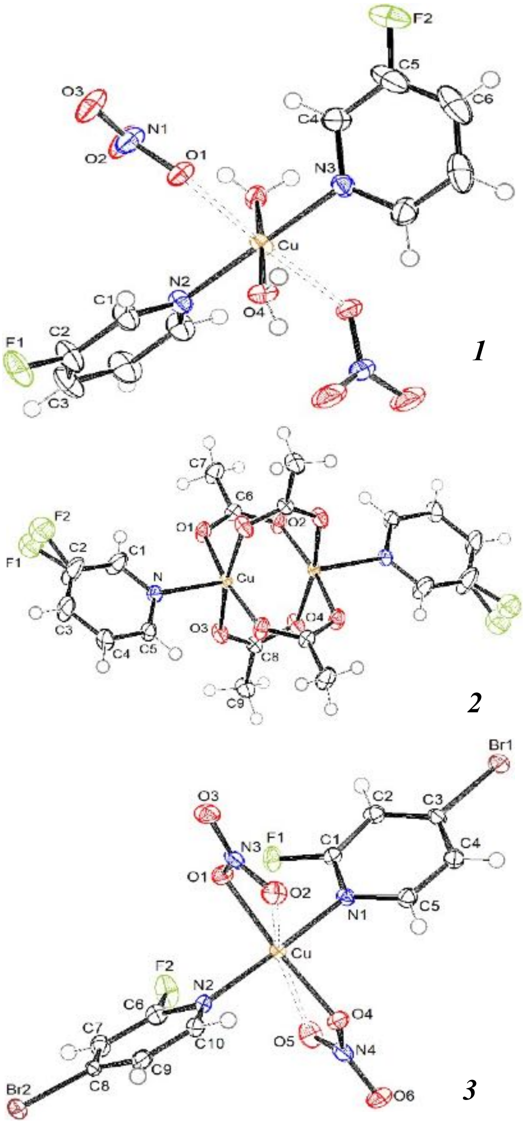
Despite increasing interest in their structural and magnetic properties, only a limited number of copper complexes containing fluorinated pyridine ligands have been structurally characterized. The preparation and characterization of novel copper coordination compounds with 3-fluoropyridine (fpy) and 4-bromo-2-fluoropyridine (fbpy) are reported.

The mononuclear coordination compound **1** with the formula $[Cu(H_2O)_2(fpy)_2(NO_3)_2]$ is characterized by a 4+2-coordinated Cu(II) ion octahedrally surrounded by two fpy ligands coordinated via the ring nitrogen atom, two solvent water molecules, and two monodentate nitrate ions. Copper atom lies on the two-fold axis. Both fluorine atoms are symmetry-disordered over two sites with 50 % occupancy.

Compound **2** with the formula $[Cu_2(\mu\text{-}Ac)_4(fpy)_2]$ forms a *paddle-wheel* dimeric centrosymmetric structure with four bridging acetate ions and two fpy ligands coordinated *via* the ring nitrogen atom. The coordination polyhedron of Cu(II) ion is slightly distorted square pyramid. The apical Cu-N distance 2.1856(1) Å is significantly longer than Cu-O distances (average 1.970(1) Å). The Cu...Cu separation within a molecule is 2.6151(1) Å. Also in this structure the fluorine atom is disordered over two sites with the occupancy of 0.553(1):0.447(1).

Compound **3** is mononuclear complex molecule, where Cu(II) is surrounded with two fbpy ligands, trans coordinated via the ring nitrogen atom and by two anisobidentate nitrate ions. Crystal structure is stabilised by the C−Br···O−N halogen bonds, with contact distances 3.043(2) and 3.192(2) Å for Br1…O3 and Br2…O5, respectively. Angle C−Br···O is 169.6(1) and 161.7(1)° for the first and second halogen bond, respectively.

All of the products were further characterized by FTIR studies, thermal analysis and magnetic measurements.



*ORTEP drawings with labelling of non-H atoms in the asymmetric unit*

**Acknowledgement**

Financial support of the Slovenian Research Agency is gratefully acknowledged (Grants P1-0175 and P2-0006)

# Coordination of $XeF_2$ to the $BrF_2^+$ Cation

Matic Lozinšek,[1] Erik Uran,[1] Miha Virant,[1] Mirela Dragomir,[2] and Kristian Radan[1]

[1] Extreme Conditions Chemistry Laboratory, Jožef Stefan Institute, Jamova cesta 39, 1000 Ljubljana, Slovenia; *E-mail*: matic.lozinsek@ijs.si
[2] Electronic Ceramics Department, Jožef Stefan Institute, Jamova cesta 39, 1000 Ljubljana, Slovenia.

Coordination compounds of the type $[M^{n+}(XeF_2)_p(AF_6^-)_n]$, in which $XeF_2$ is coordinated to a "naked" metal cation formed in reactions with metal salts of weakly coordinating anions, represent a large and structurally diverse family of noble-gas compounds [1]. In contrast, complexes in which $XeF_2$ is coordinated to a non-metal cationic center are much scarcer and are currently limited to the fluoridooxido cation $BrOF_2^+$ [2] and the oxido cations $ClO_2^+$ [3] and $BrO_2^+$ [4]. The recently reported coordination of $XeF_2$ to fluoridometal cations in the adduct cations $[PtF_3(XeF_2)_3]^+$ and $[PdF_3(XeF_2)_3]^+$ opens a new avenue for the expansion of the coordination chemistry of noble-gas fluorides [5].

In this work, the coordination of $XeF_2$ to the non-metal fluorido cation $BrF_2^+$ was explored. The $BrF_2^+$ cation features two σ-holes located on the bromine atom along the extensions of the Br−F bonds. Reactions carried out in anhydrous HF yielded the halogen-bonded complexes $[BrF_2(XeF_2)][AsF_6]$ and $[BrF_2(XeF_2)_2][AsF_6]$, which were characterized by low-temperature single-crystal X-ray diffraction and Raman spectroscopy, and further investigated by quantum-chemical calculations. These complexes constitute the first examples of $XeF_2$ coordination to a halogen(III) center.

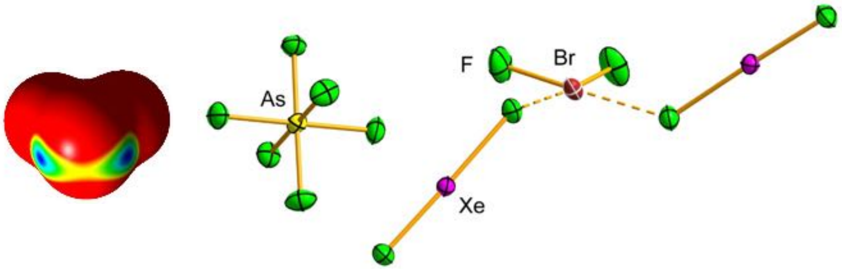


**Figure**: Molecular electrostatic potential surface of the $BrF_2^+$ cation (top 10% of positive MEP values) and the crystal structure of $[BrF_2(XeF_2)_2][AsF_6]$ (50% probability ellipsoids).

## References:

[1] Tramšek, M. & Žemva, B. (2006). *Acta Chim. Slov.* 53, 105–116.
[2] Brock, D.S., Casalis de Pury, J.J., Mercier, H.P.A., Schrobilgen, G.J. & Silvi B. (2010). *Inorg. Chem.* 49, 6673–6689.
[3] Bortolus, M.R., Ellwanger, M., Haner, J. & Schrobilgen, G.J. (2021). *J. Fluorine Chem.* 250, 109814.
[4] Bortolus, M.R., LaChapelle, G.J., Mercier, H.P.A., Haner, J. & Schrobilgen, G.J. (2023). *Inorg. Chem.* 62, 8761−8771.
[5] Motaln, K., Virant, M. & Lozinšek, M. (2026). *Inorg. Chem.* 65, 5668–5677.

**Acknowledgement**

The financial support from the Slovenian Research and Innovation Agency (ARIS) (Grant J1-60022) and the European Research Council (ERC) under the European Union's Horizon 2020 Research and Innovation Programme (Starting Grant 950625) is gratefully acknowledged.

# VARIABLE TEMPERATURE DIFFRACTION AND POLYMORPH SCREENING WITH THE XTALAB SYNERGY-ED

Emilia Buchsteiner,[1] Khai-Nghi Truong,[1] Robert Bücker,[1,2] Christian Göb,[3] Christian Schürmann,[1] Jakub Wojciechowski,[1] Michal Jasnowski,[4] Mathias Meyer,[4] Fraser White[1,2]

[1] Rigaku Europe SE, Neu-Isenburg, Germany; *E-mail:* emilia.buchsteiner@rigaku.com
[2] Rigaku Corporation, Tokyo, Japan
[3] Rigaku Asia Pacific PTE LTD, Singapore, Singapore
[4] Rigaku Polska, Wroclaw, Poland

Since its launch in 2021, the XtaLAB Synergy-ED has produced many structures, with more than 100 peer-reviewed publications and over 500 unique structures from Rigaku labs alone. While many of these structures were analysed at ambient temperature, the availability of low-temperature techniques, particularly cryo-transfer, have proven invaluable for the preservation of sensitive samples both those sensitive to vacuum and those sensitive to electron beam damage. Additionally, the instrument's enhanced automation capabilities, such as unattended measurement queues and automatic unit cell clustering, have opened new avenues for polymorph screening.

The XtaLAB Synergy-ED's compatibility with existing TEM instrument holders provides structural scientists with the ability to conduct various experiments traditionally performed in X-ray crystallography. Cryo-transfer and air-free transfer specimen holders protect samples prior to vacuum introduction [1], enabling the study of solvates and other vacuum- or air-sensitive species, and allowing for the investigation of phase behaviour. Examples of crucial findings made possible by cryo-transfer will be discussed.

Furthermore, a MEMS biasing/heating holder allows for the increase in temperature, facilitating the exploration of polymorphism of structures such as porous materials. Recent studies utilizing single-crystal data from electron diffraction on a MOF system, Cu(ta)$_2$ (Hta=1H-1,2,3-triazole), have yielded significant insights at both room temperature and 200°C. These findings are compared with previous studies by Grzywa et al. [2] using SC-XRD and PXRD, demonstrating the instrument's capability in polymorphism research.

**References:**

[1] K.-N. Truong, S. Ito et al. (2023). *Symmetry*, 15(8), 1555.
[2] M. Grzywa, D. Denysenkoet al. (2012*). Dalton Transactions*, 14, 4239.

# TAILORING THERMOSALIENT PHASE TRANSITIONS BY MOLECULAR ALLOYING

Željko Skoko,[1] Teodoro Klaser[1], Oskar Stepančić[1,2], Jasminka Popović[3], Jana Pisk[4], Luka Pavić[3], Igor Picek[5], Dubravka Matković-Čalogović[4]

[1] Department of Physics, Faculty of Science, University of Zagreb, Bijenička 32, Zagreb, Croatia; E-mail: zskoko@phy.hr

[2] Department of Physics, Division of Synchrotron Radiation Research, Lund University, Sweden

[3] Ruđer Bošković Institute, Bijenička 54, Zagreb, Croatia

[4] Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102A, Zagreb, Croatia

[5] Department of Chemistry and Biochemistry, School of Medicine, University of Zagreb, Šalata 3, Zagreb, Croatia

Thermosalient molecular crystals convert thermal energy into rapid mechanical motion through a structural phase transition. However, their practical use is limited by the fixed transition temperature of a given compound. Here, we demonstrate that molecular alloying can be used to tune the thermosalient response.

Molecular alloys of 1,2,4,5-tetrabromobenzene and 1,2,4,5-tetrachlorobenzene were prepared in different compositions and studied by DSC, hot-stage microscopy, single-crystal X-ray diffraction and variable-temperature powder X-ray diffraction. The formation of solid solutions was confirmed by the linear variation of unit-cell parameters with composition. Thermosalient behaviour was observed for alloys containing more than 90 wt% tetrabromobenzene.

The phase-transition temperature increases almost linearly with tetrabromobenzene content, from 30.13 °C for 92 wt% tetrabromobenzene to 45.33 °C for the pure compound (Figure 1). The alloys undergo the same β-to-γ transformation as pure tetrabromobenzene and retain large anisotropic thermal expansion. These results show that molecular alloying enables predictable control of thermosalient phase transitions and offers a simple strategy for designing thermally triggered molecular actuators and sensors.

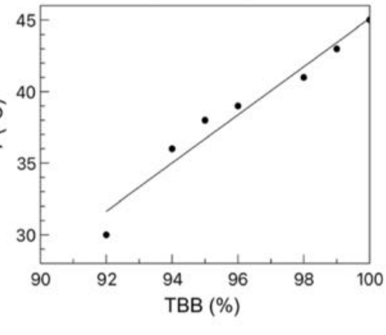


**Figure 1.** Linear dependence of the thermosalient phase-transition temperature on TBB content.

**References:**

[1] Klaser, T., Stepančić, O., Popović, J., Pisk, J., Pavić, L., Picek, I., Matković-Čalogović, D. & Skoko, Ž. (2025). *J. Mater. Chem. C*. **13**, 6539–6546.

[2] Nauha, E., Naumov, P. & Lusi, M. (2016). *CrystEngComm*. **18**, 4699–4703.

**Acknowledgement**

The authors greatly appreciate support of the European Union—NextGenerationEU through the National Recovery and Resilience Plan 2021–2026 institutional grant from University of Zagreb Faculty of Science “Encouraging competitive projects and top-tier scientific publications at the Department of Physics (ProPubFO)—ProPuBFO-1.1.3.2026”.

# HEAT IT, PUSH IT, WATCH IT MOVE: STRUCTURAL ORIGINS OF CRYSTAL DYNAMICS

Mateja Pisačić,[1] Lea Čolakić,[2] Marijana Đaković[1]

[1] University of Zagreb, Faculty of Science, Department of Chemistry, Horvatovac 102a, 10000 Zagreb, Croatia; *E-mail:* mpisacic@chem.pmf.hr
[2] Ruđer Bošković Institute, Division of Physical Chemistry, Bijenička cesta 54, 10000 Zagreb, Croatia

The remarkable ability of living organisms to adapt with dynamic movements to environmental changes, such as fluctuations in temperature and moisture, exposure to light and mechanical forces, has long been, and still is, a profound source of inspiration for scientists in the development and engineering of materials. Reproducing a perfect coexistence of mechanical properties with other functional features naturally found in biological systems, however, remains a significant challenge, particularly with respect to the precise control and deliberate fine-tuning of both structural organization and material features. With the advent of crystal engineering and the relatively recent discovery of stimuli-responsive crystalline solids, an entirely new playground in materials design has been revealed.[1−5] This rapidly evolving field offers an expansive landscape of structural and functional possibilities by harnessing the long-range order to direct and control synthetic outcomes, and consequently, tune functional properties. The number of reported crystalline materials exhibiting dynamic responses to external stimuli such as heat, light, or mechanical force has increased dramatically in recent years; nevertheless, a comprehensive structural understanding of the origins of their mechanical behavior remains unclear.

In this work, we investigated the relationship between the mechanical behavior and structural characteristics of crystals of one-dimensional cadmium(II) coordination polymer incorporating bromide and 4-pyridineoxime ligands. Our study demonstrates that the dynamic behaviour of these crystals can be actuated both thermally and by direct application of mechanical force. Notably, the mechanically induced response exhibits pronounced directionality, revealing a two-dimensional anisotropic elastic behavior that arises from distinct structural arrangements in the crystal along different directions of force application. In contrast, thermal stimulation triggers abrupt macroscopic crystal motions associated with a phase transition involving extensive structural reorganization at both the molecular and supramolecular levels. These findings advance the fundamental understanding of structure–mechanical property relationships in dynamic crystalline materials and may contribute to the rational design of emerging smart materials and crystal-based actuators, sensors, and adaptive mechanical technologies.

## References:

[1] Award, W. M. et al. (2023) *Chem. Soc. Rev*. 52, 3098.
[2] Đaković, M., et al.  (2018) *Angew. Chem. Int. Ed*. 57, 14801.
[3] Pisačić, M., et al. (2021) *Chem. Mater*. 33, 3660.
[4] Pisačić, M., et al. (2022) *Chem. Mater*. 34, 2439.
[5] Đaković, M.; et al. (2025) *J. Am. Chem. Soc*. 147, 22219.

**Acknowledgement**

This research was supported by the European Union – NextGenerationEU through the National Recovery and Resilience Plan 2021−2026. via Institutional grants of the University of Zagreb Faculty of Science (NextGenChem and CryoLab) and the Croatian Science Foundation under the project IP-2019-04-1242.

# DYNAMIC RESPONSES OF CADMIUM(II) COORDINATION POLYMER CRYSTAL TO MECHANICAL AND THERMAL STIMULI

Božena Tokić,[1] Mateja Pisačić,[1] Ivona Prša, Marijana Đaković [1]

[1] University of Zagreb, Faculty of Science, Department of Chemistry, Horvatovac 102a, 10000 Zagreb, Croatia; *E-mail:* bozena.tokic@chem.pmf.hr

Dynamic molecular crystals represent an intriguing class of crystalline materials that possess the remarkable ability to respond to a variety of external stimuli. These stimuli can include mechanical forces, heat, light, and pressure, leading to a range of potential applications and functionalities [1]. The unique reactions of these materials are often shaped by their complex structural characteristics and the subtle interplay of intermolecular forces at work within the crystal lattice [2-6]. Consequently, unravelling the intricate relationships between the structures of these materials and their resulting properties poses a significant challenge, but it is essential for advancing the development of new, functional crystalline materials that can meet specific technological needs [1-2].

To enhance our understanding of the relationship between the structure and macroscopic properties of crystals, particularly their responses to applied mechanical force, we examine coordination polymer crystals of cadmium(II) bromide with dibromopyridine, specifically $[\mathrm{CdBr_2(3,5\text{-}diBrpy)_2}]_n$. The compound crystallises in a tetragonal $P\bar{4}b2$ space group and demonstrates the targeted one-dimensional propagation of the polymeric backbone via double halogen bridging between neighbouring metal cations, further supported by two dibromopyridine ligands to complete the expected octahedral coordination. Although the ligands are rotated about the Cd–N bond, thereby closing the 70 ° angle between the pyridine-ring plane and the plane running along the polymeric backbone, symmetrically bifurcated C–H···Br(Cd) hydrogen bonds (between the pyridine and bromide ligands from two adjacent polymeric chains) propagate throughout the crystal structure. The crystals exhibited an elongated, needle-like morphology, which is essential for exploring mechanoflexible properties. Macroscopic crystal properties were evaluated using modified three-point bending and tensile tests. However, thermal characterisation of the material revealed an unexpected response to thermal stimulation, which was systematically examined using a combination of thermal and structural methods.

## References:

[1] Kusumoto, S. et al. (2023) Chem. Soc. Rev. 475, 214890.
[2] Wang, Z. et al. (2024) JACS Au 4, 279.
[3] Đaković, M., et al. (2018) Angew. Chem. Int. Ed. 57, 14801.
[4] Pisačić, M., et al. (2021) Chem. Mater. 33, 3660.
[5] Mišura, O., et al. (2022) Cryst Growth & Des. 34, 2439.
[6] Đaković, M., et al. (2025) J. Am. Chem. Soc. 147, 22219.

## Acknowledgement

This research was supported by the European Union – NextGenerationEU through the National Recovery and Resilience Plan 2021−2026. via Institutional grants of the University of Zagreb Faculty of Science (NextGenChem and CryoLab) and the Croatian Science Foundation under the project IP-2019-04-1242.

# RUTHENIUM(II) COMPLEXES WITH NOVEL PYRITHIONE LIGANDS

Katarina Lucija Lakota,[1] Uroš Rapuš,[1] Benjamin Poljanc,[1] Iztok Turel[1]

[1] University of Ljubljana, Faculty of Chemistry and Chemical Technology, Večna pot 113, 1000 Ljubljana, Slovenia; *E-mail*: iztok.turel@fkkt.uni-lj.si

Pyrithiones are organosulphur aromatic heterocyclic compounds containing a cyclic thiohydroxamate functional group. Pyrithiones and their analogues form stable metal complexes. In most cases, they act as bidentate ligands, binding to the metal through oxygen and sulphur atoms [1]. Pyrithiones and their metal complexes are potential antimicrobial, antitumour, and antiviral agents [2,3]. In most biologically active compounds, the relationship between structure and activity has been investigated. Functional groups are important for biological activity, particularly strong electron-donating or electron-accepting groups. Based on these considerations, we synthesised analogues of pyrithiones with strong electron-withdrawing groups and their corresponding metal complexes.

We prepared novel pyrithione ligands by optimising established synthetic procedures [4,5]. Using these ligands, we obtained complexes with various transition metals, most notably the ($\eta^6$-*p*-cymene)Ru(II) compounds [6]. We successfully obtained single crystals of one complex and determined its structure by X-ray diffraction.

## References:

[1] Robinson, M. A. (1964). *J. Inorg. Nucl. Chem.* 26, 1277–1281.
[2] Kladnik, J.; Coverdale, J.P.C.; Kljun, J.; Burmeister, H.; Lippman, P.; Ellis, F.G.; Jones, A.M.; Ott, I.; Romero-Canelón, I.; Turel, I. (2021). *Cancers*. 13, 2493.
[3] Kladnik, J., Ristovski, S., Kljun, J., Defant, A., Mancini, I., Sepčić, K., & Turel, I. (2020). *Int. J. Mol. Sci.* 21(16), 5628.
[4] Caron, S., Nga, M. D., Sieser, J. (2000). *Tetrahedron Lett.* 41, 2299–2302.
[5] Matsueda, R., Walter, R. (1980). *Int. J. Pept. Protein Res.* 16(5), 392–401.
[6] Kladnik, J.; Burmeister, H.; Ott, I.; Romero-Canelon, I., Turel, I. (2019). *Chem. Eur. J.* 25(62), 14169–14182

### Acknowledgement

We are grateful for the financial support from the program grant P1-0175 of the Slovenian Research and Innovation Agency (ARIS). The authors also acknowledge the support of the Centre for Research Infrastructure at the University of Ljubljana, Faculty of Chemistry and Chemical Technology, which is part of the Network of Research and Infrastructural Centres UL (MRIC UL) and is financially supported by the Slovenian Research and Innovation Agency (ARIS; Infrastructure programme No. I0-0022) for the use of dual wavelength X-ray single crystal diffractometer Rigaku Oxford Diffraction XtaLAB Synergy-S with HyPix-Arc 100 detector.

# TUNING POLARONIC PATHWAYS IN VANADATE-PHOSPHATE GLASSES BY MIXED TRANSITION METAL OXIDE SUBSTITUTION

Marta Razum,[1] Luka Pavić,[1] Jana Pisk,[2] Damir Pajić,[3] Petr Mošner,[4] Ladislav Koudelka,[4] Ana Šantić[1]

[1] Division of Materials Chemistry, Ruđer Bošković Institute, Bijenička c. 54, Zagreb, Croatia; *E-mail*: mrazum@irb.hr
[2] Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102a, Zagreb, Croatia
[3] Department of Physics, Faculty of Science, University of Zagreb, Bijenička c. 32, Zagreb, Croatia
[4] Department of General and Inorganic Chemistry, Faculty of Chemical Technology, University of Pardubice, Studentská 95, 532 10 Pardubice 2, Czechia

The short-range structure of vanadate-phosphate glasses plays a key role in defining the distribution of redox-active transition-metal sites and the connectivity of polaronic hopping pathways. Introducing a second transition metal oxide provides a way to modify the local glass structure, redox equilibria, and charge transport mechanisms. Here, we study how $MoO_3$, $WO_3$, and $Fe_2O_3$ affect the structure and polaronic transport in $x$TMO-(60-$x$)$V_2O_5$-40$P_2O_5$ glasses.

Three series of glasses were prepared by melt quenching, with $x$ = 10-60 mol% for TMO = $MoO_3$ and $WO_3$, and $x$ = 10-45 mol% for TMO = $Fe_2O_3$. The amorphous nature of the prepared samples was confirmed by powder X-ray diffraction, while changes in the local glass network were studied by Raman spectroscopy through variations in the intensity of bands associated with specific structural units. Thermal properties were studied by differential thermal analysis, and electrical transport by impedance spectroscopy. The fraction of reduced TM ions was determined using SQUID magnetometry and, for Fe-containing glasses, also Mössbauer spectroscopy.

All systems show distinct electrical transport trends. In $MoO_3$-containing glasses, conductivity decreases continuously by more than three orders of magnitude with increasing Mo content, indicating a disruption of vanadium-based hopping pathways. In the $WO_3$ series, conductivity shows a pronounced minimum at 53 mol% of $WO_3$, whereas binary $WO_3$-$P_2O_5$ glass has a high conductivity value. This suggests that in the presence of vanadium ions, tungsten ions do not tend to cluster and do not contribute to polaron transport. In contrast, $Fe_2O_3$-containing glasses show a minimum at 27 mol% $Fe_2O_3$, followed by an increase due to the participation of Fe ions in conduction pathways.

This research shows that the electrical properties of TM phosphate glasses are affected not only by the total concentration of redox-active ions, but more importantly by their distribution, local structural environment, and connectivity of hopping pathways within the glass network.

**Acknowledgement**
This work is supported by the Croatian Science Foundation (CSF) under the ECLECTIC GLASS project IP-2025-02-7124.

# ORGANORUTHENIUM(II) COMPLEXES WITH PYRITHIONE AND LIGANDS CONTAINING GROUP V. DONOR ATOMS

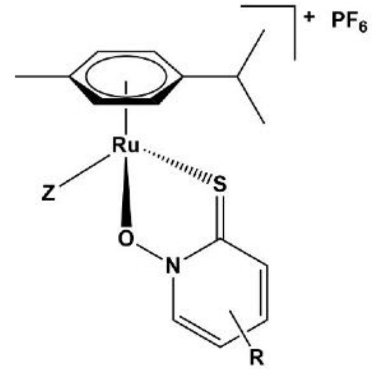
Uroš Rapuš,[1] Jakob Kljun[1], Iztok Turel[1]

[1] University of Ljubljana, Faculty of Chemistry and Chemical Technology, Večna pot 113, SI-1000 Ljubljana, Slovenia; *E-mail*: uros.rapus@fkkt.uni-lj.si

Ruthenium-based anticancer drugs have been investigated for several decades as alternatives to platinum-based chemotherapeutics. One of the more promising classes of ruthenium compounds is organoruthenium(II) complexes. The most promising representative of this class is the [dichlorido(*p*-cymene)(1,3,5-triaza-7-phosphaadamantane)ruthenium(II)] complex (RAPTA-C) [1]. While the pta ligand imparts unique properties to these complexes, several alternatives have been explored by many research groups, including ours [2].

In recent years, our research group has prepared various pyrithione analogues with different functional groups [3]. In addition, we have focused on introducing ligands containing group V. donor atoms into organoruthenium(II) complexes to influence their biological activity through their physico-chemical properties [4].

We obtained single crystals of several organoruthenium(II) complexes with fluorine-containing pyrithionato ligands and ligands with group V. donor atoms. The crystals were of sufficient quality, and we determined their structures using X-ray diffraction. Furthermore, the synthesised compounds were fully physico-chemically characterised by NMR spectroscopy, mass spectrometry, IR and UV-Vis spectroscopy, and their purity was confirmed by elemental analysis.



**Z = ligands with group V. donor atom**
**R = F containing functional groups**

**Figure 1**: General scheme of synthesised complexes.

## References:

[1] Coverdale, J. P. C., Laroiya-McCarron, T., Romero-Canelón, I., *Inorganics*, 7, 2019, 31.

[2] Kljun, J., Rebernik, M., Balsa, L.M., Kladnik, J., Rapuš, U., Trobec, T., Sepčić, K., Frangež, R., León, I.E., Turel, I., *Molecules*, 28, 2023, 2499.

[3] Kladnik, J., Kljun, J., Burmeister, H., Ott, I., Romero-Canelón, I., Turel, I., *Chem. Eur. J.*, 25, 2019, 14169–14182.

[4] Alshammari, M. M., Rapuš, U., Kljun, J., Turel, I., Romero-Canelón, I., manuscript in preparation

### Acknowledgement

We are grateful for the financial support of the Slovenian Research and Innovation Agency (ARIS): a Junior Researcher Grant to Uroš Rapuš and grant P1-0175. The authors also acknowledge the support of the Centre for Research Infrastructure at the Faculty of Chemistry and Chemical Technology, which is part of the Network of Research and Infrastructural Centres UL (MRIC UL) and is also financially supported by ARIS; Infrastructure programme No. I0-0022) for the use of the Supernova diffractometer.

# LINKING SYNTHESIS TO CRYSTAL STRUCTURE IN $LaCoO_3$: A DETAILED CRYSTALLOGRAPHIC INVESTIGATION

Dora Balen,[1] Martina Vrankić,[1] Jasminka Popović,[1] Vendula Bednaříková,[2] Serhii Tkachenko,[2] Michaela Remešová[2], Ladislav Čelko[2]

[1] Ruđer Bošković Institute, Bijenička 54, 10000 Zagreb, Croatia; *E-mail*: dobalen@irb.hr

[2] Central European Institute of Technology, Brno University of Technology, High-Performance Materials and Coatings for Industry Research Group, 61200 Brno, Czechia

Lanthanum cobaltite ($LaCoO_3$, LCO) is a rare-earth $ABO_3$ perovskite oxide whose structural complexity and sensitivity to synthesis conditions make it a model system for studying structure formation in functional oxides [1-4]. Variations in synthesis routes produce LCO with different crystallographic characteristics, often leading to subtle but significant changes in lattice distortions, oxygen sublattice configuration, and phase purity. Achieving high phase purity and precise structural control is therefore essential for reliable crystallographic analysis and for understanding the intrinsic structural degrees of freedom in this system. Despite extensive studies, the relationship between synthesis parameters and the resulting crystallographic framework, particularly at the level of local distortions and oxygen positions, remains insufficiently resolved [5,6].

In this work, we systematically investigate the evolution of the LCO crystal structure as a function of synthesis conditions. Morphology-tuned nanosized LCO powders were prepared by controlled variation of synthesis parameters followed by post-treatment. Detailed crystallographic analysis was carried out through (micro)structural refinement of powder X-ray diffraction data, with particular emphasis on key structural descriptors such as the oxygen positional parameter x(O) and the Co–O–Co bond angle. These parameters provide direct insight into octahedral tilting and lattice distortions within the perovskite framework. We demonstrate that controlled modification of synthesis conditions enables systematic tuning of these crystallographic features, establishing a clear link between preparation pathways and the resulting crystal structure of LCO.

## References:

[1] Liu, Y. et al, *J. Alloy. Compd.* (2009). 488, 204-207.
[2] Jayapandi, S. et al, *J. Sustain. Technol. Mater.* (2025). 43, e01225.
[3] Orlov, Y.S. et al, *Dalton Trans.* (2025). 54, 4530-4541.
[4] Vrankić, M. et al. *J. Alloy. Compd.* 1065 (2026) 188107.
[5] Ivanova, S. et al, *J. Alloy. Compd.* (2009). 480, 279-285.
[6] Taguchi, H. et al, *Mater. Res. Bull.* (2002). 37, 69-76.

## Acknowledgement

This work was supported by the Czech Science Foundation under project number 25-17855K and the Croatian Science Foundation under the CePrECiPe Project No. IPCZ-2024-04-8873.

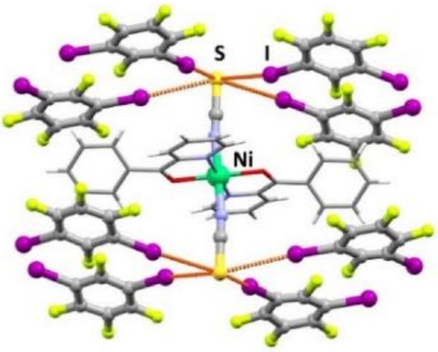
# METAL-ORGANIC HALOGEN-BONDED COCRYSTALS BASED ON THE ROBUST I···SCN SYNTHON

Lidija Posavec[1] and Dominik Cinčić[1]

[1] Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102a, Zagreb, Croatia; *E-mail:* dominik@chem.pmf.hr

Over the past three decades, studies on halogen-bonded cocrystals have mostly focused on systems with perfluorinated compounds as halogen-bond donors and a variety of organic and metal-organic acceptors involving nitrogen or oxygen atoms [1,2]. In addition, neutral metal-organic compounds containing halide or pseudohalide ligands as halogen-bond acceptors have proven to be reliable building blocks in the design and synthesis of cocrystals [3,4]. A search of the Cambridge Structural Database (CSD) [4] revealed that, for the halogen-bonding motif I···Cl–M (M = any transition metal), there are 38 entries corresponding to cocrystals of coordination compounds and perhalogenated benzenes, whereas for the motif I···SCN–M there are 15 entries,

This presentation will provide an overview of some of our recent work [5] on cocrystals based on the robust I···SCN synthon, containing $\mathrm{Ni(L^{I})_4(NCS)_2}$, $\mathrm{Ni(L^{II})_2(NCS)_2}$, and $\mathrm{Ni(L^{III})(NCS)_2}$ complexes ($\mathrm{L^{I}}$ = 4-methylpyridine or pyridine; $\mathrm{L^{II}}$ = 2,2′-bipyridine or 2-benzoylpyridine; $\mathrm{L^{III}}$ = 2-aminoethylpyrrolidine) and perfluorinated iodobenzenes. The presentation will outline: i) the evaluation of the halogen-bonding propensity of the isothiocyanate ligand, whose pendant sulfur atom enables the simultaneous formation of multiple halogen bonds, functioning either as a bi-, tri- or tetrafurcated halogen-bond acceptor; ii) the influence of cocrystallization on the *cis–trans* isomerization of the metal-organic subunit, including the possibility of directing cocrystal synthesis toward a specific isomer; and iii) the development of a general strategy for designing higher-order metal-organic halogen-bonded cocrystals based exclusively on I···S halogen bonds.



**References:**

[1] Cavallo, G., Metrangolo, P., Milani, R., Pilati, T., Priimagi, A., Resnati, G. & Terraneo, G. (2016) *Chem. Rev.*, 116, 2478–2601.

[2] Nemec, V., Lisac, K., Bedeković, N., Fotović, L., Stilinović, V. & Cinčić, D. (2021) *CrystEngComm*, 23, 3063–3083.

[3] Lisac, K. & Cinčić, D. (2018) *CrystEngComm*,20, 5955–5963.

[4] Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016) *Acta Crystallogr., Sect. B: Struct. Sci., Cryst. Eng. Mater.*, 72, 171–179.

[5] Posavec, L. & Cinčić, D. (2014) *Cryst. Growth Des.*, 24, 7514–7523.

**Acknowledgement**

This research was supported by the Croatian Science Foundation under the project IP-2019-04-1868 and IP-2025-02-6539.

# HALOGEN-BONDED COCRYSTALS OF M(NCS)$_2$(3-Xpy)$_4$ COORDINATION COMPOUNDS (M = Co, Ni, Fe, Mn; X = Cl, Br, I)

Tom Kovačić,[1] Vinko Nemec[1] and Dominik Cinčić[1]

[1] Department of Chemistry, Faculty of Science, University of Zagreb, HR-10000 Zagreb, Croatia;
*E-mail:* vnemec.chem@pmf.hr

Although less studied than halide ligands in halogen-bonded metal–organic compounds [1], isothiocyanate has proven to be a versatile halogen bond acceptor [2]. In this study we further evaluate its potential and additionally demonstrate how halogen atoms at the periphery of coordination compounds influence halogen-bonded cocrystal structures. To this end, we prepared twelve octahedral coordination compounds (M-X) of M(NCS)$_2$(3-Xpyridine)$_4$ type (M = Co, Ni, Fe, Mn; X = Cl, Br, I) and cocrystallized them with the halogen bond donor 1,4-diiodotetrafluorobenzene (**14tfib**). Characterization of (M-X)(**14tfib**)$_2$ cocrystals obtained by liquid-assisted grinding and recrystallization from solution was performed using powder and single crystal X-ray diffraction. Structural analysis of all cocrystals revealed double chains formed by I···S halogen bonds between **14tfib** and isothiocyanate ligands. In (M-I)(**14tfib**)$_2$, iodine atoms from 3-iodopyridine ligands emerged as halogen bond donors, forming weaker I···S halogen bonds between chains. In contrast, halogen-bonded chains in (M-Cl)(**14tfib**)$_2$ and (M-Br)(**14tfib**)$_2$ are connected via other non-covalent interactions. Beyond confirming the strong halogen-bonding propensity of isothiocyanate sulfur, this study demonstrates the halogen-bond donating ability of peripheral iodine atoms and shows that the metal center in (M-X)(**14tfib**)$_2$ cocrystals has no significant influence on the key features of the supramolecular architecture.

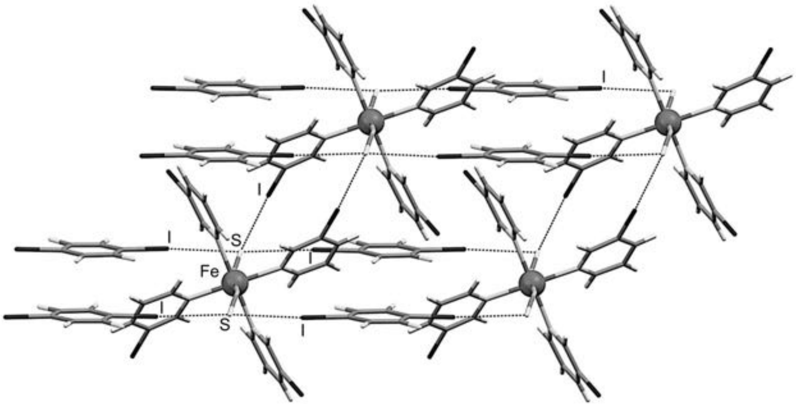


**Figure 1.** Halogen bonding in (Fe-I)(**14tfib**)$_2$

## References:

[1] Nemec, V., Lisac, K., Bedeković, N., Fotović, L., Stilinović, V. & Cinčić, D. (2021). *CrystEngComm*. 23, 3063–3083.
[2] Posavec, L. & Cinčić, D. (2024). *Cryst. Growth Des*. 24, 7514–7523.

### Acknowledgement

This research was funded by the Croatian Science Foundation under the research projects IP-2019-04-1868 and IP-2025-02-6539, and supported by the European Union – NextGenerationEU through the National Recovery and Resilience Plan 2021−2026. via Institutional grants of the University of Zagreb Faculty of Science (NextGenChem).

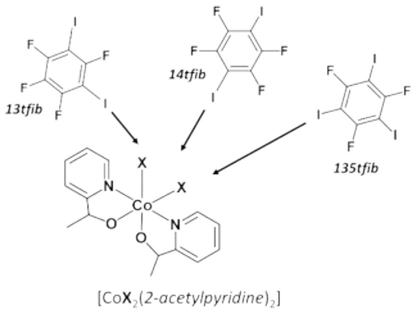
# COMPARISON OF CHLORIDE AND ISOTHIOCYANATE LIGANDS (X) AS HALOGEN BOND ACCEPTORS IN COCRYSTALS BASED ON [CO(X)$_2$(2-ACETYLPYRIDINE)$_2$] COMPLEXES

Mladen Borovina[1], Dominik Cinčić[1]

[1] Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102a, 10000 Zagreb, Croatia; *E-mail:* mborovina@chem.pmf.hr

Halogen bonds have proven to be an important tool in supramolecular chemistry and cocrystal synthesis, with perflourinated iodoarenes emerging as reliable good halogen bond donors.[1,2] Coordination compounds of transition metals containing halide or pseudohalide ligands are promising halogen bond acceptors. Due to their linear geometry and larger size, pseudohalide ligands such as thiocyanate provide greater accessibility of the acceptor site compared to halides, which may enable the formation of more complex supramolecular architectures through interactions with multiple halogen-bond donors.[3]

In this work, we prepared the octahedral coordination compound [Co(NCS)$_2$(2-acetylpyridine)$_2$] and cocrystallized it with halogen bond donors 1,3-diiodotetrafluorobenzene (**13tfib**), 1,4-diiodotetrafluorobenzene (**14tfib**), and 1,3,5-triiodotrifluorobenzene (**135tfib**) using both mechanochemical and solution-based cocrystallization methods. Our goal was to investigate the potential of the isothiocyanate ligand as a halogen-bond acceptor and to compare the obtained results with those from a previous study involving cocrystals of the analogous cobalt(II) coordination compound with chloride ligands, [CoCl$_2$(2-acetylpyridine)$_2$].[4] Three cocrystals with different acceptor:donor stoichiometries were successfully obtained: 1:1 with **13tfib**, 1:3 with **14tfib**, and 1:2 with **135tfib**, and were characterised by powder and single crystal X-ray diffraction. In all cocrystals, I···SNC-Co halogen bonds were observed, with the sulphur atoms acting as bifurcated halogen bond acceptors.



| acceptor : donor stoichiometries | | | |
|---|---|---|---|
| X | 13tfib | 14tfib | 135tfib |
| Cl⁻ | 1:2 | 1:1 | 1:2 |
| SCN⁻ | 1:1 | 1:3 | 1:2 |

## References:

[1] Walsh, R.B., Padgett, C. W., Metrangolo, P., Resnati, G., Hanks, T. W., Pennington, W. T. (2001). *Cryst. Growth Des.* 2, 165–175.

[2] Cavallo, G., Metrangolo, P., Milani, R., Pilati, T., Priimagi, A., Resnati, G., Terraneo, G. (2016). *Chem. Rev.* 4, 2478–2601.

[3] L. Posavec, D. Cinčić (2024). *Cryst. Growth Des.* 24, 7514–7523.

[4] K. Lisac, *Metal-Organic CoCl2L2 Units As Halogen Bond Acceptors In Cocrystals With Perhalogenated Compounds*, doctoral thesis, Faculty of Science, University of Zagreb.

**Acknowledgement**
This Work was funded by the Croatian-Science Foundation (IP-2025-02-6539) and supported by the European Union – NextGenerationEU through the National Recovery and Resilience Plan 2021−2026. via Institutional grants of the University of Zagreb Faculty of Science (NextGenChem).

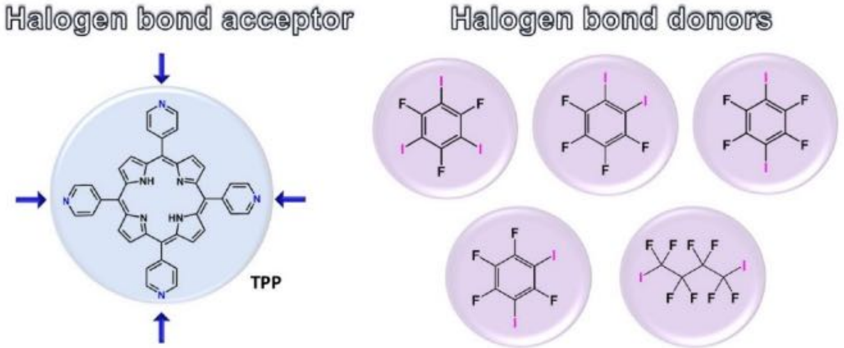
# TETRAKIS(4-PYRIDYL)PORPHYRIN AS A BUILDING BLOCK IN HALOGEN-BONDED COCRYSTALS

Lidija Posavec[1], Filip Kučas[1], Ivana Biljan[1], Dominik Cinčić[1]

[1] Department of Chemistry, Faculty of Science, University of Zagreb, Zagreb, Croatia; E-mail: lposavec@chem.pmf.hr

The development of porphyrin-based framework solids via metal coordination, hydrogen bonding, and $\pi$–$\pi$ stacking interactions has been extensively investigated over the past three decades.[1,2] In contrast, multicomponent assemblies involving porphyrin building blocks, such as cocrystals or salts, remain underexplored.[3] Porphyrins are particularly attractive supramolecular building blocks due to their rigid molecular framework, chemical stability, and readily accessible functionalization sites, which enable significant structural diversity. Strategic functionalization of porphyrins allows precise control over intermolecular connectivity, thereby directing the architecture and stability of the resulting supramolecular assemblies.

In this study, a porphyrin derivative, tetrakis(4-pyridyl)porphyrin (**TPP**), was employed as a building block for the construction of halogen-bonded cocrystals. The building unit contains four pyridyl rings with nitrogen atoms that can act as halogen-bond acceptors, enabling the design of a rigid tetratopic acceptor capable of forming complex halogen-bonded architectures. To investigate the supramolecular behavior of **TPP**, cocrystallization experiments with various halogen bond donor molecules were performed using both solution-based methods and mechanochemical synthesis. The obtained cocrystals were characterized by single-crystal and powder X-ray diffraction. Structure analysis revealed that the dominant interactions in the obtained cocrystals are I···N halogen bonds, formed with all pyridyl nitrogen atoms of **TPP**, resulting in two- and three-dimensional halogen-bonded networks. In three out of seven cocrystals, interesting supramolecular motifs are observed, where the pyridine nitrogen acts as a bifurcated acceptor, forming two halogen bonds with donor molecules.



**References:**

[1] Dar, U. A., Shahnawaz, M., Taneja, P., Dar, M. A. (2024). *ChemistrySelect*. 9, e202304817.
[2] Titi, H. M., Tripuramallu, B. K., Goldberg, I. (2016). *CrystEngComm*. 18, 3318–3339.
[3] Syssa-Magalé, J. L., Boubekeur, K., Leroy, Chamoreau, L. M., Favec, C., Schöllhorn B. (2016). *CrystEngComm.* 16**,** 10380–10384.

**Acknowledgement**

This research was supported by the Croatian Science Foundation under the project IP-2025-02-6539.

# OPERANDO XRD STUDY OF PRACTICAL BATTERY CONFIGURATIONS WITH THE DANOISE CELL

Sanja Burazer,[1] Hrvoje Tašner,[2] Grgur Mihalinec,[2] Signe S. Brummerstedt,[3] Josephine Dunker,[3] Dorthe. B. Ravnsbæk[3]

[1] Division of Materials Physics, Ruđer Bošković Institute, Zagreb, Croatia; *E-mail*: Sanja.Burazer@irb.hr
[2] Department of Electrochemistry, Faculty of Chemical Engineering and Technology, Zagreb, Croatia
[3] Department of Chemistry, Aarhus University, Aarhus, Denmark

Batteries are essential parts of modern technologies, from electric vehicles to portable devices, and the long life and reliability of batteries depend directly on understanding the mechanisms of their failure. Operando XRD is a technique that allows real-time monitoring of structural modifications during battery operation. It gives insight into the dynamic structural changes occurring during battery cycling, thus enabling a better understanding of the reasons for material degradation, including crystal lattice breakdown, phase formation and stress accumulation in the electrodes.[1]

Home-made 3D printed DANOISE cell in transmission mode was used for operando XRD measurements.[2] The results range from ex-situ XRD measurements of the graphite or NMC electrode in the DANOISE cell, without current applied, to operando XRD measurements in the half-cell, and measurements with coated electrode with the mentioned active materials. This is done to approach the industrial scale where samples are de-posited on the Cu or Al foil, respectively, and not pressed into the pellets.

The aim is to identify specific structural phenomena associated with battery failure, in order to improve the performance and stability of future battery materials and technologies and to compare the results from pellet and coated electrode. The primary focus lies on the crystallographic analysis of the operando XRD data with a sequential refinement in TOPAS. [3]

## References:

[1] Z. Wen et al. *Front. Energy Res*. (2018). 6, 66.

[2] M. Johansen et al. Batteries & Supercaps (2024). 7, e202400033J.

[3] G. W. Stinton and J. S. O. Evans*, J. Appl. Cryst*. (2007). 40, 87–95.

**Acknowledgement**

The authors greatly appreciate the support of the Ministry of Science, Education and Youth and the Croatian Science Foundation for funding this work. This work is funded by the European Union funds “National plan for Recovery and Resilience” under the number NPOO.C3.2.R3-I1.04.0187.

# MECHANOCHEMISTRY AS A ROUTE TO NOVEL SILVER(II) COMPOUNDS

Mirela Dragomir,[1] Matic Belak Vivod,[1] Matic Lozinšek,[2] and Graham King[3]

[1] Electronic Ceramics Department, Jožef Stefan Institute, Jamova cesta 39, 1000 Ljubljana, Slovenia; E-mail: mirela.dragomir@ijs.si

[2] Extreme Conditions Chemistry Laboratory, Jožef Stefan Institute, Jamova cesta 39, 1000 Ljubljana, Slovenia

[3] Canadian Light Source, 44 Innovation Blvd, Saskatoon, S7N 2V3 Saskatchewan, Canada

Systems containing $S = 1/2$ cations, such as cuprates, have long served as platforms for exploring quantum phenomena, including low-dimensional magnetism and superconductivity. In these systems, strong electronic correlations and magnetic exchange interactions give rise to a wide range of emergent behaviours. Despite their potential for similar or even more complex behaviour, silver(II)-based analogues remain far less explored. This is mainly due to difficulties in stabilising this cation, which is highly oxidising, easily hydrolysed, and thermally unstable. Silver(II) fluorides are particularly interesting, as these compounds exhibit strong covalency, significant magnetic superexchange, and low-dimensional magnetic behaviour, making them promising analogues to cuprates [1].

In this talk, I will present our recent research results on silver(II) fluorides [2]. I will show how we introduced mechanochemistry to access new (Figure 1), highly sought-after phases believed to be direct analogues to charge-doped cuprates that were impossible to obtain via conventional routes, and discuss the interplay between their structural and magnetic properties.

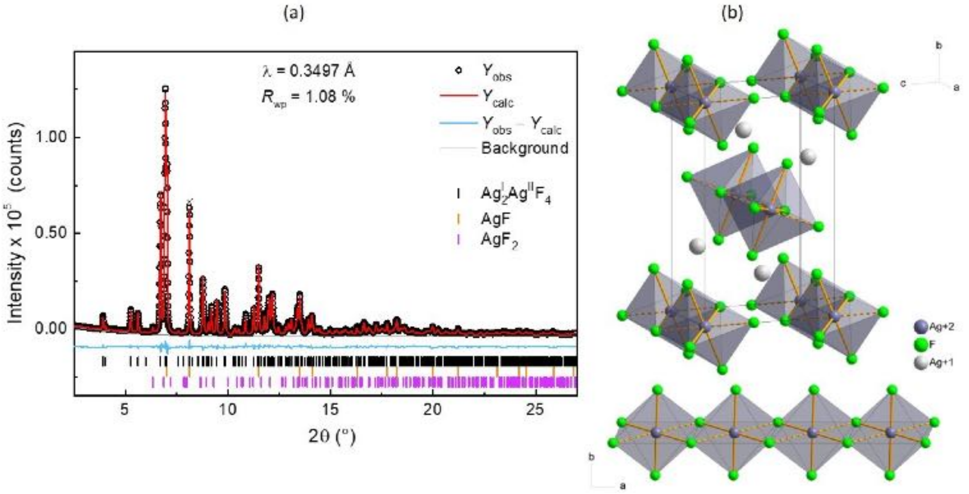


**Figure 1.** **(a)** Synchrotron PXRD of novel $Ag_3F_4$ phase obtained by mechanochemistry. **(b)** Crystal structure of $Ag_3F_4$.

## References:

[1] Grochala, W., Hoffmann, R. *Angew. Chem. Int. Ed.* (2001). 40, 2742–2781.
[2] Belak Vivod, M., King, G., Hansen, T. C., Lozinšek, M., Dragomir, M. *J. Am. Chem. Soc.* (2024). 146, 30510–30517.

## Acknowledgment

This work was supported by the Slovenian Research Agency (J2-2496 and N1-0397).

# INVESTIGATION OF AN O···π 'LAMP MOTIF' IN 2,3-DICHLORO-5,6-DICYANOBENZOQUINONE MODIFIED IN HIGHLY ACIDIC MEDIA

Nikola Jakupec,[1] Michael Bodensteiner[2] and Krešimir Molčanov[1]

[1] Department of Physical Chemistry, Ruđer Bošković Institute, Bijenička cesta 54, 10000 Zagreb, Croatia; *E-mail*: njakupec@irb.hr
[2] Faculty of Chemistry and Pharmacy, University of Regensburg, Universitätsstraße 31, 93053 Regensburg, Germany

2,3-Dichloro-5,6-dicyano-p-benzoquinone (DDQ) is a well-known oxidizing agent often used in organic synthesis for oxidation of alcohols, phenols, heterocycles etc.[1] Radical anions of DDQ have also been used for forming pancake bonded π-stacks in recent years. [2,3] Preparation of these anions is rather straightforward, as DDQ has a high redox potential and readily forms radicals after reacting as a one-electron acceptor. Furthermore, recent studies have shown DDQ reacting with π-nucleophiles to facilitate nucleophilic addition to the DDQ ring or one of the oxygen atoms.[4] However, aside from two crystal structures obtained in the mentioned work, no in-depth crystallographic study was performed on the resulting products. Therefore, the effect of the added ligand to the rest of the structure, along with the effect on crystal packing, remains unresolved.

Herein we demonstrate nucleophilic addition and substitution of organic ligands directly on the DDQ ring by using a highly acidic medium facilitated by protonated polycyanometallates. SCXRD study of the obtained products shows a persistent O···π intra- and intermolecular interaction, dubbed the 'lamp motif'. The nature of this interaction has been investigated using charge density analysis, Hirshfeld atom refinement and analysis of electrostatic potential mapped onto the Hirshfeld surface of the molecule.

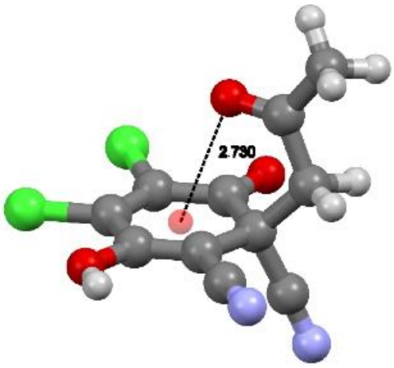


**Figure 1.** O···π 'lamp motif' present in modified DDQ, O···centroid distance is shown.

**References:**

[1] Walker, D.; Hiebert, J. D., *Chem. Rev.*, (1967) 67 153–195.
[2] Stanić, P.; Barišić, D.; Pajić, D.; Šantić, A.; Molčanov, K.; *Cryst. Growth Des.* (2022) 22 6461–6471.
[3] Stanić, P.; Poreba T.; Androš Dubraja, L.; Krawczuk, A.; Molčanov, K., *Cryst. Growth Des.* (2023) 23 3284–3296.
[4] Guo, X.; Mayr, H.; *J. Am. Chem. Soc.*, (2013) 135 12377–12387.

**Acknowledgement**
The authors would like to acknowledge the Croatian Science Foundation for funding this research under project IP-2024-05-8711.

# SYNTHESIS AND STRUCTURE OF NEW CHELATING MERCAPTOPYRIMIDINES

Blaž Antonin[1], Jakob Kljun[1]

[1] Department of Chemistry and Biochemistry, Faculty of Chemistry and Chemical Technology, University of Ljubljana, Večna pot 113, 1000 Ljubljana, Slovenia; *E-mail*: Jakob.kljun@fkkt.uni-lj.si

The synthesis of new chelating molecules possessing multiple nitrogen heterocycles is a challenging and important topic in modern coordination chemistry. Metal-catalyzed coupling reactions are generally less effective and require higher catalyst loads as they are inactivated by the final products of the reactions. In our group we have used ring-closing reactions on heterocyclic enaminone substrates which enable us to prepare multiple series of bipyridine-like ligands (Figure 1) which are used in the preparation of new biologically or catalytically active metal complexes.

Here, we will present the synthetic route for a reliable gram-scale synthesis of two families of mercaptopyrimidines (along with some happy accidents along the way) as well as their use in the synthesis of new bioactive *fac*-tricarbonylrhenium(I) complexes.[1,2]

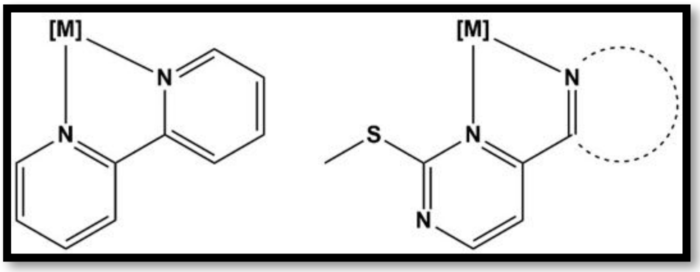


Figure 1: Metal coordination mode of 2,2’-bipyridine and the new family od mercaptopyrimidines.

**References:**

[1] Rapuš, U.; Pivarcsik, T.; Dömötör, O.; Nové, M.; Nyári, J.; Bogdanov, A.; Spengler, G.; Turel, I.; Kljun, J.; Enyedy, É.A., Structure and solution biospeciation on tricarbonylrhenium(I) complexes of mercaptopyrimidines with multifaceted biological activity (2026), *Metallomics*, article no. *mfag002*

[2] Antonin, B.; Methylations and oxidations of 2-pyrimidinethiones to stable chelating molecules for the preparation of new metal complexes of copper and rhenium (2026), *MSC thesis* (supervisor: J. Kljun)

**Acknowledgement**

We are grateful for the financial support of the Slovenian Research and Innovation Agency (ARIS) for the program grant P1-0175. The authors also acknowledge the support of the Centre for Research Infrastructure at the Faculty of Chemistry and Chemical Technology, which is part of the Network of Research and Infrastructural Centres UL (MRIC UL) and is also financially supported by ARIS (Infrastructure programme No. I0-0022) for the use of the single crystal diffractometers.

# CAERULOMYCIN K INSPIRED CHELATING PYRIDINE OXIMES

Sabi William Konsago,[1] Adrian Viveros,[1,2] Jure Jakoš,[1] Jakob Kljun[1]

[1] University of Ljubljana, Faculty of Chemistry and Chemical Technology, Večna pot 113, SI-1000 Ljubljana, Slovenia; *E-mail*: SabiWilliam.Konsago@fkkt.uni-lj.si
[2] Universidad de Alcalá, Facultad de Ciencias, Ctra Madrid-Barcelona, km.33, 600. ES-28805 Alcalá de Henares (Madrid), Spain

Recent studies on cearulomycins (Cae) and their analogues have revealed anticancer, antibacterial, and immunomodulating activities, sparking scientific interest in their potential use for drug development [1, 2]. However, the synthesis of these compounds remains largely underexplored, and the established synthetic pathways are challenging, often requiring expensive metal catalysts and multi-stage rearrangements [3].

In this work, we explore the metal-free synthesis of CaeK (Error: Reference source not found) and CaeK inspired pyridine oximes.

Furthermore, we used the synthesised compounds as ligands in Re(I) complexes, which will be studied for their potential biological activities.

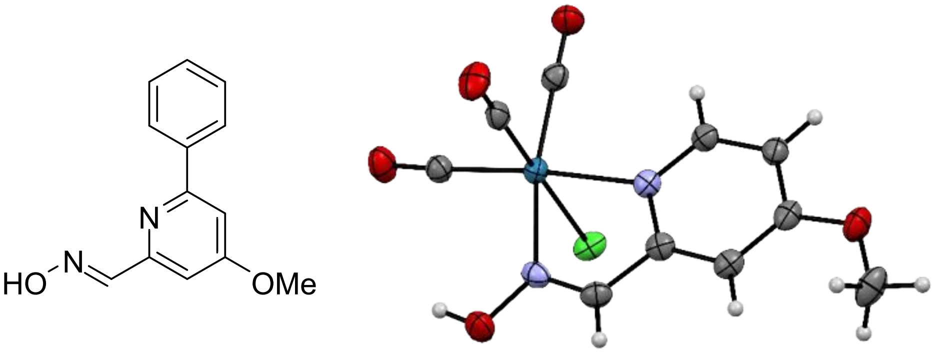


**Figure 1:** Caerulomycin K (left) and Re(I) complex with pyridineoxime (right).

**References:**

[1] Fu, P., Wang, S., Hong, K., Li, X., Liu, P., Wang, Y., & Zhu, W. (2011). *J. Nat. Prod.*, 74, 1751-1756.
[2] Tong, L.; Sun, W.; Wu, S.; Han, Y. (2022), *Eur. J. Pharmacol.*, 922, 174914.
[3] García-García, J. A., Aceña, J. L., García-García, P., & Sucunza, D. (2026). *Org. Lett.,* 28, 907−911.

**Acknowledgement**

We are grateful for the financial support of the Slovenian Research and Innovation Agency (ARIS): project grant J1-70040 and research program grant P1-0175. The authors also acknowledge the support of the Centre for Research Infrastructure at the Faculty of Chemistry and Chemical Technology, which is part of the Network of Research and Infrastructural Centres UL (MRIC UL) and is also financially supported by ARIS; Infrastructure programme No. I0-0022) for the use of the single crystal diffractometers.

# MODIFYING AND COORDINATING CAERULOMYCIN A

Jure Jakoš,[1] Jakob Kljun[1]

[1] University of Ljubljana, Faculty of Chemistry and Chemical Technology, Večna pot 113, SI-1000 Ljubljana, Slovenia; *E-mail*: jure.jakos@fkkt.uni-lj.si

As antimicrobial resistance continues to increase, the search for solutions is intensifying. To address this challenge, scientists are exploring unconventional treatments, drug modifications, and new compounds [1].

In the 50s a promising new candidate was discovered while studying the extract of *Streptomyces caerules.* This new compound was later named Caerulomycin A (CaeA) and was the first representative of an entirely new family of compounds [2]. Since then, biological studies have demonstrated good antibacterial, immunomodulating, and anticancer activity, among others [3,4].

Because of the interesting properties of this compound (Figure 1), we have decided to investigate its potential as a ligand in metal complexes. So far, we have optimized a gram-scale synthesis of CaeA and prepared several synthetic CaeA analogues. The compounds prepared were also used to synthesize the first Re(I) coordination compounds containing Caerulomycins.

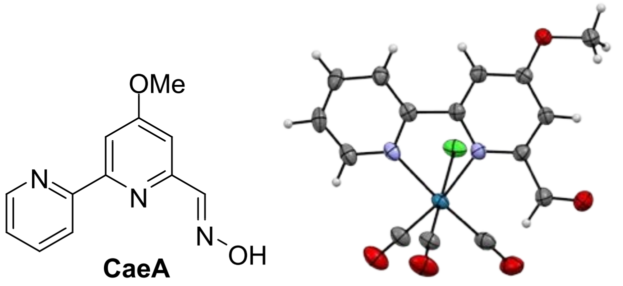


*Figure 1: Caerulomycin A (left), Re(I) complex with Caerulomycin E*

## References:

[1] Salam, M. A.; Al-Amin, M. Y.; Salam, M. T.; Sigh Pawar, J.; Akhter N.; Rabaan, A. A.; Alqumber, M. A. A. Antimicrobial Resistance: A Growing Serious Threat for Global Public Health. *Healthcare* 2023, 11, 1946.

[2] Funk, A.; Divekar, P. V. Caerulomycin, a New Antibiotic from Streptomyces Caeruleus Baldacci, I. Production, Isolation, Assay. and Biological Properties. *Can. J. Microbiol.* 1959, 5, 317–321.

[3] Tong, L.; Sun, W.; Wu, S.; Han, Y. Characterization of Caerulomycin A as a DualTargeting Anticancer Agent. *Eur. J. Pharmacol.* 2022, 922, 174914.

[4] Singla, A. K.; Krishna Gurram, R.; Chauhan, A.; Khatri, N.; Vohra, R. M.; Jolly, R. S.; Agrewala, J. N. Caerulomycin A Suppresses Immunity by Inhibiting T Cell Activity. *PLOS ONE,* 2014, 9

**Acknowledgement**:

We are grateful for the financial support of the Slovenian Research and Innovation Agency (ARIS): a Junior Researcher Grant to Jure Jakoš and grant P1-0175. The authors also acknowledge the support of the Centre for Research Infrastructure at the Faculty of Chemistry and Chemical Technology, which is part of the Network of Research and Infrastructural Centres UL (MRIC UL) and is also financially supported by ARIS; Infrastructure programme No. I0-0022) for the use of the single crystal X-ray diffractometers.

# DRUG SOLUBILITY MODIFICATION: INDOMETHACIN SALTS/COCRYSTALS WITH ISONICOTINAMIDE AND IMIDAZOLE

Marin Liović,[1] Donna Danijela Dragun,[1] Nika Rimaj,[1] Rafael Anelić,[1] Fabio Faraguna,[1] Edi Topić,[2] Ivan Halasz,[3] Ernest Meštrović[1]

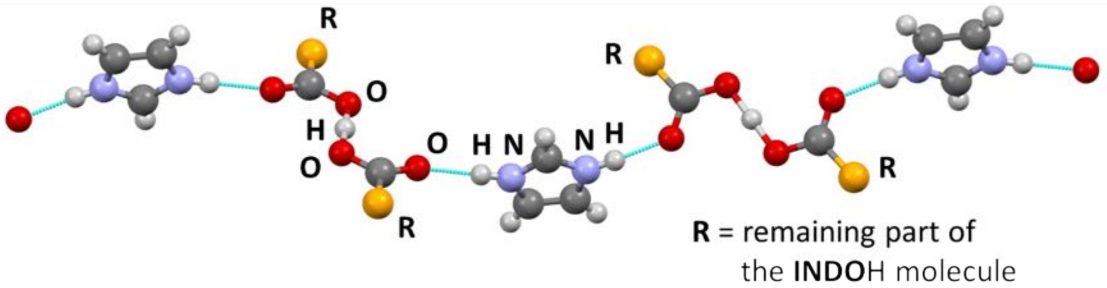
[1] Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, Zagreb; *E-mail*: mliovic@fkit.unizg.hr

[2] Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102a, Zagreb

[3] Ruđer Bošković Institute, Bijenička cesta 54, Zagreb

Cocrystallization and salt formation are powerful crystal-engineering strategies for modifying drug properties, such as solubility, while preserving the molecular scaffold of the drug molecule [1]. Indomethacin (**INDO**H), a non-steroidal anti-inflammatory drug (NSAID) [2], was selected as a candidate for such modification given its poor aqueous solubility at physiological pH which limits its oral bioavailability and therapeutic efficacy [3].

In this work, three new crystal phases were prepared by liquid-assisted grinding of **INDO**H with two pharmaceutically acceptable coformers: a 1:1 **INDO**H-isonicotinamide phase and two **INDO**H-imidazole phases with 2:1 and 1:2 stoichiometries. Suitable single crystals of the 2:1 **INDO**H-imidazole salt were prepared from ethanol solution and analysed by single-crystal X-ray diffraction. The structure contained homoconjugated $[\mathbf{INDO}\cdots\mathrm{H}\cdots\mathbf{INDO}]^{-}$ anions, a synthon previously observed in **INDO**H salts, linked by imidazolium cations into chains *via* $\mathrm{N{-}H\cdots O_{carboxylate}}$ hydrogen bonds. Finally, apparent solubilities of the prepared crystal phases were determined in the fasted-state simulated intestinal fluid (FaSSIF, pH 6.8).



A representation of the hydrogen-bonded chains in the 2:1 **INDO**H-imidazole structure.

## References:

[1] Danilovski, A. & Meštrović, E. (2024). *Croat. Chem. Acta*, 97 (4), 243-259
[2] Vane, J. R. (1971) *Nat. New Biol.*, 231, 232-235
[3] Peltonen, L. & Hirvonen, J. (2010) *J. Pharm. Pharmacol.*, 62, 1569-1579

## Acknowledgement

This work was supported by the Croatian Science Foundation under project IP-2024-05-4339, "'Coffee ring' effect in 'Lab on a Chip' environments in the development of new drug formulations" (PI: Prof. Ernest Meštrović)

# CRYSTAL STRUCTURE OF THE TERNARY GALLIDE $Zr_{10}Ru_5Ga_8$

B. Kotur[1], V. Babizhetskyy[1], O. Myakush[2], V. Smetana[3], and A.-V. Mudring[3]

[1] Department of Inorganic Chemistry, Ivan Franko National University of Lviv, Kyryla i Mefodiya Str., 6, 79005 Lviv, Ukraine; *E-mail*: bohdan.kotur@lnu.edu.ua

[2] National University of Forest and Wood Technology of Ukraine, Chuprynky Str., 103, 79057 Lviv, Ukraine

[3] Department of Biological and Chemical Engineering and iNANO, Aarhus University, 8000 Aarhus C, Denmark

Ternary intermetallic compounds of zirconium, gallium, and platinum-group metals (Ru, Rh, Pd) exhibit a remarkable synergy between their constituent elements, leading to multifunctional behavior. During a systematic study of the isothermal section of the Zr–Ru–Ga phase diagram at 870 K four ternary gallides were identified: $Zr_7Ru_{6+x}Ga_{17-x}$ ($0 \leq x \leq 2.0$) original structure type (ST) [1], $Zr_{1-x}Ga_xRu_2$ ($x = 0{,}18$) ST $MgZn_2$ [2], $ZrRu_xGa_{2-x}$ ($0.60 \leq x \leq 1.00$) ST $MgZn_2$ [3], and $Zr_{10}Ru_5Ga_8$ original ST.

The latter compound is a new one. It was synthesized by arc melting the elements under argon followed by annealing at 870 K for 720 h. Single-crystal X-ray diffraction analysis revealed that $Zr_{10}Ru_5Ga_8$ crystallizes in a new monoclinic structure type: Pearson symbol $mS46$, $Z = 2$, space group $C2/m$, $a = 7.939(4)$, $b = 13.674\ (6)$, $c = 7.963\ (3)$ Å, $\beta$=109.92(3)°. The crystal structure is composed of high-coordination Ru-centered polyhedra (CN = 14 and 12) embedded in a zirconium-gallium framework. Zirconium atoms exhibit CN of 14 and 16 and Ga atoms occupy distorted trigonal-prismatic environments formed by $Zr_6$ atoms and additional $Ru_3Ga$ units resulting in CN=10. Ga−Ga contacts are very limited. The structure is dominated by heteroatomic Zr−Ga and Ru−Ga bonding rather than extended Ga networks. This difference reflects the transition from a framework-stabilized Ga-rich structure in $Zr_7Ru_6Ga_{17}$ to a more metal-centered packing in $Zr_{10}Ru_5Ga_8$. From a crystal-chemical perspective, $Zr_{10}Ru_5Ga_8$ occupies an intermediate position between classical topologically close-packed intermetallics (e.g. Laves phases) and complex gallium-rich framework structures.

The crystal structure of $Zr_{10}Ru_5Ga_8$ can be also interpreted as consisted of flat (layers *B*, *D*, *B'*) and corrugated (layers *A*, *C*, *C'*) atomic layers perpendicular to *Z* axis, which are connected along *Z* axis in the order …*ABCDC'B'*… As a result the hexagonal channels are formed along *Z* axis inside of which there are chains of …Zr1−Ru1−Zr1… atoms with shortened interatomic distances of 2.777 Å.

Electronic structure calculations confirm metallic character of the compound and show that the bonding is dominated by Zr–Ga interactions, with additional stabilization provided by Ru–Ga and Ru–Zr contacts, while Ga–Ga interactions play only a minor role. The Fermi level lies within bands predominantly derived from Zr and Ru 4*d* states.

**References:**

[1] Babizhetskyy, V., Myakush, O., Kotur, B., Smetana, V., Kremer, R.K., Meyer, G.H. & Mudring, A.-V. (2026) *J. Alloys Compd.* 1057, 186704.

[2] Myakush, O.Y., Fedorchuk, A.A., Mokra, I.R. & Myakush, O.R. (2006) *Visnyk Lviv Univ. Ser. Chem.* 47, 36−40.

[3] Babizhetskyy, V., Myakush, O., Shatalov, B. & Kotur, B. (2025) *Visnyk Lviv Univ. Ser. Chem.* 66, 24−32.

# EXPANDING THE STRUCTURAL DIVERSITY OF 3,3’-BIPYRIDINE TO DUAL-LIGAND METAL–ORGANIC FRAMEWORKS

Darko Vušak,[1] Juraj Guraljevski,[1] and Biserka Prugovečki[1]

[1] Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102A, HR-10000 Zagreb, Croatia; *E-mail*: dvusak@chem.pmf.hr

Metal-organic frameworks (MOFs) are a class of advanced porous materials that have experienced rapid growth in research interest over the past three decades. MOF structures are easily tuned by varying metal or modifying ligand to perform targeted functionality [1–3]. Incorporation of amino acids introduces chirality into the framework, expanding the range of the potential applications of the material [3]. The Cambridge Structural Database contains over 135 000 datasets in the MOF subset of crystal structure data, of which only around 10% are crystal structures in chiral space groups. To date, only 59 entries in CSD contain 3,3’-bipyridine and no structures combining 3,3’-bipyridine and amino acidate ligands (or their derivatives) have been reported [4].

In this work, we present synthesis and crystal structures of the series of three metal-organic frameworks with copper(II), 3,3'-bipyridine (bpy) and hydrophobic amino acids – L-alanine (HAla), L-valine (HVal) and L-isoleucine (Hile): $\{[\mathrm{Cu(Ala)(NO_3)(bpy)}]\cdot\mathrm{solvents}\}_n$ ($\mathbf{1}_{\mathbf{Ala}}$), $\{[\mathrm{Cu(Val)(NO_3)(bpy)}]\cdot\mathrm{solvents}\}_n$ ($\mathbf{2}_{\mathbf{Val}}$), $\{[\mathrm{Cu_2(Ile)_2(NO_3)_2(bpy)}]\}_n$ ($\mathbf{3}_{\mathbf{Ile}}$). Alaninate and valinate form isoreticular 3D MOFs which also contain solvent molecules packed in 1D channels. Solvent molecules occupy 37.2% of unit cell volume in $\mathbf{1}_{\mathbf{Ala}}$ and 24.9% in $\mathbf{2}_{\mathbf{Val}}$ (Figures 1a and 1b). Isoleucinate direct self-assembly into a different topology, forming 2D coordination polymer without crystallization solvent molecules (Figure 1c).

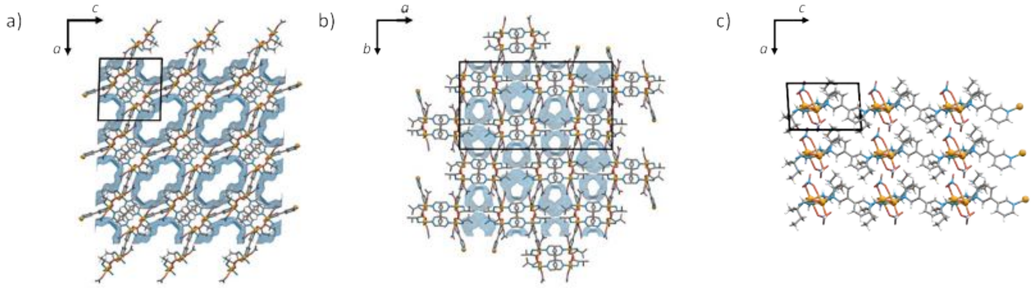


**Figure 1**. Crystal packing of 3D MOFs a) $\mathbf{1}_{\mathbf{Ala}}$, b) $\mathbf{2}_{\mathbf{Val}}$, and c) 2D chains in $\mathbf{3}_{\mathbf{Ile}}$.

## References:

[1] Barsoum, M.L., Fahy, K. M., Morris, W., Dravid, V. P., Hernandez, B. & Farha, O. K. (2025). *ACS Nano. 19(1)*, 13–20.

[2] Xu, W. & Yaghi, O. M., (2020). *ACS Cent. Sci. 6*, 1348–1354.

[3] Ren, C.-X., Ji, M., Yao, Q.-X., Cai, L.-X., Tan, B. & Zhang, J., (2014). *Chem. Eur. J. 20*, 14846–14852.

[4] Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst. B72*, 171–179.

## Acknowledgement

This research was supported by the European Union – NextGenerationEU through the National Recovery and Resilience Plan 2021−2026 via Institutional grants of the University of Zagreb Faculty of Science (*NextGenChem* and *CryoLab*).

# SALTS OF TETRACYANOQUINODIMETHANE (TCNQ) RADICAL ANION WITH LOW PARTIAL CHARGES OF −1/3 AND −2/5

Petra Stanić,[1,2] Nikola Jakupec,[1] and Krešimir Molčanov[1]

[1] Ruđer Bošković Institute, Bijenička 54, HR-10000 Zagreb, Croatia; *E-mail*: kmolcano@irb.hr
[2] Istrian University of Applied Sciences, Preradovićeva 9D, HR-52100 Pula, Croatia

7,7,8,8-tetracyanoquinodimethane (TCNQ) is a well-known electron acceptor readily reduced to a semiquinoid radical anion. However, in majority of its radical salts, it is actually partially charged, with formal charge of −1/2 and −2/3. [1,2] Full negative charge (−1) is less common. However, in some rare examples, it has other charges. Recently we described a compound in which formal charge of TCNQ moieties is −4/5. [3] In this work we present two novel salts of TCNQ with tetrabutylammonium cation and stoichiometries of 3:1 and 5:2 (implying respective partial charge of TCNQ moieties of −1/3 and −2/5). In both of them TCNQ moieties form infinite stacks bound by two-electron multicentre bonds (*pancake bonds*).

The 1:3 salt, although comprised of achiral moieties, crystallises in an unusual space group, $P1$. It is also solvable in $P\bar{1}$, but with a positional disorder of tetrabutylammonium cations and high values of $R$. Therefore, chiral crystal packing arises from a chiral arrangement of achiral moieties. The TCNQ moieties form 1D stacks of pancake-bonded trimers (short interplanar distances of <3.3 Å) separated by non-bonding stacking interactions (interplanar separations of 3.40 Å).

In 5:2 salt TCNQ moieties stack with longer interplanar separations (3.33 – 3.43 Å) and individual trimers can not be distinguished. This type of stacking implies long-range 1D antiferromagnetic ordering.

Geometry of TCNQ moieties in both salts is closer to quinoid (neutral) than to semiquinoid (radical) structure, and geometric correlations indicate that the charges of the moieties are indeed close to −1/3 and −2/5, respectively. Therefore, the structures were refined by Hirshfeld atom model (HAR) to reveal more accurate bond lengths as well as additional details of molecular structures, charges and pancake bonding.

## References:

[1] Herbstein, F. H. & Kapon, M. (2008). *Crystallogr. Rev.*, **14**, 3-74.
[2] Molčanov, K., Milašinović, V., Kojić-Prodić, B., Maltar-Strmečki, N., You, Y., Šantić, A., Kanižaj, L., Stilinović, V. & Fotović, L. (2022). *IUCrJ*, **9**, 449-467.
[3] Stanić, P., Smokrović, K., Maltar-Strmečki, N., Meurer, F., Bodensteiner, M., Hennig, C. & Molčanov, K. (2024). *Cryst. Growth Des.*, **24**, 9365-9378.

## Acknowledgement

This work was financed by the Croatian Science Foundation (HrZZ), grant IP-2024-05-8711.

# ALLYL-SUBSTITUTED PYRIDINES AS POWERFUL TOOLS FOR THE CONSTRUCTION OF NOVEL COPPER π,σ-COORDINATION COMPOUNDS

Yurii Slyvka,[1] Evgeny Goreshnik[2]

[1] Department of Inorganic Chemistry, Ivan Franko National University of Lviv, Kyryla i Mefodiya Str., 6, 79005, Lviv, Ukraine; *E-mail:* yurii.slyvka@lnu.edu.ua

[2] Department of Inorganic Chemistry and Technology, Jožef Stefan Institute, Jamova 39, SI-1000 Ljubljana, Slovenia

Copper(I)-olefin coordination compounds based on allyl-substituted heterocycles are found to be appealing objects for modern research in view of their catalytic, luminescent, nonlinear, biochemical, spin-crossover and other activities [1]. Due to the possibility of diverse ligand design and the formation of organometallic compounds with a large delocalized π-conjugated electron system with specific electronic absorption and large optical nonlinearity, copper(I) π,σ-complexes may also have a couple of potential applications in advanced laser-operated materials and in the development of novel optoelectronic devices. In our present work, we focused on the synthesis and design of novel copper(I) π-complexes with S-allyl and N-allyl substituted pyridyl-pseudothiohydantoines and 5-pyridyl-1,2,4-triazoles. π,σ-Coordination compounds were obtained in single crystalline form by means of the ac electrochemical technique starting mainly from alcohol, acetonitrile, or propylene carbonate solutions of the corresponding organic ligands and various copper(II) salts.

3-Allylthio-5-(2-pyridyl)-4*H*-1,2,4-triazoles reveal a tendency to form a dimeric building core with two copper(I) ions being coordinated with S-allyl group and two triazole N atoms. An appearance of other crystallographically independent copper(I) centers mostly is forced by the participation of the pyridyl N atom and results in a different complex architecture. For example, in the crystal structure of $[Cu_4(L1)_2(H_2O)_2(NO_3)_3](NO_3)$ ($L1$ – 3-allylthio-4-allyl-5-(2-pyridyl)-4*H*-1,2,4-triazole) there are four independent metal centers; dimeric core (based on Cu1 and Cu2) is stabilized by one bridging nitrate anion, while two other copper(I) ions form its individual trigonal-pyramidal surroundings composed of a pyridyl N atom, the C=C bond of the N-allyl group, a water molecule, and an anion. A shift of the N atom position in pyridine substituent stabilizes the formation of mixed-valence ($Cu^{I}/Cu^{II}$) complexes. In the unique structure of $[Cu^{I}_2(L2)_2(H_2O)_2Cu^{II}(H_2O)_2(NO_3)_2](NO_3)_2$ ($L2$ – 3-allylthio-4-allyl-5-(3-pyridyl)-4*H*-1,2,4-triazole) centrosymmetric dimeric cores are interconnected by $\{Cu^{II}(H_2O)_2(NO_3)_2\}$ subunits through a pyridyl bridge into the helicate. Such architectures of the obtained compounds are key for achieving large optical nonlinearity. The organization of pseudothiohydantoin complexes depends on the ligand (C=C),$N_{(imine)}$-chelate function only.

## References:

[1] Fedko, A. M., Slyvka, Yu. I., Goreshnik, E. A., Jędryka, J., Rakus, P. & Morozov, D. (2025). *J. Mol. Struct.* 1319, 139552.

## Acknowledgement

Yu. Slyvka is grateful for financial support to the President of Ukraine Grant administered by the National Research Foundation of Ukraine within the project No. 2025.02/0041 “Design and synthesis of olefin-copper complexes based on allyl derivatives of N-containing heterocycles for nonlinear optical devices.

# THE NOVEL DABCO-CHLOROCUPRATE(I) COORDINATION COMPOUNDS

Andrii Hultiaiev[1,2], Evgeny Goreshnik[1,2]

[1] Department of Inorganic Chemistry and Technology, Jožef Stefan Institute, Jamova c.39, SI-1000, Ljubljana, Slovenia;

[2] Jožef Stefan International Postgraduate School, Jamova c.39, SI-1000, Ljubljana, Slovenia;

*E-mail*: andrii.hultiaiev@ijs.si

DABCO (tryethylenediamine) has a rigid, nitrogen-based bidentate pillar structure [1]. Due to these properties, it is a known and widely used organic ligand for the formation of coordination polymers and metal-organic frameworks [2]. This study extends the known series of Cu-Cl-DABCO-containing coordination compounds [3-5] using a systematic approach based on the CuCl-DABCO-HCl composition space diagram. In this work, three Cu(I)-Cl-DABCO coordination compounds were synthesized by the solvothermal method. Their study was performed by single-crystal X-ray diffraction and Raman spectroscopy.

The **$Cu_6Cl_6(DABCO)_2$ (1)** crystallizes into infinite chains running along the 001 direction, consisting of $Cu_5Cl_6^-$ anionic clusters connected by DABCO – $Cu^+$ - DABCO bridges with 2 neutral DABCO ligands. Each $Cu_5Cl_6$ cluster is composed of a pair of Cu4 and Cu5 centres with an almost regular tetrahedral surrounding, linked by three $CuCl_2$ bridges. $Cu_5Cl_6$ clusters have 2 possible conformations due to the $CuCl_2$-bridge flexibility, which is represented as disorder at 2 positions with the occupancies of 84% and 16 %. All the chains are connected via Cl…H-C hydrogen bonds.

The **($HDABCO^+$) $Cu_5Cl_6$ (DABCO) (2)** crystallizes as yellow block crystals. Its crystal structure also contains $Cu_5Cl_6$ anionic oligomers. The Cu4 centre also coordinates the monoprotonated $HDABCO^+$ cation via the unprotonated amine group. In contrast, the Cu5 atom is bound to a neutral DABCO ligand. Both metal centres indicate an almost regular tetrahedral environment. These organic-inorganic isolated units are oriented along the 001 direction. All these units are formed into an H-bonded network via N-H…N and C-H…Cl hydrogen bonds.

The **($HDABCO^+$) CuCl (CN) (3)** contains cyanide anions, *in situ*-generated by the high-temperature decomposition of acetonitrile, each of which is disordered by rotation around the midpoint of the C-N bond by 180°, with a 50:50 ratio between domains. The crystallographically independent copper center is four-coordinated with a slightly distorted tetrahedral surrounding, containing 1 monoprotonated $HDABCO^+$, 2 bridging cyanide ligands, and a terminal chloride ion. Due to the bridging function of the cyanide ligands, the infinite cuprocyanide chains running along the 010 direction appear. A monoprotonated $HDABCO^+$ cation is coordinated to the metal via the unprotonated amine group. On the other side of DABCO, the monoprotonated quaternary ammonium group is connected via N-H…Cl hydrogen bonds with the neighbouring chloride anion, connecting the chains into a hydrogen-bonded network.

**References:**

[1] Feyziyeva, Sh., Kyritsakas-Gruber, N., et al. (2026). *J. of Solid State Chem.*, 355, 125798.
[2] Fratschko, M., Strasser, N., et al. (2025). *Cryst Growth Des.*; 25(11), 3665-3679.
[3] C. R. Groom, I. J. Bruno, M. P. Lightfoot & S. C. Ward (2016), *Acta Cryst.* B72, 171-179.

[4] Goreshnik, E. (2021), CrystEngComm., *Roy.Soc.Chem.*, 23 (40), 7171-7178.
[5] Williams, E. R., & Weller, M. T. (2013). *CrystEngComm*, 15(1), 31–33.

**Acknowledgement**: The authors acknowledge the financial support from the Slovenian Research Agency (research core funding No. P1–0045; Inorganic Chemistry and Technology).

# THE FIRST STRUCTURE OF A DISCRETE CIS-BIS(L-PROLINATO)COPPER(II) IN CO-CRYSTALS WITH UREA AND WATER. THE INFLUENCE OF CRYSTALLIZATION CONDITIONS ON THE OCCURRENCE OF UREA COCRYSTALS

Ivica Đilović*,[1] Kristina Smokrović,[1,2] Marija Leko,[1] Nenad Judaš[1]

[1] Faculty of Science, University of Zagreb, Horvatovac 102a, HR-10000 Zagreb, Croatia; E-mail: idilovic@chem.pmf.hr

[2] Jožef Stefan Institute, Jamova cesta 39, 1000 Ljubljana, Slovenia

This study explores the synthesis and structural characterization of copper(II) coordination compounds with L-proline, focusing on the transformation between *trans*- and *cis*-isomers. Using mechanochemical methods, *trans*-bis(L-prolinato)copper(II) was synthesized and subsequently employed to form co-crystals with urea and water under varying solution conditions. Notably, the introduction of urea consistently induced the formation of the *cis*-isomer, a rare configuration for such Cu(II) complexes, as confirmed by IR spectroscopy and single-crystal X-ray diffraction. Crystallographic analysis revealed that hydrogen bonding, primarily involving urea, water, and proline, plays a critical role in stabilizing the *cis*-isomer within the crystal lattice (Figure 1). Attempts to isolate pure *cis*-bis(L-prolinato)copper(II) *via* solid-state reactions to remove urea are underway, but often result in amorphization or reversion to the original complex. These findings highlight the influence of supramolecular interactions and crystallization conditions on the isomerization and stabilization of Cu(II) complexes, offering new insights into the design of supramolecular architectures in crystal engineering.[1-3]

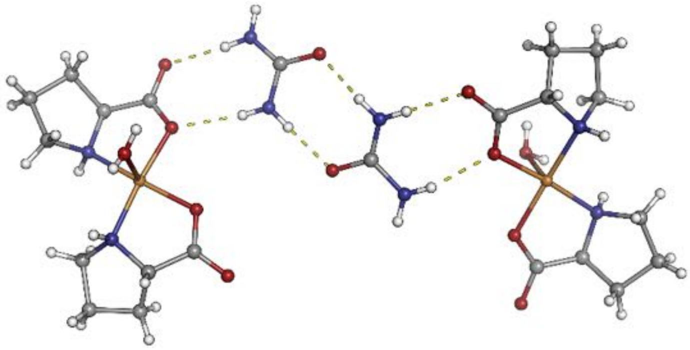


Figure 1

**References:**

[1] D. Mrvoš-Sermek, M. Tašner, D. Vušak, N. Judaš, K. Wzgarda-Raj, I. Đilović, D. Matković-Čalogović, *CrystEngComm* 2025, **27**, 356-365.

[2] K. Smokrović, S. Muratović, B. Karadeniz, K. Užarević, D. Žilić, I. Đilović, *Cryst. Growth Des.*, 2020, **20**, 2415-2423.

[3] K. Smokrović, I. Đilović, D. Matković-Čalogović, *CrystEngComm*, 2020, **22**, 4963-4968.

**Acknowledgement**

Croatian Science Foundation (grant no. IP-2014-09-4274); University of Zagreb grants for 2022-2024; CIuK project, co-financed by the Croatian Government and the European Union KK.01.1.1.02.0016.

This research was supported by the European Union – NextGenerationEU through the National Recovery and Resilience Plan 2021-2026 via Institutional grants of the University of Zagreb Faculty of Science (NextGenChem and CryoLab).

# SUPRAMOLECULAR PYRIDINIUM OXIME-FERROCYANIDE COMPLEXES: STRUCTURALLY DRIVEN CHROMIC RESPONSE

I. Picek,[1] J Popović,[2] D. Musija,[1] V. Damjanović,[1] B. Foretić [1] and D. Matković-Čalogović[3]

[1] Department of Chemistry and Biochemistry, School of Medicine, University of Zagreb, Šalata 3, Croatia; *E-mail:* ipicek@mef.hr
[2] Division of Materials Physics, Ruđer Bošković Institute, Bijenička cesta 54, Zagreb, Croatia
[3] Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102a, Croatia

Supramolecular ferocyanide–based charge-transfer complexes (CTCs) incorporating pyridinium oximes represent a versatile class of stimuli-responsive metalo-organic materials with tunable optical and redox properties [1-3]. The ferrocyanide ion with its rigid octahedral geometry, strong electron-donating and multifunctional H-bond accepting ability is an excellent building block for assembling multidimensional architectures with pyridinium oximes acting as electron acceptors and hydrogen-bond donors. These systems are characterized by a smooth interplay between crystal packing, hydrogen-bonding networks, π-π-stacking interactions and redox-activity, which collectively govern their chromic behavior [1–4].

Here, we present the comparative solid-state study of structural features of selected pyridinium oximes and their ferrocyanide CTCs to elucidate the impact of different *N*-substituent, oxime position on a pyridinium ring, and the number of oxime groups in chromic response. These include reversible hydrochromism, thermochromism, vapochromism, and redox-assisted colour switching associated with partial electron transfer and radical formation.

## References:

[1] Foretić, B., Vianello, R., Matković-Čalogović, D., Jadreško, D. & Picek, I. (2018). *New J. Chem*. 42, 16115−16126.
[2] Foretić, B., Klaser, T., Ovčar, J., Lončarić, I., Žilić, D., Šantić, A., Štefanić, Z., Bjelopetrović, A., Popović, J. & Picek, I. (2024). *Molecules*. 29, 5611−5626.
[3] Picek, I., Matković-Čalogović, D., Dražić, G., Kapun, G., Šket, P., Popović, J. & Foretić, B. (2024). *Molecules*. 29, 1698−1713.
[4] Musija, D., Picek, I., Vianello, R., Matković-Čalogović, D., Foretić, B. & Damjanović, V. (2026). *Int. J. Mol. Sci.* 27(4), 2015−2038.

# COMPARATIVE STRUCTURAL ANALYSIS OF A SERIES OF HALOGENATED THIOCARBOHYDRAZONE DERIVATIVES

Mirjana M. Radanović, Gorana S. Mrđan, Milica G. Bogdanović, Marko V. Rodić, Borko M. Matijević

[1] Department of Chemistry, Biochemistry and Environmental Protection, Faculty of Sciences, University of Novi Sad, Trg Dositeja Obradovića 3, Novi Sad, Serbia; *E-mail:* mirjana.lalovic@dh.uns.ac.rs

Monothiocarbohydrazone derivatives (compounds **1-3**) were synthesized by dissolving thiocarbohydrazide in ethanol and adding the corresponding halogen-ortho-substituted benzaldehyde. Formed monosubstituted compounds were further dissolved in acetone with slight heating to obtain asymmetrical bisthiocarbohydrazones (compounds **4-6**, Figure 1). The compounds were characterized using FT-IR and NMR spectroscopy, elemental analysis, thermal analysis, UV/Vis spectroscopy, and single-crystal X-ray diffraction. The latter revealed that compounds **1-3** adopt predominantly planar conformations stabilized by extended π-conjugation along the hydrazone backbone, while compounds **4-6** deviate from planarity. All the molecules exist in the thione form, characterized by short C=S and elongated N–N and C–N bond distances, confirming substantial electron delocalization throughout the thiocarbohydrazone fragment. Crystallographic data do not indicate significant steric distortion induced by the halogen substituent, and the molecular geometries of the three derivatives remain very similar. The principal structural differences are therefore reflected primarily in intermolecular interactions and crystal packing rather than in the intrinsic molecular planarity. The obtained results provide valuable insight into the structure–property relationships of halogenated thiocarbohydrazones and demonstrate the role of halogen substitution in determining crystal architecture and physicochemical behavior.

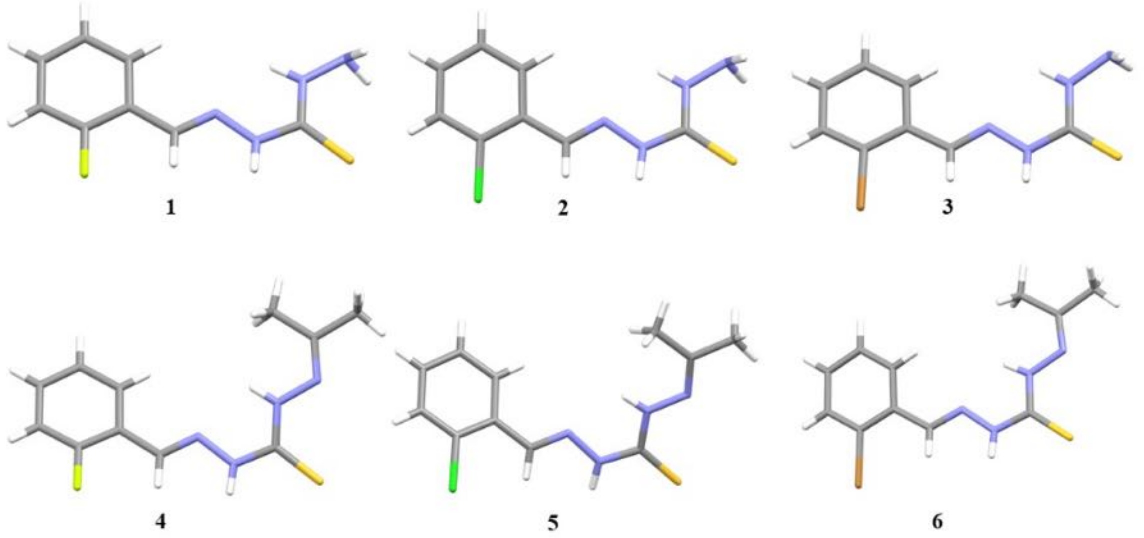


**Figure 1**. Molecular structure of derivatives **1-6**

**Acknowledgement**

The authors gratefully acknowledge the financial support of the Provincial Secretariat for Higher Education and Scientific Research (Grant No. 003864137 2025 09418 003 000 000 001 04 004).

# ENGINEERING METAGENOMIC ESTERASES: FROM ANCESTRAL RECONSTRUCTION TO CRYSTAL STRUCTURE

Ivana Kekez[1], Lucija Brtan[1] and Aleksandra Maršavelski[1]

[1] University of Zagreb, Faculty of Science, Department of Chemistry, Horvatovac 102 a, 10000 Zagreb, Croatia; *E-mail*: ikekez@chem.pmf.hr

Metagenomic enzymes represent a valuable resource for the discovery of novel biocatalysts for sustainable plastic recycling [1]. In this study, a metagenomic esterase (MGY) from the microbial community of the Venice Lagoon was investigated as a candidate enzyme for the enzymatic degradation of polyester-based bioplastics. However, the native enzyme exhibited poor solubility and limited suitability for structural studies [2]. To improve protein stability and crystallization behaviour, ancestral sequence reconstruction (ASR) was applied, yielding three ancestral variants with enhanced biochemical properties. Among them, variant 119_CLU displayed the highest thermal stability, while 118_CLU showed improved solubility. Further protein engineering involved removal of the disordered N-terminal region, generating truncated variants with reduced aggregation propensity and enhanced sample homogeneity. Extensive purification optimization and crystallization screening enabled successful crystallization of the engineered ΔN17_119_CLU variant. Crystals obtained by vapor diffusion diffracted to 2.1 Å resolution and belonged to the orthorhombic space group $P2_12_12_1$. The structure was solved by molecular replacement and revealed a conserved α/β-hydrolase fold characteristic of bacterial esterases. Structural analysis confirmed preservation of the catalytic triad (Ser160–Asp277–His300) and identified a stable dimeric assembly supported by extensive intermolecular interactions. The obtained crystal structure provides structural insight into the stabilization mechanisms introduced through ancestral reconstruction and protein engineering. These findings establish a framework for future structure-guided optimization of metagenomic esterases with potential application in sustainable bioplastic degradation and recycling.

**References:**
[1] Shalem, A., Yehezkeli, O., Fishman, A., 2024, *Appl. Microbiol. Biotechnol.* **108**:413.
[2] Kekez, I., Josić, E., Močibob, M., Mendeš, D., Maršavelski, A., 2024, *Acta Cryst. A.* **80**(a1), e122–e122.

**Acknowledgement**
This work was funded through the National Recovery and Resilience Programme (NextGenerationEU), project Enzyme engineering for sustainable recycling of bioplastics (NPOO.C3.2.R2-I1.06.0041).

# SUPRAMOLECULAR MACROCYCLES FOR WATER PURIFICATION: STRUCTURAL AND COMPUTATIONAL STUDIES OF INCLUSION COMPLEXES

Khalida Khalil[1,2] Bela Fiser[2,3*], Magdalena Małecka [1*]

[1] University of Lodz, Faculty of Chemistry, Department of Physical Chemistry, Pomorska 163/165*; E-mail:* Khalida.khalil@edu.uni.lodz.pl
[2] Doctoral School of Exact and Natural Sciences, Jana Matejki 21/23, 90-237 Lodz, Poland
[3] Institute of Chemistry, University of Miskolc, 3515 Miskolc-Egyetemváros, Hungary

The environmental persistence of chloro- and fluorocarbon compounds poses significant risks to ecosystems and human health, emphasizing the urgent need for efficient sensing and remediation strategies. Although hemicryptophane (Hm) macrocycles are well known for their applications in catalysis and energy-related systems, their potential for selective recognition of halogenated pollutants remains insufficiently explored. In this work, the host-guest interactions between hemicryptophane macrocycles and several freon-type molecules, including $CCl_4$, $CF_3Cl$, $CH_3Cl$, $CH_2Cl_2$, $CF_3Br$, $C_2F_6$, and $CF_4$, were investigated using previously successfully adapted computational methods [1] .

The study employed interaction energy calculations, natural bond orbital (NBO) analysis, frontier molecular orbital (FMO) studies, and interaction region indicator (IRI) analysis to evaluate the stability and nature of the supramolecular complexes. The results reveal that the intrinsic cavity of hemicryptophane provides a favorable environment for selective guest encapsulation. Chlorinated freons, particularly $CCl_4$ (-128.32 kJ mol$^{-1}$), $CCl_3F$ (-109.37 kJ mol$^{-1}$), and $CHCl_3$ (-92.65 kJ mol$^{-1}$), exhibited the strongest binding affinities, dominated by non-covalent interactions. Furthermore, the reduced HOMO–LUMO energy gaps indicate enhanced electronic responsiveness, highlighting the sensing potential of these systems. Overall, hemicryptophane-based macrocycles emerge as promising candidates for selective pollutant recognition and environmental remediation applications.

## References:

[1] K. Khalil, B. Fiser, and M. Małecka, *Chemosphere*, 390, 144711, 2025.

## Acknowledgement

We gratefully acknowledge Polish high-performance computing infrastructure PLGrid (HPC Center: ACK Cyfronet AGH) for providing computer facilities and support within computational grant no. PLG/2025/018935. This work is also supported by the Incentive Scholarship by NAWA STER for best foreign PhD students. BF was supported by the János Bolyai Research Scholarship of the Hungarian Academy of Sciences.

# CRYSTAL STRUCTURE AND INTERMOLECULAR INTERACTION ANALYSIS OF IMIDAZOLIUM-BASED MOLECULAR SALTS

Rehana Bano [1], Hadeer Q. Waleed [2], Olga Książkiewicz [3], Béla Viskolcz [1,2], Marcin Palusiak[3], Béla Fiser [1,2,3]

[1]Higher Education and Industrial Cooperation Centre, University of Miskolc, 3515 Miskolc-Egyetemváros, Hungary; *E-mail*: rehana.bano@uni-miskolc.hu
[2] Institute of Chemistry, University of Miskolc, 3515 Miskolc-Egyetemváros, Hungary
[3] Department of Physical Chemistry, Faculty of Chemistry, University of Lodz, 90-236 Lodz, Poland

Imidazolium-based molecular salts have attracted considerable attention due to their diverse structural architectures and the important role of intermolecular interactions in determining their physicochemical properties and supramolecular organization. Imidazolium-based molecular salts formed from imidazole derivatives and dicarboxylic acids were investigated using experimental and theoretical approaches [1]. The present study provides new structural insights into hydrogen-bonded molecular salts and their intermolecular interaction characteristics. The crystal structures were characterized by single-crystal X-ray diffraction, accompanied by detailed analyses of hydrogen-bond geometries, interaction energies, and topological features. In the investigated systems, the crystal packing is predominantly stabilized through N–H···O and C–H···O hydrogen-bonding interactions, leading to the formation of extended supramolecular networks. To obtain a deeper understanding of the intermolecular interactions and their dependence on the chemical environment, Hirshfeld surface analysis and quantum-theoretical calculations were performed. Interaction region indicator (IRI) analysis revealed distinct noncovalent interaction features with varying electron density distributions and interaction strengths among the studied molecular salts. Furthermore, quantum theory of atoms in molecules (QTAIM) analysis confirmed the presence of different bond critical paths associated with hydrogen-bonding interactions. The obtained results provide valuable insights into the structural organization and intermolecular interactions governing imidazolium-based molecular salts.

## References:

[1] Waleed, H. Q., Bano, R., Jordán, A. C., Książkiewicz, O., Palusiak, M., & Fiser, B. 2026. *Sci. Rep.* 16, 4127.

**Acknowledgement**

RB is grateful for the financial support provided by the University Research Scholarship Program of the Ministry for Culture and Innovation, funded by the National Research, Development, and Innovation Fund. We acknowledge the Digital Government Development and Project Management Ltd. for awarding us access to the Komondor HPC facility based in Hungary

# FROM MYSTERY TO MODULATION: THE STRUCTURAL STORY OF $\mathrm{RB_2[SI_2O_5]}$

Clivia Hejny[1], Volker Kahlenberg[1], and Hannes Krüger[1]

[1] Mineralogy and Petrography, University of Innsbruck, Innrain 52, 6020 Innsbruck;
*E-mail:* clivia.hejny@uibk.ac.at

Alkali silicates have been extensively studied due to their range of applications, including their use in the glass industry, bioactive ceramics, and as host materials for rare-earth-element-based silicate phosphors. Despite their importance, the structural complexity of some alkali silicates remains a challenge.

The crystal structure of $Rb_2[Si_2O_5]$ has long posed difficulties, as even the original authors of the structure noted that "with such high *R* factor the structure on itself would not be publishable" [1]. In a re-examination, a *C*-centred monoclinic cell, similar to the one previously reported was identified, but with additional reflections along the $b^{*}$-direction, which were interpreted as satellite reflections. Detailed analysis revealed satellite reflections up to the third order. In an average three-dimensionally periodic crystal structure model, that does not account for the presence of these satellite reflections, most of the oxygen atom positions are split, and rubidium atoms are six-fold coordinated and strongly underbonded.

The crystal structure was solved as an incommensurately modulated phase in the (3+1)-dimensional superspace group $C2/c(0\beta0)s0$, with $\mathbf{q} = (0,0.377(1),0)$, $a = 9.8695(6)$, $b = 8.4012(1)$, $c = 14.7701(1)$ Å, $\beta = 90.113(1)°$, and $V = 1223.4(1)$ $Å^3$. The refinement converged to an *R*-value of 0.0370, significantly lower than the previously reported value of 0.12 [1]. The $[SiO_4]$ tetrahedra adopt two distinct orientations, which were modelled using a crenel modulation function to describe the occupational modulation of atomic positions [2]. The structure consists of $[Si_2O_5]^{2-}$ - layers with intercalated rubidium atoms. The silicon layers are undulated, forming four- and eight-membered rings, a so-called $4.8^2$ net [3]. Terminal oxygen atoms of the $[SiO_4]$ tetrahedra are pulled closer into the coordination sphere of rubidium, resulting in more balanced bond valence sums for rubidium. However, this adjustment induces strain in the silicon layer, particularly in the four-membered rings, which is alleviated by the switching of tetrahedra between two orientations.

A comparison with other silicate materials featuring $4.8^2$ nets, such as $Cs_2Si_2O_5$ [1] and members of the mountainite mineral group [4], reveals that larger interlayer cations or higher interlayer content relax the silicon layer, allowing for a larger unit mesh of the silicon layer without modulation.

**References:**

[1] De Jong, B.H.W.S, Slaats, P.G.G., Supèr, H.T.J., Veldman, N, Spek, A.L. (1994). *J. Non-Crystalline Solids* 176, 164-171.
[2] Petříček, V., Eigner, V., Dusek, M., Cejchan, A. (2016). *Z. Kristallogr.* 231(5), 301-312.
[3] Hawthorne, F.C., Uvanova, Y.A., Sokolova, E. (2019). *Mineral. Mag.*, 83, 3-55.
[4] Zubkova, N.V., Filinchuk, Y.E., Pekov, I.V., Pushcharovsky, D.Y., Gobechiya, E.R. (2010). *Eur. J. Mineral.*, 22, 547–555.

# PRODUCTION OF DURABLE MULLITE-BASED CERAMICS FROM DIATOMITE

Aleksandra Šaponjić[1], Željko Skoko[3] , Marija M. Vuksanović[2], Željko Radovanović[4] Svetlana Ilić[1]

[1] Department of materials, Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, University of Belgrade, Mike Petrovića Alasa 12-14, 11000 Belgrade, Serbia; *E-mail*: acavuc@vin.bg.ac.rs; svetlanailic@vin.bg.ac.rs

[2] Department of Chemical Dynamics and Permanent Education, Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, University of Belgrade, Mike Petrovića Alasa 12-14, 11000 Belgrade, Serbia

[3] Department of Physics, Faculty of Science, University of Zagreb, Bijenička 32, 10000 Zagreb, Croatia

[4] Innovation Centre of the Faculty of Technology and Metallurgy, Karnegijeva 4, 11000 Belgrade, Serbia

Mullite-based ceramics were fabricated using diatomite consisting mainly of $SiO_2$ (70.5 wt%) and a moderately high content of $Al_2O_3$ (13.8 wt%). In order to achieve the stoichiometric mullite composition ($3Al_2O_3$-$2SiO_2$), diatomite was mixed with an appropriate amount of $Al(NO_3)_3 \cdot 9H_2O$. The crystal structure was refined by the Rietveld method by using the split-type pseudo-Voigt profile function and the polynomial background model. During the refinement, a zero shift, scale factor, half-width parameters, asymmetry and peak shape parameters were simultaneously refined. According to the X-ray diffraction analysis, mullite, quartz, cristobalite and corundum were formed at 1300 and 1400°C, while the sample sintered at 1500°C contained mullite. The microstructure of the sample sintered at 1500°C resulted in a well-developed nest-like morphology. Exceptional compressive strength—up to 188 MPa was exhibited at 1400°C. Consequently, the balance between crystalline mullite needles and intergranular glass appears to be a key parameter governing the mechanical performance of these mullite derived ceramics. Further research into mullite-based insulating materials is supported by the excellent mechanical stability of the samples sintered at 1400 C and, achieved without using binders or additives.

## References:

[1] Saponjic, A.; Maletaskic, J.; Zildzovic, S.; Radovanovic, Z.; Kuzmanovic, M.; Maslovara, S.; Ilic, S. Calcined Mullite Powder Produced from Waste Clay-Diatomite. *Sci. Sinter*. 2024, 15.

[2] Ilić, J. Maletaškić, Ž. Skoko, M.M. Vuksanović, Ž. Radovanović, I. Ristović, A. Šaponjić, Utilization of Waste Clay–Diatomite in the Production of Durable Mullite-Based Insulating Materials, *Appl. Sci*. 15 (2025) 7512. https://doi.org/10.3390/app15137512.

## Acknowledgement

This work was financially supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Contract Nos. 451-03-136/2025-03/200017, 451-03-136/2025-03/200287, and gratefully acknowledges the support of project CeNIKS co-financed by the Croatian Government and the European Union through the European Regional Development Fund—Competitiveness and Cohesion Operational Programme (Grant No.KK.01.1.1.02.0013).

# THERMAL BEHAVIOUR OF VIRGIN AND RECYCLED POLYETHYLENE TEREPHTHALATE ANALYSED BY DIFFERENTIAL SCANNING CALORIMETRY

Martina Potočnik,[1] Nataša Čelan Korošin[1]

[1] University of Ljubljana, Faculty of Chemistry and Chemical Technology, Večna pot 113, SI-1000 Ljubljana, Slovenia; *E-mail:* martina.potocnik@fkkt.uni-lj.si

Polyethylene terephthalate (PET) is one of the most widely used thermoplastic polymers and a representative semicrystalline material whose characteristics and performance depend strongly on the ratio of amorphous to crystalline phases. [1–3] The degree of crystallinity in PET affects thermomechanical resistance, rigidity, and barrier properties. [2] Mechanical recycling of PET modifies its molecular architecture through chain scission and degradation processes, affecting the crystallinity and microstructure of the material. [1, 4]

Differential scanning calorimetry (DSC) is a powerful tool for PET characterisation, enabling rapid measurement of key thermal properties, including glass transition, crystallisation, and melting processes, with their associated enthalpies and temperatures, which provide indirect insight into the polymer's history, degradation level, and crystalline structure. [3, 4] In this research, virgin and recycled PET were analysed using DSC to evaluate structural differences reflected in thermal transitions and degree of crystallinity.

Comparison of DSC curves revealed noticeable differences in thermal behaviour between virgin and recycled PET, indicating changes in crystallinity and thermal properties due to material degradation during recycling. Changes in glass transition, melting, and (cold) crystallisation temperatures and enthalpies suggest structural rearrangements associated with polymer chain conformation and crystalline organisation induced by processing history.

## References:

[1] Joseph, T. M., Azat S., Ahmadi Z., Jazani O. M., Esmaeili A., Haponiuk J. & Thomas S. (2024). *Case Stud. Chem. Environ. Eng.* 9, 100673.
[2] Di Lorenzo, M. L. (2024). *Polymers*. 16, 1975.
[3] Ronkay, F., Slezák, E., Gere, D., Lukács, N., Gyalai-Korpos, M., Molnár, A. D. & Bocz K. (2025). *Sci. Rep.* 15, 15673.
[4] La Mantia, F. P., Titone, V., Botta, L. & Glerean P. (2025). *J. Appl. Polym. Sci.* 143, 57954.

### Acknowledgement

The authors are grateful for the financial support from the junior research grant for Martina Potočnik, the Research Core Funding grant (P1-0134) provided by the Slovenian Research and Innovation Agency (ARIS), and also acknowledge the support of the Centre for Research Infrastructure at the University of Ljubljana, Faculty of Chemistry and Chemical Technology, which is part of the Network of Research and Infrastructural Centres UL (MRIC UL) and is financially supported by the Slovenian Research and Innovation Agency (ARIS; Infrastructure programme No. I0-0022).

# CRYSTAL STRUCTURE AND MAGNETIC PROPERTIES OF THE NOVEL LANGBEINITE-TYPE PHOSPHATE $BA_2FECO(PO_4)_3$

Fouad Alloun[1] Mohamed Saadi[2]

[1] Laboratory of Physical Chemistry of Applied Materials (LCPMA), Faculty of Sciences Ben M'Sick, Hassan II University of Casablanca, Morocco, *E-mail*: allounfouad@gmail.com
[2] Laboratoire de Chimie Appliquée des Matériaux, Centre des Sciences des Matériaux, Faculty of Science, Mohammed V University in Rabat, Avenue Ibn Battouta, BP 1014 Rabat, Morocco

A new mixed-metal langbeinite-type phosphate, $Ba_2FeCo(PO_4)_3$, was synthesized via solid-state reaction at 920 °C under air, and characterized by a combination of single-crystal X-ray diffraction, powder X-ray diffraction, vibrational spectroscopy, scanning electron microscopy, and magnetic measurements. Single-crystal X-ray diffraction, performed on a Bruker D8 Venture diffractometer (Mo Kα radiation), reveals that the compound crystallizes in the cubic system, space group $P2_13$, with unit cell parameter $a = 9.9081(2)$ Å and $V = 972.68(3)$ Å$^3$ ($Z = 2$). The three-dimensional framework consists of corner-sharing $FeO_6$ and $CoO_6$ octahedra interconnected through $PO_4$ tetrahedra, generating large cavities occupied by $Ba^{2+}$ cations [1,2]. Rietveld refinement of the powder diffraction data confirmed phase purity and structural consistency with single-crystal results [3]. Infrared and Raman spectroscopy confirmed the exclusive presence of slightly distorted $PO_4$ tetrahedral groups [4]. Magnetic susceptibility measurements reveal two distinct transitions at $T_1 = 14.18$ K and $T_2 = 11.98$ K in the ZFC curve, indicative of magnetic frustration. Curie-Weiss analysis yields $\theta \approx -56.6$ K, consistent with dominant antiferromagnetic super-exchange interactions along Fe–O–P–O–Co pathways, as interpreted through Goodenough-Kanamori-Anderson rules [5]. Hysteresis measurements at 8 K suggest ferrimagnetic-like behavior below $T_1$.

**References:**

[1] Zemann A., Zemann J., *Acta Crystallogr.* **10** (1957) 409.
[2] Norberg S.T., *Acta Crystallogr. B* **58** (2002) 743.
[3] Rodríguez-Carvajal J., *FullProf*, LLB-CEA, 2000.
[4] Antony C.J. et al., *Spectrochim. Acta A* **78** (2011) 415.
[5] Goodenough J.B., *Magnetism and the Chemical Bond*, Hassell Street Press, 1963.

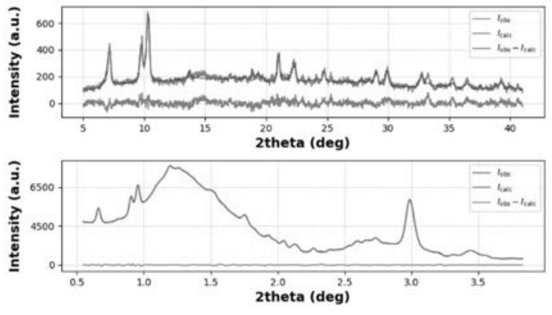
# DISCOVERY OF THE INTERMEDIATE CRYSTALLINE PHASE IN THE MECHANOCHEMICAL SYNTHESIS OF SILVER SULFADIAZINATE

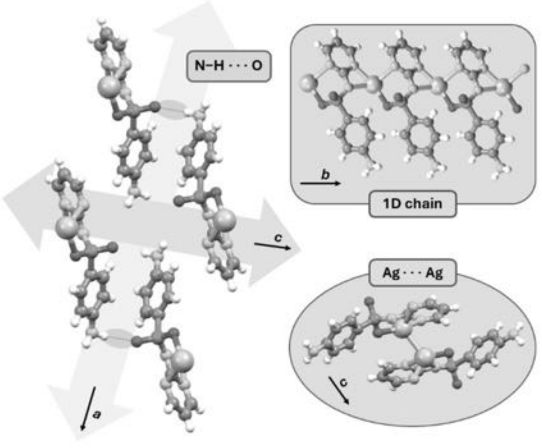
Lea Čolakić,[1] Goran Miletić,[2] Ernest Meštrović[3], Ivan Halasz[1]

[1] Division of Physical Chemistry, Ruđer Bošković Institute Bijenička cesta 54, Zagreb, Croatia;
*E-mail:* lcolakic@irb.hr
[2] Division of Materials Chemistry, Ruđer Bošković Institute, Bijenička cesta 54, Zagreb, Croatia
[3] Department of General and Inorganic Chemistry, Faculty of Chemical Engineering and Technology, Trg Marka Marulića 19, Zagreb, Croatia

Silver sulfadiazine (SSD) is a widely used active pharmaceutical ingredient for the treatment of wounds and burns. However, its conventional synthesis requires large amounts of solvents and strictly controlled conditions, which limits its environmental sustainability [1, 2]. It is known that SSD can also be prepared mechanochemically, with the catalytic addition of a solvent, which makes the synthesis faster and more environmentally friendly [3]. Monitoring of these reactions revealed a previously unknown, short-lived intermediate crystalline phase that forms at a very early stage of the reaction and disappears within minutes.

In this work, the intermediate phase was intentionally synthesized, and its crystal structure was determined using a combination of synchrotron and laboratory PXRD data, supported by computational DFT optimization. The results provide new insights into the formation mechanism of SSD, highlight the role of metastable phases in mechanochemical reactions, and open possibilities for improved control over the synthesis of this important pharmaceutical compound.





## References:

[1] World Health Organization, WHO Model List of Essential Medicines – 24th List, 2025, https://www.who.int/publications/i/item/B09474, (accessed 28 April 2026).
[2] Stöber, H. & DeWitte, W. (1982). *Anal. Profiles Drug Subst.* 11, pp. 523–551.
[3] Sović, I., Lukin, S., Meštrović, E., Halasz, I., Porcheddu, A., Delogu, F., Ricci, P. C., Caron, F., Perilli, T., Dogan, A. & Colacino, E. (2020). *ACS Omega*. 5, pp. 28663–28672.

**Acknowledgement**
This work has been supported in part by the Croatian Science Foundation under the project IP-2024-05-4339. We thank the ESRF (ID15) for beamtime.

# SURFACE PATCH CHARACTERIZATION AND CRYSTAL ORIENTATION EFFECTS ON THE PHOTOELECTRIC PROPERTIES OF GOLD-COATED SURFACES

Teodoro Klaser,[1] Antonella Cavalleri,[1] Roberto Canteri,[2] Davide Dal Bosco,[1] Rita Dolesi,[1] Rossana Dell'Anna,[2] Elena Missale,[2] Luca Pasquali,[3] Andrea Pedrielli,[2] Lorenzo Sala,[1] Francesco Venturelli,[1] and William J. Weber[1]

[1] Dipartimento di Fisica, Università di Trento and INFN, 38123 Povo, Trento, Italy; *E-mail*: tklaser@phy.hr

[2] Fondazione Bruno Kessler (FBK), Sensors and Devices Center, 38123 Povo, Trento, Italy

[3] Dipartimento di Ingegneria 'E. Ferrari', Università di Modena e Reggio Emilia, 41125 Modena, Italy.

Gold-coated surfaces exhibit spatially inhomogeneous work functions due to nanoscale variations in crystallographic orientation, surface reconstruction, step edges, and adsorbate distribution. Quantifying these surface patches is crucial for any application relying on electron photoemission.

We characterize gold-coated witness samples from the LISA Pathfinder gravitational reference system [1] — test mass (TM) and electrode housing (EH) specimens — using XPS/UPS for chemical composition and work function, ToF-SIMS for adsorbate depth profiling, and Kelvin Probe (KP) scanning to map contact potential across 100×100 µm windows with mV sensitivity.

KP measurements reveal surface potential variations of tens of mV over 0.01 mm², reflecting patches of different crystal orientations arising from reconstruction, step edges, and adsorbate-induced dipoles [2][3]. A numerical patch model — assigning each surface region a local work function from a Gaussian distribution — predicts a systematic enhancement of quantum efficiency (QE) over a uniform-surface prediction, strongest near the photoemission threshold. XPS/UPS and ToF-SIMS confirm contamination is confined to topmost layers, while heat treatment and sputtering recover the work function toward clean polycrystalline Au values.

## References:

[1] Armano, M. et al. (2009). *Class. Quantum Grav*. 26, 094001.
[2] Dowell, D.H. & Schmerge, J.F. (2009). *Phys. Rev. ST Accel. Beams*. 12, 074201.
[3] Methfessel, M., Hennig, D. & Scheffler, M. (1992). *Phys. Rev. B*. 46, 4816.

## Acknowledgement

The authors sincerely thank Fondazione Bruno Kessler (FBK, Trento) for TOF-SIMS and Kelvin Probe analyses, and Professor Pasquali (UNIMORE) for sharing data and fruitful discussions. This work is carried out in the framework of the LISA mission preparation.

# CATALYTIC BEHAVIOR AND DIELECTRIC PROPERTIES OF V-P-O-BASED GLASSES

Sara Marijan,[1] Željko Skoko,[2] Tomaš Hostinský,[3] Petr Mošner,[3] Ladislav Koudelka,[3]
Marta Razum[1], Josipa Sarjanović,[4] Jana Pisk[4] and Luka Pavić[1]

[1] Division of Materials Chemistry, Ruđer Bošković Institute, Zagreb, Croatia; *E-mail*: smarijan@irb.hr
[2] Department of Physics, University of Zagreb, Zagreb, CroatiaB
[3] Department of General and Inorganic Chemistry, Department of General and Inorganic Chemistry, University of Pardubice, Pardubice, Czech Republic
[4] Department of Chemistry, University of Zagreb, Zagreb, Croatia

Vanadium-containing mixed oxides are among the most important catalysts for selective oxidation reactions due to their exceptional activity and selectivity in functionalization of organic substrates, particularly in the conversion of olefins and paraffins into value-added compounds [1]. Their catalytic performance is closely related to the presence of V=O bonds, which act as active sites for substrate activation, and to the ability of vanadium to adopt multiple oxidation states, enabling efficient electron transfer during catalytic processes [1]. Particularly important are V–P–O-based materials, such as vanadyl pyrophosphate, widely known for their high selectivity in oxidation reactions of industrial relevance [1]. Compared to their crystalline analogs, V–P–O-based glasses represent an attractive but still insufficiently explored class of catalytic materials. Besides their simple and efficient preparation by the conventional melt-quenching technique, which ensures high reproducibility and facilitates large-scale production, these materials exhibit high catalytic activity and selectivity in epoxidation reactions [2], highlighting their potential for industrial catalytic applications. In addition to catalytic activity, dielectric properties of these materials are also important due to their potential application in electrochemical energy storage systems, as they both reflect underlying charge transport processes, with improvements in dielectric response strongly correlating with enhanced catalytic performance and observed structural features [3]. In this work, glasses from V–P–O-based system are investigated with respect to their dielectric and catalytic properties. Dielectric response is studied by solid-state impedance spectroscopy, while catalytic activity is evaluated in oxidation reactions of selected organic substrates. The relationship between composition, dielectric behavior, and catalytic activity is discussed through structure-property relationship.

## References:

[1] Duprez, D. & Cavani, F. (2014) Handbook of Advanced Methods and Processes in Oxidation Catalysis: From Laboratory to Industry, Imperial College Press, London.
[2] Pisk, J., Marijan, S., Klaser, T., Mošner, P., Koudelka, L., Agustin, D., Skoko, Ž. & Pavić, L., (2024) *J. Non-Cryst. Solids* 626, 122780.
[3] Marijan, S., Mošner, P., Koudelka, L., Skoko, Ž., Pavić, L. & Pisk, J., *J. Non-Cryst. Solids* 651 (2025) 123386.

**Acknowledgement**

This work is supported by the Croatian Science Foundation (CSF) under the ECLECTIC GLASS project IP-2025-02-7124.

# FROM STRUCTURE TO TRANSPORT: PHOSPHATE GLASSES CONTAINING TRANSITION METAL-OXIDES

Sara Marijan,[1] Marta Razum,[1] Teodoro Klaser[2], Željko Skoko,[2] Damir Pajić,[2] Shiro Kubuki,[3] Tomaš Hostinský,[4] Petr Mošner,[4] Ladislav Koudelka,[4] Jana Pisk[5] and Luka Pavić[1]

[1] Division of Materials Chemistry, Ruđer Bošković Institute, Zagreb, Croatia; *E-mail*: lpavic@irb.hr
[2] Department of Physics, Faculty of Science, University of Zagreb, Zagreb, Croatia
[3] Graduate School of Science, Tokyo Metropolitan University, Tokyo, Japan
[4] Department of General and Inorganic Chemistry, Faculty of Chemical Technology, University of Pardubice, Pardubice, Czech Republic
[5] Department of Chemistry, Faculty of Science, University of Zagreb, Zagreb, Croatia

Phosphate-based glasses and glass-ceramics are promising materials for electrochemical energy storage due to their tunable structural, thermal, and electrical properties. Incorporation of transition metal oxides (TMOs) into alkali phosphate glass networks strongly affects charge transport by modifying network connectivity and enabling electronic conduction via the small polaron hopping mechanism (SPHM). Depending on composition, these materials may exhibit ionic, electronic, or mixed conduction, making them attractive for battery-related application. [1]

Among the TM-containing phosphate glasses and glass-ceramics to be presented, particular attention is given to sodium vanadium phosphate (NVP) glasses prepared by the conventional melt-quenching technique. Vanadium exhibits a dual role, acting as both a network former/modifier and an electronically conductive species, depending on its concentration and oxidation state distribution. [2,3] Structural changes induced by compositional variations are investigated using infrared and Raman spectroscopy, while thermal behaviour and crystallisation tendency are analysed by differential thermal analysis (DTA). Solid-state impedance spectroscopy measurements performed over a broad frequency and temperature range provide detailed insight into charge transport processes. Through electrical equivalent circuit (EEC) analysis and model-free conductivity scaling approaches, charge carrier dynamics, relaxation phenomena, and the interplay between ionic and electronic conduction are elucidated. The results obtained contribute to a better understanding of structure-property relationships in phosphate-based glassy materials for advanced electrochemical applications

## References:

[1] Gandi, S., Vaddadi, V. S. C. S., Panda, S. S. S., Goona, N. K., Parne, S. R., Lakavat, M., Bhaumik, A., (2022*) J. Power Sources* 521, 230930.
[2] Marijan, S., Klaser, T., Mirosavljević, M., Mošner, P., Koudelka, L., Skoko, Ž., Pisk, J., Pavić, L., (2024) *Int. J. Mol. Sci*. 25, 3005.
[3] Barczyński, R. J., Król, P., Murawski, L., (2010*) J. Non-Cryst. Solids* 356, 1965.

### Acknowledgement

This work is supported by the Croatian Science Foundation (CSF) under the ECLECTIC GLASS project IP-2025-02-7124.

# VALORISATION OF INDUSTRIAL COMBUSTION BY-PRODUCTS AS ALTERNATIVE BINDERS FOR LOW-CARBON CONSTRUCTION

Vesna Zalar Serjun,[1] Anton Meden,[2] Romana Cerc Korošec,[2] Marta Počkaj,[2] Primož Oprčkal[1]

[1] Slovenian National Building and Civil Engineering Institute, Dimičeva ulica 12, SI-1000 Ljubljana, Slovenia; *E-mail*: vesna.zalar@zag.si
[2] Faculty of Chemistry and Chemical Technology, University of Ljubljana, Večna pot 113, SI-1000 Ljubljana, Slovenia

Industrial residues that display binder-like behaviour are key enablers of a circular and lower-carbon construction sector. Ashes generated in high-temperature combustion vary widely in composition and reactivity depending on the fuel and the air-pollution-control device that collects them, so each stream must be evaluated individually before it can be regarded as a recycled binder.

In this work, eight ashes originating from coal, co-combustion, paper-mill and biomass combustion were examined in order to establish how their phase assemblage governs their hydration response. Bulk chemistry was obtained by X-ray fluorescence, and the crystalline and amorphous fractions were quantified by Rietveld-refined powder X-ray diffraction; the data were then placed against the compositional fields of conventional supplementary cementitious materials. Pastes were prepared without any chemical activator at water-to-ash ratios of 1:1 and 1:1.2, and the secondary phases were followed by X-ray diffraction between 2 and 180 days, while the early heat release was recorded by isothermal calorimetry. Reactivity was additionally rated against the supplementary-binder criteria of SIST EN 450-1 and ASTM C1897.

Calcium aluminate hydrates were the dominant reaction products in every sample: the calcareous paper-mill ashes reacted most vigorously, the amorphous-rich coal and co-combustion ashes developed relevant phases over longer periods, and the ashes not captured by electrostatic precipitation proved least reactive.

The findings indicate that even weakly reactive streams can be activated when blended with more reactive ones, supporting the design of ash-based binder mixtures for geotechnical use [1,2].

## References:

[1] Zalar Serjun, V. (2024). *Materials*. 16, 5065.
[2] Snellings, R., Suraneni, P. & Skibsted, J. (2023). *Cem. Concr. Res*. 171, 107199.

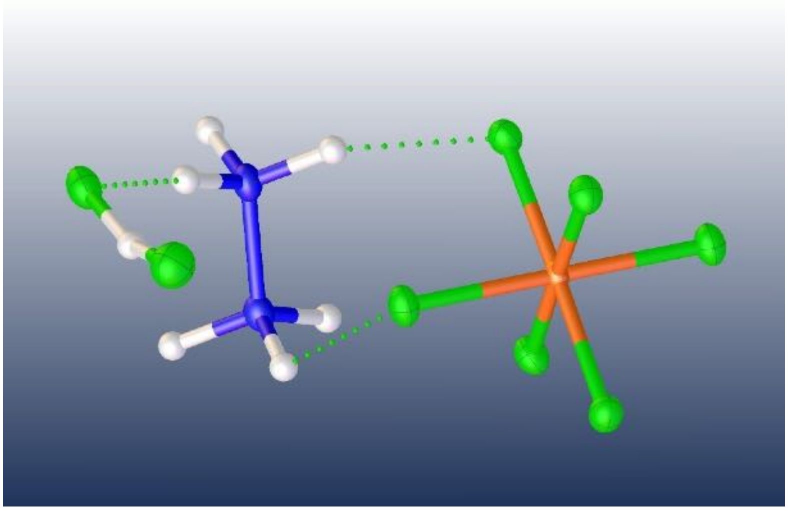
**Funding Information:**
P2-027 and J1-4413, J7-50228 Slovenian Research and Innovation Agency (ARIS), Slovenia

# NEW HYDRAZINIUM SALTS WITH BIFLUORIDE ANION

Evgeny Goreshnik [1]

[1] Department of Inorganic Chemistry and Technology, Jožef Stefan Institute, Jamova 39 1000 Ljubljana Slovenia; *E-mail*: Evgeny.goreshnik@ijs.si

$N_2H_6(HF_2)$ salt (I) was synthesized by the reaction of hydrazinium hydrate and HF aqueous solutions. Due to the well-known etching properties [1] of bifluoride-containing solutions, the $(N_2H_6)(HF_2)_2SiF_6$ (II) compound formed on the glass plate covered by a solution of I. Both compounds were structurally studied by single-crystal X-ray diffraction. For more accurate determination of hydrogen atoms positions, non-spherical atom refinement was performed for both structures. Both compounds contain doubly protonated hydrazinium (+2) cations. In both compounds, cations and anions form a complex system of N–H···F hydrogen bonds. The bifluoride anions in both compounds show noticeable asymmetry, which is likely related to specific effects of hydrogen bonding.



**References:**
[1] Williams, K.R., Muller, R.S. (1996). *Journal of Microelectromechanical Systems*. 5, 256–269.

# FROM DISCRETE COMPLEXES TO COORDINATION POLYMERS IN COBALT COORDINATION CHEMISTRY

Nives Kitanovski[1]

[1] Faculty of Chemistry and Chemical Technology, University of Ljubljana, Večna pot 113, SI-1000 Ljubljana, Slovenia; *E-mail*: nives.kitanovski@fkkt.uni-lj.si

Two cobalt(II) coordination compounds were synthesized under aqueous reaction conditions. The compounds were obtained as single crystals suitable for X-ray diffraction analysis, which provided insight into their coordination environments and intermolecular interactions. Complementary spectroscopic, magnetic, and elemental analyses were employed to support their characterization.

The crystal structures reveal octahedral coordination environments around the cobalt centres and different modes of coordination in the solid state.

Intermolecular interactions, including hydrogen bonding and π–π stacking interactions, contribute to the stabilization of the crystal packing.

**Acknowledgement**
Financial support from the Slovenian Research and Innovation Agency (ARIS) under grant P1-0175 is gratefully acknowledged. The author also thanks the Centre for Research Infrastructure at the Faculty of Chemistry and Chemical Technology, University of Ljubljana (IC UL FKKT), for providing access to the SuperNova diffractometer

# From Crystal Structures to Solid Forms – Exploring CSD Tools for Interactions, Morphology and Particle Properties

Matthew Lightfoot[1], Ilaria Gimondi [2], Andrew Peel[2]

[1] Cambridge Crystallographic Data Centre, Cambridge UK; E-mail:lightfoot@ccdc.cam.ac.uk
[2] Cambridge Crystallographic Data Centre, Cambridge UK

Understanding the relationship between crystal structures and solid forms is crucial in fields ranging from pharmaceuticals to materials science. This workshop introduces participants to the Cambridge Structural Database (CSD)[1] and the suite of tools developed by the Cambridge Crystallographic Data Centre (CCDC) to explore intermolecular interactions, crystal morphology and particle properties.

Beginning with a brief introduction to the CCDC and an overview of the CSD, attendees will gain insight into the wealth of structural data available for analysis. The session will include a guided introduction to Mercury[2], the CCDC's powerful visualisation tool, with a short hands-on demonstration to familiarise users with its interface and core functionalities.

The workshop will then explore key concepts in solid form assessment, followed by a practical overview of Mercury tools for analysing intermolecular interactions, enabling participants to identify and interpret packing motifs and interaction patterns within crystal structures.

Participants will also be introduced to CSD-Particle for examining particle-level properties, and to morphology prediction methods including BFDH Morphology and VisualHabit, with hands-on demonstrations illustrating how these approaches can be used to predict and rationalise crystal habit.

The workshop concludes with an interactive session where attendees can apply the tools to their own structures or provided examples, reinforcing learning through practical exploration.

This session is designed for users seeking to enhance their understanding of how crystal structure data can inform solid form design, particle behaviour and materials performance.

**References:**

[1] Groom, C.R., Bruno, I.J, Lightfoot, M.P. & Ward, S.C. (2016) *Acta Cryst.*, B72, 171-179
[2] Macrae, C.F., Sovago, I., Cottrell, S.J., Galek, P.T.A., McCabe, P., Pidcock, E., Platings, M., Shields, G.P., Stevens, J.S., Towler, M. & Wood, P.A. (2020) *Appl. Cryst.*, 53, 226-235

# LIST OF PARTICIPANTS

**ALLOUN, Fouad**
Hassan II University of Casablanca, Faculty of Sciences Ben M'Sick
Morocco

**BALEN, Dora**
Ruđer Bošković Institute
Zagreb, Croatia

**BANO, Rehana**
University of Miskolc, Higher Education and Industrial Cooperation Centre
Miskolc-Egyetemváros, Hungary

**BOROVINA, Mladen**
University of Zagreb, Faculty of Science, Department of Chemistry
Zagreb, Croatia

**BOŽIN, Emil S.**
Center for Solid State Physics and New Materials, Institute of Physics Belgrade
Belgrade, Serbia

**BUCHSTEINER, Emilia**
Rigaku Europe SE
Germany

**BURAZER, Sanja**
Ruđer Bošković Institute
Zagreb, Croatia

**CETINA, Mario**
University of Zagreb, Faculty of Textile Technology
Zagreb, Croatia

**CINČIĆ, Dominik**
University of Zagreb, Faculty of Science, Department of Chemistry
Zagreb, Croatia

**ĆUŽIĆ, Lucija**
Aparatura d.o.o.
Zagreb, Croatia

**ČAVLINA, Ana**
Aparatura d.o.o.
Zagreb, Croatia

**ČOLAKIĆ, Lea**
Ruđer Bošković Institute
Zagreb, Croatia

**DOHNÁLEK, Jan**
Institute of Biotechnology of Czech Academy of Sciences
Vestec, Czech Republic

**DRAGOMIR, Mirela**
Jožef Stefan Institute
Ljubljana, Slovenia

**ĐAKOVIĆ, Marijana**
University of Zagreb, Faculty of Science, Department of Chemistry
Zagreb, Croatia

**ĐILOVIĆ, Ivica**
University of Zagreb, Faculty of Science
Department of Chemistry
Zagreb, Croatia

**ERTL, Andreas**
Mineralogisch-Petrographische Abt., Naturhistorisches Museum
Wien, Austria

**GIESTER, Gerald**
Universität Wien, Institut für Mineralogie und Kristallographie
Wien, Austria

**GORESHNIK, Evgeny**
Jožef Stefan Institute
Ljubljana, Slovenia

**GOTIĆ, Marijan**
Ruđer Bošković Institute
Zagreb, Croatia

**GUERIN, Sarah**
University of Limerick, Bernal Institute, Department of Chemical Sciences
Limerick City, Ireland

**HEJNY, Clivia**
University of Innsbruck, Institute of Mineralogy and Petrography
Innsbruck, Austria

**HULTIAIEV, Andrii**
Jožef Stefan Institute
Ljubljana, Slovenia

**JAKOŠ, Jure**
University of Ljubljana, Faculty of Chemistry and Chemical Technology
Ljubljana, Slovenia

**JAKUPEC, Nikola**
Ruđer Bošković Institute
Zagreb, Croatia

**KEKEZ, Ivana**
University of Zagreb, Faculty of Science,
Department of Chemistry
Zagreb, Croatia

**KHALIL, Khalida**
University of Lodz, Faculty of Chemistry,
Department of Physical Chemistry
Lodz, Poland

**KITANOVSKI, Nives**
University of Ljubljana, Faculty of Chemistry and
Chemical Technology
Ljubljana, Slovenia

**KLASER, Teodoro**
Università degli Studi di Trento / INFN
Trento, Italy

**KLJUN, Jakob**
University of Ljubljana, Faculty of Chemistry and
Chemical Technology
Ljubljana, Slovenia

**KONSAGO, Sabi William**
University of Ljubljana, Faculty of Chemistry and
Chemical Technology
Ljubljana, Slovenia

**KOTUR, Bohdan**
Ivan Franko National University of Lviv
Lviv, Ukraine

**KRISTL, Matjaž**
University of Maribor, Faculty of Chemistry and
Chemical Engineering
Maribor, Slovenia

**LAKOTA, Katarina Lucija**
University of Ljubljana, Faculty of Chemistry and
Chemical Technology
Ljubljana, Slovenia

**LIGHTFOOT, Matt**
Cambridge Crystallographic Data Centre (CCDC)
Cambridge, United Kingdom

**LIOVIĆ, Marin**
University of Zagreb, Faculty of Chemical
Engineering and Technology
Zagreb, Croatia

**LOZINŠEK, Matic**
Jožef Stefan Institute
Ljubljana, Slovenia

**MARIJAN, Sara**
Ruđer Bošković Institute
Zagreb, Croatia

**MARUŠIĆ, Jani**
ITR-LAB d.o.o.
Ljubljana, Slovenia

**MATKOVIĆ-ČALOGOVIĆ, Dubravka**
University of Zagreb, Faculty of Science,
Department of Chemistry
Zagreb, Croatia

**MEDEN, Anton**
University of Ljubljana, Faculty of Chemistry and
Chemical Technology
Ljubljana, Slovenia

**MEGLIČ, Barbara**
ITR-LAB d.o.o.
Ljubljana, Slovenia

**MOLČANOV, Krešimir**
Ruđer Bošković Institute
Zagreb, Croatia

**NEMEC, Vinko**
University of Zagreb, Faculty of Science,
Department of Chemistry
Zagreb, Croatia

**PAVIĆ, Luka**
Ruđer Bošković Institute
Zagreb, Croatia

**PICEK, Igor**
University of Zagreb, School of Medicine
Zagreb, Croatia

**PISAČIĆ, Mateja**
University of Zagreb, Faculty of Science,
Department of Chemistry
Zagreb, Croatia

**POČKAJ, Marta**
University of Ljubljana, Faculty of Chemistry and
Chemical Technology
Ljubljana, Slovenia

**PODJED RIHTARŠIČ, Nina**
University of Ljubljana, Faculty of Chemistry and Chemical Technology
Ljubljana, Slovenia

**POSAVEC, Lidija**
University of Zagreb, Faculty of Science,
Department of Chemistry
Zagreb, Croatia

**POTOČNIK, Martina**
University of Ljubljana, Faculty of Chemistry and Chemical Technology
Ljubljana, Slovenia

**RADANOVIĆ, Mirjana**
University of Novi Sad, Faculty of Sciences
Novi Sad, Serbia

**RAPUŠ, Uroš**
University of Ljubljana, Faculty of Chemistry and Chemical Technology
Ljubljana, Slovenia

**RAZUM, Marta**
Ruđer Bošković Institute
Zagreb, Croatia

**SKOKO, Željko**
University of Zagreb, Faculty of Science,
Department of Physics
Zagreb, Croatia

**SLYVKA, Yurii**
Ivan Franko National University of Lviv
Lviv, Ukraine

**STILINOVIĆ, Vladimir**
University of Zagreb, Faculty of Science,
Department of Chemistry
Zagreb, Croatia

**STRUKAN, Neven**
RENACON d.o.o.
Zagreb, Croatia

**ŠAPONJIĆ, Aleksandra**
University of Belgrade, National Institute of the Republic of Serbia, Vinča Institute of Nuclear Sciences
Belgrade, Serbia

**ŠEBALJ, Nikola**
Anton Paar Croatia
Zagreb, Croatia

**ŠTEFANIĆ, Goran**
Ruđer Bošković Institute
Zagreb, Croatia

**TOKIĆ, Božena**
University of Zagreb, Faculty of Science
Department of Chemistry
Zagreb, Croatia

**VUŠAK, Darko**
University of Zagreb, Faculty of Science,
Department of Chemistry
Zagreb, Croatia

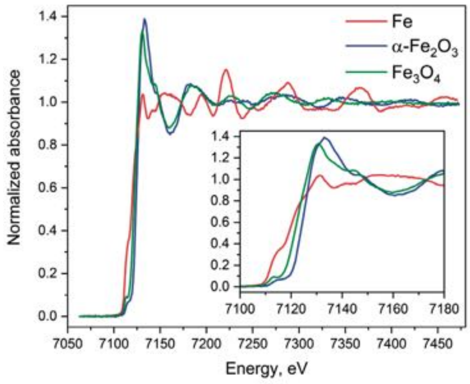
**ZALAR SERJUN, Vesna**
Slovenian National Building and Civil Engineering Institute (ZAG)
Ljubljana, Slovenia

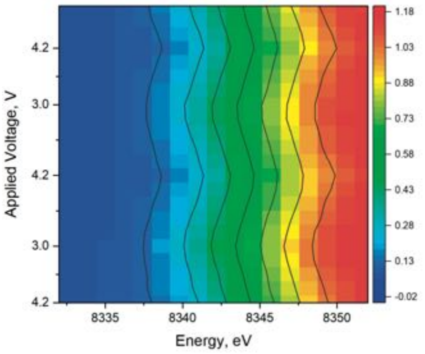
**Accompanying persons:**

Katharina Ertl
Oksana Goreshnik
Slyvka Ivanna-Kateryna
Lidija Molčanov
Lucija Molčanov
Dominik Molčanov
Danilo Radanović
Žarko Radanović
Relja Radanović
Viesta Pryimak
Mihaela Matovina
Branka Ropac-Gotić
Svetlana Ilić
Mateja Klaser
Gordan Klaser
Viktor Klaser
Dr Cian McKeown
Josip Cetina
Tomaž Serjun

# SPONSOR'S PAGES

Rigaku oxford diffraction
XtaLAB Synergy-ED
Powered by JEOL
Rigaku oxford diffraction
HyPix inside


Fe
α-$Fe_2O_3$
$Fe_3O_4$
Normalized absorbance
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
7050
7100
7150
7200
7250
7300
7350
7400
7450
Energy, eV
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
7100
7120
7140
7160
7180


Applied Voltage, V
4.2
3.0
4.2
3.0
4.2
8335
8340
8345
8350
Energy, eV
1.18
1.03
0.88
0.73
0.58
0.43
0.28
0.13
-0.02

# Your partner of choice in intergrated research

Selvita

Having experience in both **pharma and biotech R&D,** we are well aware of what it means to discover a hit and transform it into a drug. You can best benefit from this "insider" experience through our integrated drug discovery services.

### TARGET VALIDATION

- Target validation with genetic and pharmacological approach
- Biomarker expression and post-tranlational modifications
- Cellular processes

### HIT IDENTIFICATION

- Assay development and screening
- HTS/vHTS/HCS
- Priopㅤrietary macrocycle library
- Fragment-based drug design
- Structure- and ligand-based drug design
- Biophysical methods

### HIT TO LEAD AND LEAD OPTIMIZATION

- Medicinal and synthetic chemistry
- CADD
- In vitro pharmacology
- ADME/DMPK
- Protein production an X-ray crystallography
- Early toxicology
- In vivo pharmacology
- Translational research

### PRECLINICAL/CLINICAL CANDIDATE

- Non-GLP tox studies
- Solid state
- GLP bioanalysis
- Ex vivo analysis for biomarker research
- Batch release for clinical trials (GMP)

## WHY WORK WITH US

- ✓ **Multiple client-serving projects** undertaken from hit identification, H2L and LO start points
- ✓ **Diverse modalities applied:** small molecule enzyme inhibitors to target covalent inhibitors and PROTACs
- ✓ **Proven expertise & track record:** over 700 clients in 40 countries, completing over 4000 different projects to date

## VISIT OUR WEBSITE

www.selvita.com

## CONTACT US

sales@selvita.com

**Anton Paar develops, produces, distributes, and provides support for analytical instruments used in research, development, and quality control worldwide, as well as highly accurate process measuring systems and custom-tailored automation and robotics solutions.**

The Anton Paar GmbH Group currently has more than 4,200 employees and is active in over 110 countries across the globe.

Customers include the biggest international soft drink producers and breweries as well as petroleum, food, chemical, and pharmaceutical companies, and many more.

Anton Paar is committed to long-term partnerships with our customers and employees as well as responsibility towards society in general.

Since 2003, the Anton Paar GmbH Group, as part of the Anton Paar Group AG, has been owned by the Santner Foundation, a non-profit organization exclusively and directly aimed at charitable work. The foundation supports non-commercial scientific work and research in the field of natural science and technology for public utility, addiction prevention, and the rehabilitation of drug addicts.

# ELECTRON MICROSCOPY

## Thermo Scientific™ Helios™ 5 Laser PFIB

Fastest high-quality subsurface and 3D characterization at millimeter scale with nanometer resolution.

ThermoFisher
SCIENTIFIC

## Phenom XL G3 Desktop SEM

Discover the new **Thermo Scientific™ Phenom™ XL G3 Desktop SEM,** the longer-lasting CeB6 electron source reduces downtime and costs, while the improved backscatter electron detector delivers higher contrast, better compositional analysis, and superior signal-to-noise ratio—ideal for both industry and academia.

**NEW**

**LONGER LIFE, SHARPER INSIGHTS**

**High performance and efficiency in a compact design.**

OPTIKA®
ITALY

### Professional Stereo Microscopes

SLX SERIES - Stereomicroscopes For Higher Education & Laboratory
SZ SERIES - Stereozoom Microscopes For Laboratory & Industry
CL SERIES - Cold Light Illuminators
GEM SERIES - Stereozoom Microscopes For Gemology

### Industrial Microscopes

MET SERIES - Metallurgical Microscopes
IS SERIES - Inspection Video Microscopes

WWW.ITR-LAB.SI

---

**ALL YOU NEED FOR ELECTRON MICROSCOPY**
ULTIMATE EQUIPMENT SOLUTIONS ▪ CUSTOM SERVICE ▪ HIGH QUALITY FOR OUR CUSTOMERS
PERSONAL PROFESSIONAL APPROACH ▪ COMMITMENT TO YOUR SUCCESS

ITRLAB

# PREVIOUS MEETINGS

# PREVIOUS MEETINGS

*Slovenian-Croatian and Croatian-Slovenian Crystallographic Meetings*

## VENUES

| | | | | | |
|---|---|---|---|---|---|
| 1st | Otočec | Slovenia, 1992 | 17th | Ptuj | Slovenia, 2008 |
| 2nd | Stubičke Toplice | Croatia, 1993 | 18th | Varaždin | Croatia, 2009 |
| 3rd | Kranjska Gora | Slovenia, 1994 | 19th | Strunjan | Slovenia, 2010 |
| 4th | Trakošćan | Croatia, 1995 | 20th | Baška | Croatia, 2011 |
| 5th | Zreče | Slovenia, 1996 | 21st | Pokljuka | Slovenia, 2012 |
| 6th | Umag | Croatia, 1997 | 22nd | Biograd na Moru | Croatia, 2013 |
| 7th | Radenci | Slovenia, 1998 | 23rd | Logar Valley | Slovenia, 2014 |
| 8th | Rovinj | Croatia, 1999 | 24th | Bol | Croatia, 2016 |
| 9th | Gozd Martuljek | Slovenia, 2000 | 25th | Ljubljana | Slovenia, 2017 |
| 10th | Lovran | Croatia, 2001 | 26th | Poreč | Croatia, 2018 |
| 11th | Bohinj | Slovenia, 2002 | 27th | Rogaška Slatina | Slovenia, 2019 |
| 12th | Plitvice | Croatia, 2003 | 28th | Poreč | Croatia, 2022 |
| 13th | Bovec | Slovenia, 2004 | 29th | Topolšica | Slovenia, 2023 |
| 14th | Vrsar | Croatia, 2005 | 30th | Veli Lošinj | Croatia, 2024 |
| 15th | Jezersko | Slovenia, 2006 | 31st | Rogla | Slovenia, 2025 |
| 16th | Petrčane | Croatia, 2007 | | | |

## INVITED AND PLENARY LECTURES

### 1st Slovenian-Croatian Crystallographic Meeting, Otočec ob Krki, Slovenia.

*October 1–2, 1992.*

| | |
|---|---|
| **A. Kalman (Budapest, Hungary)** | *On the nature of hypervalent S-O bonds in sulfuranes* |
| **B. Kojić-Prodić et al. (Zagreb Croatia)** | *The biological significance of conformational changes of beta-D-glucopyranose moiety in peptidoglycans* |
| **C. Kratky (Graz, Austria)** | *Crystallography of B12-coenzymes* |
| **V. Kraševec (Ljubljana, Slovenia)** | *Crystallography of 2D precipitates caused by a minor phase additions in some ceramic systems* |

### 2nd Croatian-Slovenian Crystallographic Meeting, Stubičke Toplice, Croatia.

*September 30–October 1, 1993.*

| | |
|---|---|
| **L. Randaccio (Trieste, Italy)** | *Structural and solution properties of rhodoximes: the Rh analogues of cobaloximes, a vitamin B12 model* |
| **V. Kaučič (Ljubljana, Slovenia)** | *The structure of zeolite and aluminophosphate molecular sieves* |
| **K. Huml (Prague, Czech Republic)** | *Crystallography in drug design* |

| | |
|---|---|
| **B. Gržeta and H. Toraya (Zagreb, Croatia)** | *Powder-pattern-fitting methods in structure determination* |

## 3rd Slovenian-Croatian Crystallographic Meeting, Kranjska gora, Slovenia.

*September 29–30, 1994.*

| | |
|---|---|
| **W. Fuller, A. Mahendrasingam, and V. T. Forsyth (Keele, UK)** | *Structural studies of biological and industrial fibres using X-ray synchrotron radiation sources and neutron beams* |
| **A. Rečnik and D. Kolar (Ljubljana, Slovenia)** | *Local structure of planar faults in oxide ceramics* |
| **T. Schirmer (Basel, Switzerland)** | *Crystal structures of porins: proteins that form transmembrane pores* |
| **M. Luić and N. Brničević (Zagreb, Croatia)** | *Stereochemistry of hexanuclear niobium clusters with the [Nb6Cl12]2+ unit* |

## 4th Croatian-Slovenian Crystallographic Meeting, Trakoščan, Croatia.

*September 28–30, 1995.*

| | |
|---|---|
| **I. Hargittai and M. Hargittai (Budapest, Hungary)** | *Structure of molecules and assemblies* |
| **V. Marinkovič (Ljubljana, Slovenia)** | *Scanning tunneling microscopy of surface structures* |
| **H. Fuess (Darmstadt, Germany)** | *Contributions of crystallography to material science* |
| **D. Balzar (Zagreb, Croatia)** | *Diffraction line broadening - nuisance or lattice-imperfections fingerprints* |

## 5th Slovenian-Croatian Crystallographic Meeting, Zreče, Slovenia.

*June 13–15, 1996.*

| | |
|---|---|
| **H. D. Flack (Geneve, Switzerland)** | *Mastering least-squares refinement* |
| **J. V. Brenčič (Ljubljana, Slovenia)** | *Structural studies of the halopyridine complexes of trivalent elements* |
| **P. Panjan (Ljubljana, Slovenia)** | *Interfacial reaction in multilayer structures studied with XTEM and XRD* |
| **H. Follner (Lienz, Austria)** | *Correspondence between structure and morfology and twin formation* |
| **Z. Blažina (Zagreb, Croatia)** | *The rare earth based intermetallics - a scientist's paradise* |

## 6th Croatian-Slovenian Crystallographic Meeting, Umag, Croatia.

*June 19–21, 1997.*

| | |
|---|---|
| **A. Meden (Ljubljana, Slovenia)** | *Crystal structure solution from powder diffraction data - state of the art and perspectives* |
| **B. Ya. Kotur (Lviv, Ukrayina)** | *Scandium binary and ternary alloy systems and intermetallic compounds* |
| **P. Orioli (Firenze, Italy)** | *Structural studies on the interactions between metal ions and biological macromolecules* |
| **M. Vinković (Zagreb, Croatia)** | *Synergy between crystallography and computational chemistry* |

## 7th Slovenian-Croatian Crystallographic Meeting, Spa Radenci, Slovenia.

*June 18–20, 1998.*

| | |
|---|---|
| **M. Kaftory (Haifa, Izrael)** | *Three decades of chemical reactions in the solid state from photodimerization to methyl transfer* |
| **A. M. Tonejc (Zagreb, Croatia)** | *High-resolution electron microscopy (HREM): image processing analysis of defects and grain boundaries in nanocrystalline materials* |
| **E. Tillmanns (Vienna, Austria)** | *How to avoid unnecessarily low symmetry in crystal structure determinations* |
| **K. Djinović Carugo (Ljubljana, Slovenia)** | *Protein function through crystallography* |

## 8th Croatian-Slovenian Crystallographic Meeting, Rovinj, Croatia.

*June 17–19, 1999.*

| | |
|---|---|
| **D. Yu. Pushcharovsky (Moscow, Russia)** | *Recent contribution and modern perspectives in XRD studies of minerals* |
| **G. Jovanovski (Skopje, Macedonia)** | *Metal sacharinates and their complexes with N-donor ligands* |
| **M. Bolognesi et al. (Pavia, Italy)** | *The high resolution structure of GDP-4-keto-6-deoxy-D-mannose epimerase/reductase* |
| **G. G. Dodson (York, UK)** | *The chemistry and evolution of the catalytic structures in serine hydrolases* |
| **A. Demšar (Ljubljana, Slovenia)** | *The inclusion of the ionic fluorides in soluble organometallics* |

## 9th Slovenian-Croatian Crystallographic Meeting, Gozd Martuljek, Slovenia,

*June 17–19, 2000.*

| | |
|---|---|
| **C. Giacovazzo (Bari, Italia)** | *Phasing: from powders to proteins* |
| **Ch. Baerlocher (Zuerich, Switzerland)** | *The texture approach to structure solution from powder data* |
| **A. Tonejc (Zagreb, Croatia)** | *Crystallographic features of mechanically milled and alloyed nano-sized crystalline and amorphous materials* |
| **I. Turel (Ljubljana, Slovenia)** | *The crystal structures of quinolones and their metal compounds* |

## 10th Croatian-Slovenian Crystallographic Meeting, Lovran, Croatia.

*June 21–24, 2001.*

| | |
|---|---|
| **K. Prout (Oxford, UK)** | *Molecules in motion* |
| **G. Zanotti (Padova, Italy)** | *The transport of vitamin A in mammals: a crystallographer's view* |
| **B. Kobe (Brisbane, Australia):** | *Protein-peptide binding and its regulation* |
| **O. Milat (Zagreb, Croatia) and G. Calestani (Parma, Italy):** | *Crystallography of composite crystals* |

## 11th Slovenian-Croatian Crystallographic Meeting, Bohinj Lake, Slovenia.

*June 27–30, 2002.*

| | |
|---|---|
| **H. Boehm (Mainz, Germany)** | *Phase transitions in modulated structures* |
| **G. Giester (Vienna, Austria)** | *Five years of CCD X-ray data collection at Vienna University* |
| **E. R. T. Tiekink (Singapore, Singapore)** | *Adventures in engineering molecular solids* |
| **D. Matković-Čalogović (Zagreb, Croatia)** | *Some protein crystallography examples - a small molecule crystallographers view* |
| **B. Modec (Ljubljana, Slovenia)** | *Oxomolybdenum(V) clusters built of dinuclear metal-metal bonded units* |

## 12th Croatian - Slovenian Crystallographic Meeting, Plitvice Lakes, Croatia.

*June 19–22, 2003.*

| | |
|---|---|
| **B. Kojić-Prodić (Zagreb, Croatia)** | *Hydrogen bonding and supramolecular architecture* |
| **G. Vlaic (Trieste, Italy)** | *XFAS spectroscopies and chemistry: some selected results* |
| **J. P. Abrahams, N. Ban (Zuerich, Switzerland)** | *X-ray crystallographic structure determination of large asymmetric macromolecular assemblies* |
| **A. Golobič (Ljubljana, Slovenia)** | *Solving structural problems of ceramic materials* |
| **A. Danilovski (Zagreb, Croatia)** | *Biological and pharmaceutical solids in the crystallographic arena* |

## 13th Slovenian-Croatian Crystallographic Meeting, Bovec, Slovenia.

*June 16–20, 2004.*

| | |
|---|---|
| **R. Loris (Brussel, Belgium)** | *Structural basis of plasmid addiction and programmed cell death in bacteria* |
| **D. Turk (Ljubljana, Slovenia)** | *Roles of papain-like cathepsins in immune system response: exclusive interactions as the other face of selectivity* |
| **K. Domasevitch, J. Sieler (Leipzig, Germany)** | *Architecture and design of new porous networks* |
| **A. Moguš-Milanković (Zagreb, Croatia)** | *Structure and properties of phosphate glass* |

## 14th Croatian-Slovenian Crystallographic Meeting, Vrsar, Croatia.

*June 15–17, 2005.*

| | |
|---|---|
| **N. Lah (Ljubljana, Slovenia)** | *Structural diversity of copper carboxylate complexes* |
| **L. R. MacGillivray (Iowa, USA)** | *Molecular crystals as media for constructing molecules* |
| **R. Cerny (Geneva, Switzerland)** | *Crystal structures of inorganic compounds from powder diffraction* |
| **M. Milun (Zagreb, Croatia)** | *Atomic structure of surfaces and thin films* |
| **E. Libowitzky (Vienna, Austria)** | *Dynamics of crystal structures: results between diffraction and spectroscopy* |

## 15th Slovenian-Croatian Crystallographic Meeting, Jezersko, Slovenia.

*June 14–18, 2006.*

| | |
|---|---|
| **W. L. Duax (Buffalo, USA)** | *The genes and amino acid sequences and crystal structures of short chain oxireductase enzymes* |
| **R. E. Dinnebier (Stuttgart, Germany)** | *Powder diffraction at non-ambient conditions using 2D-detectors* |
| **G. Štefanić (Zagreb, Croatia)** | *Formation of high-temperature ZrO2 polymorphs at room temperature* |
| **M. Kosec (Ljubljana, Slovenia)** | *Ferroelectrics: from bulk to nano* |

## 16th Croatian-Slovenian Crystallographic Meeting, Petrčane, Croatia.

*June 13–17, 2007.*

| | |
|---|---|
| **C. Giacovazzo et al. (Bari, Italy)** | *EXPO2007: A tool for crystal structure solution and refinement from powder data* |
| **N. Tomašić (Zagreb, Croatia)** | *Metamict minerals: Insight into relic crystal structuires* |
| **R. Kužel et al. (Prague, Czech Republic)** | *Structural studies of submicrocrystalline materials obtaind by severe plastic deformation* |
| **B. Kozlevčar (Ljubljana, Slovenia)** | *Structural analysis of copper(II) coordination compounds and correlation with their magnetic properties* |

## 17th Slovenian-Croatian Crystallographic Meeting, Ptuj, Slovenia.

*June 19–22, 2008.*

| | |
|---|---|
| **M. Jaskolski, K. Michalska (Poznan, Poland)** | *L-Asparaginases, their friends and relations* |
| **G. Pavlović (Zagreb, Croatia)** | *Mercury(II) coordination chemistry in the environment* |
| **B. Kobe et al. (Brisbane, Australia)** | *Two hotdogs are better than one: The structure of acy-coa thioesterase and the complementarity of structural methods* |
| **P. Strauch (Potsdam, Germany)** | *Solid state EPR: a structure-spectroscopy relationship* |
| **B. Orel et al. (Ljubljana, Slovenia)** | *Synthesis of polyhedral oligomeric silsesquioxane (POSS) hybrids and their applications as surface modifiers* |

## 18th Croatian-Slovenian Crystallographic Meeting, Varaždin, Croatia.

*June 17–21, 2009.*

| | |
|---|---|
| **K. Rissanen (Jyvaeskylae, Finland)** | *Weak intermolecular interactions in the solid state, the supramolecular chemistry perspective* |
| **S. Petriček (Ljubljana, Slovenia)** | *Complexes with ethers and polyethers P. Naumov Direct observations of dynamic processes in crystals: from the topochemical postulate to ultrafast time-resolved diffraction* |
| **F. Antson et al. (York, England)** | *How viruses fill their capsids with DNA: crystallography of a DNA-translocating molecular motor* |
| **P. Dubček (Zagreb, Croatia)** | *Small angle probe into thin film* |

## 19th Slovenian-Croatian Crystallographic Meeting, Strunjan, Slovenia.

*June 16–20, 2010.*

| | |
|---|---|
| **A. L. Spek (Utrecht, The Netherlands)** | *Why Crystal Structure Validation?* |
| **Z. Dauter (Argonne National Lab., USA)** | *Nobel Prizes Related to Crystallography* |
| **A. Višnjevac (Zagreb, Croatia)** | *Single Crystal X-ray Crystallography as a Method of Choice in Biomimetic Modelling* |
| **I. Arčon (Nova Gorica, Slovenia)** | *Structural Analysis of Ordered and Disordered Materials with X-ray Absorption Spectroscopy* |

## 20th Croatian-Slovenian Crystallographic Meeting, Baška, Island Krk, Croatia.

*June 15–19, 2011.*

| | |
|---|---|
| **V. Holy (Prague, Czech Republic)** | *Synchrotron-related methods of investigatio of nanostructures* |
| **A. Šantić (Zagreb, Croatia)** | *Charge carrier transport in materials with disordered structures* |
| **T. Friščić (Cambridge, UK)** | *How to be efficient and environmentally-friendly at the same time: solid-state routes to materials and molecules* |
| **A. Pevec (Ljubljana, Slovenia)** | *Structural studies of some organotitanium(IV) complexes* |
| **M. Cetina (Zagreb, Croatia)** | *From self-inclusion and host-guest complexes to channel structures* |

## 21st Slovenian-Croatian Crystallographic Meeting, Pokljuka, Slovenia.

*June 14–17, 2012.*

| | |
|---|---|
| **L. B. McCusker (ETH Zürich, Switzerland)** | *Powder diffraction, electron microscopy and microdiffraction - meeting the challenge of zeolite structure analysis* |
| **K. R. Koch (Univ. of Stellenbosch, South Africa)** | *Deceptively simple, rich platinum(II/IV) and rhodium(III) chemistry viewed through new eyes: What secrets can the 195Pt/103Rh nuclei reveal about their molecular disguise in the solution and solid-state?* |
| **Z. Popović (Zagreb, Croatia)** | *Correlation between supramolecular interactions and structural characteristics of Ag(I) complexes* |
| **F. Perdih (Ljubljana, Slovenia)** | *Structural aspects of organotitanium fluorides* |

## 22nd Croatian-Slovenian Crystallographic Meeting, Biograd na Moru, Croatia.

*June 12–16, 2013.*

| | |
|---|---|
| **C. B. Aakeröy (Kansas State University, USA)** | *From molecular sociology to functional materials* |
| **A. Altomare (Bari, Italy)** | *The challenge of the ab-initio crystal structure solution by powder diffraction data: the EXPO software* |
| **V. Bermanec (Zagreb, Croatia)** | *The importance of collecting and investigation of mineral samples from ore deposits - example of Stari Trg (Trepča) mine* |
| **M. Jeršek (Ljubljana, Slovenia)** | *Inclusions in gemstones - origin, identification and valuation* |
| **J. Popović (Zagreb, Croatia)** | *Nanocrystalline metal oxides: synthesis, structure and properties* |

## 23rd Slovenian-Croatian Crystallographic Meeting, Logar Valley, Slovenia.

*June 19–22, 2014.*

| | |
|---|---|
| **I. R. Evans (Durham, UK)** | *Structural chemistry of functional materials: mobility in the solid state* |
| **J. S. O. Evans (Durham, UK)** | *Functional inorganic materials: synthesis, structure, properties and methods development* |
| **M. Đaković (Zagreb, Croatia)** | *From molecular structure to crystalline solids: non-covalent interactions as a structure directing force in supramolecular assemblies* |
| **T. Balić-Žunić (Copenhagen, Denmark)** | *Crystallography in mineralogy in the XXI century* |
| **G. Gunčar (Ljubljana, Slovenia)** | *A structural view of nanobodies* |

## 24th Croatian-Slovenian Crystallographic Meeting, Bol, Croatia.

*September 21–25, 2016.*

| | |
|---|---|
| **L. Brammer (Sheffield, UK)** | *Flexibility, Dynamics and Chemical Reactions in Solids: Molecular Crystals to Framework Materials* |
| **G. Dražić (Ljubljana, Slovenia)** | *Direct imaging and quantification of crystal structures at the atomic level using Cs corrected scanning transmission electron microscope* |
| **M. Jaskolski (Poznan, Poland)** | *Handling crystal pathologies in macromolecular crystallography* |
| **Ž. Skoko (Zagreb, Croatia)** | *Thermosalient crystals – acrobatics on the nanoscale* |
| **M. Zema (Pavia, Italy)** | *Crystallography and Society: outcomes of IYCr2014* |

## 25th Slovenian-Croatian Crystallographic Meeting, Ljubljana, Slovenia.

*June 14–17, 2017.*

| | |
|---|---|
| **D. Stalke, (Göttingen, Germany)** | *100 years of Lewis diagram – still valid in the light of charge density?* |
| **E. V. Boldyreva (Novosibirsk, Russia)** | *High-pressure studies of organic and coordination compounds* |
| **M. Marinšek (Ljubljana, Slovenia)** | *3D microstructure reconstruction from stack of 2D images demonstrated in Ni-SDC cermets* |
| **J. K. Cockcroft (London, UK)** | *Powder diffraction: an essential complementary tool for those skilled in the art but one with pitfalls for the unwary* |
| **K. Molčanov (Zagreb, Croatia)** | *Stacking of planar conjugated rings – beyond aromatics* |

## 26th Croatian-Slovenian Crystallographic Meeting, Poreč, Croatia.

*June 13–17, 2018.*

| | |
|---|---|
| **A. Katrusiak (Poznan, Poland)** | *High-pressure effects in hydrogen-bonded crystals* |
| **P. Scardi (Trento, Italy)** | *SRXRD of metal nanocrystals: learning from mistakes* |
| **S. C. Tarantino (Pavia, Italy)** | *Crystals' warm-up, stretching and ... workout!* |
| **Z. Štefanić (Zagreb, Croatia)** | *Purine nucleoside phosphorylases: a quest for enzyme mechanism and allosteric pathways* |
| **N. Zabukovec Logar (Ljubljana, Slovenia)** | *Crystallography in Microporous Materials Research* |

## 27th Slovenian-Croatian Crystallographic Meeting, Rogaška Slatina, Slovenia.

*June 19–23, 2019.*

| | |
|---|---|
| **P. Bombicz (Budapest, Hungary)** | *Synthon/property-engineering of calixarenes (supramolecular interactions, shape and symmetries)* |
| **M. Vrankić (Zagreb, Croatia)** | *Ambient and non-ambient driven X-ray powder diffraction: Insights into the structure-property relationship in powders* |
| **P. Macchi (Bern, Switzerland)** | *Are there molecules in crystals?* |
| **M. Lozinšek (Ljubljana, Slovenia)** | *Noble-gas chemistry in 21st century* |

## 28th Croatian-Slovenian Crystallographic Meeting, Poreč, Croatia.

*September 7–11, 2022.*

| | |
|---|---|
| **A. Bacchi (Parma, Italy)** | *Smart materials for the release of liquid ingredients* |
| **A. Moliterni (Bari, Italy)** | *Crystallography, a powerful lens for Materials Science* |
| **M. Klementová (Prague, Czech Republic)** | *Structure determination of nanomaterials from electron diffraction data* |
| **J. Kljun (Ljubljana, Slovenia)** | *Development of bioactive metal compounds: structural insights into design and molecular modes of action* |

## 29th Slovenian-Croatian Crystallographic Meeting, Topolšica, Slovenia.

*June 14–18, 2023.*

| | |
|---|---|
| **D. Cinčić (Zagreb, Croatia)** | *Crystal engineering of organic and metal-organic multicomponent halogen-bonded solids* |
| **K. Djinović Carugo (Grenoble, France)** | *Order from Disorder: Towards molecular architecture of the muscle Z-disk assembly* |
| **A. Kokalj (Ljubljana, Slovenia)** | *DFT modeling of materials and crystal structures using periodic-boundary conditions* |
| **S. Parsons (Edinburgh, UK)** | *High pressure phase transitions in molecular crystals* |

## 30th Croatian-Slovenian Crystallographic Meeting, Veli Lošinj, Croatia.

*June 12–16, 2024.*

| | |
|---|---|
| **I. Halasz (Zagreb, Croatia)** | *In situ powder X-ray diffraction and Raman spectroscopy for monitoring of ball-milling mechanochemistry* |
| **L. Cendron (Padua, Italy)** | *A structural view of SOS response in bacteria: how it works and how to block it* |
| **D. Pelc (Zagreb, Croatia)** | *Diffuse scattering and nanoscale correlations in quantum materials* |
| **C. Esterhuysen (Stellenbosch, South Africa)** | *The role of intermolecular interactions in chemical processes* |
| **M. Dragomir (Ljubljana, Slovenia)** | *Synthesis and structure-property relationships of selected quantum materials* |

## 31st Slovenian-Croatian Crystallographic Meeting, Rogla, Slovenia.

*June 18–22, 2025.*

| | |
|---|---|
| **R. Boehler (Tennessee, USA)** | *The power of the laser-heated diamond cell combined with electron microscopy* |
| **A. Čobić (Zagreb, Croatia)** | *Complete recrystallization of metamict allanite matrices under hydrothermal conditions* |
| **M. Gemmi (Pontedera, Italy)** | *Single crystal electron diffraction on hard and softmatter* |
| **M. Mazaj (Ljubljana, Slovenia)** | *Exploring dynamics and interactions in metal organic frameworks* |
| **E. E. McCabe (Durham, United Kingdom)** | *Designing functional materials: mechanisms and consequences of broken inversion symmetry* |

**Croatian Crystallographic Association**

**Slovenian Crystallographic Society**

# Thirty-Second Croatian–Slovenian Crystallographic Meeting

Vodice, Croatia
17–21 June 2026

## Book of Abstracts and Programme

*Edited and prepared by*

Željko Skoko

Marijana Đaković

Teodoro Klaser

Luka Pavić