

CROATIAN CRYSTALLOGRAPHIC ASSOCIATION
SLOVENIAN CRYSTALLOGRAPHIC SOCIETY

The twenty-second Croatian-Slovenian crystallographic meeting - CSCM22

Biograd, Croatia, June 12 - 16, 2013

The twenty-second Croatian-Slovenian crystallographic meeting will be held in
the HOTEL Ilirija, Biograd, Croatia,
from Wednesday to Sunday, June 12-16, 2013.
The opening of the Meeting will take place on Thursday at 8.30.

ORGANIZING COMMITTEE

Chairs

Stanko Popović, Zagreb
Ivan Leban, Ljubljana

Committee Members (in alphabetical order)

Mirjana Bijelić, Zagreb
Mario Cetina, Zagreb
Marijana Đaković, Zagreb
Amalija Golobič, Ljubljana
Nina Lah, Ljubljana
Marija Luić, Zagreb
Dubravka Matković-Čalogović, Zagreb
Anton Meden, Ljubljana
Jasminka Popović, Zagreb
Željko Skoko, Zagreb
Zoran Štefanić, Zagreb
Antun Tonejc, Zagreb
Aleksandar Višnjevac, Zagreb
Martina Vrankić, Zagreb

The Meeting is organized jointly by the *Croatian Crystallographic Association* and the *Slovenian Crystallographic Society*,
with cooperation of the *Croatian Association of Crystallographers*

The twenty-second Croatian-Slovenian crystallographic meeting - CSCM22

is financially supported by





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Thursday, June 13, 2013

7 ⁰⁰ – 8 ³⁰	Registration of participants	
8 ³⁰	Opening of the meeting	S. Popović I. Leban
8 ⁴⁰	Boris Kamenar - In memoriam	S. Popović


INVITED KEYNOTE LECTURE	Chairperson:	A. Višnjevac
9 ⁰⁰ – 9 ⁴⁵	<u>Andreas Roodt</u> Kinetics and other systematic probing of electron density at transition metal centres for application in chemical processes	1

PLENARY LECTURE	Chairperson:	J. Popović
9 ⁵⁰ – 10 ³⁵	<u>Angela Altomare</u> The challenge of crystal structure solution by Powder Diffraction Data: the EXPO software	2

10⁴⁰ – 11⁰⁰ **Coffee break****ORAL PRESENTATIONS***

Chairpersons: T. Đorđević, I. Đerđ
 *only name of the presenting author is given
 ☼ young crystallographers section

11 ⁰⁰ – 11 ¹⁰	Matic Lozinšek ☼ Structural investigations of vanadium(V) oxyfluorides	7
11 ¹⁰ – 11 ²⁰	Marijana Đaković Oxoanions in supramolecular assemblies of tridentate diamide complexes of Ni(II)	8
11 ²⁰ – 11 ³⁰	Aleksandar Višnjevac Biomimetic modelling of a mononuclear metallopeptidases active site with the triazole based tridentate ligands	9
11 ³⁰ – 11 ⁴⁰	Tanja Koleša Dobravec ☼ Diversity in supramolecular architecture of [M(acac)₂(dpa)] complexes (M = Co, Ni, Zn)	10

11 ⁴⁰ – 11 ⁵⁰	Nina Lah Copper coordination compounds with metronidazole	11
11 ⁵⁰ – 12 ⁰⁰	Marta Kasunič Isostructural series of [MII(bdmpza)₂]\cdot2H₂O compounds (bdmpza = bis(3,5-dimethylpyrazol-1-yl)acetate) with first row transition metals	12
12 ⁰⁰ – 12 ¹⁰	Milica Kosović Cobalt complexes with biologically active dithiocarbamate derivative	13
12 ¹⁰ – 12 ²⁰	Anna Moliterni The random-model-based method (RAMM) in EXPO2013	14
12 ²⁰ – 12 ³⁰	Rosanna Rizzi The Hybrid Big Bang Big Crunch in the EXPO2013 program	15
12 ³⁰ – 12 ⁴⁰	Corrado Cuocci Crystallographic study of PET radiotracers in clinical evaluation for early diagnosis of Alzheimer	16
12 ⁴⁰ – 12 ⁵⁰	Dubravka Šišak Jung High(er) accuracy in structure determination from X-ray Powder Diffraction (XPD) data using MYTHEN 24K detector	17
12 ⁵⁰ – 13 ¹⁵	Welcome drink	
14 ³⁰ – 15 ⁰⁰	Additional registration	

15⁰⁰ – 16⁰⁰ **EXPO2013 workshop**

PLENARY LECTURE		Chairperson:	M. Đaković
16 ⁰⁰ – 16 ⁴⁵	Christer B. Aakeröy From molecular sociology to functional materials		3

16⁵⁰ – 17¹⁰ **Coffee break**



ORAL PRESENTATIONS

Chairpersons: N. Lah, K. Molčanov

17 ¹⁰ – 17 ⁴⁰	Gligor Jovanovski Comprehensive study of minerals from the Republic of Macedonia	18
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17 ⁴⁰ – 17 ⁵⁰	Tamara Đorđević Mineral-like arsenates: crystal structure of $\text{Cd}_{0.77}\text{Co}_{2.73}(\text{AsO}_4)_{1.5}(\text{HAsO}_4)(\text{H}_2\text{AsO}_4)_{0.5}$	19
17 ⁵⁰ – 18 ⁰⁰	Igor Djerdj Interplay between the structural and magnetic probes in elucidation of the structure of novel 2D layered $\text{V}_4\text{O}_4(\text{OH})_2(\text{O}_2\text{CC}_6\text{H}_4\text{CO}_2)_4 \cdot \text{DMF}$	20
18 ⁰⁰ – 18 ¹⁰	Nikola Biliškov ☼ Structural and hydrogen sorption properties of $\text{SmNi}_{5-x}\text{Ga}_x$ system – an experimental and theoretical study	21
18 ¹⁰ – 18 ²⁰	Ognjen Milat Electron diffraction study of disorder in $\text{Al}_{.63}\text{Cu}_{.24}\text{Co}_{.13}$ decagonal quasiperiodic crystal	22
18 ²⁰ – 18 ³⁰	Tomče Runčevski ☼ Gymnastics in the crystal state: irreversible photodimerisation of GFP chromophore-like molecule	23
18 ³⁰ – 18 ⁴⁰	Andrej Pevec Crystal structures of carboxypyridinium hexafluoridotitanates	24
18 ⁴⁰ – 18 ⁵⁰	Marcus J. Winter Advances in X-ray Crystallography	25
18 ⁵⁰ – 19 ⁰⁰	Luca Russo Rigaku brings photon counting, shutterless detection technology to the broad Crystallographic user community: The P200 Series presented	26
19 ⁰⁰ – 19 ¹⁰	Jörg Wiesmann Beam conditioning in cutting edge X-ray analytical equipment	27

Friday, June 14, 2013

PLENARY LECTURE	Chairperson:	P. Šegedin
8 ³⁰ – 9 ¹⁵	Vladimir Bermanec	4
	The importance of collecting and investigation of mineral samples from ore deposits - example of Stari Trg (Trepča) mine	

MEETING EXCURSION

10⁰⁰



Excursion by boat to Kornati Archipelago for all participants and accompanying persons

Saturday, June 15, 2013

PLENARY LECTURE	Chairperson:	Ž. Skoko
8 ³⁰ –9 ¹⁵	Jasminka Popović Nanocrystalline metal oxides: synthesis, characterisation and application	5

PLENARY LECTURE	Chairperson:	I. Leban
9 ²⁰ – 10 ⁰⁵	Miha Jeršek Inclusions in gemstones – origin, identification and valuation	6

10¹⁰ – 10³⁰ Coffee break

ORAL PRESENTATIONS

Chairpersons: I. Brekalo, D. Cinčić

10 ³⁰ – 10 ⁵⁰	Mariusz Jaskolski Modulated protein structure with 28 molecules in the asymmetric unit solved for a tetartohedrally twinned crystal	28
10 ⁵⁰ – 11 ⁰⁰	Dubravka Matković-Čalogović Crystallographic studies of three dioxomolybdenum(VI) polymorphs and a supramolecular square complex	29
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11 ²⁰ – 11 ³⁰	Joanna Sliwiak ☼ Crystal structure of Hyp-1 protein from St John's wort in complex with melatonin	32
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11 ⁴⁰ – 11 ⁵⁰	Franka Miriam Brueckler Origami and space groups	34
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12 ⁰⁰ – 12 ¹⁰	Vladimir Stilinović Competition between charge assisted hydrogen and halogen bonding in pyridinium trichloroacetates	36

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12 ³⁰ – 12 ⁴⁰	Krištof Kranjc 1-Trityl-1H-pyrrole-2,5-dione and its derivatives as bulky dienophiles for Diels–Alder reactions	39
12 ⁴⁰ – 12 ⁵⁰	Martina Vrankić Structural study of Cr-doped barium aluminate	40

ORAL PRESENTATIONS

Chairpersons:

F. M. Brueckler, N. Biliškov

16 ⁰⁰ – 16 ¹⁰	Evgeny Goreshnik Copper(I) salts π-complexes with some allyl-derivatives of tetrazoles and thiadiazoles	41
16 ¹⁰ – 16 ²⁰	Dominik Cinčić 1:1 and 1:2 cocrystals of 4,4-bipyridine and N-bromosuccinimide: the complexes with a very short N...Br halogen bond	42
16 ²⁰ – 16 ³⁰	Ivana Brekalo ☀ Gas-solid interconversion of metalloorganic salts and coordination compounds of copper(ii) with aromatic amines	43
16 ³⁰ – 16 ⁴⁰	Nuša Hojnik ☀ Novel lanthanide(III) coordination compounds with nicotinic acid	44
16 ⁴⁰ – 16 ⁵⁰	Krešimir Molčanov Mononuclear complexes of copper(II) with chloranilic acid	45
16 ⁵⁰ – 17 ⁰⁰	Katja Krančan ☀ Novel ruthenium(II) complexes with 2-substituted 4,5-bis(methoxycarbonyl)pyridines	46
17 ⁰⁰ – 17 ¹⁰	Matjaž Kristl Preparation and crystal structures of some transition metal coordination compounds with hydroxylamine	47
17 ¹⁰ – 17 ²⁰	Saša Petriček Complexes of cobalt(II) bromide with O-donor ligands	48
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17 ⁴⁰ – 17 ⁵⁰	Elizabeta Tratar-Pirc A trinuclear nickel(II) xanthurenate complex	49

17 ⁵⁰ – 18 ⁰⁰	Miha Trdin ✨ Two new trinuclear nickel(II) halides with 2-pyridineethanol	50
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19 ²⁰ – 19 ³⁰	Nenad Judaš Controlling the outcome of mechanochemical synthesis	59

19³⁰ **Closing remarks**

Chairpersons: I. Leban, S. Popović

20⁰⁰ **Meeting Dinner**



Boris Kamenar (1929 – 2012)

Professor Emeritus Boris Kamenar, a fellow of the Croatian Academy of Sciences and Arts (CASA), a distinguished Croatian professor in Chemistry and an internationally recognized scientist and eminent intellectual, suddenly passed away in Premantura, near Pula, Croatia, on July 12, 2012.

Professor Boris Kamenar was a dedicated teacher of Inorganic Chemistry and Crystallography at all levels of study at the Faculty of Science, University of Zagreb. He was a supervisor to about thirty MSc and PhD students. He participated in many professional and public activities. He served as President of the Croatian Chemical Society and of the Union of Chemical Societies of Yugoslavia (1976–1980), Secretary of the Yugoslav Centre of Crystallography (1966–1990), President of the Croatian Crystallographic Association (1991–2005), Vicepresident and President of the European Crystallographic Committee (1978–1984). He was the representative of CASA in the Governing Board of the European Science Foundation, serving also as President of the Board for international collaboration of CASA. He was a member of World Academy of Sciences and Arts and of Macedonian Academy of Sciences and Arts. Boris Kamenar received several awards for his scientific and teaching contributions: the *Ruđer Bošković* Award, the Award of Zagreb, the State Award for Lifetime Achievements, the Medal of Božo Težak and the Medal of Chemistry Department, Faculty of Science, Zagreb.

Boris Kamenar was born on February 20, 1929 in Sušak (now Rijeka, where he attended primary and secondary school. He graduated in chemical technology at the University of Zagreb and began his professional career as an engineer at The Cranes Factory and Foundry, *Vulkan* in Rijeka, where he established the Laboratory for Chemical and Mechanical Investigations. In 1956 he joined the group of Professor Drago Grdenić at the Ruđer Bošković Institute in Zagreb working on problems of silicon and boron chemistry. In 1960 he defended PhD thesis entitled *A new method for obtaining pure silicon and boron* at the University of Zagreb. Afterwards, he was appointed Assistant, Associate and Full Professor at the Chemistry Department, Faculty of Science, University of Zagreb. He retired in 1999, and in 2000 he was awarded the status of Professor Emeritus of the University of Zagreb. In 1991 he was elected a Full Member of CASA.

B. Kamenar spent his postdoctoral research (1964/65) in the Chemical Crystallography Laboratory of Professor Dorothy C. Hodgkin, later Nobel Prize winner, in Oxford. He returned to the same Laboratory as a Visiting Fellow of All Souls College of Oxford University (1971/72). He was appointed Visiting Professor at universities of New Zealand, in 1980, 1989/90 and 1995/96. During his career, he served as Head of the Chemistry Department, Faculty of Science, as Head of Laboratory of General and Inorganic Chemistry, Chemistry Department and as Vice Dean and Dean of the Faculty of Science in Zagreb.

The scientific interest of Boris Kamenar was X-ray structural analysis of inorganic, coordination and organometallic compounds, as well as organic compounds of pharmacological importance. His scientific research began with a pioneering development of new methods of semiconductor production. He developed a new method for obtaining pure silicon and boron which was described in his PhD thesis. The results of his scientific research were published in 160 scientific papers, 20 professional papers, reported at a number of international conferences, and many of them found a place in textbooks and monographs. As an internationally renowned scientist, Boris Kamenar chaired or co-chaired a large number of national and international conferences, committees, symposia. He was initiator, principal investigator of national and international research projects.

Boris Kamenar's first structural studies were related to structures of tin(II), arsenic(III) and antimony(III) compounds with aim to elucidate the stereochemical function of the unshared electron pair. Results of these studies confirmed that Sidgwick-Powell rule could be also applied to heavy atoms. He solved a number of charge transfer complexes, and in 1973 he published, with Professor K. Prout, a review article *Crystal Structures of Electron-Donor-Acceptor Complexes* in a book *Molecular Complexes*, edited by R. Foster. Boris Kamenar was involved in the X-ray structure determination of a large number of mercury(I) and mercury(II) compounds and complexes of iron, nickel, copper, niobium and molybdenum. He and his co-worker Branko Kaitner wrote a review article on iron complexes in the book *Structural Studies on Molecules of Biological Interest* in honour of Dorothy Hodgikin (Clarendon Press, Oxford 1981). Boris Kamenar was primarily engaged in investigation of molybdenum complexes and polyoxomolybdates, which can serve as models for understanding the structure and function of enzymes and also as catalysts in a vast number of chemical processes. He and his coworkers solved a significant number of such structures containing molybdenum in different oxidation states and surrounded by different type of ligands, especially those containing nitrogen, sulfur and oxygen.

Boris Kamenar was involved in investigations of biologically and pharmacologically important organic compounds and their structures. His first result in this area, published in 1965, was the molecular structure of Eschenmoser's *pseudo-corrin*, a compound obtained from the final stage of Eschenmoser's synthesis of corrin. A very nice research in which he participated was the determination of the crystal structure of a class of new azalide macrocyclic antibiotics (azitromycin) (1987) and potential antihyperglycemics from the class of dioxepino-azirines. This research was the result of his long-term cooperation with the Research Institute of the PLIVA Pharmaceutical Company. He solved the crystal and molecular structure of histamine H₂-receptor antagonist Burimamid, a new type of drug. This investigation was performed in collaboration with Smith, Klein and French Laboratories Ltd.

All of those who knew Professor Boris Kamenar will remember him as a meritorious scientist and professional. His colleagues and co-workers will miss much his strong, pleasant and optimistic personality.

Marina Cindrić, Chemistry Department, Faculty of Science, University of Zagreb