

## THURSDAY, June 15, 2017

8<sup>00</sup> - 9<sup>40</sup> **REGISTRATION OF PARTICIPANTS**

9<sup>45</sup> **OPENING REMARKS**

Chairpersons: A. Meden  
D. Matković-Čalogović

### **MORNING SESSION**

10<sup>00</sup> **PLENARY LECTURE**

Chairperson: D. Matković-Čalogović

**DIETMAR STALKE**

100 YEARS LEWIS DIAGRAM - STILL VALID IN THE LIGHT OF  
CHARGE DENSITY?

11<sup>00</sup> **COFFEE BREAK**

**ORAL PRESENTATIONS**

Chairpersons: M. Lozinšek  
M. Jurić

11<sup>20</sup> **Horst Puschmann, Oleg V. Dolomanov**  
WHAT'S NEW IN OLEX2?

11<sup>40</sup> **Sabina Grabner, Barbara Modec**  
ZINC COMPLEXES WITH CURCUMINATE

11<sup>50</sup> **Luka Šmital, Mladen Borovina, Marijana Đaković**  
FINE-TUNING THE SUPRAMOLECULAR SYNTHETIC  
CONDITIONS OF ACAC-BASED CU(II) COMPLEXES WITH A  
SERIES OF PYRIDILOXIMES

12<sup>00</sup> **Darko Vušak, Inka Kirasić, Biserka Prugovečki, Dubravka Matković-Čalogović**  
SYNTHESES AND CRYSTAL STRUCTURES OF THE ESSENTIAL  
METAL COMPLEXES WITH 2,2'-IMINODIACETAMIDE

12<sup>10</sup> **Marta Počkaj, Matjaž Mazaj, Venčeslav Kaučič, Nataša Zabukovec Logar**  
TWO-DIMENSIONAL MAGNESIUM COORDINATION  
COMPOUND WITH 4,4'-BIPHENYLDICARBOXYLATO LIGAND

12<sup>20</sup> **Martin Adam**  
THE D8 ADVANCE FAMILY OF XRD SOLUTIONS

12<sup>30</sup> LUNCH BREAK

## AFTERNOON SESSION

13<sup>30</sup> PLENARY LECTURE Chairperson: J. Stare

**ELENA BOLDYREVA**

HIGH-PRESSURE STUDIES OF ORGANIC AND  
COORDINATION COMPOUNDS

14<sup>30</sup> COFFEE BREAK

ORAL PRESENTATIONS

Chairpersons: F. Perdih  
N. Judaš

14<sup>50</sup> **Andreas Roodt, Carla Pretorius, Alice Brink, Ferdi Groenewald,**  
**Pennie P. Mokolokolo, Jeanet Conradie, Dumisani V. Kama**  
METALS 'COMMUNICATING' IN DINUCLEAR Rh(I)  
COMPLEXES?

15<sup>10</sup> **Luka Fotović, Vinko Nemec, Vladimir Stilinović, Dominik Cinčić**  
INFLUENCE OF EXPERIMENTAL CONDITIONS ON THE  
CRYSTALLIZATION OF A SCHIFF BASE COPPER(II) COMPLEX

15<sup>20</sup> **Neven Strukan**  
AERIS - NEW BENCHTOP X-RAY DIFFRACTOMETER FROM  
PANALYTICAL

15<sup>35</sup> **Marijana Đaković, Ivan Kodrin, Željka Soldin, Christer B. Aakeröy**  
TOWARDS TAILORING OF METAL-CONTAINING BENDING  
CRYSTALS

15<sup>45</sup> **Miha Virant, Martin Gazvoda, Andrej Pevec, Janez Košmrlj**  
PALLADIUM(II) COMPLEX WITH PYRIDINE-SUBSTITUTED  
MESOIONIC LIGANDS

15<sup>55</sup> **Mihael Eraković, Vladimir Stilinović, Dominik Cinčić**  
MODELLING THE POSITION OF HALOGEN ATOMS IN THE  
CRYSTALS CONTAINING HALONIUM IONS

16<sup>05</sup> **Martin Gazvoda, Andrej Pevec, Janez Košmrlj**  
X-RAY DIFFRACTION ANALYSIS AS A KEY TOOL TO  
DETERMINE STEREOCHEMICAL OUTCOME OF ALDOL  
REACTION ON  $\beta$ -AMINO ACIDS

- 16<sup>15</sup> Andrej Jaklin, Željko Skoko, Stanko Popović, Sanda Rončević, Ivan Nemet, Frederic Marin, Davorin Medaković  
BIOMINERALIZATION IN THE EMBRYOS OF  
SEA SLUG *APLYSIA CALIFORNICA* COOPER, 1863
- 16<sup>25</sup> **BREAK**
- 16<sup>40</sup> Vladimir Stilinović, Dominik Cinčić  
SYNTHON CONSERVATION UPON CHANGING THE CONTACT  
ATOM IN SACCHARIN AND *N*-HALOGENOSACCHARIN  
COCRYSTALS
- 16<sup>55</sup> Evgeny Goreschnik, Andrii Vakulka  
SOME PRODUCTS OF COPPER DISSOLVING IN A  
CHAL<sub>4</sub> - DMSO MIXTURE
- 17<sup>05</sup> Ivica Đilović, Krunoslav Užarević  
COORDINATION PREFERENCES OF PERCHLORATE ANIONS  
IN COMPLEXES WITH FLEXIBLE RECEPTOR
- 17<sup>15</sup> Kristian Radan, Boris Žemva  
CRYSTALLIZATION AND STRUCTURAL PECULIARITIES OF  
XENON(II) COMPOUNDS WITH POLYMERIC FLUORIDO  
ANIONS
- 17<sup>25</sup> Jernej Stare  
ENRICHING CRYSTALLOGRAPHIC STUDIES WITH THEORY:  
QUANTUM CHEMISTRY
- 17<sup>40</sup> Ivan Kodrin, Vedran Barbarić, Marijana Đaković  
CALCULATION OF MOLECULAR ELECTROSTATIC POTENTIAL  
OF COORDINATION POLYMERS
- 17<sup>50</sup>-18<sup>00</sup> Matjaž Mazaj, Gregor Mali, Nataša Zabukovec Logar  
STRUCTURE DYNAMICS OF CALCIUM TEREPHTHALATE  
MOF-TYPE MATERIAL UPON HEATING AND HYDRATION
- 18<sup>15</sup> **OLEX2 WORKSHOP (PART I)**

**FRIDAY, June 16, 2017**

**MORNING SESSION**

9<sup>00</sup> **PLENARY LECTURE** Chairperson: A. Meden

**MARJAN MARINŠEK, GREGOR KAPUN, TINA SKALAR**  
3D MICROSTRUCTURE RECONSTRUCTION FROM STACK OF  
2D IMAGES DEMONSTRATED ON Ni-SDC CERMETS

10<sup>00</sup> **COFFEE BREAK**

**ORAL PRESENTATIONS**

Chairpersons: A. Pevec  
M. Gotić

10<sup>20</sup> **Franc Perdih, Simona Pavlin, Matic Šobak**  
STRUCTURAL DIVERSITY IN SILVER COMPLEXES WITH  
4,4,4-TRIFLUORO-1-PHENYLBUTANE-1,3-DIONATO LIGAND

10<sup>30</sup> **José Fernandes, Teodor Klaser, Željko Skoko**  
NEW INSIGHTS ABOUT THE THERMOSALIENT EFFECT

10<sup>40</sup> **Bor Lucijan Turek, Marijan Kočever, Franc Perdih, Krištof Kranjc**  
SYNTHESIS OF A MACROCYCLE DERIVED FROM 2H-PYRAN-2-  
ONE DERIVATIVE AND A DOUBLE DIENOPHILE BASED ON  
MALEIMIDE

10<sup>50</sup> **Nikola Bedeković, Vladimir Stilinović, Dominik Cinčić**  
NEW HALOGEN BONDED COCRYSTALS OF 1,3-  
DIIODOTETRAFLUOROBENZENE WITH ORGANIC BASES

11<sup>00</sup> **Andrej Hoivik, Franc Perdih, Krištof Kranjc**  
2H-PYRAN-2-ONES AS DIENES IN THE FORMATION OF  
BICYCLO[2.2.2]OCTENES AND FURTHER TRANSFORMATIONS

11<sup>10</sup> **Marcus J. Winter**  
ADVANCES IN X-RAY CRYSTALLOGRAPHY

11<sup>30</sup> **BREAK**

- 11<sup>40</sup> **Anton Gradišek**  
WHAT CAN NMR TELL US ABOUT MOLECULAR DYNAMICS IN HYDROGEN-STORAGE MATERIALS?
- 11<sup>50</sup> **Kristina Smokrović, Ivica Đilović, Dubravka Matković-Čalogović**  
MOLECULAR RECOGNITION OF AMINO ACIDS IN THE SOLID STATE: A MIXED CU(II) COMPLEX AND CO-CRYSTALS WITH UREA AND PYRIDINE DERIVATIVES
- 12<sup>00</sup> **Katja Traven, Jure Stojan, Jakob Kljun, Sara Seršen, Tea Lanišnik Rižner, Iztok Turel**  
RUTHENIUM(II) COMPOUNDS AS POTENTIAL INHIBITORS OF ALDO-KETO REDUCTASES
- 12<sup>10</sup> **Tomislav Piteša, Vladimir Stilinović, Gordan Horvat**  
EXPERIMENTAL STUDY AND MD SIMULATIONS OF ACETONE VAPOR EFFECTS ON POLYMORPHIC PHASE TRANSITION IN DIBENZOYLMETHANE
- 12<sup>20</sup> **Tamara Đorđević, Sabrina Gerger, Marko Jagodič, Zvonko Jagličić**  
MAGNETOSTRUCTURAL CORRELATIONS OF SELECTED DIVALENT TRANSITION METAL ARSENATES: AN UPDATE
- 12<sup>30</sup> **Jakob Kljun, Katja Traven, Jure Stojan, Tea Lanišnik Rižner, Iztok Turel**  
RUTHENIUM COMPLEXES OF LIGAND PYRITHIONE WITH POTENT INHIBITION OF AKR1C ENZYMES AND ANTICANCER ACTIVITY
- 12<sup>40</sup> **Vesna Zalar Serjun, Ana Mladenović**  
CHARACTERIZATION OF MINERAL PHASES FORMED DURING THE HYDRATION OF DIFFERENT RECYCLED MATERIALS
- 12<sup>50</sup> **Matic Lozinšek**  
A RARE EXAMPLE OF XENON DIFLUORIDE COORDINATION TO SODIUM ION
- 13<sup>00</sup> **LUNCH BREAK**
- AFTERNOON**
- 15<sup>00</sup> Conference trip with dinner at Ljubljana castle (19<sup>00</sup>).

## SATURDAY, June 17, 2017

### MORNING SESSION

- 9<sup>00</sup> **OLEX2 WORKSHOP (PART II)**
- 10<sup>00</sup> **PLENARY LECTURE** Chairperson: A. Golobič
- JEREMY KARL COCKCROFT**  
POWDER DIFFRACTION: AN ESSENTIAL COMPLEMENTARY  
TOOL FOR THOSE SKILLED IN THE ART BUT ONE WITH  
PITFALLS FOR THE UNWARY
- 11<sup>00</sup> **COFFEE BREAK**
- ORAL PRESENTATIONS** Chairpersons: M. Počkaj  
I. Đilović
- 11<sup>20</sup> **Andrej Pevec, Patricija Hribar, Janez Košmrlj**  
COORDINATION COMPOUNDS WITH  
METHOXYCARBONYLMETHYL-N-(2-PYRIDYL)THIOUREA AS  
A LIGAND
- 11<sup>30</sup> **Marijana Jurić, Lidija Androš Dubraja, Filip Torić, Damir Pajić**  
STRUCTURAL AND MAGNETIC INVESTIGATIONS OF  
[CR<sup>III</sup>NB<sup>V</sup>] COMPOUNDS; ANTIFERROMAGNETIC COUPLING  
OF CR<sup>III</sup> THROUGH -O-NB<sup>V</sup>-O- BRIDGES
- 11<sup>40</sup> **Mateja Štefančič, Anton Meden, Ana Mladenovič**  
THE QUANTITATIVE ANALYSIS OF HYDRATING PORTLAND  
CEMENT INVESTIGATED BY MEANS OF IN-SITU XRD
- 11<sup>50</sup> **Lidija Kanižaj, Krešimir Molčanov, Marijana Jurić**  
1D HETEROMETALLIC [CU<sup>II</sup>CR<sup>III</sup>] OXALATE- AND  
CHLORANILATE-BRIDGED CHAINS
- 12<sup>00</sup> **Amalija Golobič, Leja Erzin**  
A HYDRATE OF NEW COPPER(II) COMPLEX WITH PYRIDINE,  
CARBONATO AND METHANOATO LIGANDS

12<sup>10</sup> **Ivan Marić, Goran Štefanić, Marijan Gotić**  
STRUCTURAL AND PHOTOCATALYTICAL PROPERTIES OF  
HYDROTHERMALLY SYNTHESIZED IRON/TITANIUM OXIDE  
NANOPARTICLES

12<sup>20</sup> **Saša Petriček**  
COMPLEXES OF MANGANESE(II) OR NICKEL(II) CHLORIDES  
AND 3-HYDOXYPYRIDIN-2-ONE

12<sup>30</sup> **LUNCH BREAK**

## AFTERNOON SESSION

13<sup>30</sup> **PLENARY LECTURE** Chairperson: M. Đaković

**KREŠIMIR MOLČANOV**  
STACKING OF PLANAR CONJUGATED RINGS - BEYOND  
AROMATICS

14<sup>30</sup> **COFFEE BREAK**

**ORAL PRESENTATIONS** Chairpersons: S. Petriček  
V. Stilinović

14<sup>50</sup> **Till A. Samtleben**  
STOE - TRADITION OF INNOVATION SINCE 1887

15<sup>00</sup> **Aleksandar Meštrić, Nenad Judaš**  
TETRA- $\mu$ -BENZOATO- $k^8O_8$ -BIS[(*N,N*-  
DIETHYLFORMAMIDE- *KO*)DICOPPER(II)]

15<sup>10</sup> **Jean Marcel Ateba Mba, Robert Dominko**  
A NEW CLASS OF POWERFUL MATERIALS FOR  
ELECTROCHEMICAL ENERGY STORAGE: LITHIUM-RICH  
OXYFLUORIDES WITH CUBIC DENSE PACKING

- 15<sup>20</sup> Andraž Krajnc, Jure Varlec, Matjaž Mataj, Alenka Ristić, Nataša Zabukovec Logar, Gregor Mali  
STRUCTURAL INVESTIGATION OF HYDRATED ALUMINOPHOSPHATES
- 15<sup>30</sup> Aleš Štefančič, Gyöngyi Klupp, Tilen Knaflič, Dmitry S. Yufit, Anton Potočnik, Denis Arčon, Andrew Beeby  
ALKALI-METAL TRIPHENYLIDES: STRUCTURE MAGNETISM RELATIONSHIP
- 15<sup>45</sup> Valentina Milašinović, Krešimir Molčanov  
NITRANILIC ACID - A NOVEL LIGAND FOR CONSTRUCTION OF COORDINATION POLYMERS
- 15<sup>55</sup> Nejc Rozman, David M. Tobaldi, Robert C. Pullar, João A. Labrincha, Andrijana Sever Škapin  
PHOTOCATALYTIC AND PHOTOCHROMIC Cu-TiO<sub>2</sub> HYBRID NANOMATERIAL
- 16<sup>05</sup> Matija Uršič, Tanja Lipec, Anton Meden, Iztok Turel  
A STRUCTURAL STUDY OF SOME RUTHENIUM-DIKETONATE COMPLEXES
- 16<sup>15</sup> Teodoro Klaser, Željko Skoko, Serena C. Tarantino, Michele Zema  
IS NEGATIVE THERMAL EXPANSION GOVERNING FORCE FOR THERMOSALIENT EFFECT?
- 16<sup>25</sup> **BREAK**
- 16<sup>35</sup> Andraž Oštrek, Matic Lozinšek  
VANADIUM(V) OXYFLUORIDES DERIVED FROM VOF<sub>3</sub> AND SMALL NITROGEN BASES
- 16<sup>45</sup> Mladen Borovina, Ivan Kodrin, Marijana Đaković  
COMPUTATIONALLY AUGMENTED CRYSTALLOGRAPHIC STUDY OF HYDROGEN/HALOGEN BOND SWITCHING IN SELECTED CO<sup>II</sup> AND NI<sup>II</sup> PENTANE-2,4-DIONATO COMPLEXES
- 16<sup>55</sup> Marko Tomić, Mladen Borovina, Marijana Đaković  
COPPER(II) HALIDE COMPLEXES WITH PYRIDINE-OXIME LIGANDS

- 17<sup>05</sup> **Valentina Borko, Goran Štefanić**  
IMPACT OF SYNTHETIC ROUTE ON THE STRUCTURAL AND  
MICROSTRUCTURAL CHANGES IN THE ZrO<sub>2</sub>-CaO SYSTEM
- 17<sup>15</sup> **Bojan Kozlevčar, Marta Počkaj**  
TRIAZOLE LIGANDS WITH BULKY SIDE GROUPS IN  
COORDINATION COMPOUNDS' ARCHITECTURE
- 17<sup>25</sup> **Ivica Petar Čališ, Mladen Borovina, Marijana Đaković**  
ONE-POT MECHANOCHEMICAL SYNTHESIS OF ACAC-BASED  
COPPER(II) COMPLEXES WITH OXIMES
- 17<sup>35</sup> **Mario Cetina, Zoran Džolić**  
INTERMOLECULAR INTERACTIONS IN TWO  
CONSTITUTIONALLY ISOMERIC ANTHRACENE-BASED  
OXALAMATES FORM TWO-DIMENSIONAL NETWORKS
- 17<sup>45</sup> **Ivan Leban, Stanko Popović**  
COMMON CRYSTALLOGRAPHIC MEETINGS  
(CROATIA-SLOVENIA-ITALIA-EUROPE) 1966-2017

18<sup>00</sup> **CLOSING REMARKS**

Chairpersons: D. Matković Čalogović  
A. Meden