

XXIX. INTERNATIONAL CONFERENCE
ON COORDINATION AND BIOINORGANIC CHEMISTRY

SCIENTIFIC PROGRAM

MONDAY, 3 June 2024


Room 1

9:00 **OPENING**

**9:15 – 11:30 Plenary Lectures A
ELECTRONIC, MOLECULAR AND CRYSTAL STRUCTURES**

Room 1

Chairman: M. Yamashita

9:15 – 10:00 R. Herchel (*Czech Republic*)  34
**Molecular Nanomagnets – a Perspective Playground for Theorists and
Experimentalists**

10:00 – 10:30 P. Baran (*USA*)  17
Back to My N-oxide Roots

10:30 – 11:00  *Coffee break*

11:00 – 11:30 S. Hsu (*Taiwan*)  35
**Understanding Nitrite Reduction Through Bio-Inspired Copper
Complexes**


**14:30 – 16:30 Section Lectures A
ELECTRONIC, MOLECULAR AND CRYSTAL STRUCTURES**

Room 1

Chairman: R. Herchel

14:30 – 14:45 M. Breza (*Slovakia*)  20
**DFT Studies of Triangulo Cobalt-Hydride Clusters with
Trimethylphosphine and Carbonyl Ligands**




14:45 – 15:00 M. Gall (*Slovakia*)  29
Neural Networks Prediction of Docking Scores

15:00 – 15:15 I. Jelemenská (*Slovakia*)  37
**Comparative DFT Study of the Effectiveness of p-phenylenediamine
Antioxidants Through Their Coordination Ability Towards the Selected
Transition Metals**

15:15 – 15:45  *Coffee break*

Room 1

Chairman: P. Baran

- 15:45– 16:00 J. Moncol' (*Slovakia*)  60
Common and Unusual Isomerism of Copper(II) Carboxylate Complexes
- 16:00 – 16:15 J. Pavlik (*Slovakia*)  68
Pentacoordinate Co(II) SIMs: Chlorides Over Bromides?
- 16:15 – 16:30 J. Švorec (*Slovakia*)  88
Multinuclear Copper(II) Complexes of Pyridine-2,6-dicarboxamide Based Ligands

TUESDAY, 4 June 2024

8:30 – 11:45 Plenary Lectures B SOLUTION AND SOLID STATE REACTIVITY

Room 1 *Chairman: I. Pantcheva*

8:30 – 9:15 J. Krzystek (*USA*) 📖 44
Single-Molecule Magnetism: History and Current Trends

9:15 – 9:45 B. Kutus (*Hungary*) 📖 47
The Chemistry of Bauxite Residue Neutralization

9:45 – 10:15 N. N. Murthy (*India*) 📖 61
O₂ and t-BuO₂H Reactivity of Cobalt and Iron Complexes with Anisole-Appended Tetradentate Ligand: Impact of Coligands

10:15 – 10:45 ☕ *Coffee break*

Room 1 *Chairman: B. Drahoš*

10:45 – 11:15 R. Routaboul (*France*) 📖 77
Post-Synthetic Modification Mechanism for 1-D Spin Crossover Coordination Polymers

11:15 – 11:45 I. Pantcheva (*Bulgaria*) 📖 66
Sodium Monensin and its Divalent Metal Complexes with Different Coligands

14:00 – 16:15 Section Lectures B SOLUTION AND SOLID STATE REACTIVITY





Room 1 *Chairman: J. Krzystek*

14:00 – 14:15 Z. Baranová (*USA*) 📖 18
Syntheses of Schiff-Base Ligands Derived from Pyridine *N*-oxides and Their Transition Metal Complexes










14:15 – 14:30 B. Drahoš (*Czech Republic*) 📖 27
Tuning of Magnetic Properties in Pentagonal Bipyramidal Complexes with Macrocyclic Ligands

14:30 – 14:45 Y. Lai (*France*) 📖 49
From PSM Reaction on Iron-Triazole Spin-Crossover Complexes to Their Use in Catalysis

14:45 – 15:15 ☕ *Coffee break*

- 15:15 – 15:30 R. Szabados Mészáros (*Hungary*)  57
Continuous Flow Synthesis of Furanic Ethers by Etherification of Furanic Alcohols Catalysed by Kaolinite
- 15:30 – 15:45 J. Papp (*Hungary*)  67
Synthesis, Characterization and HCl Titration Studies of Al-substituted Fe-(oxi)-hydroxide Phases
- 15:45 – 16:00 G. Peintler (*Hungary*)  69
Solubility Measurements in Solutions of Ca(II) Gluconate Hydroxide Complexes
- 16:00 – 16:15 P. Sipos (*Hungary*)  79
The Conversion of Li_2CO_3 to LiOH Using $\text{Ca}(\text{OH})_2$

20:00 – 21:30 Posters

- 1 S.-H. Chen (*Taiwan*)  21
Synthesis and Reactivity of the Unsymmetrical β -Diketiminato Nickel Complexes
- 2 M. Červeňáková (*Slovakia*)  25
Exploring the Structural, Spectral, and Magnetic Properties of Metal Complexes with Biologically Active Ligands: Insights into Complex-DNA Interactions
- 3 H. Fedorenko (*Ukraine*)  28
Dinuclear Ln(III) Complexes with p-tert-butylcalix[4]arene: Structure and Luminescence
- 4 L. Habala (*Slovakia*)  32
Fluorine-Containing Schiff Bases and Their Metal Complexes: Structure and Bioactivity
- 5 I. Ivanov (*Bulgaria*)  36
Divalent Metal Complexes of Sodium Monensin Bearing Thiocyanate Ligands
- 6 M. Kepeňová (*Slovakia*)  39
Palladium(II) Complexes with Derivatives of 8-hydroxyquinoline and Dimethyl Sulfoxide
- 7 M. L. Kis (*Hungary*)  40
Complexes of Monensin A with Divalent Metal Ions – A Solution Study
- 8 A. Koščíková (*Slovakia*)  42
On the 3d/4f Heterobimetallic Complexes Based on Bicompartmental Schiff Base Type Ligands
- 9 J. Kurjan (*Slovakia*)  45
Cu(II) and Ag(I) Complexes of 4-hydroxycoumarin Derivative: Synthesis, Structure and Biological Activity






- 10 L. Kurowski (*Poland*)  46
Strength in Weakness – Nitrile Silver(I), Copper(I) and Copper(II) Complexes for Organic-Inorganic Electronics
- 11 G. Kuzderová (*Slovakia*)  48
Structural and Biological Evaluation of Silver(I) Complexes with Proline and Hydroxyproline
- 12 M. Matiková Mařarová (*Slovakia*)  56
Simple Iron Complexes with Sulfato Ligands and Their Thermal Behavior and Magnetic Properties
- 13 K. Musza (*Hungary*)  62
Reaction Kinetics in the Secondary School Chemistry Teaching: Experimental Determination of the Partial Reaction Order
- 14 N. Petkov (*Bulgaria*)  70
Two-directional Approach in the Study of Cerium Monensinates – Experimental Evaluation and Molecular Modelling
- 15 K. Petrželová (*Czech Republic*)  71
Half-Sandwich Ru, Os, Rh, Ir Complexes with 2-(2-(diphenylphosphino)ethyl)-pyridine
- 16 E. Pivovarova (*Poland*)  72
Metal-Based Compounds: Synthesis and Characterization of New Thiazole-based Iridium and Palladium Complexes with Potential Anticancer Properties
- 17 M. Puchoňová (*Slovakia*)  75
Study of Benzoatocopper(II) Complexes with Benzimidazole Derivatives
- 18 R. Smolko (*Slovakia*)  80
Pentacoordinate Ni(II) Complexes Using a 3+2 Approach: Synthetic Strategy and Crystal Structures
- 19 S. Šterbinská (*Czech Republic*)  87
Novel Multicomponent Os and Ru Compounds as Potential Anticancer Drugs
- 20 S. Stoykova (*Bulgaria*)  81
X-ray Structures and Spectral Properties of Heteronuclear Monensinates [Co(MonNa)₂(NO₃)₂] and [Mn(MonNa)₂(NO₃)₂]
- 21 J. Tomičová (*Slovakia*)  90
Octahedral Iron Complexes with Halogen Derivatives of 1,10-phenanthroline
- 22 S. Vitushkina (*Slovakia*)  94
Di- and Trinuclear Complexes of Co(II) with 1,3-phenylenediamine-Based Schiff Bases
- 23 E. Zahradníková (*Czech Republic*)  97
Chemistry of Macrocyclic Ligands and Their Co(II) Complexes: Preparation, Structure and Magnetism

WEDNESDAY, 5 June 2024

8:30 – 10:45 Plenary Lectures C APPLIED INORGANIC AND COORDINATION CHEMISTRY

Room 1




Chairman: P. Sipos

- 8:30 – 9:15 M. Yamashita (*Japan*)  95
Molecular Spin Qubits toward Quantum Computer and High-Density Memory Devices Based on Molecular Magnets
- 9:15 – 9:45 M. Onani (*South Africa*)  65
Gold Nanoparticles Synthesized by Red Wine Extracts Promote Growth of Skin Fibroblast, Implicating Their Application in Wound Healing
- 9:45 – 10:15 R. Podgajny (*Poland*)  73
New Synthons for Shaping Optical Properties: Charge Transfer, Second Harmonic Generation, and Photoluminescence
- 10:15 – 10:45 M. Szabados (*Hungary*)  82
Modification of the Framework of Layered Double Hydroxides by Mechanical Stresses
- 10:45 – 11:15  *Coffee break*

11:15 – 12:00 Section Lectures C APPLIED INORGANIC AND COORDINATION CHEMISTRY

Room 1




Chairman: B. Kutus

- 11:15 – 11:30 A. Dołęga (*Poland*)  26
Structural Considerations of Thiazolothiazoles and Bithiazoles: Evaluating Planar Systems in the Formation of Complexes with *d*-block Metals
- 11:30 – 11:45 A. Romanov (*UK*)  76
Carbene-Metal-Amide Energy Materials for Application in Organic Light-Emitting Devices
- 11:45 – 12:00 D. Taher (*Jordan*)  89
Synthesis of Chloro-Substituted β -Ketimate Palladium Complexes, Spectral and Thermal Investigation of Their Structures

11:15 – 12:00 Section Lectures C
APPLIED INORGANIC AND COORDINATION CHEMISTRY

Room 2

Chairman: M. Onani

- 11:15 – 11:30 M. Malček (*Slovakia*)  52
Computational Study of Carbon Nanomaterials as Hydrogen Adsorbents
- 11:30 – 11:45 M. Malček Šimunková (*Slovakia*)  53
TiO₂/Taxifolin as Interfacial Charge Transfer (ICT) Complex
- 11:45 – 12:00 R. Šípoš (*Slovakia*)  85
Photocatalytic Degradation of Diclofenac in Water by Modified g-C₃N₄ and Biochar Under UV-A and Visible Light




15:15 – 18:30 Excursion to the Castle ČERVENÝ KAMENŤ

THURSDAY, 6 June 2024

9:00 – 10:15 Plenary Lectures D COMPLEXES IN HUMAN MEDICINE AND THE ENVIRONMENT

Room 1






Chairman: B. Gyurcsik

- 9:00 – 9:45 N. Metzler-Nolte (*Germany*)  58
Bioinorganic Approaches to Overcome Antimicrobial Resistance
- 9:45 – 10:15 T. Marzo (*Italy*)  55
Unveiling the Mechanism of Action of Pharmaceutical Inorganic Compounds: Challenges and Future Prospects
- 10:15 – 10:45  Coffee break

10:45 – 12:00 Section Lectures D COMPLEXES IN HUMAN MEDICINE AND THE ENVIRONMENT

Room 1

Chairman: N. Metzler-Nolte




- 10:45 – 11:00 B. Gyurcsik (*Hungary*)  31
Double Selection of the Metal Ions by the TEM-1 Beta-Lactamase/Ampicillin System
- 11:00 – 11:15 F. Jozefíková (*Slovakia*)  38
Flufenamato-/Niflumato-copper(II) Complexes with Very Akin Chemical Composition but Diametrically Different Molecular Structure. What About Their Biological Activity?
- 11:15 – 11:30 P. Kopel (*Czech Republic*)  41
Biologically Active Benzimidazole Complexes
- 11:30 – 11:45 Y.-F. Lin (*Taiwan*)  50
DFT Mechanistic Insights into Nitric Oxide Generation from Nitrite via O-atom Transfer in the Unsymmetrical β -Diketiminato Copper(II) Complexes
- 11:45 – 12:00 J. Valentová (*Slovakia*)  92
Copper(II) Complexes with Schiff Bases Derived from 2-pyridinecarbaldehyde N-oxide and Amino Acids: Studies on DNA Binding, Nuclease Activity, and Cytotoxicity

10:45 – 11:45 Section Lectures D COMPLEXES IN HUMAN MEDICINE AND THE ENVIRONMENT

Room 2

Chairman: T. Marzo

- 10:45 – 11:00 R. Křikavová (*Czech Republic*)  43
Can Ta(V) Half-Sandwich Complexes Compete with the Established 5d Metal-based Anticancer Agents?

- 11:00 – 11:15 I. Potočník (*Slovakia*)  74
Zirconium Complexes with 8-hydroxyquinoline Derivatives
- 11:15 – 11:30 P. Štarha (*Czech Republic*)  86
Transition Metal Complexes for Cancer Therapy
- 11:30 – 11:45 N. Tsaulwayo (*South Africa*)  91
Role of Heterocyclic Atom and Steric Effect of Mononuclear $N^{\wedge}N$ - Ru(II) Towards Biological Activities









14:00 – 14:15 Special Wiley Lecture

Room 1 *Chairman: M. Breza*

- 14:00 – 14:15 K. Glatz (*Germany*)
Opening the Editor's Black Box: Insider Tips for Successful Submissions

14:15 – 17:15 Young Scientists Section

Room 1 *Chairman: M. Breza*

- 14:15 – 14:25 K. Chmur (*Poland*)  22
Potential Antitumour Properties of Oxidovanadium(IV) Compounds on a Human Osteosarcoma
- 14:25 – 14:35 B. Cieřla (*Poland*)  23
Zinc and Cadmium Silanethiolates in Search of New Approaches for Luminescent Materials
- 14:35 – 14:45 A. Climova (*Poland*)  24
New Zn(II) Complexes as Potential Anticancer Agents: From Synthesis to Structure
- 14:45 – 14:55 K. Gutmańska (*Poland*)  30
New Pathways for Synthesis of Thiazolothiazoles, Bithiazoles, and Their Metal Complexes: Investigating Properties and Applications
- 14:55 – 15:05 P. Halař (*Czech Republic*)  33
Photomagnetically Active Molecular Magnets
- 15:05 – 15:15 M. Liřtiak (*Slovakia*)  51
New Copper(II) and Palladium(II) Salicylate Complexes with Chelating N,N -donor Ligands
- 15:15 – 15:25 N. Malinová (*Slovakia*)  54
Penta- and Heptacoordinated Cobalt(II) Single-Ion Magnets with Tridentate N -donor Ligand
- 15:25 – 15:35 T. Mgijima (*South Africa*)  59
Green Synthesis of Gold Nanoparticles for Wound Healing

15:35 – 16:05  *Coffee break*

Room 1

Chairman: P. Kopel

- 16:05 – 16:15 S.-B. Nagy (*Hungary*)  63
Lanthanum-Based Cuprate Perovskites for Catalytic Triazine Formation via Acceptorless Dehydrogenative Coupling
- 16:15 – 16:25 A. Nemčovič (*Slovakia*)  64
Synthesis and Photoswitchable Properties of New Tridentate Arylazopyridine-substituted Benzothiazole Ligands and Their Cobalt(II) Complexes
- 16:25 – 16:35 V. Szabó (*Hungary*)  83
Incorporation of Mn, Ni, Cu and Zn Ions into CoAl₄ Layered Double Hydroxide Catalyst Precursors
- 16:35 – 16:45 Y. Szabó (*Hungary*)  84
Synthesis of Katoite Phases, Their Characterization and Neutralization Reactions
- 16:45 – 16:55 R. Varga (*Slovakia*)  93
Hirshfeld Surface Analysis of Nickel(II) Complexes with 2-aminomethylbenzimidazole
- 16:55 – 17:05 T.-S. Yang (*Taiwan*)  96
Ligand Control on the Geometry and Spin-State of Unsymmetrical β -Diketiminato Nickel(II) Complexes
- 17:05 – 17:15 B. Zowiślok (*Poland*)  98
From Stimuli-Responsive Emission to Rare AIE Phenomenon in Platinum(II) Terpyridyl Complex

Room 1

17:15 **CLOSING**