

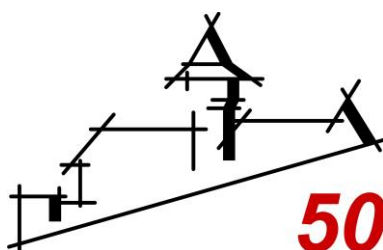
**XXV. INTERNATIONAL CONFERENCE
ON COORDINATION AND BIOINORGANIC CHEMISTRY**

**Advancing Coordination, Bioinorganic and Applied
Inorganic Chemistry**

The 50th Anniversary of ICCBIC

*May 31 – June 5, 2015
Smolenice, Slovakia*

BOOK OF ABSTRACTS



PROGRAM

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**Slovak Chemical Society
Radlinského 9, 812 15 Bratislava
Slovakia**

**Advancing Coordination, Bioinorganic and Applied Inorganic Chemistry
The 50th Anniversary of ICCBIC
M. Melník, P. Segľa, and M. Tatarko (Eds.)**

**Book of Abstracts
Monograph**

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Abstracts of papers published in the Book of Abstracts are printed as submitted. Full papers published in USB-monograph were reviewed and the opinion of the referees was deciding for incorporating a paper into the monograph.

The contributions have been edited by the editors only to the extent considered necessary and according to recommendations of the referees, naturally with the consent of the authors. The experimental data given in particular abstracts and/or papers, the conclusions expressed and the general style adopted remain, however, the responsibility of the named authors. Great care has been taken to maintain the accuracy of the information contained in the volume. However, neither Slovak Chemical Society nor the editors can be held responsible for errors, linguistic or numerical. Authors were themselves responsible for referring to appropriate and complete references and for obtaining the necessary permission to reproduce copyright materials and data from other sources.

PREFACE

The XXV. International Conference on Coordination and Bioinorganic Chemistry is organized in the Congress Centre of the Slovak Academy of Sciences in Smolenice Castle by the

Slovak Chemical Society
Slovak Academy of Sciences
Slovak University of Technology in Bratislava
Alexander Dubček University in Trenčín

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This publication contains a complete scientific and social program. Moreover, the abstracts of the papers contributed to the Conference and presented as lectures and posters are contained in it and arranged in the alphabetical order according to the presenting authors. The name of the author presenting the contribution is underlined. At the end a list of authors is attached.

The Conference is organized with the support of the Ministry of Education, Science, Research and Sport of the Slovak Republic within the Research and Development Operational Programme for the project “University Science Park of STU Bratislava”, ITMS 26240220084, co-funded by the European Regional Development Fund.

XXV. INTERNATIONAL CONFERENCE
ON COORDINATION AND BIOINORGANIC CHEMISTRY

TIME TABLE

MONDAY, June 1, 2015

8:00	Breakfast
9:00	Opening
9:15 – 9:45	Opening Lecture
9:45 – 12:00	Plenary Session A
13:00	Lunch
14:30 – 17:45	Concurrent Sessions A, B
18:00	Official Ceremony
18:30	Dinner
19:30	Get-together Party

TUESDAY, June 2, 2015

7:30	Breakfast
8:15 – 12:30	Plenary Session C
13:00	Lunch
14:30 – 17:30	Concurrent Session C, D
18:30	Dinner

WEDNESDAY, June 3, 2015

7:30	Breakfast
8:15 – 11:30	Plenary Session B
12:00	Lunch
13:15 – 17:45	Excursion
18:30	Dinner
20:00 – 21:30	Poster Session

THURSDAY, June 4, 2015

7:30	Breakfast
8:15 – 12:30	Plenary Session D
13:00	Lunch
14:30 – 17:30	Young Session
17:30	Closing
19:30	Banquet and Farewell Party

FRIDAY, June 5, 2015

7:30	Breakfast
8:00	Departure (bus 1)
9:00	Departure (bus 2)

A

Electronic, molecular, and crystal structures

New theoretical approaches and experimental techniques applied in structural investigation of inorganic compounds and materials, coordination compounds and biocomplexes

C

Applied inorganic and coordination chemistry

Nanomaterials, magnetic materials, optomaterials, exploitation of physical and chemical properties of inorganic and coordination compounds and composites, supramolecular devices, superconductors

B

Solution and solid state reactivity

Synthesis and characterization, spectral and magnetic properties of coordination compounds, electrochemistry, thermochemistry, photochemistry, catalysis, speciation of complexes in solutions

D

Complexes in human medicine and the environment

Preparation, structure, chemical, biological properties and function of therapeutical agents and enzymes, natural and model biocomplexes, catalyzed destruction of environmental pollutants

Monday		8	9	10	11	12	13	14	15	16	17	18	19	20	21
Room 1	Room 2	Breakfast 8:00	Opening	Opening Lecture	Plenary Session A Part 1	Plenary Session A Part 2	Taking Photography	Lunch 13:00	Concurrent Session B Part 1	Concurrent Session B Part 2	Concurrent Session B Part 3	Official Ceremony (18:00)	Diner 18:30	Get-together Party 19:30	
									Concurrent Session A Part 1	Concurrent Session A Part 2					
Tuesday		8	9	10	11	12	13	14	15	16	17	18	19	20	21
Room 1	Room 2	Breakfast 7:30	Plenary Session C Part 1	Plenary Session C Part 2	Plenary Session C Part 3		Lunch 13:00		Concurrent Session D Part 1	Concurrent Session D Part 2	Concurrent Session D Part 3		Diner 18:30		
									Concurrent Session C						
Wednesday		8	9	10	11	12	13	14	15	16	17	18	19	20	21
Room 1	Room 2	Breakfast 7:30	Plenary Session B Part 1	Plenary Session B Part 2		Lunch 12:00		→ The Castle Dolná Krupá 13:45 – 14:45 13:15	← Concert in Dolná Krupá 14:45 – 15:15	← Mead tasting Smolenice 15:15 – 16:45 15:15	← Mead tasting Smolenice 16:15 – 17:45 16:15		Diner 18:30	Poster Session 20:00 – 21:30	
								↑ 14:15							
Thursday		8	9	10	11	12	13	14	15	16	17	18	19	20	21
Room 1	Room 2	Breakfast 7:30	Plenary Session D Part 1	Plenary Session D Part 2	Plenary Session D Part 3	Plenary Session D Part 4	Lunch 13:00		Young Session Part 1	Young Session Part 2	Young Session Part 3	Closing		Banquet and Farewell Party 19:30	
									Young Session Part 4	Young Session Part 5					

XXV. INTERNATIONAL CONFERENCE
ON COORDINATION AND BIOINORGANIC CHEMISTRY

SCIENTIFIC PROGRAM

MONDAY, June 1, 2015

9.00 **Opening (Room 1)**

Room 1 Opening lecture

9:15 – 9:45 M. Melník (*Slovakia*)  86
Purine alkaloids as drugs and ligands

**9.45 – 12.00 Plenary Session A
ELECTRONIC, MOLECULAR, AND CRYSTAL STRUCTURES**

Room 1 Part 1 *Chairman: M. Melník*

9:45 – 10:30 A. Hauser (*Switzerland*)  59
Photophysics of d^6 transition metal complexes

10.30 – 11.00  *Coffee Break*

Room 1 Part 2 *Chairman: A. Hauser*

11:00 – 11:30 M. Haga (*Japan*)  54
Development of surface coordination chemistry toward functional devices

11:30 – 12:00 N. Kojima (*Japan*)  69
**Dynamical behaviour of the charge transfer phase transition
in dithiooxalato-bridged iron mixed-valence system**

**14.30 – 17.45 Concurrent Session B
SOLUTION AND SOLID STATE REACTIVITY**

Room 1 Part 1 *Chairman: T. Pintauer*

14:30 – 14:45 P. Baran (*USA*)  27
Structural study of oxidovanadium complexes with pyrazoles

14:45 – 15:00	M. Bortoluzzi (<i>Italy</i>) Mononuclear and heterodinuclear phenanthroline-dione complexes of <i>d</i>- and <i>f</i>-block elements	 32
15:00 – 15:15	M. Breza (<i>Slovakia</i>) On magnetic properties of Cu(II) and Cr(II) "paddle-wheel" acetates	 34
15:15 – 15:30	A. Burdukov (<i>Russia</i>) Functionalized iron(II) tris-dioximate clathrochelates: Redox-innocent metal and non-innocent ligand	 35

Room 1	Part 2	Chairman: M. Saphier
---------------	---------------	----------------------

15:30 – 15:45	F. G. Gelalcha (<i>USA</i>) Novel iron catalysts for biomimetic asymmetric epoxidations	 50
15:45 – 16:00	S. A. Kuznetsov (<i>Russia</i>) Electrochemical study of rhenium complex formation in halide and oxohalide melts	 77
16:00 – 16:15	M. Mikuriya (<i>Japan</i>) Nickel(II) complex with 1,4,7-tris(2-aminoethyl)-1,4,7-triazacyclononane	 89
16:15 – 16:30	K. Nakajima (<i>Japan</i>) Structure conversion and chromic behaviour of the metal-hydrazone complexes in solution and in the solid state	 95

Room 1	Part 3	Chairman: P. Strauch
---------------	---------------	----------------------

16:30 – 16:45	I. Pantcheva (<i>Bulgaria</i>) Application of circular dichroism spectroscopy to assess coordination ability of natural polyether ionophores	 103
16:45 – 17:00	I. Šalitroš (<i>Slovakia</i>) Photoactive mononuclear and polynuclear iron(II) spin crossover compounds	 114
17:00 – 17:15	R. Šipoš (<i>Slovakia</i>) Nucleophilic, electrophilic reactivity, some spectral and electrochemical properties of iron(II) clathrochelates	 119
17:15 – 17:30	J. C. Swarts (<i>South Africa</i>) Polysiloxanes as carriers for rhodium-ferrocenyl complexes with potential catalytic applications	 125
17:30 – 17:45	M. Vershinin (<i>Russia</i>) Molecular design of iron(II) clathrochelates carrying annulated rib heterocycles	 133

14.30 – 16.45	Concurrent Session A ELECTRONIC, MOLECULAR, AND CRYSTAL STRUCTURES
----------------------	---

Room 2	Part 1	<i>Chairman: M. Haga</i>
---------------	---------------	--------------------------

- | | | |
|---------------|---|--|
| 14:30 – 14:45 | M. Gall (<i>Slovakia</i>)
Ab initio simulation of crack propagation in pure and Y-doped β-S₃N₄ |  48 |
| 14:45 – 15:00 | L. Jeremias (<i>Czech Republic</i>)
Synthesis and coordination chemistry of R₃PE (E = S, Se, Te) ligands |  65 |
| 15:00 – 15:15 | M. Koman (<i>Slovakia</i>)
Structural study of new Mn(III) and Fe(III) dipicolinate complexes |  70 |
| 15:15 – 15:30 | J. Moncol' (<i>Slovakia</i>)
Supramolecular structure and isomerism of new copper(II) halogenobenzoate complexes with nicotinamide |  93 |

Room 2	Part 2	<i>Chairman: N. Kojima</i>
---------------	---------------	----------------------------

- | | | |
|---------------|---|---|
| 15:30 – 15:45 | G. Ondrejovič (<i>Slovakia</i>)
Structures of Cu₄OCl₆L₄ complexes studied by vector analysis |  101 |
| 15:45 – 16:00 | J. Pavlik (<i>Slovakia</i>)
DFT approach to spin crossover in embedded systems |  104 |
| 16:00 – 16:15 | P. Segl'a (<i>Slovakia</i>)
Study of copper(II) and cobalt(II) furancarboxylate and thiophencarboxylate complexes |  117 |
| 16:15 – 16:30 | J. Švorec (<i>Slovakia</i>)
EPR spectroscopy of Cu(II) complexes. What we have learned |  124 |
| 16:30 – 16:45 | D. Valigura (<i>Slovakia</i>)
An unusually wide spectrum of 3-methylsalicylatocopper(II) complexes with ronicol |  130 |

TUESDAY, June 2, 2015

8.15 – 12.30	Plenary Session C APPLIED INORGANIC AND COORDINATION CHEMISTRY
---------------------	---

Room 1	Part 1	<i>Chairman: M. Abe</i>
---------------	---------------	-------------------------

8:15 – 9:00	T. Mizokawa (<i>Japan</i>) Electronic structure of transition-metal compounds with various spin-charge-orbital instabilities	 91
-------------	--	--

Room 1	Part 2	<i>Chairman: T. Mizokawa</i>
---------------	---------------	------------------------------

9:00 – 9:30	M. Abe (<i>Japan</i>) Synthesis and guest binding studies on coordination giant capsules containing cofacial bis(porphyrin) motifs	 19
-------------	--	--

9:30 – 10:00	F. Mohr (<i>Germany</i>) Golden opportunities: New aspects of the chemistry of gold	 92
--------------	---	--

10:00 – 10:30	P. Day (<i>United Kingdom</i>) Molecular nano-materials: The long road from basic science to technological innovation	 40
---------------	---	--

10.30 – 11.00	 <i>Coffee Break</i>	
---------------	---	--

Room 1	Part 3	<i>Chairman: F. Mohr</i>
---------------	---------------	--------------------------

11:00 – 11:30	M. O. Onani (<i>South Africa</i>) Synthesis and characterization of iminopyridyl complexes with thiophene based ligands for heck coupling reactions	 100
---------------	---	---

11:30 – 12:00	P. Sobota (<i>Poland</i>) Organometallic compounds in the synthesis of new materials: Old ligands, new tricks	 122
---------------	---	---

12:00 – 12:30	J. D. E. T. Wilton-Ely (<i>United Kingdom</i>) Molecular and nanoscale assemblies as highly sensitive and selective sensors of toxic species	 135
---------------	--	---

14.30 – 17.30	Concurrent Session D COMPLEXES IN HUMAN MEDICINE AND THE ENVIRONMENT
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Room 1	Part 1	<i>Chairman: J. Darkwa</i>
---------------	---------------	----------------------------

- | | | |
|---------------|---|--|
| 14:30 – 14:45 | A. Ahmedova (<i>Bulgaria</i>)
First experimental evidences for the anticancer activity of anthracene-based coordination nano-capsules |  20 |
| 14:45 – 15:00 | S. A. Drweesh (<i>Egypt</i>)
Synthesis, crystal structure and biological activities of Pd(II) complexes with quinolin-8-ol derivatives as ligands and 8-hydroxyquinolinium cation |  43 |
| 15:00 – 15:15 | M. Fiallo (<i>France</i>)
Permeable reactive barriers: Degradation of organic molecules by Fe(0) |  45 |
| 15:15 – 15:30 | D. Gambino (<i>Uruguay</i>)
New organometallic compounds of bioactive ligands as prospective antiparasitic agents |  49 |

Room 1	Part 2	<i>Chairman: P. Day</i>
---------------	---------------	-------------------------

- | | | |
|---------------|--|--|
| 15:30 – 15:45 | B. Gyurcsik (<i>Hungary</i>)
New generation of chimeric nucleases based on colicin E7 nuclease domain |  53 |
| 15:45 – 16:00 | M. Gál (<i>Slovakia</i>)
Degradation of pharmaceuticals by ferrate(VI) |  47 |
| 16:00 – 16:15 | S. C. N. Hsu (<i>Taiwan</i>)
Study on bio-inspired polypyrazolylborate copper nitrite complexes |  61 |
| 16:15 – 16:30 | E. V. Lider (<i>Russia</i>)
Synthesis and cytotoxic activity of new Cu(II) and Pt(II), Pd(II) complexes with nitrogen-containing ligands |  78 |

Room 1	Part 3	<i>Chairman: Y. Hisaeda</i>
---------------	---------------	-----------------------------

- | | | |
|---------------|--|---|
| 16:30 – 16:45 | P. Mikuš (<i>Slovakia</i>)
Bio-medical aspects of theophylline and its metal complexes |  90 |
| 16:45 – 17:00 | I. Potočník (<i>Slovakia</i>)
Characterization and <i>in vitro</i> antimicrobial and cytotoxic activity of complexes with 5-chloro-quinolin-8-ol |  107 |
| 17:00 – 17:15 | N. S. Rukk (<i>Russia</i>)
REE complexes with antipyrine: Structural and cytotoxic studies |  112 |

17:15 – 17:30 P. Sharrock (*France*)  118
Radiation-sensitive phantoms with paramagnetic metal ions for 3-D MRI dosimetry of radiotherapy

14.30 – 15.45	Concurrent Session C APPLIED INORGANIC AND COORDINATION CHEMISTRY
---------------	--

Room 2

Chairman: P. Sobota

14:30 – 14:45 M. Drábik (*Slovakia*)  42
Common & nontraditional cements in the syntheses of MDF materials.

14:45 – 15:00 C. Hahn (*USA*)  55
Alkene and alkyne activation in a bisphosphine monoxide gold(I) complex

15:00 – 15:15 M. Mazur (*Slovakia*)  85
EPR spectroscopy of copper(II) complexes with *N*-donor ligands and 3,5-dichlorosalicylic acid in frozen solutions

15:15 – 15:30 C. Rajnák (*Slovakia*)  110
Pentacoordinate cobalt(II) complexes as single molecule magnets

15:30 – 15:45 J. Titiš (*Slovakia*)  129
Structural tunability of single-molecule magnet behaviour in Co(II) complexes

WEDNESDAY, June 3, 2015

8.15 – 11.30	Plenary Session B SOLUTION AND SOLID STATE REACTIVITY
---------------------	--

Room 1	Part 1	<i>Chairman: J. Krzystek</i>
---------------	---------------	------------------------------

8:15 – 8:45	R. Boča (<i>Slovakia</i>) Field induced single-ion magnets	📖 31
8:45 – 9:15	J. Krzystek (<i>USA</i>) How to measure extremely large zero-field splitting in high-spin coordination complexes?	📖 73
9:15 – 9:45	T. Pintauer (<i>USA</i>) Towards development of highly active copper catalysts for activation of monohalogenated substrates in atom transfer radical addition (ATRA)	📖 106
9.45 – 10.15	☕ <i>Coffee Break</i>	

Room 1	Part 2	<i>Chairman: R. Boča</i>
---------------	---------------	--------------------------

10:15 – 10:45	M. Saphier (<i>Israel</i>) π-Complexes of copper(I) with aromatic rings – applications	📖 115
10:45 – 11:15	P. Strauch (<i>Germany</i>) Flexibility of copper(II) – structure and EPR spectroscopy	📖 123
11:15 – 11:30	S. Chorazy (<i>Poland</i>) Charge transfer and spin transition phenomena in cyanido-bridged $\{M_9[M'(CN)_8]_6\}$ ($M = 3d$ metal ion, $M' = W, Re$) molecules	📖 38

- 01 L. Yu. Alikberova (*Russia*)  22
Amide complexes of lanthanide bromides and chlorides: Syntheses and structure
- 02 A. Bakalova (*Bulgaria*)  24
Synthesis and characterization of new mixed Pt(II) complexes with 3-thiolanespiro-5'-hydantoin and 4-thio-1*H*-tetrahydropyranespiro-5'-hydantoin
- 03 S. Belaid (*Algeria*)  28
Synthesis, characterization and biological activities of oxovanadium(IV) complexes with reduced schiff bases derived from *N,N'*-*O*-phenylenebis(salicylideneimine)
- 04 A. Bieńko, D. Bieńko (*Poland*)  30
Synthesis, crystal structure and magnetic properties of homo- and heterometallic, multi-core materials.
- 05 V. Farkasová (*Slovakia*)  44
Preparation and biological properties of Pd(II) complexes with quinolin-8-ol halogenderivatives and K^+ , Cs^+ or 5-chloro-7-iodo-quinolinium cations
- 06 J. Gülzow (*Germany*)  52
Mono- and dinuclear Cu(II) complexes of new ligands with N_3O_x donor sets
- 07 J. Halaška (*Slovakia*)  56
New copper(II) chloro- and dichlorobenzoate complexes with isonicotinamide
- 08 L. Hanousková (*Czech Republic*)  57
Organometallic dichlorido ruthenium(II) complexes
- 09 Z. Harmatová (*Slovakia*)  58
Kinetic study of thermal decomposition of some Cu(II) complexes with biologically important *N,N*-diethylnicotinamide
- 10 J. Hutýra (*Czech Republic*)  62
Gold(I) complexes as potent *in vitro* anticancer agents
- 11 K. Jomová (*Slovakia*)  66
Iron-induced oxidative stress and human disease
- 12 J. Kasparkova (*Czech Republic*)  67
A dual-targeting, apoptosis-inducing organometallic half-sandwich iridium anticancer complex
- 13 L. Krivosudský (*Slovakia*)  72
Peroxidovanadium complexes in non-aqueous solvents

- 14 D.-Y. Ma, X. Li, H.-F. Guo, X.-Y. Hao (*China*)  82
A hydrostable and nitril/methyl-functionalized metal-organic framework for drug delivery and highly selective CO₂ adsorption
- 15 J. Mihalčiak (*Slovakia*)  87
Synthesis, spectral properties and crystal structures of cobalt(II) dipicolinates with melamin
- 16 J. Miklovič (*Slovakia*)  88
Synthesis, crystal structure and spectral properties of nickel(II) hydroxy-pyridinecarboxylates
- 17 D. Motoyama (*Japan*)  94
Energy storage by proton-coupled electron transfer reactions of Ru complexes
- 18 B. Nikolova-Mladenova (*Bulgaria*)  97
Synthesis and characterization of new gallium(III) complexes with 5-bromo-salicylaldehyde benzoylhydrazones
- 19 T. V. Petrasheuskaya (*Belarus*)  105
Redox-active zinc(II) complexes with Mannich bases: Synthesis, physico-chemical characterization and biological evaluation
- 20 L. Saghatforoush (*Iran*)  113
Synthesis and crystal structures of two new Hg(II) and Cd(II) complexes with 2,3,5,6-tetrakis-(2-pyridyl) pyrazine
- 21 A. Scrivanti (*Italy*)  116
New heteroscorpionate lanthanide complexes for ring opening polymerization
- 22 A. Yu. Skryabina (*Russia*)  120
Neodymium complexes with antipyrine: Dependence of cytotoxicity on anion type and size
- 23 J. Vančo (*Czech Republic*)  131
Ternary copper(II)-lawsone complexes
- 24 M. Witwicki (*Poland*)  136
EPR and DFT insight into interaction between o-semiquinone radicals and metal ions

THURSDAY, June 4, 2015

8.15 – 12.30		Plenary Session D	
		COMPLEXES IN HUMAN MEDICINE AND THE ENVIRONMENT	
Room 1	Part 1	<i>Chairman: S. M. Aldoshin</i>	
8:15 – 9:00	C. J. Rhodes (<i>United Kingdom</i>)		111
	Zeolites: Fundamental features and environmental implications.		
Room 1	Part 2	<i>Chairman: C. J. Rhodes</i>	
9:00 – 9:30	S. M. Aldoshin (<i>Russia</i>)		21
	Functional nitrosyl iron complexes as models of the active sites of non-heme proteins: Structure, unusual electronic and magnetic properties, and prospects of their application in human medicine and engineering		
9:30 – 10:00	V. Brabec (<i>Czech Republic</i>)		33
	Insights into the molecular and epigenetic mechanisms of antitumor effects of Pt(IV)-valproic acid conjugates		
10:00 – 10:30	J. Darkwa (<i>South Africa</i>)		39
	Theraupetic potential of gold dithiocarbamates as anticancer agents		
Room 1	Part 3	<i>Chairman: V. Brabec</i>	
10:30 – 11:00	Y. Hisaeda (<i>Japan</i>)		60
	Bio-inspired catalysts learned from B₁₂ enzyme for degradation of environmental pollutants		
11:00 – 11:30	M. Tacke (<i>Ireland</i>)		127
	Novel carbene-metal complexes as anticancer drugs and antibiotics – potential and limitations		
Room 1	Part 4	<i>Chairman: M. Tacke</i>	
11:30 – 12:00	E. Lodyga-Chruscinska (<i>Poland</i>)		80
	Coordinating and biological activities of some flavonoids and their Schiff base analogs		
12:00 – 12:30	J. A. Thomas (<i>United Kingdom</i>)		128
	Tuning in <i>cellulo</i> targeting and function of metal complex bioprobes		

14.30 – 17.30	Young Session
----------------------	----------------------

Room 1	Part 1	<i>Chairman: N. Kojima</i>
---------------	---------------	----------------------------

- | | | |
|---------------|--|---|
| 14:30 – 14:40 | H. Bálint (<i>Hungary</i>)
A possible method of gene editing using Ni(II)-induced zinc finger nucleases |  25 |
| 14:40 – 14:50 | R. K. Balogh (<i>Hungary</i>)
The potential application of CueR protein in detection of selective detection of toxic metal ions |  26 |
| 14:50 – 15:00 | P. Bertová (<i>Slovakia</i>)
Copper(II) carboxylate complexes with ethylnicotinate: Synthesis, spectral properties and crystal structures |  29 |
| 15:00 – 15:10 | A. S. Bushmeleva (<i>Russia</i>)
Syntheses and structure of lanthanide halides complexes with bidentate amide ligands |  36 |
| 15:10 – 15:20 | D. Čechová (<i>Slovakia</i>)
Crystal structure and EPR spectra of new manganese(II) halogenbenzoate complexes with neocuproine |  37 |
| 15:20 – 15:30 | O. Dömötör (<i>Hungary</i>)
Complexes of Rh(III)(η^5-Cp*) with (N,O)- and (N,N)-donor bidentate ligands: Solution equilibrium and interaction with human serum albumin |  41 |

Room 1	Part 2	<i>Chairman: J. D. E. T. Wilton-Ely</i>
---------------	---------------	---

- | | | |
|---------------|---|--|
| 15:30 – 15:40 | A. Forgácssová (<i>Slovakia</i>)
Study of gallium(III) aminocarboxylates with sulfonamides |  46 |
| 15:40 – 15:50 | M. Gozzi (<i>Germany</i>)
Metal-<i>nido</i>-carbaborate complexes as metallocene analogues: Strategies, syntheses and characterization |  51 |
| 15:50 – 16:00 | T. Inui (<i>Japan</i>)
Mononuclear cobalt(III) complexes with <i>N</i>-salicylidene-2-hydroxy-5-bromobenzylamine and <i>N</i>-salicylidene-2-hydroxy-5-chlorobenzylamine |  63 |
| 16:00 – 16:10 | V. Janíková (<i>Slovakia</i>)
The study of the formation of coordination compounds with aniline in the interlayer space of Ca²⁺-, Cu²⁺- and Fe³⁺-exchanged montmorillonite |  64 |
| 16:10 – 16:20 | T. Klemens (<i>Poland</i>)
Rhenium complexes incorporating 2,2':6',2''-terpyridine derivatives – synthesis and photoluminescence properties. |  68 |

16:20 – 16:30 D. Krajčiová (Slovakia)  71
Study of copper(II) aminocarboxylates with sulfonamides

Room 1 **Part 3** *Chairman: P. Baran*

16:30 – 16:40 E. Kubiňáková (Slovakia)  74
Electrochemical generation of ferrate(VI) from molten hydroxides

16:40 – 16:50 V. Kuchtanin (Slovakia)  75
Nickel(II) Schiff base complexes: Synthesis, characterization and catalytic activity in Kumada cross-coupling reaction

16:50 – 17:00 L. Kucková (Slovakia)  76
A charge density study of biologically active copper complex

17:00 – 17:10 M. Litecká (Slovakia)  79
Cyclen like a perspective chelating agent for toxic Hg(II) ion

17:10 – 17:20 Z. Lukačovičová (Slovakia)  81
Tetrachloridoiron(III) and thiocyanatoiron(II) complexes with pyridine derivatives – syntheses, infrared spectra and structures

17:20 – 17:30 P. Augustín (Slovakia)  23
Synthesis and properties of novel iron(III) Schiff-base compounds

14.30 – 16.30 Young Session

Room 2 **Part 4** *Chairman: M. Drábik*

14:30 – 14:40 P. Masárová (Slovakia)  83
Synthesis, structural and magnetochemical study of the iron(III) Schiff base complexes

14:40 – 14:50 K. Matelková (Slovakia)  84
Copper carboxylate complexes – synthesis and structural characterization

14:50 – 15:00 K. Nasri (Tunisia)  96
Calcium phosphates and their applications

15:00 – 15:10 Y. N. Nosova (Russia)  98
Anticancer ruthenium compounds with biologically active ligands

15:10 – 15:20 M. Omote (Japan)  99
Synthesis and properties of dinuclear oxidovanadium(IV) complexes with cyclam-based macrocyclic ligands having four Schiff-base pendant arms

15:20 – 15:30 A. Packová (*Slovakia*)  102
Magnetic properties and magnetostructural d-correlation of hexacoordinate Ni(II) complexes

Room 2 **Part 5** *Chairman: P. Segl'a*

15:30 – 15:40 M. Puchonová (*Slovakia*)  108
SOD mimetic activity of some salicylatocopper complexes

15:40 – 15:50 I. Puškárová (*Slovakia*)  109
On the efficiency of PPD antioxidants

15:50 – 16:00 L. Smolko (*Slovakia*)  121
Mononuclear tetracoordinate Co(II) complexes as field-induced single-molecule magnets

16:00 – 16:10 A. Świtlicka-Olszewska (*Poland*)  126
Structural, spectroscopic and DFT study of rhenium(I) carbonyls incorporating 1,10-phenanthroline derivatives

16:10 – 16:20 F. Varga (*Slovakia*)  132
Synthesis, structural and magnetic properties of Co(II) complexes: Investigation of potential single-molecule magnets

16:20 – 16:30 S. Werner (*Germany*)  134
Platinum(II) and palladium(II) dithiocarbamates with water-soluble phosphine ligands

17.30 **Closing (Room 1)**

**Synthesis and guest binding studies on coordination giant capsules containing cofacial
bis(porphyrin) motifs**

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Recent development of metallosupramolecular chemistry has afforded a series of interesting high-molecular-weight discrete complexes with distinct structures, electronic properties, and chemical functions.¹⁻³⁾ Molecular capsules are one of such supramolecular compounds that provide a unique feature for molecular recognition by incorporating guest molecules into the cavity. In this presentation, we report that a new, remarkably large molecular cavity can be prepared by employing a pyridyl-appended porphyrin and trimetallic clusters as molecular building blocks.

New molecular capsules have been structurally identified by single-crystal X-ray diffraction analysis. The compounds contain two cofacially-oriented porphyrin motifs which are supported by four triangular Ru₃O clusters through the Ru–pyridyl bonds. The face-to-face porphyrin was separated by 17.3 Å, giving an exceptionally large cavity as a host molecule. Indeed, the Zn-metallated capsule has shown a highly selective guest-binding ability for long alkyl-chain diamine molecules H₂N(CH₂)_nNH₂ confirmed by UV-vis titration experiments. VT-NMR and DOSY studies have further addressed the guest-binding structures of the giant capsules in solution.

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First experimental evidences for the anticancer activity of anthracene-based coordination nano-capsules

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The anticancer activity of coordination nano-capsules, providing a spherical shell and confined cavity, was evaluated. The anticancer activity of the Pt and Pd capsules was tested on three types of human cancer cell lines (HL-60, SKW-3 and T-24) and the cisplatin resistant line HL-60/CDDP. In order to indirectly assess the potential of the Pt-capsule for drug delivery and its activity modulation index (AMI), cytotoxicity tests of the host-guest complexes including caffeine or triphenylene guest molecules were performed in combination with cisplatin. It was found that the Pt-capsule, empty or loaded with guest molecules, significantly enhances the anticancer activity of cisplatin, with AMI > 5 in some cases. Notably, the anticancer activity of the **empty Pt-capsule alone** is comparable to that of cisplatin. The results from the performed in vitro tests on the cytotoxicity against the resistant cells HL-60/CDDP indicated an additional positive trend – the empty Pt-capsule, in presence or absence of cisplatin, show a resistance factors RF < 1 in contrast to the capsules with filled cavity. This suggests that the capsule's cavity does play a role not only in increasing the cisplatin activity (against the non-resistant cancer cells) but also in overcoming the acquired drug resistance.

Acknowledgements: The authors are grateful to the National Science Fund of Bulgaria (DFNI-B02/24), and the Japanese Ministry of Education, Culture, Sports, Science and Technology (MEXT) through Grants-in-Aid for Scientific Research on Innovative Areas “Soft Molecular Systems”, as well as to the “BeyondEverest” project FP7-REGPOT-2011-1.

**Functional nitrosyl iron complexes as models of the active sites of non-heme proteins:
Structure, unusual electronic and magnetic properties, and prospects of their application
in human medicine and engineering**

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The method for synthesis has been developed and dinitrosyl iron complexes of a new class (DNIC) have been obtained, which contain functional sulfur-containing ligands and are mimetics of the active sites of nitrosyl non-heme proteins. The structure of cationic, neutral and anionic forms of paramagnetic mononuclear, binuclear diamagnetic of μ -S type and paramagnetic of μ -S-CN type nitrosyl complexes has been studied. Based on precision X-ray data and quantum-chemical calculations, specific features of the electronic structure of the basic $(\text{NO})_2\text{Fe}^-$ unit of these complexes have been studied, as well as the influence of ligand surrounding on NO donating properties and mechanism of decomposition of the complexes in various solvents at different pH values of the solutions. The obtained results open possibilities for development of promising medicines on their base, i.e., NO donors for the therapy of socially important diseases.

DNIC with two, four and eight NO groups in the molecule have been obtained. Molecular-genetic mechanisms of their impact in vivo have been studied, preclinical tests have been performed and substances-leaders have been selected for the further investigations and creation of medicines.

Amide complexes of lanthanide bromides and chlorides: Syntheses and structure

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Lanthanide complexes are used for the preparation of materials required by various areas of novel technology. Interest of researchers in complexes containing carbamide $\text{CO}(\text{NH}_2)_2$ (Ur), and acetamide CH_3CONH_2 (AA) causes by ability of these ambidentate ligands to form a developed system of hydrogen bonds. So they are convenient model systems of the supramolecular type.

The aim of the present work is synthesis and study (IR, single crystal XRD, TGA) of $[\text{Nd}(\text{Ur})_6(\text{H}_2\text{O})_2]\text{Br}_3$ and $[\text{Ln}(\text{AA})_4(\text{H}_2\text{O})_4]\text{X}_3 \cdot (\text{H}_2\text{O})$ ($\text{Ln} = \text{La}, \text{Nd}, \text{Ho}, \text{Er}$; $\text{X} = \text{Cl}$ or Br). Ligands coordinated Ln through the oxygen atoms, and the coordination polyhedra of the Ln atoms are distorted tetragonal antiprisms or two-capped trigonal prism ($\text{CN} = 8$).

All the complexes on study are characterized by the developed system of hydrogen bonds with bromides or chloride ions (and outer-sphere water molecules) in the cavities of the structure formed by the complex cations. We compared the degree of ligand distortion and ionicity of metal-ligand interaction in the lanthanide series and depending on the nature of halide ions.

Synthesis and properties of novel iron(III) Schiff-base compounds

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A series of mononuclear iron(III) compounds of general formula $[\text{FeL}^5\text{X}]$ (L^5 is a pentadentate Schiff-base ligand, and X is an anionic thiocyanato or chlorido ligand) has been synthesized and structurally characterized. The magnetic data have been taken with a SQUID apparatus (QD, MPMS-XL7) in the temperature range 2 – 300 K and field up to 7 T.

We tried to prepare a series of complexes exhibiting the spin crossover (SCO) [1]. For the synthesis with iron(III) and potassium thiocyanate we used amines *dpt* (N-(3-aminopropyl)-1,3-propanediamine) and *dptm* (N-(3-aminopropyl)-N-methyl-1,3-propanediamine) and as a source of aldehyde we used 2-hydroxynaphtaldehyde (abbr. *na*). In this way three complexes were obtained $[\text{Fe}(\text{nadpt})\text{NCS}]$ (**1a**), $[\text{Fe}(\text{nadptm})\text{NCS}] \cdot (\text{CH}_3)_2\text{CO}$ (**2a**) and $[\text{Fe}(\text{nadptm})\text{NCS}]$ (**2b**). Unfortunately, the SCO properties were not observed as in the whole temperature range the compounds are high-spin.

Another prepared compound is the high-spin chlorido precursor $[\text{Fe}(\text{3EtOSalpet})\text{Cl}]$ (**3a**) which will be combined with pseudohalido coligands (NCS^- , NCO^- , N_3^-) and 4f elements to get complexes with interesting magnetic properties.

This work was supported by Slovak grant agencies (VEGA 1/0522/14, APVV-0014-11) and by Program to support young researchers SUT No. 1344.

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Synthesis and characterization of new mixed Pt(II) complexes with 3-thiolanespiro-5'-hydantoin and 4-thio-1H-tetrahydropyranespiro-5'-hydantoin

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Cisplatin is one of the most successful used anticancer drugs in the treatment of wide variety of solid tumors(head and neck, lung, bladder etc.), testicular and ovarian cancers. Because of its severe toxicity profile and spontaneous development of drug resistance in tumors, numerous Pt(II) complexes have been synthesized and tested for antitumor activity. Some of the investigations have focused on utilizing of the ligands bearing other donor atoms than N (e.g. S, P, O). Two new mixed Pt(II) complexes with general formula *cis*-[PtL(NH₃)Cl₂] where L is 3-thiolanespiro-5'-hydantoin and 4-thio-1H-tetrahydropyranespiro-5'-hydantoin were synthesized. The complexes were studied by elemental analysis, melting points, IR, ¹H, ¹³C NMR spectra and DTA analysis. The experimental data showed that the coordination mode of the ligands with the Pt ions was realized by sulphur atom from the cyclic ring. The obtained complexes were chemically examined in comparison with previously synthesized and published *cis*-[PtL₂Cl₂](**1**) with the same ligands which structures were calculated and proved by DFT method. The new compounds as well as previously investigated complexes(**1**) were analyzed for cytotoxicity *in vitro* on SKW-3 and HL-60 human tumour cell lines. The results showed that all complexes exerted concentration dependent antiproliferative activity.

A possible method of gene editing using Ni(II)-induced zinc finger nucleases

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The goal of our experiments was to design new type of artificial nucleases to specifically recognize, bind and cleave DNA for wide variety of purposes. Zinc finger proteins are modular specific DNA binders that can be designed to target any desired DNA base sequence. As such, they can control the function of genes, but they also can be turned into specific DNA manipulating agents. A hydrolytic reaction by means of which we can specifically cleave proteins by nickel(II) ions – results in a square planar metal complex at the N-terminus of the C-terminal cleavage product. The latter complex is known as ATCUN motif, which is able to cleave DNA. Based on these facts, the combination of the two experiments will, according to our expectations, will lead to the development of in situ prepared specific nucleases.

For this purpose, we established the optimal conditions of the specific cleavage of the zinc finger proteins both in the absence and presence of DNA. We elaborated a test system and a precise protocol to study the specific cleavage of the P-1MEY# zinc finger protein - which is modified to contain only one cleavage site for nickel(II)ions. Combined electrophoretic, HPLC, CD and MS measurements were applied to monitor the reaction and to determine the solution structure of the complexes formed.

**The potential application of CueR protein in detection of selective detection
of toxic metal ions**

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Some transition metal ions are essential for the living cells, but their large amounts cause toxic effects. Therefore, metal ions are under strict regulation. Better understanding of these mechanisms may help to establish selective and sensitive metal binding or detecting systems. The CueR protein regulates the intracellular amount of Cu^I-ion in several strains of bacteria. The regulation by CueR is based on the conformational change of the protein upon metal binding, influencing the bound DNA structure. Consequently, the transcription of the regulated gene(s) starts and proteins are produced to remove the excess metal ions from the cell.

During this work modified bacteria were established that produce a fluorescent protein in the presence of the appropriate metal ions. The CueR protein provides biological response only to single-charge transition metal ions (Cu^I-, Ag^I- and Au^I). To better understand the selectivity, so the structure and the metal-binding features of the CueR protein, the expression in *E. coli* BL21 cells and the optimization of the purification procedure of the CueR were performed. The purity was checked with SDS-PAGE, the CueR protein was characterized with nano-ESI-MS. The solution structure and the metal ion coordination features were investigated by spectroscopic methods.

Structural study of oxidovanadium complexes with pyrazoles

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As a continuation of our study on pyrazole and pyrazolato complexes with transition metals, reactions of vanadyl sulfate with pyrazole and its 4- and 3-substituted derivatives were studied. Vanadium complexes attract attention mainly for their anticancer and insulin-mimicking characteristics. Regardless of the used stoichiometry of reactants, only complexes of the composition $[V(O)(pzH^*)_4(SO_4)]$ (pzH^* = pyrazole, 4-, or 3-methyl, phenyl, t-butyl, or halogen-substituted pyrazole) were isolated. Crystal structures revealed monomeric neutral species with vanadium atom coordinated in apically distorted octahedron. Its equatorial plane is formed by four nitrogen atoms from terminally coordinated pyrazole ligands. The oxido ligand and one oxygen atom from the sulfato group fill the apical positions. Orientation of individual pyrazole ligands reflects the most efficient possible intramolecular hydrogen bonding with the sulfato ligand. Deprotonation of pyrazole with triethylamine resulted in the formation of a heptanuclear pyrazolato vanadium complex of the composition $(Et_3NH)_2[V^{IV}_6(O)_6V^V(OMe)(\mu_3-O)_3(\mu-OMe)_6(\mu-pz)_6] \cdot 3/2H_2O$ in which tetrahedrally coordinated V^V atom uses three bridging oxido ligands to support a peripheral ring of six V^{IV} atoms linked together via alternating double-pyrazolato and double-methoxido bridges.

Synthesis, characterization and biological activities of oxovanadium(IV) complexes with reduced Schiff bases derived from *N,N'*-*O*-phenylenebis(salicylideneimine)

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A new oxovanadium (IV) complexes with reduced Schiff bases derived from *N,N'*-*O*-phenylenebis(salicylideneimine) has been synthesized and characterized by elemental analysis, thermogravimetry, FTIR, ESR, magnetic measurements, UV-Visible spectra and conductivity.

The complexes were found to be [ML](H₂O) species, where the deprotonated ligands are coordinated to metal ion by N₂O₂ donor atoms.

The antioxidant activity of ligands and complexes was evaluated by dpph method and reveals that the complexes exhibit a higher scavenging activity than corresponding ligands.

The antifungal activity was evaluated on different human fungi including yeasts of the *Candida* genus (*C.albicans* and *C.glabrata*) and an opportunistic mould *Aspergillus fumigatus*. The complexes exhibit a low activity toward *C.albicans*.

Copper(II) carboxylate complexes with ethylnicotinate: Synthesis, spectral properties and crystal structures

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Synthesis and characterization of eight new complexes of various structural types are reported. Furancarboxylic and thiophencarboxylic acids were used as heterocyclic acids. With 5-nitro-2-furancarboxylic acid (5-NO₂-2-fucH), which is the most acidic of the used acids, we have prepared two monomeric complexes [Cu(5-NO₂-2-fuc)₂(H₂O)₂] (*II*) and [Cu(5-NO₂-2-fuc)₂(H₂O)₄] (*III*), as well as one dimeric complex [Cu(5-NO₂-2-fuc)₂(Etnic)₂]₂ (*V*) (where Etnic is ethylnicotinate). On the other hand, with 2,5-dimethyl-3-furancarboxylic acid (2,5-Me₂-3-fucH), 2-thiophencarboxylic acid (2-tpcH), 3-methyl-2-thiophencarboxylic acid (3-Me-2-tpcH) and 5-methyl-2-thiophencarboxylic acid (5-Me-2-tpcH), we have prepared dimeric complexes of the acetate type [Cu(2,5-Me₂-3-fuc)₂(H₂O)]₂ (*I*), [Cu(2,5-Me₂-3-fuc)₂(Etnic)]₂ (*IV*), [Cu(2-tpc)₂(Etnic)]₂ (*VI*), [Cu(3-Me-2-tpc)₂(Etnic)]₂ (*VII*) and Cu(5-Me-2-tpc)₂(Etnic)]₂ (*VIII*). The characterizations were based on elemental analysis, infrared, electronic and EPR spectra, and magnetic measurements over a temperature range of 1.9–300 K. Moreover, complexes *III*, *V*, *VII* and *VIII* were also studied by monocystal X-ray structure analysis. The structure of the Cu(II) furancarboxylate and thiophencarboxylate complexes is dependent upon acidity constant of the heterocyclic acids and the coordinating and steric properties of the added base.

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**Synthesis, crystal structure and magnetic properties of homo- and heterometallic,
multi-core materials**

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Molecular Magnets belong to the group of intensely tested nano-objects due to their interesting physical properties and the expected technological applications. One way to design this type of magnetic materials is a method of building blocks and self-assembly process. In the framework of this work we investigate the structure and magnetism of multi-core homo- and heterometallic compounds composed of building blocks, cationic and anionic metal complexes, which were connecting by bridge. To create heterometallic compounds we used the cationic complexes of Cu (II) and Ni(II) with macrocyclic ligands of different number of substituents and anionic cyanometalate complexes $[M(CN)_6]^{3-}$ [$M = Fe, Cr$]. For the synthesis of homometallic, multi-core materials we applied mononuclear compounds of Cu (II), Ni (II) and Co (II) with two possible coordination place. Trithiocyanuric acid (ttcH₃) or 1,3,5-benzenetricarboxylic acid attracted our attention because in the structure, there are six atoms which can be applied for coordination to central atoms and thus form bridges connecting central atoms. Using the synthetic strategies of molecular building blocks approach, the new framework was obtained with different topology: dimeric systems $[Ni_2(pmdien)_2(H_2O)_2(\mu\text{-tdga})](ClO_4)_2 \cdot 2H_2O$, trimers $[M_3(pmdien)_3(\mu\text{-ttc})](ClO_4)_3$ ($M = Ni^{2+}, Co^{2+}$), pentamers $[NiL_1]_3[M(CN)_6]_2$, heptamer $[Ni_7(pmdien)_6(H_2O)_2(\mu\text{-ttc})_3](ClO_4)_5 \cdot 3H_2O$ and 3D-dimensional spin glass material. Magnetic susceptibility measurements of cyanometalate compound revealed ferromagnetic interactions among the central atoms with transition temperature determined from ZFC and FC measurement at about $T_c = 6 - 8$ K and strong anisotropy effect at lower temperature.

Field induced single-ion magnets

R. Boča

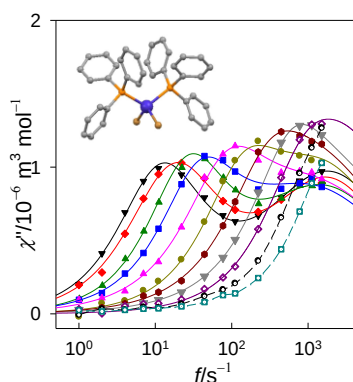
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A number of mononuclear Co(II) complexes was investigated by the AC susceptibility measurements in order to identify a slow magnetic relaxation based upon the temperature and frequency dependence of the out-of-phase magnetic susceptibility. Typically, 20 AC frequencies ($f = 0.1$ to 1500 Hz) were set-up with 10 scans for one external field B_{DC} and 12 temperature points ranging between 1.9 and 4.1 K (when χ'' usually vanishes) [1-3].

The studied systems cover $[\text{CoBr}_2(\text{PPh}_3)_2]$, three tetracoordinate $[\text{CoX}_2(\text{bqu})]$ complexes ($X = \text{Cl}, \text{Br}, \text{I}$), five pentacoordinate $[\text{CoCl}_2(\text{L}^{\text{Cn}})]$ complexes, and a well known magnetochemical standard $\text{HgCo}(\text{NCS})_4$. The slow magnetic relaxation has been found irrespective of the sign of the D-parameter (axial zero-field splitting), e.g. for $D/hc = +10 \text{ cm}^{-1}$ for $[\text{CoX}_2(\text{bqu})]$ systems.

To a big surprise, two relaxation processes were identified in the reported cases. The frequency dependence of χ'' has been analyzed in terms of the extended Debye model adapted for two relaxation processes giving rise to the adiabatic susceptibility χ_s , two isothermal limits χ_{T1} and χ_{T2} , two distribution parameters α_1 and α_2 , and two relaxation times τ_1 and τ_2 . The existence of two branches of the relaxation is ascribed to the solid-state packing giving rise to either dimeric units or chain-like structures.



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**Mononuclear and heterodinuclear phenanthroline-dione complexes
of *d*- and *f*-block elements**

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1,10-phenanthroline-5,6-dione (Phd) complexes of Group 3 and lanthanide elements having formulae $\text{Ln}(\text{hfac})_3(\text{Phd})$ ($\text{Ln} = \text{Y}, \text{Eu}, \text{Yb}$; hfac = hexafluoroacetylacetonate) have been synthesized and characterized. Complexes of *d*-block elements of the type $[\text{MCl}(\text{Phd})-(\text{p-cymene})]^+$ ($\text{M} = \text{Ru}, \text{Os}$) have been also prepared. In all these species the coordination of the polydentate ligand occurs by the N-donor moieties, as indicated by DFT calculations. The novel compounds have been tested, together with *fac*- $\text{ReBr}(\text{Phd})(\text{CO})_3$, as precursors for the preparation of heterobimetallic *d/f* derivatives. The reaction of the rhenium complex with yttrium or lanthanide anhydrous triflate salts led to the formation of the complexes $\text{ReBr}(\text{CO})_3(\text{N,N'-Phd-O,O'})\text{Ln}(\text{OTf})_3(\text{THF})$ ($\text{Ln} = \text{Y}, \text{Eu}, \text{Yb}$), where the trivalent ions interact with the quinonoid moiety. The redox properties of the rhenium centre resulted strongly affected by the coordination of $\text{Ln}(\text{OTf})_3$, as observed by comparing cyclic voltammetry measurements carried out on *fac*- $\text{ReBr}(\text{Phd})(\text{CO})_3$ and on $\text{ReBr}(\text{CO})_3(\text{N,N'-Phd-O,O'})\text{Y}(\text{OTf})_3$.

**Insights into the molecular and epigenetic mechanisms of antitumor effects
of Pt(IV)-valproic acid conjugates**

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Platinum prodrugs, such as Pt(IV) derivatives of antitumor cisplatin containing axial valproic acid (VPA) ligands, destroy cancer cells with greater efficacy than either conventional cisplatin or its Pt(IV) derivatives containing biologically inactive axial ligands. The activity of the inert Pt(IV) prodrugs is connected with their intracellular Pt(IV)→Pt(II) reduction resulting in a release of axial ligands and active Pt(II) drug. Moreover, the major mechanism of action of cisplatin comprises its coordinative binding to DNA whereas VPA inhibits histone deacetylase (HDAC) activity. In this study, we examined the molecular mechanisms of enhanced toxic effects in tumor cells of the Pt(IV) conjugates with VPA. We demonstrate that (i) Pt(IV)-VPA conjugates decondense chromatin in cells markedly more effectively than free VPA; (ii) of the total Pt inside the cells, a considerably higher fraction of Pt from the Pt(IV)-VPA conjugates is bound to DNA than from the conjugates with biologically inactive ligands. The results indicate that the enhanced cytotoxicity of the Pt(IV)-VPA conjugates is a consequence of several processes involving enhanced cellular accumulation, downregulation of HDACs, and yet other biochemical processes (not involving HDACs) which potentiate antitumor effects.

On magnetic properties of Cu(II) and Cr(II) "paddle-wheel" acetates

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Geometries of neutral complexes $M_2(O_2CCH_3)_4 \cdot 2H_2O$, $M = Cu$ or Cr , in various spin states were optimized within C_i symmetry in vacuo as well as in aqueous solution at DFT level of theory using B3LYP functional, B97D functional with Grimme's D2 dispersion scheme, B3LYP-D hybrid functional with Petersson-Frisch dispersion model and long-range corrected CAM-B3LYP functional using the Coulomb-attenuating method. Singlet spin states were treated within a "broken symmetry" approach using an unrestricted formalism. All functionals indicate antiferromagnetic copper(II) acetate whereas the same property of chromium(II) acetate is predicted by the B97D and B3LYP-D ones only. Room-temperature Gibbs free energy data suggest a high sensitivity of the preferred spin state on the environment. Cu-Cu distances do not differ substantially from the experimental value unlike the Cr-Cr ones. The calculated values of exchange coupling constants significantly depend on the DFT functional used as well as on the environment. The best agreement with experimental data for copper(II) acetate exhibit the vacuum data obtained by B3LYP and B3LYP-D functionals and for chromium(II) acetate the analogous data obtained by B97D and B3LYP-D functionals.

Functionalized iron(II) tris-dioximate clathrochelates: redox-innocent metal and non-innocent ligand

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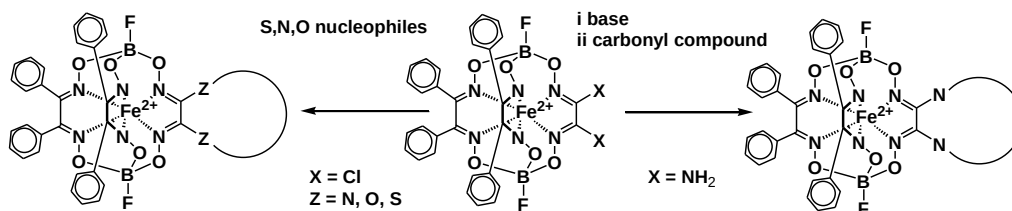
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Boron-capped tris-dioximate cage complexes (clathrochelates) are a specific type of coordination compounds with high chemical stability and diverse physico-chemical properties. The nature of their macrobicyclic cage ligands causes strong stabilization of particular oxidation states of the central metal ion thus essentially limiting their redox chemistry. We work on extending the redox chemistry of the iron(II) cage complexes using the ligand-centered redox processes. The synthetic approaches (nucleophilic and electrophilic) to the clathrochelates with redox non-innocent rib-annulated heterocyclic fragments will be discussed, as well as electrochemical and spectral properties of the synthesized compounds.



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Syntheses and structure of lanthanide halides complexes with bidentate amide ligands

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Lanthanide compounds are of interest due to their variable applications, e.g., materials required by different areas of technology (catalysts, X-ray protectors, etc.). The aim of this research is to synthesise new complexes of acetylurea (AcUr) and biuret (BU) with lanthanide halides and to study them by IR spectroscopy, thermal and X-ray diffraction analyses.

We found that complexes of AcUr with LaBr₃, PrBr₃, NdCl₃ and SmCl₃ are built of the [Ln(AcUr)₂(H₂O)₅]³⁺ complex cations (coordination number 9), while the same complexes with parent amide ligand BU have another structure of inner sphere. Recently we obtained complex [Tb(BU)₂(H₂O)₄]Cl₃, which is similar to the previously studied biuret complexes of lanthanide halides. We have also found a new type of AcUr complex [Ho(AcUr)₂(H₂O)₄]Cl₃·H₂O. Structure of its complex cation is similar to that of biuret complexes (coordination polyhedron is two-capped trigonal prisms). The presence of outer-sphere water is first discovered in this type of complexes. The AcUr and BU molecules are bidentate ligands and, on coordination, they change their conformation due to rotation around the C–N single bond. The coordinated acetylurea and biuret molecules are joined to the halide ions and water molecules of the adjacent complex cations by hydrogen bonds.

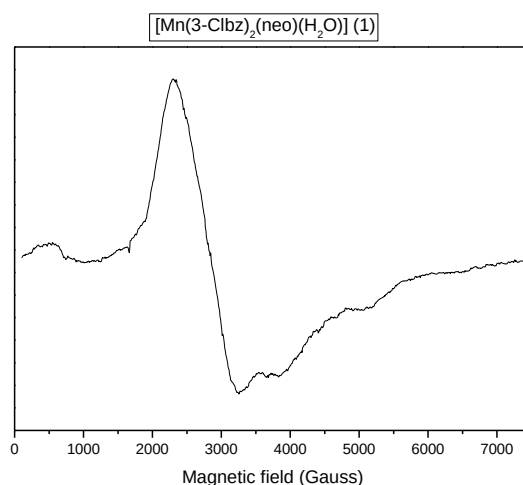
Crystal structure and EPR spectra of new manganese(II) halogenbenzoate complexes with neocuproine

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Four new Mn(II) complexes with the neocuproine as a ligand have been prepared. Compounds [Mn(3-Clbz)₂(neo)(H₂O)] (1), [Mn(4-Clbz)₂(neo)(H₂O)] (2), [Mn((3-NO₂)bz)₂(neo)(H₂O)] (3), [Mn((4-NO₂)bz)₂(neo)(H₂O)] (4) were subsequently studied by Electron Paramagnetic Resonance spectroscopy (EPR) and their crystal structures by determined by single-crystal X-ray analysis.



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**Charge transfer and spin transition phenomena in cyanido-bridged $\{M_9[M'(CN)_8]_6\}$
($M = 3d$ metal ion, $M' = W, Re$) molecules**

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Phase transitions related to the changes in the oxidation and/or spin states of metal centers can be realized through a spin crossover (SCO) effect, or a charge transfer induced spin transition (CTIST) as found in some bimetallic mixed-valence materials. Both SCO and CTIST phenomena can be induced by changes in temperature, pressure, or light irradiation in heterometallic cyanido-bridged coordination systems. In this context, we present cyanido-bridged $\{M_9[M'(CN)_8]_6\}$ ($M = Co, Fe$; $M' = W, Re$) clusters of a six-capped body-centered cube topology revealing thermally induced CTIST and SCO. $\{Fe_9[Re(CN)_8]_6\}$ exhibits the spin crossover phase transition at $T_{1/2} = 195$ K which occurs exclusively for a single Fe^{II} embedded in the center of a cluster core. The analogous $\{Fe_9[W(CN)_8]_6\}$ reveals the thermal phase transition at $T_c = 211$ K connected with a charge transfer (CT) between Fe and W ions. The $^{HS}Fe^{II} - W^V$ isomer dominates at high temperatures, while the $^{HS}Fe^{III} - W^{IV}$ redox pair is observed below phase transition, giving the reversed thermal hysteresis loop in magnetic measurements. The addition of Co^{II} results in the trimetallic $\{Fe_6Co_3[W(CN)_8]_6\}$ which combines the Fe – W CT with the CTIST phenomenon between $^{HS}Co^{II} - W^V$ and $^{LS}Co^{III} - W^{IV}$ electronic isomers dominated above and below 200 K, respectively.^[1-3]

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Therapeutic potential of gold dithiocarbamates as anticancer agents

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Gold complexes have been studied as alternatives to *cis*-platin following the discovery of the serious side effects of *cis*-platin. As results several gold(I) and gold(III) complexes have been investigated as non-platinum based anticancer drugs. Most of these gold complexes have been designed to have thiolato ligands in a similar manner that resemble well-known gold drugs like Auranofin, Solganol and Myocrisin that have phosphine and thiolate ligands.

However, since the discovery by Fregona and coworkers that gold(III) dithiocarbamate as potential antineoplastic agents [1], several research groups, including ours [2], have investigated gold(I) and gold(III) dithiocarbamate complexes for their activity against several forms of cancer. Examples of some of these gold dithiocarbamate complexes are: $[\text{Au}(\text{DMDTC})\text{X}_2]$ (DMDTC = N,N-dimethyldithiocarbamate, X = Cl or Br) and $[\text{Au}\{(\text{Ph}_2\text{P}(\text{CH}_2)_n\text{PPh}_2(\text{PDTC}))\}]$ (PDTC = pyrazolyldithiocarbamate, $n = 2 - 6$). This presentation will outline how gold(I) and gold(III) dithiocarbamates are emerging as new therapeutic agents for the fight against several forms of cancer.

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Molecular nano-materials: The long road from basic science to technological innovation

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Encouraging technological innovation and its connection with basic science is important for governments and business. It is therefore interesting to ask how this has played out in the field of molecular nano-materials. I will refer to three examples: molecule-based magnets, molecular information processing and (a recent arrival) organic-inorganic composites.

1. Till late in the last century the words ‘molecular’ and ‘magnet’ were never found written together. The notion that a molecule-based solid, crystallisable from solution near room-temperature, could behave as a magnet was quite alien. Now, molecular or ‘molecule-based’ magnets constitute an important area of nano-science, with increasing ramifications in technology. But where did this new field spring from? I will address the motivations of the earliest research, emphasising the unique nature of the organisation where it took place – Bell Telephone Laboratories in New Jersey, USA.

2. In the IT industry Moore’s Law has held sway for more than 50 years. In the 1970s it was already realised that this implies that the IT switching platforms would soon be the size of molecules. I will summarise a few of the ideas that emerged and show why, up till now, they have still not been implemented!

3. Organic-inorganic composite salts were recognised some 30 years ago as combining physical properties characteristic of both organic molecular and inorganic continuous lattices but direct applications were slow to come. Now they turn out to be ideal materials for building solar photovoltaic cells with remarkably high efficiencies up to 15%. Start-up companies are already in existence.

**Complexes of Rh(III)(η^5 -Cp^{*}) with (N,O)- and (N,N)-donor bidentate ligands:
Solution equilibrium and interaction with human serum albumin**

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Recently, the interest in metal based anticancer research shows a pronounced shift towards compounds possessing mode of actions different from Pt based compounds. Complexes of the neighbouring transition metals such as Ru, Os, Ir and Rh can be attractive alternatives, since intra- or extracellular proteins are their presumed biological targets besides DNA. Simple Rh(III) salts showed antitumor activity, but their kinetic inertness and tendency to hydrolyze hindered their further application. Rh(III)(η^5 -arenyl) complexes can overcome these disadvantages. Here we present the solution equilibrium aspects of complexes formed between [Rh(III)(η^5 -Cp^{*})]²⁺ fragment and (N,O)-donor (picolinic acid, (iso)quinaldic acid, 6-methylpicolinic acid) or (N,N)-donor (2,2'-bipyridine, ethylenediammine) ligands in pure aqueous solution. Complexation processes were studied by pH-potentiometry, UV-Vis and ¹H NMR spectroscopy. Our investigations are also focused on the interaction of these Rh(III) complexes with human serum albumin to reveal their distribution in blood serum studied by means of ¹H NMR spectroscopy, ultrafiltration and spectrofluorometry.

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Common & nontraditional cements in the syntheses of MDF materials

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Current advances in cement-based chemically bonded ceramics and composites are making a vital impact on the progress of materials chemistry, materials science and associated technologies; macro-defect-free (MDF) materials also belong to this category. The raw materials for the case studies of MDF processes have comprised a. o. Portland cement or new challenging cementitious compositions and polyphosphates of formula $(\text{NaPO}_3)_n$ or $\text{Na}_5\text{P}_3\text{O}_{10}$. The synthesis procedure complied with that generally accepted in the field.

The scope of cross-linking as a key item of the successful MDF synthesis has been studied by two independent experimental methods – thermal analysis and IR spectroscopy. Thermoanalytical data confirm (i) the substantial scope of cross-links formation in the system based on a new challenging cementitious composition and (ii) by one third higher content of cross-links in MDF materials synthesized from mechanochemically activated raw mixtures than that in probes formed after a standard mixing of raw materials. Reported and discussed is also the effect of phosphorus atoms from positions in P–O–Al cross-links upon the indicative vibrations in the IR spectral range – the vibration shifted by 16 - 26 cm^{-1} from a value of entire Al–O group. Similar sensitivity of IR vibrations reports reference data for Si–O–Al linkages.

Synthesis, crystal structure and biological activities of Pd(II) complexes with quinolin-8-ol derivatives as ligands and 8-hydroxyquinolinium cation

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Four new palladium(II) complexes based on quinolin-8-ol ligands (XQ) have been prepared as potential anticancer agents: HQH[PdCl₂(CQ)]·2H₂O (**1**) (HQ = quinolin-8-ol, CQ = 5-chloro-7-iodo-quinolin-8-ol), HQH[PdCl₂(ClQ)] (**2**) (ClQ = 5-chloro-quinolin-8-ol), HQH[PdCl₂(NQ)] (**3**) (NQ = 5-nitro-quinolin-8-ol) and HQH[PdCl₂(dBrQ)]·2H₂O (**4**) (dBrQ = 5,7-dibromo-quinolin-8-ol). All complexes have been characterized by IR spectroscopy, elemental analysis and X-ray structure analysis. The differences in the stretching $\nu(\text{O-H})$ and $\nu(\text{C=N})$ vibrations of ligands and prepared complexes proved that the ligands are coordinated to the palladium atom in a bidentate manner *via* oxygen and nitrogen atoms. This was confirmed by X-ray structure analysis which revealed that the prepared complexes are ionic coordination compounds with Pd(II) central atoms square-planarly coordinated by nitrogen and oxygen atoms of the bidentate molecule of XQ, the other two *cis*-positions are occupied by chlorido ligands. Negative charges of these complex anions are balanced by uncoordinated hydroxyquinolinium cations. The structures of **1** – **4** are stabilized by hydrogen bonds and π - π interactions. Cytotoxic and antimicrobial activities of **1** – **4** are currently evaluated.

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**Preparation and biological properties of Pd(II) complexes with quinolin-8-ol
halogenderivatives and K⁺, Cs⁺ or 5-chloro-7-iodo-quinolinium cations**

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NH₂(CH₃)₂[PdCl₂(XQ)] complexes were used to prepare anticancer coordination compounds of general formula Cat[PdCl₂(XQ)] by cationic exchange between NH₂(CH₃)₂⁺ and Cat⁺ cations, where XQ are halogenderivatives of quinolin-8-ol (5-chloro-7-iodo-quinolin-8-ol (CQ), 5,7-dibromo-quinolin-8-ol and 5,7-dichloro-quinolin-8-ol) and Cat is K⁺, Cs⁺ or protonated molecule of CQ. All complexes were characterized by IR spectroscopy which showed that ν(N–H) and ν(C–H) vibrations from NH₂(CH₃)₂⁺ cations were missing in Cat[PdCl₂(XQ)] complexes thus confirming successful cationic exchange. Elemental analyses corroborated the composition of the prepared complexes. Moreover, X-ray structure analysis was performed on HCQ[PdCl₂(CQ)]. Its structure contains square-planar *cis*-[PdCl₂(CQ)][–] complex anions in which CQ molecule is bidentately coordinated to Pd(II) atom by nitrogen and oxygen atoms of CQ pyridine and deprotonated phenolic part, respectively. Negative charges of the anions are balanced by uncoordinated HCQ cations. The structure is stabilized by hydrogen bonds and π–π interactions. Anticancer and antimicrobial activities of the prepared compounds are currently studied.

This work was supported by the Slovak Research and Development Agency under contract No. SK-SRB-2013-0004, by the VEGA grant 1/0598/14, and by the Ministry of Education, Science and Technological Development of the Republic of Serbia (grant No. 41010 and projects Nos. 175069 and 175103). S.A.D. thanks The National Scholarship Programme of the Slovak Republic for the financial support during his stay at P.J. Šafárik University in Košice.

Permeable reactive barriers: Degradation of organic molecules by Fe(0)

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Permeable reactive barrier (PRB) is a technology that has been recognized as being a cost-effective technology for “in situ passive method” groundwater remediation. It is an implementation of filtration consisting in a permeable zone, which passively captures a plume of contaminants through immobilization or transformation of the pollutants, releasing decontaminated water to the other side of the barrier. PRB’s are composed of inexpensive filler materials which may be doped with reagents specific for the remediation of particular compounds. It is reported that zero valent iron (ZVI) is particularly effective in the chemical degradation of persistent chlorinated compounds into non-toxic and harmless by-products.

We have elaborated porous plaster compositions doped with ZVI in order to control the flux of water to be treated. Our interest was to test the PRB with ZVI in reacting with organic nitro compounds and we used nitroaniline as the model pollutant. The nitroaniline was quantified by UV spectroscopy by measuring the absorption at 430 nm. The nitro compound is reduced to phenylenediamine and the rate of the reduction depends on the molecular structure of the organic compound.

Study of gallium (III) amino carboxylates with sulphonamides

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Gallium complexes has shown efficacy in the treatment of several apparently diverse disorders. Gallium has some medically useful radionuclides which have made extensive contribution in both the diagnosis and therapy of some diseases especially with usage in oncology, for example ⁶⁷Ga, ⁶⁸Ga. Besides platinum, gallium is also very promising for the treatment of some cancer diseases. Specificity of the Ga pharmaceuticals toward the target is usually applied as a complex. Complexation with organic ligands has been recognized as a promising strategy for creating new diagnostic and tumour-inhibiting compounds with a number of advantages. Chelating agents like macrocyclic chelators (DOTA, NOTA) are used to form more stabile complexes. Radiolabeled amino acids and peptides are of increasing interest in nuclear medicine with special emphasis to peptides labelled with positron emitters. Our research was aimed at the development of ternary Ga complexes with selected amino carboxylates and sulphonamides as potential diagnostic and/or therapeutic agents in nuclear medicine and oncology.

Acknowledgement: This work was supported by the projects VEGA 1/0873/15, KEGA 022UK-4/2015, FaF UK/14/2015 and carried out in the Toxicological and Antidoping Center and at the Department of Pharmaceutical Analysis and Nuclear Pharmacy, Faculty of Pharmacy, Comenius University in Bratislava.

Degradation of pharmaceuticals by ferrate(VI)

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Oxidation potential of chemical compounds containing iron(VI) is in the acidic environment the second highest after fluorine. This unique feature can be utilized in the wastewater treatment. Chemical and biological pollutants (e.g. pesticides, hormones, drugs, pharmaceuticals, viruses, resistant germs, heavy metals etc.) are usually present in wastewater. Some of them are not completely removed using “traditional” methods. Therefore innovative and alternative approaches are required. In this study, ferrate was electrochemically prepared in the strong alkaline NaOH/KOH environment. The degradation power of ferrate was tested on the group of 120 pharmaceuticals. Various ferrate concentrations ranging from hundredths of micrograms to hundredths of milligrams per liter were used in the weak basic system. Water samples were taken from the waste water treatment plant nearby Oncological Institute in Bratislava. After the treatment with iron(VI) majority of the drugs found in this wastewater were completely removed. Compounds with higher oxidation potentials were only partially removed. In this case it was necessary to adjust pH slightly below 6.

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***Ab initio* simulation of crack propagation in pure and Y-doped β - Si_3N_4**

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In this paper, we report the results of a theoretical tensile experiment on a new intergranular glassy film (IGF) models in polycrystalline β - Si_3N_4 with prismatic planes with pure and Y-doped SiO_2 in three different concentrations of doped metal in IGF. The models consist of 308 atoms in the cell, which contains two blocks of Si_3N_4 with prismatic planes and IGF formed by SiO_2 layer between them. This model with periodic boundary conditions was optimized by molecular dynamics, fully relaxed and calculated using the Vienna ab initio simulation package VASP, where for all atoms we used ultrasoft GGA PAW potentials.

The results of simulations show complicated deformation and failure mechanisms in IGF during crack propagation. In pure SiO_2 the crack propagation occurs only in IGF what indicates that interactions between SiO_2 and Si_3N_4 layers are stronger than Si-O bonds in IGF. In the case of Y-doped SiO_2 we observe all yttrium atoms located in IGF without any interactions with Si_3N_4 layer and no Y-Y bonds. Our results show weaker Y-O interactions than Si-O bonds in SiO_2 what leads to crack propagation mainly between Y and O atoms in IGF.

New organometallic compounds of bioactive ligands as prospective antiparasitic agents

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Chagas disease constitute a major health concern in Latin America. Currently available treatments are decades old and suffer from limited efficacy, undesirable collateral effects and development of resistance. Inorganic Medicinal Chemistry offers an innovative approach for the development of new antiparasitic drugs.

We have designed prospective antichagasic metal compounds by including in a single chemical entity ligands bearing antitrypanosomal activity and pharmacologically active metals, as an attempt to provide drugs capable of modulating multiple targets simultaneously. Among the bioactive ligands we have extensively studied a family of thiosemicarbazones whose main mode of trypanosomicidal action is the intraparasite bioreduction of their 5-nitrofuryl pharmacophore leading to toxic free radical species. We have rationally designed classical and organometallic metal compounds and evaluated the effect of complexation and nature of co-ligands on the pharmacological profile of these ligands.

In this work we report new {RuCp}, *fac*-Re(CO)₃ and heterobimetallic Pd and Pt ferrocene compounds and compare their biological behavior and probable mechanism of action with those of previously developed compounds.

Novel iron catalysts for biomimetic asymmetric epoxidations

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Despite their potential as versatile, sustainable and environmentally benign alternatives to precious and heavy metals iron catalysts have been less frequently exploited in asymmetric synthesis in general and epoxidations in particular. Highly successful iron catalyzed asymmetric epoxidations of alkenes using O₂/air or H₂O₂ in aqueous media are particularly rare.

We have previously described a novel green approach for achieving high asymmetric inductions in biomimetic aromatic alkene epoxidations. Using in situ generated iron complexes of novel optically pure diamine ligands, additives and with H₂O₂ as the oxidant high ee-values of epoxides were observed in some cases. The in addition to discussion of the underlying concepts, the scope and limitations, and insights into the mechanism of the novel catalytic system, the talk will disclose our more recent and promising results for the first time.

**Metal-*nido*-carbaborate complexes as metallocene analogues: Strategies,
syntheses and characterization**

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Metal-*nido*-carbaborate complexes are attracting interest in pharmacological applications mostly thanks to the parallels between metallacarbaboranes and metallocenes in the binding mode to the metal center.^[1] In addition, anionic *nido*-carbaborate (Dcb^{-2}) ligands greatly stabilize both high and low formal metal oxidation states, conferring high chemical and metabolic stability to the complexes, and generally low toxicity.^[2]

Our focus is on the synthesis of half-sandwich Ti^{IV} - and V^{IV} -*nido*-carbaborate complexes, containing as second ligand an alkyl-substituted cyclopentadienyl (Cp) ring, as hybrid organic-inorganic analogues of the metallocenes of titanium and vanadium.^[3]

We are using a one-pot synthetic strategy to introduce the ligands, i.e. Dcb^{-2} and Cp, simultaneously at the metal center. As metal complex precursor, MCl_3 ($\text{M} = \text{Ti}, \text{V}$) is used. As substituents on the cyclopentadienyl ring, alkyl amines (R-NH_2 , R-NMe_2) are being studied. The products are characterized by NMR, EPR, UV-vis spectroscopy and mass spectrometry.

Electrochemical and conductometric experiments are expected to elucidate the aqueous stability and kinetic lability of the synthesized metal-*nido*-carbaborate complexes.

Mono- and dinuclear Cu(II) complexes of new ligands with N₃O_x donor sets

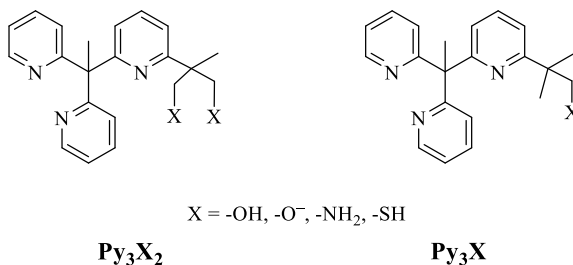
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It is well known that copper has a high relevance in metalloenzymes. In nature copper is coordinated in mononuclear or multinuclear fashion, as in the quercetin 2,3-dioxygenase [1] or the hemocyanin [2]. Copper based enzymes catalyses many different redox processes. Nowadays, inspired by nature, it is a common research strategy to coordinate copper with aromatic nitrogen ligands [3, 4, 5]. This motivated us to develop new model systems with our ligands.

Our ligand Py₃X₂ (X = –NH₂) is already well studied with respect to its iron chemistry. We investigated the analogous ligand Py₃(OH)₂ and its coordination behaviour towards Cu(II) ions. For comparison, we also synthesised the new modular ligand Py₃X. The position X is available for hydroxyl, amine or sulfide functions. Thus we have a high variability of the donor set.



On this poster the mono- and dinuclear Cu(II) complexes of the two ligands Py₃(OH)₂ and Py₃OH are presented and discussed with respect to their coordination behaviour. All compounds have been characterised by UV/Vis spectroscopy, mass spectrometry and single-crystal X-ray crystallography.

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New generation of chimeric nucleases based on colicin E7 nuclease domain

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Zinc-finger or TALE nucleases including – FokI catalytic domain are useful tools for targeted cleavage of genomic DNA. They can induce gene repair by homologous recombination mechanism in the presence of a suitable DNA template – predicting the possibility of their application in gene therapy of monogenetic diseases. However, the presently available chimeric nucleases show toxicity preventing their use in human therapy.

Our research is focused on the design of controlled artificial nucleases, the active conformation of which is induced by binding to the specific DNA target. Instead of the commonly used FokI domain, in this novel approach, we fuse the separated N-terminal and inactive catalytic C-terminal segments of the Colicin E7 nuclease domain to different termini of a specific DNA binding zinc finger protein to achieve the substrate dependent control.

Computational methods were applied to design the linker sequences and to identify the suitable C- and N-terminal units. The four designed proteins have been expressed in *E. coli* cells, without cytotoxic effect. The protein folding, DNA-binding affinity, specificity and the nuclease activity were studied. We also attempted to obtain similar construct with a TALE protein and collected their advantages and disadvantages.

Development of surface coordination chemistry: Toward functional devices

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Surface coordination chemistry directed to the fabrication of well-defined nanostructures on a surface is an important approach to develop functional devices. As a modular unit, we used redox- and photo-active complexes with coordination sites, which act as not only a building unit but also a functional module. We designed novel rod-shaped Ru complexes with four phosphonate groups, in which the functionality of modular complexes was tuned by the selection of peripheral ligands. First, for the fabrication of DNA-template nanowire on a solid surface, DNA trapping was achieved by use of an acridine group for a double-strand DNA intercalator in the Ru complex. Secondly, redox potentials were tuned by changing auxiliary ligands. In the layer-by-layer (LbL) films fabricated by coordination induced LbL growth method, the potential gradient was controlled by the sequential order of the Ru units. For the homo multilayer films, the small transparent coefficients for the electron transfer processes were ca. $0.013 \sim 0.027 \text{ \AA}^{-1}$, suggesting that the Ru complex layers have long-range electron transport ability. For the hetero layer film, current rectification and charge trapping were observed only for the layer number above 2. Since the charge trapping on the outer layer took place by the change of potential between -0.5 V and 0.7 V, the heterolayer film acts as a memory device having a write/erase operation by applied potential.

Alkene and alkyne activation in a bisphosphine monoxide gold(I) complex

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Gold(I) complexes have become very important as catalyst for alkene and alkyne functionalization with wide applications in organic synthesis. We have recently prepared a new gold(I) complex containing a bisphosphine monoxide ligand of the type [Au(PPO)Cl] (PPO = 1,2-bis(diphenylphosphino)benzene monoxide), which showed moderate catalytic efficiency for the hydration and hydroamination of alkynes. Whereas the new gold(I) complex is a very active catalyst for the hydroarylation of ethylpropiolate.

In order to understand the alkene and alkyne functionalization, it is important to study the coordination chemistry of substrate complexes in more detail. The information gained from structurally characterized alkene and alkyne gold(I) complexes help to rationalize selectivities of hydrofunctionalization reactions. The synthesis and characterization of series of cationic gold(I) complexes of the type [Au(PPO)(alkene)]BF₄ and [Au(PPO)(alkyne)]BF₄ will be discussed.

New copper(II) chloro- and dichlorobenzoate complexes with isonicotinamide

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The isonicotinamide (ina), which can be coordinated as N-donor monodentate terminal ligand or N,O-donor bidentate bridging ligand, presents useful ligand for construction hydrogen-bonding coordination polymers. The nine new monomeric and dimeric complexes of chloro- and dichlorobenzoato copper(II) complexes with isonicotinamide (ina) with various formulas: $[\text{Cu}(\text{3-Clbz})_2(\text{ina})_2]\{[\text{Cu}(\text{3-Clbz})(\text{ina})_2(\text{3-ClbzH})]\}_2$, $[\text{Cu}(\text{2-Clbz})_2(\text{ina})_2] \cdot 2\text{H}_2\text{O}$, $[\text{Cu}(\text{2,6-Cl}_2\text{bz})_2(\text{ina})_2] \cdot 2\text{H}_2\text{O}$, $[\text{Cu}(\text{2,4-Cl}_2\text{bz})_2(\text{ina})_2(\text{H}_2\text{O})_2]$, $[\text{Cu}(\text{4-Clbz})_2(\text{ina})_2]_2$, $[\text{Cu}(\text{2,3-Cl}_2\text{bz})_2(\text{ina})_2]_2$, $[\text{Cu}(\text{2,5-Cl}_2\text{bz})_2(\text{ina})_2]_2$, $[\text{Cu}(\text{2,6-Cl}_2\text{bz})_2(\text{ina})_2]_2$, $[\text{Cu}(\text{3,5-Cl}_2\text{bz})_2(\text{ina})_2]$ and $[\text{Cu}(\text{3-NO}_2\text{bz})_2(\text{ina})(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$ (where 2-Clbz = 2-chlorobenzoate, 3-Clbz = 3-chlorobenzoate, 4-Clbz = 4-chlorobenzoate, 2,3-Clbz = 2,3-dichlorobenzoate, 2,4-Clbz = 2,4-dichlorobenzoate, 2,5-Clbz = 2,5-dichlorobenzoate, 2,6-Clbz = 2,6-dichlorobenzoate and 3,5-Clbz = 3,5-dichlorobenzoate) were prepared and characterized by single-crystal X-ray structural analysis. The isonicotinamide in all three monomeric complexes is coordinated as N-donor terminal ligand.

The molecules of all compounds are linked through N—H $\cdots$ O and/or O—H $\cdots$ O hydrogen bonds into supramolecular hydrogen-bonding-coordination chains and networks.

Organometallic dichlorido ruthenium(II) complexes

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Ruthenium-based antitumor complexes represent a promising alternative to the clinically used platinum(II) compounds (e.g. *cisplatin*) showing activity and different mechanism of action against different human cancer cell lines. The ruthenium complexes, such as NAMI-A, KP1019/NKP-1339 and/or RAPTA-C, may serve as representatives of these complexes. The latter one belongs to the group of organometallic complexes with incorporated arene ligands, e.g. *p*-cymene (*p*-cym) in this case.

The results showing the biological perspective of the above mentioned compounds motivated us to prepare a series of eight new organometallic ruthenium complexes of the general formula $[\text{Ru}^{\text{II}}(\text{p-cym})(\text{L}^{\text{n}})\text{Cl}_2]$ (where L^{n} = monodentate *N*-coordinated 7-azaindole derivatives). These complexes were fully characterized by various techniques, such as elemental analysis, mass spectrometry, infrared and NMR (multinuclear, 2D) spectroscopy. All the prepared complexes were screened for their *in vitro* cytotoxicity against human ovarian cancer cell lines A2780 and moreover. Their ability to interact with small biologically relevant molecules (e.g. glutathione) and cell uptake were also studied.

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**Kinetic study of thermal decomposition of some Cu(II) complexes with biologically
important *N,N*-diethylnicotinamide**

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Thermogravimetry (TG) and derivative thermogravimetry (DTG) have been applied to evaluating non isothermal kinetic parameters (the apparent activation E_a , the pre-exponential factor A in the Arrhenius equation and rate constant k) for thermal decomposition reactions of solid complexes: $\text{Cu}_2(2\text{-Clbz})_4(\text{denia})_2$ (I), $\text{Cu}_2(2\text{-Brbz})_4(\text{denia})_2$ (II) and $\text{Cu}_2(2\text{-Brbz})_2(\text{denia})_2(\text{H}_2\text{O})$ (III).

Thermal decomposition of complexes I and II proceeds in two steps and in three steps for complex III. The final product of thermal decomposition of studied complexes was CuO. The kinetic stability of the complexes (on the basis of E_a for 1st step) can be ordered in the sequence $\text{I} < \text{III} < \text{II}$.

Photophysics of d^6 transition metal complexes

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Transition metal complexes possess excited states of very different character, that is, metal-centred ligand-field states, charge transfer states, and ligand centred $\pi\pi^*$ states for complexes with conjugated organic ligands. This results in an incredible diversity in physical and photophysical properties, as for instance the phenomena of thermal and light-induced spin crossover in iron(II) complexes, or the luminescence and electron donor/acceptor properties of excited ruthenium(II) polypyridyl complexes. The two classes of d^6 complexes, in fact, constitute model systems for the elucidation of a large number of elementary photophysical processes. The rate and efficiency of these processes are not only related to the ground and excited electronic structures, but also to the nuclear structures of the different states. Excited state electronic and nuclear structures can be probed with different time-resolved spectroscopic and structural techniques over many orders of magnitude ranging from picoseconds to days. In this contribution, the photophysical properties of iron(II) spin-crossover complexes will be presented and compared to those of analogous ruthenium(II) complexes with to aim to elaborate common principles leading nevertheless to very different behaviour.

**Bio-inspired catalysts learned from B₁₂ enzyme for degradation
of environmental pollutants**

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We have been interested in vitamin B₁₂-dependent enzymes, involving the cobalt species as a catalytic center, and dealing with a hydrophobic vitamin B₁₂, heptamethyl cobyrinate perchlorate, which has ester groups in place of the peripheral amide moieties of the naturally occurring vitamin B₁₂. In order to construct a good catalytic system, we prepared various nanomaterials with vitamin B₁₂ activities. These bio-inspired catalysts are very interesting from the viewpoint of green chemistry. 1,1-bis(4-chlorophenyl)-2,2,2-trichloroethane (DDT) is characterized by a pronounced insecticidal property and has been used worldwide for the last several decades despite hazardous effects on human health and wildlife. Because of recent environmental concerns, there is pressing need for efficient methods for degradation of such chlorinated compounds accumulated in the soil. DDT was degraded effectively by the bio-inspired catalysts with vitamin B₁₂ function. Such vitamin B₁₂ derivatives also can apply the detoxification of inorganic arsenic by the methylation. These bio-inspired catalysts are very interesting from the viewpoint of green chemistry.

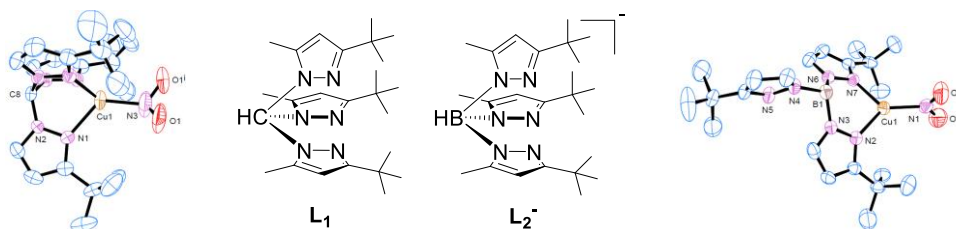
Study on bio-inspired polypyrazolylborate copper nitrite complexes

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Copper-containing nitrite reductases (Cu-NIRs) active site contains a type II copper catalytic center. The reaction mechanisms of Cu-NIRs have been proposed on the basis of the results of numerous spectroscopic and crystallographic studies. The key challenge for synthetic inorganic chemist is the synthesis of a copper(I)-nitro adduct. Herein we report the synthesis and structural characterization of two different kinds of copper(I)-nitro species stabilized by tripodal scorpionate: a neutral sterically hindered tris(3-tertiary-butylpyrazolyl)methane (L_1) ligand and an anion sterically hindered hydrotris(3-tertiary-butylpyrazolyl)borate (L_2^-) ligand. These ligand sets contain a facially coordinating group of pyrazole that closely mimic the pyramidal array of histidine imidazoles coordinated to the type II active site copper ion in the enzyme. Our approach will give a set of synthetic modeling system to imitate the electronic property of reduced nitrite bound type II copper center by two different charges of ligands. The study shows that the nitrite reductase reactivity of neutral and anion copper(I)-nitro complexes are influenced by the electron density around copper(I)-nitro core and their ligand steric concern.



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Gold(I) complexes as potent *in vitro* anticancer agents

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Gold-based metallotherapeutics have been clinically used for the treatment of rheumatoid arthritis since the first half of 20th century. Gold(I) complexes Auranofin (triethylphosphine-(2,3,4,6-tetra-*O*-acetyl-1-*D*-thiopyranosato-*S*)gold(I)) and gold thiolate salts, e.g. Solganol and Myochrysin, can be named as representatives of this group of anti-arthritis drugs. Moreover several studies revealed that these gold(I) complexes do not exhibit only anti-rheumatic properties, but additionally can act as anticancer agents.

In this work, a series of nine Auranofin-inspired gold(I) complexes with the general composition [Au(L)(PPh₃)] (**1-9**), where L stands for a deprotonated hypoxanthine derivative and PPh₃ for triphenylphosphine, were prepared, fully characterized and screened for their *in vitro* cytotoxicity against nine human cancer cell lines. Complexes **4**, **5** and **6** exhibit the best IC₅₀ values in the range between ca. 1,9 to 6,3 μM against MCF-7, A2780, A2780R, 22Rv1, G-361 and THP-1 cancer cell lines.

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**Mononuclear cobalt(III) complexes with *N*-salicylidene-2-hydroxy-5-bromobenzylamine
and *N*-salicylidene-2-hydroxy-5-chlorobenzylamine**

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Cobalt(III) complexes with *N*-salicylidene-2-hydroxy-5-bromobenzylamine (H₂sbba) and *N*-salicylidene-2-hydroxy-5-chlorobenzylamine (H₂scba), [*n*-(C₄H₉)₄N][Co(sbba)₂] (**1**) and [*n*-(C₄H₉)₄N][Co(scba)₂] (**2**), were synthesized. The crystal structure of **2** was determined by the single-crystal X-ray diffraction method at 90 K. It crystallizes in the monoclinic space group *P*2₁/*n* with *a* = 11.729(2) Å, *b* = 16.901(3) Å, *c* = 21.483(4) Å, *β* = 98.840(4)°, *V* = 4208.2(14) Å³, *D_x* = 1.295 g/cm³, and *Z* = 4. The *R*1 [*I* > 2σ(*I*)] and *wR*2 (all data) values are 0.0644 and 0.1920, respectively, for all 9521 independent reflections. The compound is composed of tetra(*n*-butyl)ammonium cation and octahedral cobalt(III) complex anion with two scba²⁻ ligands in meridional coordination. The electronic spectral features of **1** and **2** are consistent with the octahedral cobalt(III) ion with an N₂O₄ donor set.

**The study of the formation of coordination compounds with aniline in the interlayer space
of Ca²⁺-, Cu²⁺- and Fe³⁺-exchanged montmorillonite**

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The influence of Ca²⁺-, Cu²⁺- and Fe³⁺-exchanged montmorillonite (MMT) on the type of interaction with aniline in the interlayer space of MMT were studied by means of X-ray powder diffraction and infrared spectra. The results of X-ray diffraction show that aniline is successfully intercalated in the interlayer space of montmorillonite. From IR spectra follow that in Ca²⁺- and Fe³⁺-MMT is aniline indirect coordinated through water-bridge, in Cu²⁺-MMT is aniline also protonated (the spectrum of protonated aniline shows deformation and rocking NH₃⁺ absorption at ~1521cm⁻¹). In Cu²⁺-MMT indirect coordination and protonation is obtained simultaneously.

Synthesis and coordination chemistry of R_3PE (E = S, Se, Te) ligands

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The interest in phosphine chalcogenides R_3PE (E = O, S, Se or Te) is based on their selective complexation properties towards ‘hard/soft’ metal cations.¹ Their metal complexes are one of the most common chalcogenide sources used in colloidal nanocrystal syntheses.² Several studies have been reported on phosphine oxides, sulfides and selenides, while only a few complexes with the phosphine tellurides have been described.¹

The successful syntheses of $EtPh_2PE$ and Et_2PhPE (E = S, Se and Te) ligands by direct oxidation of starting phosphorous compounds ($EtPh_2P$ and Et_2PhP , respectively) by elemental chalcogen are reported.

The reaction conditions, X-ray structures of the compounds, NMR spectra (^{31}P and ^{125}Te) and their complexation reaction with Pd^{2+} salts will be discussed in detail.

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Iron-induced oxidative stress and human disease

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Iron is one of the most important elements in human body. It participates in many metabolic pathways and both an iron deficiency and iron overload may have various damaging effects to living organisms. Many studies discussing the role of iron in the etiology of several human diseases such as neurological diseases (e.g. Alzheimer disease, Parkinson disease, Huntington disease, Friedrich ataxia), cancer, as well as aging have been reported. A great effort has been devoted to identify intake, regulation, storage and homeostasis of iron. The aim of this review is to discuss recent findings related to proteins involved in iron homeostasis, iron-induced oxidative stress, and iron-related diseases. Attention will be devoted to the ability of some antioxidants either to prevent damage from reactive oxygen species (ROS) generated in the presence of iron or to prevent formation of ROS by iron chelation.

**A dual-targeting, apoptosis-inducing organometallic half-sandwich
iridium anticancer complex**

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The cellular mechanism of action of an iridium(III) half-sandwich complex $[(\eta^5\text{-C}_5\text{Me}_4\text{C}_6\text{H}_4\text{C}_6\text{H}_5)\text{Ir}(\text{phen})\text{Cl}]\text{PF}_6$ (phen = phenanthroline) (**1**) was examined. Complex **1** was used to treat several cell lines, including cisplatin-sensitive, cisplatin-resistant (with intrinsic and acquired resistance) carcinoma cells with wild type p53 status as well as the cells with no intact p53 gene, and nontumorigenic cells. Complex **1** preferentially kills cancer cells over nontumorigenic cells and exhibits no cross-resistance with cisplatin. It appears to retain significant activity in human tumor cell lines that are refractory or poorly responsive to cisplatin. Complex **1** exhibits dual effects in killing cancer cells causing nuclear DNA damage and mitochondrial dysfunction involving ROS production simultaneously. Flow cytometric studies and impedance-based monitoring of cellular responses to **1** demonstrated that **1** acts more quickly than cisplatin to induce cell death and that **1** is a more effective apoptosis inducer than cisplatin in particular in early stages of treatment, when the apoptotic effects predominate over necrosis. Overall, our findings confirm that **1** and its iridium derivatives represent promising candidates for further pre-clinical studies and new additions to the growing family of nonplatinum metal-based anticancer complexes.

**Rhenium complexes incorporating 2,2':6',2''-terpyridine derivatives – synthesis
and photoluminescence properties.**

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The influence of the coordination sphere on the photophysical and photochemical properties of transition metal complexes has been the subject of intense research. Particularly attention has been paid to Re(I) tricarbonyl complexes with 1,10-phenanthroline or 2,2'-bipyridine derivatives. Most of these compounds exhibit good phosphorescence properties, which make them attractive for solar energy conversion, luminescence sensing, for photosensitization of organic substrates, organic light-emitting diodes (OLEDs) and in other fields such as catalysis, and medicinal chemistry.

On contrary, [Re(CO)₃(terpy)Cl] was found to be nonluminescent and a more limited number of studies on the rhenium(I) tricarbonyl complexes incorporating 2,2':6',2''-terpyridine derivatives can be found in the literature. The recent studies, however, have revealed the possibility of improving the emission performance and application potential of these complexes by insertion of *terpy* ligand structural modifications.

In this communication, synthesis, structure and photoluminescent properties of series of complexes of general formula [ReCl(CO)₃(4'-R-terpy)] will be presented.

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Dynamical behaviour of the charge transfer phase transition in dithiooxalato-bridged iron mixed-valence system

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In the case of mixed-valence system whose spin states are situated in the spin crossover region, conjugated phenomena coupled with spin and charge are expected. Based on this viewpoint, we have developed a ferromagnetic mixed-valence system, $[\text{Fe}^{\text{II}}\text{Fe}^{\text{III}}(\text{dto})_3]$ ($A = (n\text{-C}_n\text{H}_{2n+1})_4\text{N}$, spiropyran), and investigated their multifunctional properties induced by the synergetic effects between spin, charge and photon. In the cases of $(n\text{-C}_n\text{H}_{2n+1})_4\text{N}[\text{Fe}^{\text{II}}\text{Fe}^{\text{III}}(\text{dto})_3]$, a charge transfer phase transition (CTPT) takes place at 122 K and 143 K for $n = 3$ and 4, respectively, where an electron transfers reversibly between the t_{2g} orbitals in the Fe^{II} and Fe^{III} sites. At the CTPT, the iron valence state is dynamically fluctuated with a frequency of about 0.1 MHz, which was confirmed by means of muon spin relaxation. Moreover, an anomalous enhancement of dielectric constant with thermal hysteresis was observed at CTPT in the whole measuring frequency range between 1 Hz and 1 MHz, which is attributed to the dynamical fluctuation of electrons between Fe^{II} and Fe^{III} sites associated with the CTPT. This anomaly becomes striking as the frequency is lowered, which is quite similar to the dielectric relaxation in relaxor ferroelectrics. Such frequency dependence is likely to be caused by the electron hopping on the grain boundary of domains.

**Structural study of new Mn(III) and Fe(III) dipicolinate complexes for enhancement
of ozonation treatment process**

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The chemistry of manganese and iron complexes has been investigated recently since these metals are present in a various biological redox systems including peroxidases, catalases, superoxide dismutases, dioxygenases and lipoxidases. The manganese is also present in the oxygen evolving complex (OEC) in photosystem II of green plants which consists of a tetranuclear manganese cluster. Dipicolinic acid is known to be a major component of bacterial spores. The metal dipicolinate complexes are also used in environmentally friendly “green” catalysis. The most common include heterogeneous catalysis, oxidation reactions and degradation reactions of waste water. The structural characterization of a new Manganese(III) and Iron(III) dipicolinate complexes with selected cations of pyridinecarboxamides is reported ($[M(\text{dipic})_2]^{-1}$ ($M = \text{Mn(III)}$ or Fe(III))). Each of the dipic anions are coordinate to M atom in a terdentate fashion manner, via two O atoms and the N atom (dipic = pyridine-2,6-dicarboxylate anion). The respective complex anions contained the following cations, pyridinium, isonicotinamidium, nicotinamidium, etc. Basic compounds $(\text{H}_5\text{O}_2)[\text{Fe}(\text{dipic})_2]$ and $(\text{H}_3\text{O})_2\{[\text{Mn}(\text{dipic})_2]\}_2 \cdot 3\text{H}_2\text{O}$ were used for testing of the wastewater degradation reactions enhancement.

Study of copper (II) aminocarboxylates with sulfonamides

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There have been some notable developments in several areas of organometallic pharmaceuticals that have potentially far-reaching importance for future medical applications and a research as well. One of the significant developments in the field of oncology and hematology is the application of copper complexes. The chemistry of copper compounds has been extensively investigated, and the relationship between structure and reactivity is of a major importance. Copper creates stable complexes with a wide variety of organic molecules (in our review work they are amino carboxylates and sulfonamides in the presence of macrocyclic chelators). The aim of our experimental investigation is designing and preparation of ternary copper (II) complexes with selected amino carboxylates and sulfonamides. Although such ternary complexes have not been prepared and characterized so far, one can expect of their inhibition activity toward carbonic anhydrase IX.

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Peroxidovanadium complexes in non-aqueous solvents

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Peroxidovanadium complexes represent an important group of vanadium compounds thanks to their bioinorganic properties under physiological conditions (insulin mimetic properties, model compounds for vanadium haloperoxidases, antineoplastic properties) as well as their intervention in vanadium-catalyzed oxidations in non-aqueous solvents (CH₃CN, CH₂Cl₂, CHCl₃). However, speciation of peroxido complexes of vanadium in non-aqueous solvents has not been thoroughly and sufficiently studied so far.

In our work, we focused on speciation of peroxidovanadium complexes in a mixed CH₃CN/H₂O solvent. Besides [VO(O₂)₂(H₂O)][–] we identified in such solutions dinuclear and novel trinuclear species. We confirmed their oxidizing properties in sulfoxidation and epoxidation reactions in various solvents. ⁵¹V NMR spectroscopy showed that the trinuclear species is most likely one of the oxidizing agents in vanadium-catalyzed oxidation with H₂O₂ in different solvents.

How to measure extremely large zero-field splitting in high-spin coordination complexes?

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The recent developments in the field of molecular magnetism, namely discovery of mononuclear single-molecule magnets (as opposed to polynuclear clusters) has necessitated a quantitative determination of the zero-field splitting (zfs) as the main property underlying their magnetic behavior. The zfs of the ground spin state in high-spin coordination complexes of such ions as Co(II), Fe(II), Ni(II) or Re(IV) can reach 100 cm^{-1} and beyond. As such, it is no longer amenable to measurement by our preferred method, high-frequency and -field EPR (HFEPR), at least not in the usual range of frequencies/fields available (up to 1 THz / 35 T). In my talk I will review the alternative experimental methods to measure extremely large zfs, including magnetometry, magnetic circular dichroism, inelastic neutron scattering, Mössbauer spectroscopy, frequency-domain FT-IR spectroscopy, and terahertz EPR.

Electrochemical generation of ferrate(VI) from molten hydroxides

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Ferrate(VI) can be prepared chemically or electrochemically. Electrochemical synthesis proceeds in a concentrated solution of alkali metal hydroxides or their melts, where either an iron anode or Fe^{3+} ions are oxidized. The objective of this work was to determine basic parameters of electrochemical preparation of ferrate(VI) in molten sodium hydroxide, potassium hydroxide and their mixtures. An effect of working temperature, current density and duration of electrolysis in different type of electrolytes was examined.

In the case of molten systems the lowest possible working temperature and maximum acceptable current density are the most important parameters. If the electrolyte contains KOH it was found that increasing amount KOH caused increase in the concentration of produced ferrate(VI). The reason probably is in the formation of solid potassium ferrate(VI) salt (much lower solubility than sodium ferrate(VI)). After appropriate product separation process a stable form of ferrate(VI) with high purity can be prepared.

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**Nickel (II) Schiff base complexes: Synthesis, characterization and catalytic activity
in Kumada cross-coupling reactions**

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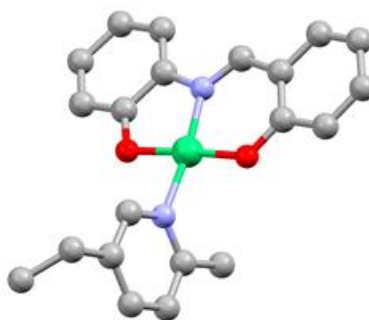
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Schiff base ligands have been extensively studied in coordination chemistry mainly due to their facile syntheses, easily tuneable steric and electronic properties, as well as good solubility in common solvents. Transition metal complexes with Schiff bases, which contain oxygen and nitrogen as donor atoms are of particular interest, because of their ability to possess square-planar or octahedral stereochemistry.

The reaction of nickel(II) acetate with tridentate *ONO*-chelating Schiff base (L) lead to the distorted monomeric square planar [NiLB] complexes (where B are derivatives of pyridine, piperidine, imidazole or phosphine).

Square-planar complexes under study have been characterized by spectral methods (IR, UV-VIS and NMR spectroscopy) and the magnetic data have been taken with a SQUID apparatus in the temperature range 2 – 300 K and field up to 7 T.

Some [NiLB] complexes under study were tried for their catalytic activity in Kumada cross-coupling reactions.



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A charge density study of biologically active copper complex

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The charge density and topological analysis of studied compound, (5-chlorosalicylate)-(2,9-dimethylphenanthroline)-(aqua) copper complex [1], was studied from experimental (XD suite of programs, [1]) and theoretical (BLYP/6-311G** level of theory, TONTO program [2]) point of view.

The copper atom in the studied complex has a deformed square pyramidal coordination with four equatorial atoms and one oxygen atom in the apical position. The copper oxidation state based on d-electron populations is most probably 1.3 with approximately 9.7 electrons in d orbital. The analysis of the d-orbital population furthermore reveals that the bonding orbital is dx^2-y^2 and non-bonding dxy one. All coordination bonds in the complex have positive values of Laplacian, where a higher value is related to a stronger coordination bond, hand in hand with a shorter bond distance. In this respect, the bond of copper with oxygen atom of hydroxyl group, Cu-O(3) is the strongest one.

The preliminary study on the DNA cleavage activity has shown that the complex under study behave as the chemical nuclease itself and also in the presence of added hydrogen peroxide.

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Electrochemical study of rhenium complex formation in halide and oxohalide melts

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The electrochemical behaviour of rhenium chloride complexes in alkali metal chlorides has been studied. Both in the NaCl melt and in the NaCl-KCl equimolar mixture rhenium was found to be present only in the form of Re(III) complexes. However, in the NaCl (40 mol.%) – KCl (60 mol.%) melt Re(IV) complexes were observed to appear. Electroreduction in the given salt mixture as well as in KCl, CsCl melts occurs in two stages with a sequential transition of one and three electrons.

Discharge of rhenium fluoride complexes ReF_6^{2-} to the metal in chloride and chloride-fluoride melts occurs in two stages too.

Introduction of oxygen anions into the CsCl melt containing Cs_2ReCl_6 results in Re(V) stabilization in the ReOCl_5^{2-} composition. At different Re/O ratios, the complexes formed in oxofluoride melts were ReOF_5^- , $\text{ReO}_2\text{F}_4^{2-}$ and ReO_4^- . Thus, in oxofluoride melts the oxidation states stabilized were Re(VI) and Re(VII).

**Synthesis and cytotoxic activity of new Cu(II) and Pt(II), Pd(II) complexes with
nitrogen-containing ligands**

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This work is devoted to new coordination compounds of copper(II), platinum(II), and palladium(II) with pyridine and isothiazole derivatives, their X-ray crystal structure and study of their cytotoxic activity in comparison with cisplatin in several cell lines. It is considered that cisplatin is the most active chemotherapeutic agent among of the existing chemotherapeutic drugs. However, due to its efficient cytotoxic effects, cisplatin has adverse drug effects and chemo-resistance.

The cytotoxicity some of the complexes in comparison with cisplatin was investigated *in vitro* against human cancer cell lines: HEK 293 (human embryonic kidney) and U937 (leukemic). Our results showed that cisplatin and complexes inhibit HEK 293 cell line in a dose and time dependent manner, toxicity of complexes is similar to that of cisplatin. The U937 cell line is significantly less sensitive to complexes compared to cisplatin. However, this selective sensitivity can be useful for the selection of drugs with reduced sensitivity to normal cells.

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Cyclen like a perspective chelating agent for toxic Hg(II) ion

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To heavy metals detoxication N, O, S – polydentate ligands are commercially used. Complexing properties of perspective chelating agent, cyclen (1,4,7,10- tetraazacyclododecane, L), toward to Hg(II) ion by potentiometric titrations were determined. System was studied in aqueous solution ($25 \pm 0.1^\circ\text{C}$, $I(\text{KNO}_3) = 0.1 \text{ M}$) and as a titrant was used potassium hydroxide solution with accurate concentration. Potentiometric results were correlated with ^1H NMR experiments.

Coordinating and biological activities of some flavonoids and their Schiff base analogs

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The dietary flavonoids are gaining attention as potential protectors against a variety of human diseases. Among them there are flavones and flavonones. Fisetin and hesperetin belong to these classes of compounds, respectively. Both are the group of natural products possessing a broad spectrum of biological activities and important therapeutic applications. In our studies we have investigated acid-base, spectroscopic and binding to DNA properties of fisetin and its copper(II) complexes. Potentiometric and UV-Vis titrations revealed that fisetin and Cu(II) complexes can be present in different protonation states depending on the pH region. Several forms can coexist together at the same pH. Electronic absorption and emission spectra showed strong interactions of the studied systems with DNA. Both intercalative and electrostatic mechanism is possible. We have also undertaken studies on a new Schiff base analogue of hesperetin. Schiff bases and their metal complexes are known to be biologically important, hence our interest in the subject. Hydrazone hesperetin Schiff base (HHSB) has been synthesized and used for Cu(II) complex formation. The compounds were characterized using different spectroscopic methods. Studies on antioxidant activities were undertaken to gain information on the biological significance of HHSB and Cu(II)/HHSB complex.

**Tetrachloridoiron(III) and thiocyanatoiron(II) complexes with pyridine derivatives –
syntheses, infrared spectra and structures**

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New tetrachloridoiron(III) complexes with several pyridine derivatives of the composition $(LH)[FeCl_4]$ (L = nicotinamide (*nia*), *N,N*-diethylnicotinamide (*dena*), 2-pyridylmethanol (*2pm*) or methyl-3-pyridylcarbamate (*mpc*) and two thiocyanatoiron(II) complexes of the composition $(mpcH)_2[Fe(NCS)_4(mpc)_2]$ and $[Fe(NCS)_2(2pm)_2]$ have been prepared and characterized by elemental analysis, infrared spectroscopy, and (*denaH*)[FeCl₄] and $(mpcH)_2[Fe(NCS)_4(mpc)_2]$ also by X-ray structure analysis.

The structure of (*denaH*)[FeCl₄] consists of *denaH*⁺ cations and [FeCl₄][−] anions. The [FeCl₄][−] anions exhibit rotational disorder, as approximated by two [FeCl₄][−] tetrahedrons. There is also a hydrogen bond between the pyridine nitrogen atom of one *denaH*⁺ cation and the carbonyl oxygen atom of a neighboring *denaH*⁺ cation (N–H...O=C). The corresponding equivalent hydrogen bonds interconnect two *denaH*⁺ cations and lead to the formation of polymeric zig-zag 1-D chains.

The $(mpcH)_2[Fe(NCS)_4(mpc)_2]$ is built from two *mpcH*⁺ cations and one $[Fe(NCS)_4(mpc)_2]^{2-}$ anion which are held together also by two hydrogen bonds between the pyridine nitrogen atoms of two *mpcH*⁺ cations and O atoms of two carbamate groups from coordinated *mpc* molecules in the anion (N–H...O=C). In the anion four N atoms from NCS groups and two N atoms from pyridine rings about iron(II) atom form a slightly distorted octahedral environment.

From the spectral and published data follows that in $[Fe(NCS)_2(2pm)_2]$ complex the thiocyanate groups are coordinated to Fe(II) atom through nitrogen atoms. We suppose that coordinated *2pm* molecules act as chelate bidentate *N,O*-ligands.

In this paper structural parameters and infrared spectra of similar complexes are compared and discussed.

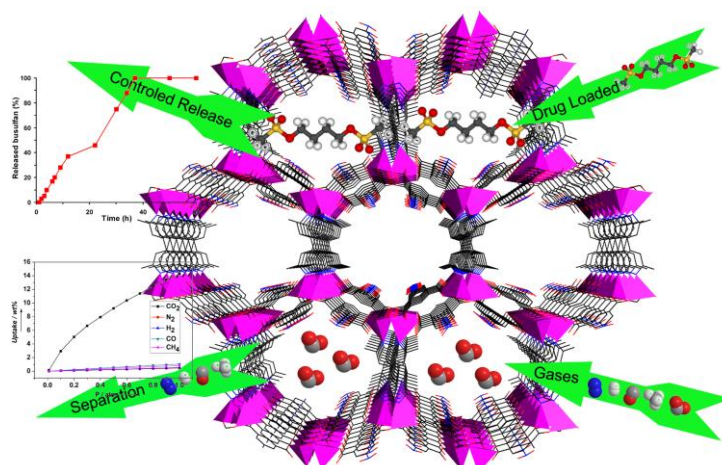
A hydrostable and nitril/methyl-functionalized metal-organic framework for drug delivery and highly selective CO₂ adsorption

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By using a strategy of introducing hydrophobic groups to the linkers, a hydrostable MOF was constructed based on 5-nitroisophthalate and 2,2'-dimethyl-4,4'-bipyridine coligands, revealing a 3D dia topology structure with a 1D channel parallel to the c axis. TGA, PXRD, and water vapor sorption studies reveal high thermal and water stability for the framework. The framework is very porous and possesses not only high busulfan payloads with an encapsulation efficiency up to 21.5% but also very high CO₂ selective capture compare with other small gases (*i.e.* CH₄, N₂, O₂, CO and H₂) at 298 K based on molecular simulations due to the pore surface being populated by methyl and nitril groups. Furthermore, *in vitro* MTT assays were conducted on four different cells lines in contact with increasing concentrations of the framework and the results showed that the framework was nontoxic (cell viability > 80%) up to concentrations of 500 µg/mL.



Synthesis, structural and magnetochemical study of the iron(III) Schiff base complexes

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The twelve iron(III) complexes consisting of the Schiff condensation products and chlorido or pseudohalido coligands have been prepared, structurally and magnetochemically characterized. The expected coordination chromophores - {Fe(N₃O₂)Cl} or {Fe(N₃O₂)N'} were confirmed by X-ray diffraction analysis, at which nitrogen donor atoms are either in *fac* or in *mer* arrangement and oxygen donor atoms have *cis* configuration, with exception of one compound, that was successfully prepared as pure *cis* isomer and pure *trans* isomer. The structurally determined compounds were investigated by SQUID magnetometry. In the first pseudohalido complex was observed an abrupt and complete spin crossover accompanied by 2 K thermal hysteresis ($T_c = 83$ K) [1]. The crystal structure of this complex has been solved for both possible spin states: low-spin and high-spin to detect the changes of the unit cell. The second pseudohalido compound exhibits gradual and incomplete spin crossover ($T_c = 250$ K), but this magnetic properties strongly depends on the presence of lattice solvent molecules. Once, molecules of the acetone are incorporated into the structure, complex becomes high-spin. The high-spin state behavior over the temperature range 2 – 300 K has been observed for all remaining compounds.

[1] P. Masárová, P. Zoufalý, J. Moncol', I. Nemec, J. Pavlik, M. Gembický, Z. Trávníček, R. Boča, I. Šalitroš; *New J. Chem.*, **2015**, 39, 508-519

Copper carboxylate complexes – synthesis and structural characterization

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Six copper(II) oxalate complexes, namely $K_2[Cu(ox)_2]$ (**1**), $(Hiz)_2[Cu(ox)_2]$ (**2**), $[Cu(ox)(N-Bzliz)_2]$ (**3**), $(HMeiz)_2[Cu(ox)_2(H_2O)]$ (**4**), $[Cu(ox)(Meiz)_2]$ (**5**) and $[Cu(ox)_2](1-Bzliz)(H_2O)]$ (**6**), where ox = oxalate ion, iz = imidazole, N-Bzliz = N-benzylimidazole, Meiz = 2-methylimidazole, have been synthesized and characterized by single crystal or powder X-ray diffraction.

Coordination polyhedron in structures **1**, **2**, **3** and **6** is tetragonal bipyramidal arrangement with central atom in centre of symmetry. The square-planar coordination of the copper(II) central atom in **4** is provided by four oxygen donor atoms of the oxalate chelating ligand. In **5**, the Cu(II) atom is pentacoordinated by three donor oxygen atoms of oxalate groups and the remaining two sites are occupied by the nitrogen atoms of the 2-methylimidazole.

In the last few years, several structural – magnetic correlations have been proposed and the influence of Jahn – Teller distortion effect in oxalate – bridged copper(II) sites was described (Jenniefer & Muthiah (2013); Kang (2005); Murphy & Hathaway (2003)).

EPR spectroscopy of copper(II) complexes with *N*-donor ligands and 3,5-dichlorosalicylic acid in frozen solutions

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In the present contribution, the chemical environments of copper(II) ions in the copper(II) complexes containing 3,5-dichlorosalicylic acid (3,5-diClSalH) and Cu(II) salts (Cu(ac)₂ or CuSO₄) and *N*-donor ligands (3-pyridylmethanol (ronicol) or *N,N'*-diethylnicotinamide (denia), with varying ligand-to-metal ratio, x , [Cu(ac)₂(aq) or CuSO₄(aq) + 2 (3,5-diClSalH(solv)) + x (ronicol or denia (solv))], where $x = 0, 1, 2, 4, 6, 8, 12, 16$, were studied by EPR spectroscopy in the frozen solutions at low temperature. The effects of two copper(II) salts (containing anions of different basicity), 3,5-dichlorosalicylic acid and two *N*-donor ligands with varying ligand-to-metal ratio on the formation of resulting complexes in the solutions are discussed. Well-resolved ¹⁴N superhyperfine splitting lines in the parallel and perpendicular part of the second- and third-derivative axially symmetric Cu(II) EPR spectra indicate that nitrogen atoms could be coordinated to the central Cu(II) ion in the equatorial plane. The trend in *g*-values ($g_{\parallel} > g_{\perp} > 2.0023$) indicates that the unpaired electron is localized on the d_{x²-y²} orbital on copper ion. Such rich data cannot be obtained by EPR spectroscopy of power samples of the given copper(II) complexes.

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Purine alkaloids as drugs and ligands

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Purine alkaloids are one of the most fascinating organic compounds. These alkaloids possess wide range of pharmaceutical activities as therapeutic agents. They potentiate the cytotoxicity of a variety of DNA damaging agents, especially caffeine. They inhibited the carcinogenetic activity of cigarette smoke, as well as enhanced the cytotoxicity of some cancerostatic drugs. Possesses anti-inflammatory and anti-asthmatic effects especially theophylline, affects the central nervous system, etc.

Purine alkaloids as a ligands are variable as well: caffeine prefer coordinated via its N9, however there is an example in which coordinated via its O10 atom which is rarity. Theophylline prefer coordinated via N7 (as anion) there are also examples in which coordinated via N7 + C8 and even via N7 + N9 + O10 donor sites, which are varieties. Theobromine prefer coordinated via N2 (as anion) and even via N9 (as molecule).

Selected Cu(II) complexes were tested against some rheumatic arthritis and will be discussed.

**Synthesis, spectral properties and crystal structures of cobalt(II) dipicolinates
with melamin**

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This study is dealing with several new cobalt(II) complexes with pyridine-2,6-dikarboxylic acid (dipicolinic acid – PDCH₂) and 1,3,5-triazine-2,4,6-triamine (melamine - mel). So far, only two complexes with given composition were reported, where one contains coordinated mel and in the other, uncoordinated mel is bonded through hydrogen bonds.

We describe the syntheses, their molecular structures and included the description of their infrared and electron spectra of the three new complexes. This work has been done with the intention to further study the magnetic properties and biologic activity of said complexes. For this, several complexes have been synthesized and their structure was affirmed using monocrystal RTG structural analysis.

Our complexes contain uncoordinated melamin and tridentate coordinated PDC dianion. They have extensive systems of hydrogen bonds, creating supramolecular 3D structures. Effort has also been made towards finding a model for synthesizing complexes with predicted properties and structure.

The financial support of Slovak grant agency VEGA 1/0472/13 is gratefully acknowledged.

**Synthesis, crystal structure and spectral properties of nickel(II)
hydroxypyridinecarboxylates**

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Synthesis and characterization of six new complexes Ni(II) with 2-hydroxynicotinic acid (2-OHnicH) composition $[\text{Ni}(\text{2-OHnic})_2\text{L}_2]$ {where L = furo[3,2-c]pyridine – FP; [1]benzofuro[3,2-c]pyridine – BFP; isoquinoline – IQ; 3,5-dimethylpyridine – 3,5-DMpy; isonicotinic amide – INA} and $\text{Ni}(\text{2-OHnic})_2(\text{MFP})_2(\text{H}_2\text{O})_4$ {where MFP = 2-methylfuro[3,2-c]pyridine} are reported. The characterizations were made on elemental analyses, infrared and electronic spectra. The 2-hydroxynicotinate anion in prepared complexes coordinates by salicylate type O,O-chelation (through oxygen atom of the carboxyl group and deprotonated phenolate oxygen atom) to the Ni(II) ions as shown by infrared spectroscopy results. Molecular structure of the complex $[\text{Ni}(\text{2-OHnic})_2(\text{FP})_2]$ was determined by X-ray powder diffraction analyses and confirm above assumption.

Acknowledgments: Grant agencies (Slovakia: VEGA 1/0233/12; VEGA 1/0472/13; APVV-0014-11) are acknowledgment for financial support.

Nickel(II) complex with 1,4,7-tris(2-aminoethyl)-1,4,7-triazacyclononane

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A nickel(II) complex with 1,4,7-tris(2-aminoethyl)-1,4,7-triazacyclononane (taetacn), [Ni(taetacn)](ClO₄)₂·H₂O, was synthesized. The crystal structure was determined by the single-crystal X-ray diffraction method at 293 K. The compound is composed of octahedral nickel(II) cation with three pendant groups of taetacn, tetrahedral ClO₄[−] anion, and crystal water molecule. The electronic spectral feature is consistent with the octahedral geometry. The temperature dependence of the magnetic susceptibility (4.5–300 K) could be interpreted by taking into consideration the zero-field splitting of the nickel(II) ion ($g = 2.14$, $D = 3.72 \text{ cm}^{-1}$, and $N\alpha = 300 \times 10^{-6} \text{ cm}^3 \text{ mol}^{-1}$). The cyclic voltammetry in DMF showed quasi-reversible and irreversible oxidation waves ($E_{\text{pa}} = 0.54$, $E_{\text{pc}} = 0.45 \text{ V}$; $E_{\text{pa}} = 1.16$, $E_{\text{pc}} = 0.71 \text{ V}$ versus Ag/Ag⁺).

Bio-medical aspects of theophylline and its metal complexes

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Alkaloids are most fascinating organic compounds and many researches pay much attention to them. From the very wide range of alkaloids is chosen one of them – theophylline. Theophylline (1,3-dimethylxanthine) possess pharmacological activities as therapeutic agent. Theophylline has expressive antiinflammatory and antiasthmatic effect, enhanced mobilization of lipid reduces the brain regional adenylate cyclase activity, facilitate glucose inhibition. Theophylline is muscle relaxant, vasodilator, diuretic and cardiac stimulant.

Theophylline is very attractive as ligand and selected crystal structures of theophylline – metal complexes are presented and discussed, as well as some results of bioactivity tests are also discussed. The theophylline complexes of copper, zinc, mercury, platinum, palladium, rhodium, gold and cobalt are known. Crystal structures of theophylline – metal complexes showed variable stereochemistry about the respective metal central atoms. Monomeric structures are most common with the following chromophores: HgNC; AuNP; ZnN₄, ZnO₂N₂; PdN₂P₂, PdP₂NS, PdP₂NC; CoN₅Cl; PtN₂P₂, PtP₂NS; and CuO₂N₂, CuN₃O, CuN₅, CuO₃N₂, CuN₃O₂ and CuN₄O₂. Dimeric structures contain the following chromophores: PtP₂NS and RhO₄NRh'. There is even polymeric structure: PtC₄ON. These structures are analyzed not only from structural parameters, oxidation states of the respective metal atoms, but also from their bio-activities.

**Electronic structure of transition-metal compounds with various
spin-charge-orbital instabilities**

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Transition-metal compounds show surprisingly rich physical and chemical properties due to strongly correlated *d* electrons with spin, charge, and orbital degrees of freedom. The electronic structure of transition-metal compounds is characterized by two parameters: Coulomb interaction *U* between transition-metal *d* electrons and charge-transfer energy Δ from the ligand *p* to transition-metal *d* orbitals (Zaanen-Sawatzky-Allen scheme). In insulating transition-metal compounds with relatively large Δ , the ligand *p* orbitals are fully occupied and the spin-orbital orderings of *d* electrons can be described by combination of Jahn-Teller and Kugel-Khomskii mechanisms. On the other hand, it is known that transition-metal compounds with small or negative Δ exhibit unique spin-charge-orbital instabilities induced by ligand *p* holes. Here we present experimental and theoretical studies on negative- Δ transition-metal compounds including NaCu³⁺O₂, PrNi³⁺O₃, CaFe⁴⁺O₃, CsAu²⁺Br₃, Ir²⁺Te₂, and Au²⁺Te₂. The surface or interface of such transition-metal compounds tends to show dramatic physical and chemical functionalities that may find applications as future orbitronics devices, strongly-correlated photocatalysts, etc.

The authors would like to thank the long term collaborations with Prof. D. I. Khomskii (Univ. of Köln), Prof. G. A. Sawatzky (Univ. of British Columbia), and Prof. N. L. Saini (Univ. of Roma La Sapienza).

Golden opportunities: New aspects of the chemistry of gold

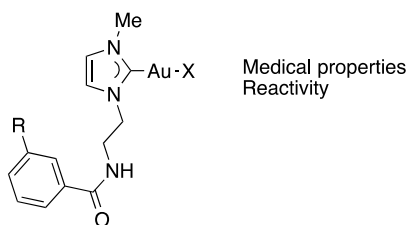
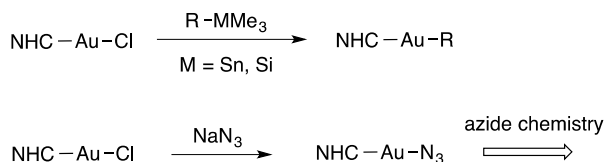
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We present here our latest research on the chemistry of gold in both the +1 and +3 oxidation states. First we show how organotin- and, in some cases, organosilicon compounds can be used to transfer organic groups to gold under very mild conditions. The structures, reactivity and photophysical properties of the compounds have also been studied in detail.

In the second part of the presentation we will discuss the synthesis and reactivity of carbene stabilised gold azido compounds. Finally, we disclose some new *N*-heterocyclic carbene ligands containing amide-substituents and their behaviour as ligands for gold and platinum. These compounds are of interest for their medical application, for which we will present some preliminary data.



**Supramolecular structure and isomerism of new copper(II) halogenobenzoate complexes
with nicotinamide**

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Nicotinamide has been employed as a supramolecular reagent [1] in the synthesis of fifteen copper(II) halogeno- and dihalogenobenzoate complexes. Compounds show various crystal structures of formulas $[\text{Cu}(\text{X-bz})_2(\text{nia})_2]$, $[\text{Cu}(\text{X-bz})_2(\text{nia})_2(\text{H}_2\text{O})]$ and $[\text{Cu}(\text{X-bz})_2(\text{nia})_2(\text{H}_2\text{O})_2]$. The crystal structures of all ones were determined by the single-crystal X-ray structural analysis. All these compounds are monomeric complexes with a square-pyramidal or square-bipyramidal coordination sphere around Cu^{2+} ion.

The two polymorphs of $[\text{Cu}(2,6\text{-Cl}_2\text{bz})_2(\text{nia})_2]$ are examples of coordination compounds, which are conformation and supramolecular isomers. Additionally, the $[\text{Cu}(\text{X-bz})_2(\text{nia})_2(\text{H}_2\text{O})_2]$ and $[\text{Cu}(\text{X-bz})_2(\text{nia})_2] \cdot 2\text{H}_2\text{O}$ present examples of coordination isomerism.

The molecules of all compounds are connected by $\text{N} \cdots \text{H} \cdots \text{O}$ and/or $\text{O} \cdots \text{H} \cdots \text{O}$ hydrogen bonds from NH_2 groups of nicotinamide and water molecules, which create supramolecular hydrogen-bonding-coordination chains and networks.

[1] J. Halaška, A. Pevec, P. Strauch, B. Kozlevčar, M. Koman, J. Moncol', Polyhedron 61 (2013) 20. J. Moncol', J. Maroszová, M. Koman, M. Melník, M. Valko, M. Mazúr, T. Lis, J. Coord. Chem. 61 (2008) 3740.

Energy storage by proton-coupled electron transfer reactions of Ru complexes

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Proton gradient in biomembrane plays an important role for energy generation through the ATP synthesis. Here, we proposed new energy storage system based on the proton-coupled electron transfer (PCET) reactions of two Ru complexes by mimicking the energy transducing principle of proton gradient in the biomembrane. We synthesized novel Ru complexes with tridentate bis(benzimidazolyl)pyridine (Ru-N) and benzene ligands (Ru-C), which showed large differences on the Ru(II/III) oxidation potentials and pKa values. By introducing cyclometalated bond in the Ru-C complex, the Ru(II)/Ru(III) oxidation potentials were shifted to a negative direction and the pKa values became higher compared to those of the Ru-N. In the two half-cell device, each cell included Ru(II)-N and Ru(III)-C complexes as PCET active materials. Starting from neutral pH, the charging process induced not only the increase of voltage but also a large pH difference between two half-cells under chronopotentiometric measurement. The two half-cell device revealed repeated charging-discharging cycles, accompanied by the changes of both voltage and pH. Therefore, an electric energy can be stored as a proton gradient, which was generated by the PCET reaction of the Ru complexes. We will discuss the design of new type of rechargeable energy storage devices based on the PCET reaction of metal complexes.

**Structure conversion and chromic behaviour of the metal-hydrazone complexes
in solution and in the solid state**

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We have focused our attention to the chemical and physical stimuli-responsive transition-metal complexes in solution and in the solid state. A wide variety of hydrazone-metal complexes has been reported, and the structures and properties of the complexes have been investigated in order to explore their fascinating functionalities. In this work, we prepared hydrazone-palladium(II) complexes of $[\text{PdCl}_2(\text{HL})]$ and $[\text{PdCl}(\text{L})]$ (HL and L^- denote protonated and deprotonated hydrazone ligands, respectively), and determined their structures by X-ray analysis. The thermal and/or photochemical structure conversion of the complexes proceeded in acetonitrile, and the thermochromic and/or vapochromic structure conversion also occurred even in the solid state. We would also report on the reactivity of the related hydrazone-platinum(II) complexes.

Calcium phosphates and their applications

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The major use of calcium phosphates is for making industrial fertilizers to supplement farm land with phosphate which is an essential but limiting element for plant growth. The natural ores are mined for apatites (mainly $\text{Ca}_5(\text{PO}_4)_3\text{F}$), that are transformed into phosphoric acid by use of sulfuric acid leaching. The produced H_3PO_4 can then be added to raw ore to produce TSP (triple superphosphate), which contains a large amount of soluble phosphate in the form of MCPM, monocalcium phosphate monohydrate ($\text{Ca}(\text{H}_2\text{PO}_4)_2 \cdot \text{H}_2\text{O}$). When heated this compound gives an acid pyrophosphate which is less soluble than MCPM. The crystal structures vary depending on drying conditions, and we have experimented spray drying as a fast way to obtain a reproducible product, well characterized, by IR, NMR, TG-DSC methods and SEM observations. The other applications of calcium phosphates will be mentioned with examples.

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**Synthesis and characterization of new Gallium(III) complexes with
5-bromosalicylaldehyde benzoylhydrazones**

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New Gallium (III) complexes with 5-bromosalicylaldehyde-4-hydroxy-benzoylhydrazone and 5-bromosalicylaldehyde isonicotinoylhydrazone have been synthesized. All compounds were characterized by elemental analysis, IR and ¹H NMR spectroscopy. According to the experimental data the formulas [Ga(L)₂](NO₃) were suggested. The complexes are mononuclear with the Ga(III) ions being surrounded by two tridentate ligands. The analysis revealed coordination binding through deprotonated phenolic-oxygen, azomethine-nitrogen and amide-oxygen atoms.

The cytotoxic properties of the ligands and newly synthesized complexes were tested by MTT-dye reduction assay on two human tumor cell lines: T-cell leukemia SKW-3 and the acute myeloid leukemia HL-60 cell lines. The compounds exhibited concentration-dependent cytotoxic effects with low micromolar IC₅₀ values.

Financial Support: The presented work has been financially supported by the Medical Science National Fund at the Medical University of Sofia (Grant 15/2014).

Anticancer ruthenium compounds with biologically active ligands

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The development of metal-based anticancer compounds has traditionally focused on cytotoxic platinum-based compounds, however, in recent years there has been much of interest in the development of ruthenium-based anticancer drugs and it was shown that the ligand sphere strongly influences their anticancer and antimetastatic properties.

The tumor specificity of ruthenium compounds can be increased by linking Ru part to the biologically active organic molecules. Lonidamine is known to inhibit the aerobic glycolysis in cancer cells while simultaneously enhancing glycolysis in the normal cells. Bexarotene is agonist of the retinoid X receptor and specific against T-cell lymphoma.

This presentation will focus on synthesis and characterization of the hybrid complexes based on lonidamine and bexarotene tethered to the ruthenium unit via an imidazole group. Ru(II) compounds found to be highly cytotoxic against number of the human cancer cell lines. Importantly, lonidamine-modified complexes were remarkable active against brain cancer cell lines and the hybrid bexarotene-ruthenium compound, showed high cytotoxicity against cancer cells, while showed no cytotoxicity against non- tumorigenic cell lines.

This work was supported by Russian Science Foundation (14-13-00483)

**Synthesis and properties of dinuclear oxidovanadium(IV) complexes with cyclam-based
macrocyclic ligands having four Schiff-base pendant arms**

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Dinuclear oxidovanadium(IV) complexes with tetrakis(5-bromosalicylideneaminoethyl)cyclam (cyclam = 1,4,8,11-tetraazacyclodecane) ($H_4tbsaec$), tetrakis(3,5-dibromosalicylideneaminoethyl)cyclam ($H_4tdbsaec$), tetrakis(5-chlorosalicylideneaminoethyl)cyclam ($H_4tcsaec$), tetrakis(3,5-dichlorosalicylideneaminoethyl)cyclam ($H_4tdcsaec$), tetrakis(3-methoxysalicylideneaminoethyl)cyclam ($H_4tmtsaec$), and tetrakis(5-methylsalicylideneaminoethyl)cyclam ($H_4tmsaec$), $[(VO)_2(L)]$ ($L = tbsaec^{4-}$, $tdbsaec^{4-}$, $tcsaec^{4-}$, $tdcsaec^{4-}$, $tmtsaec^{4-}$, and $tmsaec^{4-}$), have been synthesized and characterized by elemental analysis, infrared and electronic spectra, and temperature dependence of magnetic susceptibilities (4.5 – 300 K). The magnetic interaction between the two metal ions is very weak with the J values of $-0.44 - -1.2 \text{ cm}^{-1}$. These data are in accordance with that two oxidovanadium(IV) ions are bound by the chelating of the two Schiff-base pendant arms outside the central tetraazacyclotetradecane ring forming a square-pyramidal coordination geometry.

**Synthesis and characterization of iminopyridyl complexes with thiophene based ligands
for Heck coupling reactions**

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The new ligands, (5-methyl-2-thiophene-2-pyridyl(R))imine [R = methyl (**L1**); R = ethyl (**L2**)] and (5-bromo-2-thiophene-2-pyridyl(R))imine [R = methyl (**L3**); R = ethyl (**L4**)] were successfully synthesized via Schiff base condensation reaction and obtained in good yields. The ligands were reacted with PdCl₂(COD) and PdClMe(COD) to give their corresponding palladium(II) complexes **1-8**. All compounds were characterized by IR, ¹H and ¹³C NMR spectroscopy, elemental analysis and mass spectrometry. The molecular structures of **6** and **8** were confirmed by X-ray crystallography. Both compounds crystallized in monoclinic *P2₁/n* space system. The coordination geometry around the palladium atom exhibited distorted square planar geometry at the metal center. The complexes were evaluated as catalyst precursors for standard Heck coupling reactions and showed remarkable catalytic activity with steric and electronic influences.

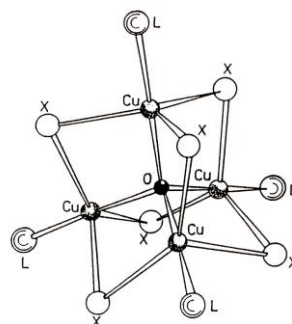
Structures of $\text{Cu}_4\text{OCl}_6\text{L}_4$ complexes studied by vector analysis

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The complex $\text{Cu}_4\text{OX}_6\text{L}_4$ ($\text{X} = \text{Cl}, \text{Br}$) molecule (fig. below) can be regarded as a supramolecular model of interactions between ligand substrates L and hypothetical round-shaped coordination tetra-receptor Cu_4OX_6 that provides four exactly oriented OCuCl_3 receptors. The tetra-receptor Cu_4OX_6 of the molecule is thermodynamically stable, its shape is relatively rigid, but simultaneously soft, to be distorted by interactions coming from inside and outside of the molecule that is located in the structure of the $\text{Cu}_4\text{OX}_6\text{L}_4$ complex. These structural properties inspired us to elaborate a vector model for quantitative characterization of structural dynamics by lengths of bond, distance, polyhedral and molecular vectors, including their direction in the structure. Structures of $\text{Cu}_4\text{OX}_6\text{L}_4$ complexes are interest to researchers, since above fifty structures are known until now.



The results of structural vector analysis of $\text{Cu}_4\text{OX}_6\text{L}_4$ complexes are discussed with respect to: structure (crystallographic system, Bravais lattice, point group, space group, Schoenflies index), physico-chemical properties (electron interactions by covalent bonds, hydrogen bonds, van der Waals interactions, intra- and intermolecular electron flows), biochemical aspects (substrates L = coordinated bioactive molecules).

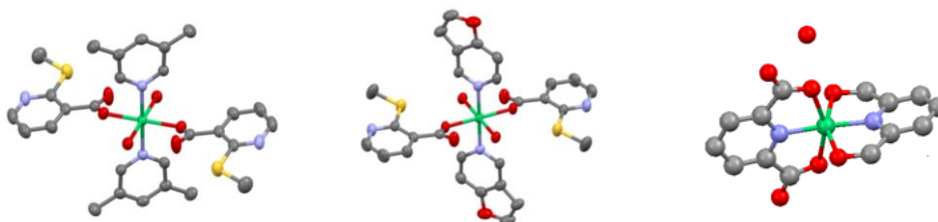
Magnetic properties and magnetostructural *D*-correlation of hexacoordinate Ni(II) complexes

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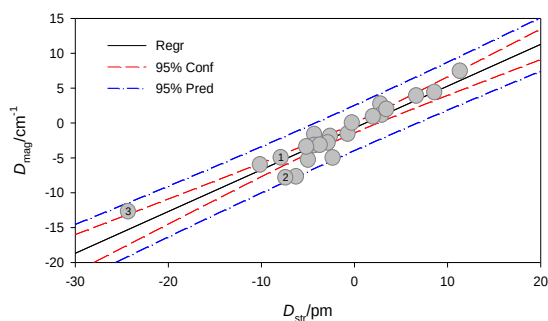
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New Ni(II) complexes [Ni(2-Me-Snic)₂(3,5-lut)₂(H₂O)₂] (**1**), [Ni(2-Me-Snic)₂(FP)₂(H₂O)₂] (**2**) and [Ni(pydc)(pydm)]·(H₂O) (**3**) have been synthesized, structurally and spectrally characterized. The {NiN₂O₄} chromophore refers to a compressed tetragonal bipyramid for which a negative zero-field splitting is expected.



SQUID magnetic measurements of complexes **1-3** revealed that they behave magnetically as typical $S = 1$ spin systems with considerable zero-field splitting parameter $D/hc = -7.8 \text{ cm}^{-1}$ for the complex **1**, $D/hc = -5.0 \text{ cm}^{-1}$ for **2** and $D/hc = -12.7 \text{ cm}^{-1}$ for **3**. The complexes **1-3** conform the magnetostructural *D*-correlation for hexacoordinate Ni(II) complexes with negative structural and magnetic anisotropy [1].

This work was supported by Slovak grant agencies (VEGA 1/0233/12 and APVV-0014-11).



[1] J. Miklovič, A. Packová, P. Segľa, J. Titiš, M. Koman, J. Moncol', R. Boča, V. Jorík, H. Krekuzska, D. Valigura; Inorg. Chim. Acta 429 (2015) 73-80.

**Application of circular dichroism spectroscopy to assess coordination ability
of natural polyether ionophores**

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Natural polyether ionophorous antibiotic Monensin (MonH) forms isostructural complex species $[M(\text{Mon})_2(\text{H}_2\text{O})_2]$ (**1**, $M = \text{Mg}^{2+}, \text{Ca}^{2+}, \text{Mn}^{2+}, \text{Co}^{2+}, \text{Ni}^{2+}, \text{Zn}^{2+}$) characterized by X-ray diffraction on single crystals, IR, NMR, EPR, FAB-MS spectroscopies, etc. Complexes **1** possess enhanced antimicrobial and antitumor activity as compared to the non-coordinated ligand.

The ability of MonH to bind divalent metal ions was evaluated by means of circular dichroism spectroscopy in methanolic solutions. The data revealed that Monensinate anion (Mon^-) forms two types of metal complexes depending on metal-to-ligand molar ratio. Known complexes **1** were detected in the presence of ligand excess ($M^{2+} : \text{Mon}^- = 1:10 - 1:2$). The increase of metal(II) ion concentration led to the formation of $[\text{MMon}(\text{H}_2\text{O})]^+$ species (**2**, $M^{2+} : \text{Mon}^- = 1:1 - 6:1$) observed for the first time.

The experimental data showed that the coordination of divalent metal ions influences significantly the spectral pattern of Monensin despite of the structural similarities between compounds studied.

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DFT Approach to spin crossover in embedded systems

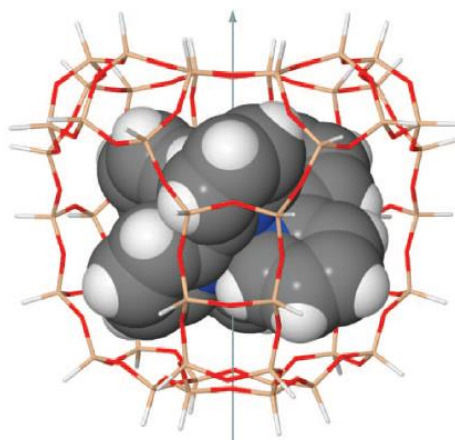
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The spin state energetics, structural properties and guest-host interactions of the benchmark spin crossover systems $[\text{Fe}(\text{bipy})_3]^{2+}$ and $[\text{Co}(\text{bipy})_3]^{2+}$ (bipy = 2,2'-bipyridine) embedded into the zeolite Y cavity were studied theoretically. The PBE functional was employed within the STO 3- ζ or STO 2- ζ basis sets, respectively, for all atoms. On top of our previous study [1] the performance of the recently defined dispersion correction by Grimme et al [2] was examined here as well.



[1] A. Vargas, A. Hauser and L.M. Lawson Daku, *J. Chem. Theory. Comput.*, **2009**, 5 (1), 97.

[2] S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.*, **2010**, 132, 154104.

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**Redox-active zinc(II) complexes with Mannich bases: synthesis, physico-chemical
characterization and biological evaluation**

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Zn(II) complexes with 4,6-di-*tert*-butyl-3-(pyrrolidine-1-ilmethyl)-1,3-dihydroxybenzene (L^I), 4,6-di-*tert*-butyl-3-(piperidine-1-ilmethyl)-1,3-dihydroxybenzene (L^{II}), 4,6-di-*tert*-butyl-3-(azetidine-1-ilmethyl)-1,2-dihydroxybenzene (L^{III}), 4,6-di-*tert*-butyl-3-(morpholine-1-ilmethyl)-1,2-dihydroxybenzene (L^{IV}), and 4,6-di-*tert*-butyl-3-(methylpiperazine-1-ilmethyl)-1,2-dihydroxybenzene (L^V), have been synthesized and characterized by means of elemental analysis, TG/DTA, FT-IR, UV-Vis, ESR, and conductivity measurements. Antifungal activity of these ligands and their respective Zn(II) complexes has been determined against *Aspergillus niger*, *Fusarium spp.*, *Penicillium lividum*, *Mucor spp.*, *Sclerotinia sclerotiorum*, *Botrytis cinerea* and *Alternaria alternata*. Zn(II) complexes exhibit pronounced antifungal activity, which in a number of cases is comparable with that of Nystatin and Terbinafine or even higher. Spectrophotometric investigation was carried out in order to estimate the rate of the reduction of bovine heart cytochrome *c* with these compounds. A low reducing ability of the compounds L^I – L^V and their Zn(II) complexes (even to the point of its absence) upon interaction with Cyt *c* was found.

Towards development of highly active copper catalysts for activation of monohalogenated substrates in atom transfer radical addition (ATRA)

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Fundamentals of copper catalyzed atom transfer radical addition (ATRA) and mechanistically similar polymerization (ATRP) were discussed. Special emphasis was placed on structural characterization and electrochemical properties of copper complexes. Recent advances in the area of development of highly active copper complexes for both processes were also reviewed. It was found that the systematic incorporation of electron donating groups in currently among the most active tris(2-pyridylmethyl)amine (TPMA) based ligands significantly increases the catalytic activity in copper mediated ATRA/ATRP. The presented results could have significant implications in the area of activation of monohalogenated substrates in copper catalyzed ATRA because the halide functionality in the addition product can be selectively reduced, eliminated, displaced, or potentially converted to a Grignard reagent.

Characterization and *in vitro* antimicrobial and cytotoxic activity of complexes with 5-chloro-quinolin-8-ol

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With the aim to follow a biological activity of 5-chloro-quinolin-8-ol (ClQ) complexes with 3d metals we have prepared eight complexes: [Mn(ClQ)₂] (**1**), [Fe(ClQ)₃] (**2**), [Co(ClQ)₂(H₂O)₂] (**3**), [Ni(ClQ)₂(H₂O)₂] (**4**), [Cu(ClQ)₂] (**5**), [Zn(ClQ)₂(H₂O)₂] (**6**), [Mn(ClQ)₃]·DMF (**7**) and [Co(ClQ)₃]·DMF·(EtOH)_{0.35} (**8**). Complexes were characterized by IR and UV-VIS spectroscopy and thermal analysis; X-ray structure analysis was carried out for complexes **7** and **8**, too. Their structures consist of octahedral [M(ClQ)₃] complexes (M = Mn(III) and Co(III), respectively) and solvated DMF and EtOH molecules. Antimicrobial activity of **1** – **6** and ligand ClQ was tested against 12 strains of bacteria and 5 strains of fungi. According to the strength of their antimicrobial activity, compounds can be sorted: **1** > ClQ > **6** > **3/4** > **2** > **5**. The analysis of cancer cell viability showed that these complexes were cytotoxic on human breast carcinoma (MDA-MB), human colon carcinoma (HCT-116) and on human lung carcinoma epithelial cells (A549). Cytotoxic effect was dose dependent: concentration decrease of all tested compounds was followed by markedly increase of tumor cell viability. Complex **2** seems to be a good candidate for future pharmacological evaluation, particularly in the field of breast cancer research.

SOD mimetic activity of some salicylatocopper complexes

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The investigation of salicylatocopper complexes in presence of nitrogen donor ligand is recently growing research area for the interesting mimetic activity of those complexes. We present here three X-salicylatocopper (where X = 3-methyl, or 4-methoxy) complexes with three different N-donor ligand of the formula $[\text{Cu}(\mu\text{-menia})(3\text{-Mesal})_2(\text{menia})(\text{H}_2\text{O})]_2$ **1**, $\text{Cu}(3\text{-Mesal})_2(\text{denia})_2(\text{H}_2\text{O})_2$ **2**, $\text{Cu}(4\text{-MeOsal})_2(2\text{-pyme})_2$ **3**. The complexes were characterized by elemental analysis, IR, UV-VIS spectrophotometry. The cyclic voltammetry study, as well as the superoxide dismutase activity of prepared complexes in solution have been measured. The SOD activity was compared with parent ligand copper acetate, native SOD enzyme, as well as with related copper complex containing non-steroidal anti-inflammatory drugs. The best inhibition value has been found for the complex **1** ($\text{IC}_{50} = 2.24 \mu\text{M}$), that allows to place the complex **1** into a group of good superoxide scavengers. The SOD activity together with the redox stability are related to the composition, structure of the complexes.

On the efficiency of PPD antioxidants

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Structures of four *N*-phenyl-*N'*-alkyl-*p*-phenylenediamine (PPD) antioxidants with Cu²⁺ ions at possible reaction sites were optimized at B3LYP/6-311G* level of theory. No Cu-C bonds formation at tertiary carbon sites was concluded. The complexes with copper atoms at aliphatic nitrogen sites are energetically preferred which is connected with shorter copper-nitrogen bonds in this case.

Molar Antioxidant Effectiveness (AEM) very well correlates with spin density of copper atoms at the nitrogen reaction site between aromatic rings. Fairly good AEM correlation with copper and nitrogen atomic charges at this nitrogen site may be concluded as well.

This work was supported by Slovak Grant Agency VEGA under the contract No. 1/0327/12. We thank the HPC center at the Slovak University of Technology in Bratislava, which is a part of the Slovak Infrastructure of High Performance Computing (SIVVP Project No. 26230120002, funded by the European Region Development Funds), for computing facilities.

Pentacoordinate cobalt(II) complexes as single molecule magnets

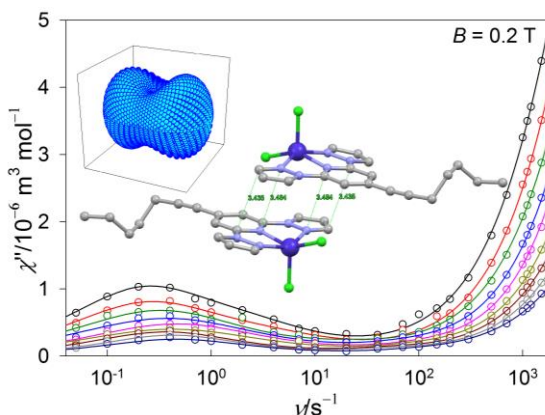
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The class of single-molecule magnets (SMM's) could represent one of the key roles for high-density information storage in the future¹. The investigation and rational modification of novel ligands along with alteration of central atoms are promising tools which could allow the tuning of relaxation time of SMM's. For this study we synthesized and characterized a set of mononuclear pentacoordinate Co(II) complexes made

up from “antennae” ligand e.g. L^{C0} = 4-iodo-2,6-di-pyrazol-1-yl-pyridine; L^{C7} = 4-hept-1-ynyl-2,6-di-pyrazol-1-yl-pyridine; L^{C10} = 4-dec-1-ynyl-2,6-di-pyrazol-1-yl-pyridine; L^{C12} = 4-dodec-1-ynyl-2,6-di-pyrazol-1-yl-pyridine; L^{C14} = 4-tetradec-1-ynyl-2,6-di-pyrazol-1-yl-pyridine. The complex $[CoL^7Cl_2]$ forms a dimer held by short π - π stacking with head-to-head contacts at 3.4 Å. At $B_{DC} = 0.2$ T a low-frequency peak at the out-of-phase susceptibility is seen ($\nu \sim 0.3$ Hz) whereas the second peak appears at $\nu > 1500$ Hz confirming two slow relaxation processes².



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[1] G. Christou et. al, *Angew. Chem. Int. Ed.*, 2004, 43, 2117-2121.

[2] R. Boča et. al, *Inorg. Chem.*, 2014, 53, 8200-8202.

Zeolites: Fundamental features and environmental implications

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A critical review is presented of zeolites and their use in practical applications. Specifically considered are their role as media for selective light-induced oxidations using molecular O₂, and the relationship between this phenomenon and the surface electric fields that exist in zeolites. Methods for determining the strength of the zeolite surface fields are discussed, using sorbed molecules such as CO with IR detection, and the spin-probes, di-tert-butyl nitroxide and NO, as detected using ESR spectroscopy. The relationship between these surface fields and molecular reorientation energetics for free radicals sorbed in zeolites, obtained using muonium as a spin-label, is explored. Finally, results obtained from exposing the naturally occurring zeolite, clinoptilolite, to high energy electrons as a means for activating the material toward the selective removal of radioactive caesium and strontium cations from the wastewaters of nuclear power plants are presented.

REE complexes with antipyrine: Structural and cytotoxic studies

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Complexes of transition-metals with bioactive ligands, in particular those of lanthanides, appear to have considerable promise due to their possible application in medicine as anticancer drugs. The aim of the present work consists in the synthesis and studies (IR-spectroscopy, single crystal XRD, cytotoxicity assay (mouse fibroblasts NCTN L929 and human larynx epidermoid carcinoma HEP 2 cells)) on $[\text{Ln}(\text{AP})_6]\text{X}_3$ (AP: 2,3-dimethyl-1-phenyl-3-pyrazolin-5-one, antipyrine; $\text{X} = \text{I}^-, \text{ClO}_4^-$) complexes. Compounds of both series are the isostructural ones. They contain $[\text{Ln}(\text{AP})_6]^{3+}$ complex cations and I^- or ClO_4^- anions in the outer sphere, but in the respective perchlorate series the coordinated antipyrine molecules are more planar and $[\text{Ln}(\text{AP})_6](\text{ClO}_4)_3$ are more cytotoxic ($c = 1 \cdot 10^{-3}$ mol/L) relative to $[\text{Ln}(\text{AP})_6]\text{I}_3$. As to $[\text{Ln}(\text{AP})_6]\text{I}_3$ at 10^{-3} mol/L, they demonstrate higher cytotoxic effect with respect to the cancer cells in comparison with the normal ones. All the studied compounds are noncytotoxic in the concentration range 10^{-7} - 10^{-4} mol/L. Cytotoxicity of both series complexes is superior to free antipyrine and slightly below that of inorganic starting compounds showing non-monotonous dependence along the Ln row. Influence of anion size and structure on bioactivity of complexes is discussed as well.

**Synthesis and crystal structures of two new Hg(II) and Cd(II) complexes
with 2,3,5,6-tetrakis-(2-pyridyl) pyrazine**

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Under thermal gradient in solution phase, reaction of Hg(II) and Cd(II) salts with 2,3,5,6-tetrakis -(2-pyridyl) pyrazine (tppz) in 1:1 molar ratio afforded dinuclear [Hg₂I₄(tppz)] (**1**) and mononuclear [CdI₂(tppz)] (**2**) complexes. The complexes have been characterized by elemental analyses, FTIR, ¹H-NMR spectroscopy. Solid state structures of both complexes have been determined by single crystal X-ray diffraction analyses. Single crystal X-ray diffraction structural analysis reveals that tppz acts as bis-tridentate and tridentate chelating ligand in **1** and **2**, respectively. Metal(II) ions adopt a distorted square pyramid geometry and have the same coordination environment in both complexes. Weak C–H···I, C–H···I and C–H···π interactions contribute to the stabilization of the crystal packing of both complexes, which results in formation of 1D supramolecular chains. Based on the ¹H NMR spectroscopy measurements, both complexes decompose in solution and releases free tppz in solution.

Comparison of the thermogravimetric curves for both complexes shows that the complex **1** is more thermally stable than **2**. Decomposition of both complexes ended with formation of corresponded metal oxide

Photoactive mononuclear and polynuclear iron(II) spin crossover compounds

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The phenomenon of spin crossover (SCO) between low-spin (LS) and high-spin (HS) state presents probably one of the most spectacular examples of molecular bistability. Until now, the most investigated is thermally activated transition of spin, which can be influenced also by other triggers like pressure, magnetic or electric field. Moreover, in the last three decades, the light induced LS↔HS photoconversion (LIESST, reverse LIESST effect and ligand driven light induced SCO) attracts the research interest.

The iron(II)-bis(pyrazolyl)pyridine compounds represents class of materials which often exhibits the room temperature, abrupt and hysteretic SCO accompanied by intense thermochromism. Herein we present thermal and light-induced ST investigation in series of mononuclear iron(II)-bis(pyrazolyl)pyridine complexes [1]. The photomagnetic experiments revealed LS→HS conversion, slow relaxation of metastable photoinduced HS states and presence of light induced thermal hysteresis loops. In addition to the mononuclear compounds, new anthracene-contained photoactive bis(pyrazolyl)pyridine organic ligands were synthesized. The consecutive iron(II) complexation resulted in the formation of oligomeric polynuclear complexes with grid-like or hexagone-like molecular architecture.

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π -Complexes of copper(I) with aromatic rings – Applications

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The apparent stability constants of the complexes of Cu(I)_{aq} with several aromatic compounds have been published.

From the experimental published results (N.M.R, E.S.R, UV-vis and electrochemistry) it is clear that the complexes formed are due to $d \rightarrow \pi^*$ interactions between the copper d orbitals and the aromatic π system.

Recent results show that copper(I) facilitate selective ortho nitration of phenol. These results support a quantum mechanical calculation indicating that copper (I) is bound mainly to one carbon-carbon bond of the ring, the ring structure is distorted and the carbon hydrogen length ortho to the hydroxyl group becomes longer.

It seems that these kind of complexes resemble an excited state of the aromatic system due to charge transfer from the bonding orbital of the aromatic system to the Cu^+ , and back donation to the π^* anti bonding of the aromatic system.

The finding that $\text{Cu}^+_{(\text{aq})}$ forms $d \rightarrow \pi^*$ complexes with aromatic compounds might explain the catalytic activity of copper(I) in Electrophilic aromatic substitution and in copper catalyzed oxidation of aromatic compounds.

New heteroscorpionate lanthanide complexes for ring opening polymerization

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Yttrium and lanthanum amido-complexes with bis(pyrazol-1-yl)acetates in their coordination spheres were studied as the catalysts in ϵ -caprolactone and lactide ring-opening polymerization. High-weight poly(ϵ -caprolactone) (PCL) was obtained in almost quantitative yield under mild conditions, while lactide polymerization was less efficient. The average chain length of PCL was dependent upon the choice of the metal centre and the presence of substituents on the pyrazole rings of the ancillary ligand. The ground-state geometries of the complexes and the first stages of ϵ -caprolactone polymerization were computationally modelled by means of DFT calculations.

**Different structural types of copper(II) and cobalt(II) furan- and thiophencarboxylates:
X-ray structural, spectral and magnetic analysis**

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Preparation, spectral properties, magnetic properties and crystal structures of copper(II) and cobalt(II) furancarboxylate and thiophencarboxylate complexes with nicotinamide, isonicotinamide and *N*-methylnicotinamide have been described in our previous papers [1-3].

In the present work, furan- and thiophencarboxylatecopper(II) and cobalt(II) complexes with ethylnicotinate, 3-hydroxymethylpyridine and 4-hydroxymethylpyridine are reported. The complexes under study were characterized by electronic, IR, EPR spectroscopy, magnetic susceptibility over the temperature range and X-ray structure analysis. Spectral and magnetic behaviours are discussed in regard to X-ray parameters.

The financial supports of Slovak grant agencies VEGA (1/0472/13) and APVV (APVV-0014-11) are gratefully acknowledged.

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**Radiation-sensitive phantoms with paramagnetic metal ions for 3-D MRI dosimetry
of radiotherapy.**

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At the University Hospital in Toulouse in 2006, 145 patients treated for cerebral tumors by radiotherapy, were over-irradiated and twenty of them died. In fact, radiotherapy is computer defined and regulated, but only the direct detection in tissue-equivalent material phantoms can give the true adsorbed dose in a human body in three dimensions. This is partly due to inhomogeneity of body tissues with different densities such as lung or bone which make it difficult to predict radiation diffusion in a complex volume.

In order to develop three dimensional dosimetry techniques with suitable spatial and dose resolutions to assess treatment quality controls, we have prepared radiation-sensitive phantoms with paramagnetic metal ions, such as iron or manganese, for 3-D MRI dosimetry.

These phantoms are made with biopolymer protein gels with the same electronic density as the human body, acceptable mechanical properties and a reduced diffusion of the paramagnetic species inside the material. This allows conserving the 3-D information derived from the MRI image and producing isodosimetric data to confirm or not that the planned radiation therapy corresponds to the doctor's order. A priori verification of radiation doses should help prevent radiotherapy accidents by better adjustment of irradiation intensities.

Nucleophilic, electrophilic reactivity, some spectral and electrochemical properties of iron(II) clathrochelates

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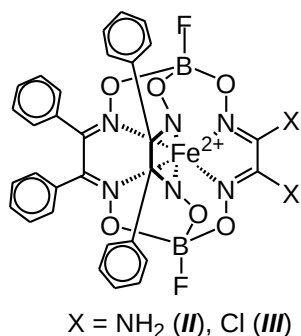
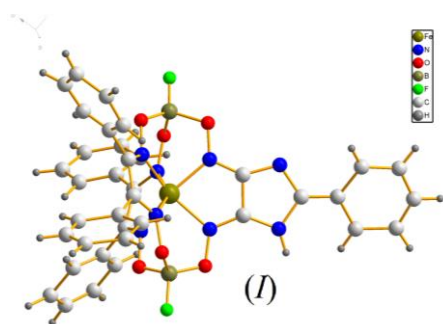
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Several different clathrochelates were prepared by nucleophilic substitution and electrophilic addition in boron-capped tris-dioximate iron(II) clathrochelates. Clathrochelate **I** was prepared i) by electrophilic addition of PhC(O)H to the diamino iron(II) clathrochelate **II**; ii) by nucleophilic substitution of chlorine with PhC(NH)NH₂ in the dichloroglyoximate analog **III**. Some other clathrochelates were derived from **III**; the products were characterized by UV-VIS, NMR spectroscopy and X-ray crystallography. Some electrochemical and spectral properties of the synthesized compounds are discussed.



This study was supported by VEGA Agency project 1/0543/15 and RFBR grants 13-03-90907, 13-03-00702 and 12-03-90706.

Neodymium complexes with antipyrine: dependence of cytotoxicity on anion type and size

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Complexes of rare earth elements (REE) with a number of bioactive ligands often demonstrate promising anticancer activity both *in vitro* and *in vivo*. Early we have shown non-monotonous dependences of the NCTN L929 and Hep-2 cells survivability on the lanthanide atomic number for $[\text{Ln}(\text{AP})_6]\text{I}_3$ (AP: antipyrine, 2,3-dimethyl-1-phenyl-3-pyrazolin-5-one). The aim of the present work is to consider influence of the anion type, structure and size on the cytotoxic properties of complexes with the same cation. As an example we have studied $[\text{Nd}(\text{AP})_6]\text{X}_3$ ($\text{X} = \text{I}^-$, ClO_4^- , BPh_4^-). Both iodide- and perchlorate compounds are the isostructural ones differing only in anion size and its disorder degree. We have demonstrated that $[\text{Nd}(\text{AP})_6](\text{BPh}_4)_3$ is the most cytotoxic compound at $c=0.001$ mol/L, the NCTN L929 cells survivability being equal to ca. 20%. The cytotoxicity decreases in the row $[\text{Nd}(\text{AP})_6](\text{BPh}_4)_3$ – $[\text{Nd}(\text{AP})_6](\text{ClO}_4)_3$ – $[\text{Nd}(\text{AP})_6]\text{I}_3$ similar to the anion size decrease along the BPh_4^- – ClO_4^- – I^- sequence. It is possibly related with the electrostatic interactions between the charged species and the phosphate backbone of DNA, π – π stacking interactions between the DNA bases and the 5- or 6-membered rings of the ligand molecule as well as by steric hindrances due to large-size anions.

Mononuclear tetracoordinate Co(II) complexes as field-induced single-molecule magnets

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Tetrahedral Co(II) complexes have recently become one of the most interesting classes of compounds in the field of single-molecule magnets (SMMs), since they exhibit slow magnetic relaxation. As a part of our larger study on complexes with composition $[\text{Co}(\text{L})\text{X}_2]$ (L = chelate N-donor ligand, X = halide) we report syntheses, crystal structures and magnetic properties of three novel complexes $[\text{Co}(\text{biq})\text{X}_2]$ (biq = 2,2'-biquinoline); X = Cl (**1**), Br (**2**) and I (**3**). Single-crystal X-ray structure analyses revealed molecular structures of the complexes in which the complex molecules interact by weak C-H...X hydrogen bonding interactions leading to a chain-like arrangements of complex molecules. In addition, π - π interactions between the biq ligands enhance dimensionalities of the formed supramolecular structures. Although the complexes are isostructural, the system of π - π interactions in **3** differs from those observed in **1** and **2**. The results of temperature variable magnetic studies of **1-3** revealed the existence of two magnetic relaxation processes for spin reversal. The DC magnetic data of **1** and **2** are similar, while slightly different for **3**; the observed difference can be explained on the basis of the above mentioned differences in the crystal structures.

Slovak grant agencies (APVV-0014-11, VEGA 1/0075/13, VVGS-2014-164) are acknowledged for the financial support.

Organometallic compounds in the synthesis of new materials: Old ligands, new tricks

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Organometallic compounds and their derivatives, especially those containing alkoxide and aryloxy ligands, represent an enormous family of species featuring broad structural diversities and their chemistry has significantly expanded recently. The development of modern technologies and synthetic approaches has allowed desired products to be produced under mild conditions and has provided more versatility over the stoichiometry, composition, structure, and morphology of the produced inorganic materials than can be obtained using conventional methods such as solid-state reactions [1]. For instance, these compounds are perfect candidates for sol–gel synthesis and various chemical vapor deposition techniques to produce highly phase-pure oxide products. Interest in the field of mixed-metal alkoxo-organometallic and alkoxide chemistry has significantly expanded, largely because of their attractive structural chemistry, catalytic properties, and potential for industrial applications. The applicability of such compounds is related to the cooperation of two different metals in a single complex, which can result in interesting properties that are not the simple sum of the individual metal ions, and are often crucial to achieve the desired activity from a system. In the lecture we present three relatively unexplored synthetic methods for obtaining functional materials using organometallic-derived compounds aimed at producing heterometallic precursors for a wide range of oxide materials.

Acknowledgement: The author wish to thanks the National Science Centre (Poland) under grant no 2011/03/B/ST/01040

[1] L. John, P. Sobota, *Accounts of Chemical Research*, 2014, **47**, 470–481.

Flexibility of copper(II) – Structure and EPR spectroscopy

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Copper (II) is a workhorse not only in coordination chemistry to be studied by EPR spectroscopy. Very often the question of diamagnetic dilution arises. This can be achieved by e.g. organic solvents or in solid state by suited crystalline host lattices. In both cases the geometric and electronic situation around the copper center might be influenced.

In coordination compounds copper (II) might coordinate tetrahedral (CN 4), square planar (CN 4) or octahedral (CN 6) or somehow inbetween. The square planar coordination is usually preferred, but depending on the structural situation around Cu(II) shows a high degree of structural flexibility. This structural flexibility influences also the electronic situation around the paramagnetic copper center ($S = \frac{1}{2}$) and this can be monitored by EPR spectroscopy.

In the presentation the variation of the measured EPR parameters of some copper (II) complexes with CuS_4 , CuS_2N_2 , CuCl_4 and CuBr_4 coordination spheres and the influences of different hosts will be discussed.

EPR spectroscopy of Cu(II) complexes. What we have learned.

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EPR spectroscopy represents a very powerful spectroscopic method for investigation and elucidating of many structural properties of transition metal complexes. A careful analysis of EPR spectra often provide information about the local structure of paramagnetic centre that could be conveniently compared with x-ray structural analysis data. In addition, it is always worthwhile when the interpretation of the obtained results is supported by recent quantum chemical calculation to improve of our understanding of studied topic.

Presented contribution will summarize some of our last results that we have achieved during our study of copper complexes with different types of biologically active ligands.

**Polysiloxanes as carriers for rhodium-ferrocenyl complexes
with potential catalytic applications**

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Rhodium complexes are used as catalysts in many organic transformations such as hydrogenation of olefins, hydroformylation reactions and the carbonylation of methanol. The rate determining step in the Monsanto process, where methanol is converted to acetic acid, involves oxidative addition of methyl iodide to the catalyst, $[\text{Rh}(\text{CO})_2\text{I}_2]^-$.

The rhodium(I) complexes $[\text{Rh}(\text{CO})(\text{PPh}_3)(\text{FcCOCHCOR})]$ with $\text{R} = \text{CF}_3$, CH_3 , Ph (phenyl) and Fc (ferrocenyl), have been shown to undergo oxidative addition with methyl iodide. By anchoring these complexes on a polymeric support, here polysiloxanes, entire new systems may be designed having different properties than the original complexes.

Here we report the synthetic protocols, electrochemical and spectroscopic characterisations, and the kinetics of oxidative addition of methyl iodide to the rhodium(I) core of $[\text{Rh}(\text{CO})-(\text{R-PPh}_2)(\text{FcCOCHCOR})]$ where R-PPh_2 = a polysiloxane bearing PPh_2 -containing side chains. The PPh_2 functionality of the polysiloxane, R-PPh_2 , is the anchoring site of the rhodium moiety to the polymer.

The authors acknowledge the UFS for financial support.

**Structural, spectroscopic and DFT study of rhenium(I) carbonyls incorporating
1,10-phenanthroline derivatives**

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Since the first observation of electronically excited luminescence in [ReCl(CO)₃(phen)], reported by Wrighton and Morse in 1974, a great variety of luminescent Re(I) diimine tricarbonyls have been intensively studied. These compounds have attracted a considerable attention due to their potential applicability in devices for luminescence sensing, organic light-emitting diodes (OLEDs) and in other fields such as catalysis and medicinal chemistry. The rhenium(I) diimine tricarbonyl complexes are ³MLCT emitters typified by a broad structureless emission band sensitive to changes in the nature of the environment. As a consequence, variations in the structure of the non-carbonyl ligands can provide considerable effects on the luminescence (energies, lifetimes and quantum yields), excited-state properties, and other physical properties of the rhenium(I) diimine tricarbonyls

A novel tricarbonyl rhenium(I) complex of 5-amine-1,10-phenanthroline has been synthesized and characterized by IR, NMR, UV-Vis spectroscopy and single crystal X-ray analysis. The luminescent properties of [ReCl(CO)₃(5-NH₂-phen)] were studied in solution at 298 and 77 K and compared with the free ligand. To get detailed insight into the electronic structure and spectroscopic properties of [ReCl(CO)₃(5-NH₂-phen)], the density functional theory (DFT) and time-dependent DFT (TD-DFT) calculations were performed.

Acknowledgment: The research was co-financed by the National Research and Development Center (NCBiR) under Grant ORGANOMET No: PBS2/A5/40/2014

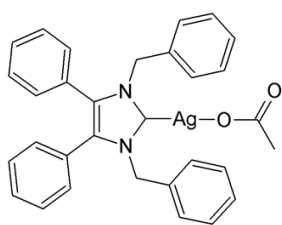
**Novel carbene-metal complexes as anticancer drugs and antibiotics –
Potential and limitations**

M. Tacke

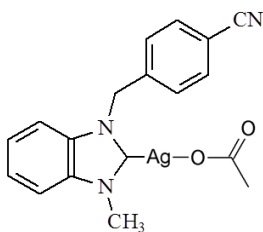
*UCD School of Chemistry and Chemical Biology, University College Dublin, Belfield,
Dublin 4, Ireland*

✉ Dr. Matthias Tacke; e-mail: matthias.tacke@ucd.ie

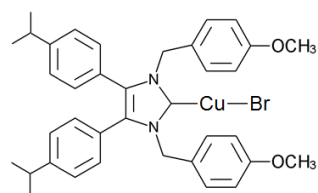
The synthesis of N-heterocyclic carbene (NHC) silver(I) acetate complexes with varying lipophilic benzyl-substituents at the 1 and 3 positions of the (benz)imidazole ring was achieved by reaction of silver(I) acetate with the corresponding (benz)imidazolium halide salts [1]. These NHC-silver(I) acetate derivatives exhibit interesting structural motifs in the solid state and proof to be soluble and stable in biological media. Some derivatives like SBC3 show strong antibacterial activity against Gram-negative and Gram-positive bacteria, while others are cytotoxic. Here, NHC-silver(I) acetate complexes were found to have IC₅₀ values as low as 1.2 micromolar against the human renal cancer cell line Caki-1 and (1-methyl-3-(p-cyanobenzyl) benzimidazole-2-ylidene) silver(I) acetate has become the anticancer lead structure SBC1. The synthesis and biological evaluation of SBC1 and novel Ag, Au, Ru and Cu complexes like WBC4 will be communicated.



SBC3



SBC1



WBC4

[1] F. Hackenberg, M. Tacke, Dalton, 43 (2014) 8144

Tuning in *cellulo* targeting and function of metal complex bioprobes

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Ruthenium(II) polypyridyl complexes that interact reversibly with DNA can display high binding affinities. We are constructing complexes with specific sequence binding preferences, as well as interesting biophysical and photophysical properties. Although such complexes offer potential as *in cellulo* probes for luminescence microscopy, poor cellular uptake by live cells generally restricts the use of many such systems..

In recent studies we have developed complexes that are taken up by live eukaryotic and prokaryotic cells where they bind to specific biomolecules. These complexes function as multifunctional probes imaging intracellular structures and biomolecules through a number of different high-resolution microscopy techniques, including conventional and time-domain optical microscopy and transmission electron microscopy.

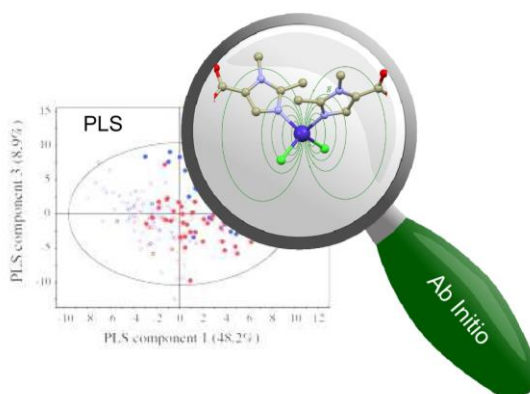
Structural tunability of single-molecule magnet behaviour in Co(II) complexes

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Modern electronics is on the brink of revolutionary change, since special molecular entities, so called single-molecule magnets (SMMs), attractive for high-density information storage and quantum computing were developed. SMMs are metal complexes (large polynuclear or simple mononuclear) that, beside other interesting quantum phenomena, exhibit slow relaxation of the magnetization.



We have studied a series of mononuclear tetracoordinate Co(II) complexes in which a large diversity of the magnetic anisotropy (measured by the axial zero-field splitting parameter D) was observed. We have applied statistical methods (such as partial least-squares regression PLS) and *Ab Initio* calculations to investigate the structural aspects of this diversity. On the basis of these findings we have defined the magnetostructural correlations which provide simple rules for tuning the SMM properties in this family of compounds.

This work was supported by Slovak grant agencies (VEGA 1/0233/12 and APVV-0014-11).

An unusually wide spectrum of 3-methylsalicylatocopper(II) complexes with ronicol

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Ronicol (3-pyridylmethanol, abbreviated as ron) is known for its anti-inflammatory and in coordination chemistry for extraordinary tendency to act as bridging ligand, so most of its known complexes are polymeric ones. Moreover, the most of the polymeric copper(II) complexes are 1D “doubly bridged” ones or they form 2D layered structures and only few give other structural pattern. In this contribution four different 3-methylsalicylatocopper(II) complexes containing ronicol ligand will be presented. In addition to the most common 2D layered $[\text{Cu}(\text{3-Mesal})_2(\text{ron})_2]_n$ (**1**) structure, the molecular $[\text{Cu}(\text{3-Mesal})_2(\text{ron})_2]$ (**2**) was obtained and characterized. Moreover solvent containing $[\text{Cu}(\text{3-Mesal})_2(\text{ron})_2(\text{H}_2\text{O})] \cdot \text{H}_2\text{O}$ (**3**), $\text{Cu}(\text{3-Mesal})_2(\text{ron})(\text{H}_2\text{O})_2$ (**4**) were prepared and characterized spectral methods and by elemental analysis. For complexes (**1**), (**2**) and (**3**) their crystal structures were solved and will be analyzed.

The obtained results will be analysed in relation to the all other known copper(II) complexes with this ligand.

Ternary copper(II)-lawsone complexes

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2-Hydroxy-1,4-naphthoquinone (lawsone) belongs to a group of secondary metabolites of plants, fungi and some bacteria, and shows very interesting pharmacological activities, such as antibiotic, antiviral, antifungal, anti-inflammatory, and antiproliferative. Recently, it has been found that octahedral copper(II) aquacomplexes of 2-hydroxy-1,4-naphthoquinone and its derivatives show interesting magnetic properties and remarkable biological activities, such as antimicrobial, fungicide, and antitumor. With the aim to evaluate the effects of the *N*-donor ligands, substituting the apical coordination places in the octahedral polyhedra of the copper(II)-lawsone aquacomplexes, on the magnetic properties and biological activities, we prepared and thoroughly characterized a series of seven ternary complexes with the general formula $[\text{Cu}(\text{lawsone})_2(\text{L})_x(\text{H}_2\text{O})_y]$, where $x = 1$ or 2 ; $y = (2-x)$; and *L* = pyridine, imidazole, 2-amino-, 3-amino-, 4-amino-pyridines, 3-hydroxypyridine, and 3,5-dimethylpyrazole. This work was funded by OP VK - ESF (CZ.1.07/2.3.00/30.0041), and NPU I (LO1305) of the MŠMT ČR.

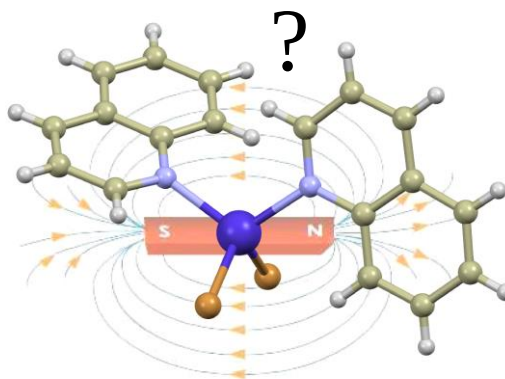
**Synthesis, structural and magnetic properties of Co(II) complexes:
Investigation of potential single-molecule magnets**

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Detection of slow magnetic relaxation in mononuclear 3d metal complexes is an important task in the emerging field of molecular magnetism. Single-molecule magnets (SMMs), as the main objects of interest, show relaxation effects as a consequence of the energy barrier ($E_b \approx |D|S^2$, where D is axial zero-field splitting (ZFS) parameter) for the magnetization reversal between the two lowest $M_S = \pm S$ states. SMMs are a major scientific target because of their potential applications in high-density magnetic memories and quantum-computing devices. New tetracoordinate Co(II) complexes have been prepared, structurally and spectrally characterized. Magnetic properties of these compounds were investigated using SQUID magnetometry and contemporary methods of quantum chemistry in order to determine and understand their potential SMM behavior.



Molecular design of iron(II) clathrochelates carrying annulated rib heterocycles

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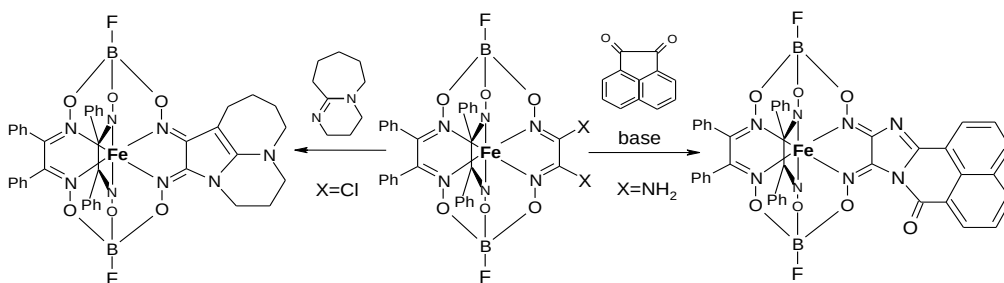
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Tris-dioximate transition metal clathrochelates are promising molecular scaffolds for design of the polytopic molecules and polyfunctional materials with high chemical stability and diverse physico-chemical properties. Nowadays one of the main methods of preparation of novel clathrochelates consists in modification of the macrobicyclic cage by the reactions of the coordinated dioxime ligand. Currently we are developing synthetic approaches to the design of heterocycles annulated to the dioximate rib fragment. In our research we use two different synthetic tactics: nucleophilic and electrophilic. Synthesis and characterization (single crystal X-ray crystallography and NMR spectroscopy) of the compounds obtained as well as possible mechanisms of reactions will be discussed in this work.



This study was partly supported by RFBR (grants 13-03-00702).

Platinum(II) and palladium(II) dithiocarbamates with water-soluble phosphine ligands

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Six platinum and palladium compounds with high water solubility of the type *cis*-[M(PTA)₂(S₂CNR₂)] (M = Pt, Pd) were prepared with several dithiocarbamate ligands, starting from *cis*-[MCl₂(PTA)₂] complexes. Five of the synthesized platinum and palladium compounds were screened against a panel of neuroblastoma cell lines. While the platinum derivatives show anti-cancer efficacy in picomolar to nanomolar concentrations, the palladium compounds are completely inactive.

The platinum complex with the dithiocarbamate ligand derived from isonipecotic acid was furthermore coupled with an amine, glycine methyl ester, by using a mixture of DCC and HOBt as coupling reagents, to form a bioconjugate.

All synthesized compounds were characterized by NMR- and IR-spectroscopy and, in some cases, by mass and elemental analysis. Crystal structures could be obtained for a couple of complexes.

**Molecular and nanoscale assemblies as highly sensitive and selective sensors
of toxic species**

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Metal-based systems can be designed to give a selective response for a range of analytes and the stepwise, modular construction of complex systems, often containing more than one metal centre, offers a powerful methodology to achieve this aim. This contribution will describe how inexpensive, simple building blocks can be employed to generate systems of much greater complexity, ranging from molecular metal compounds to functional materials on the nanoscale [1-4].

The presentation will describe how the design and modification of molecular systems can be extended to their immobilisation on supports suitable for applications in the real world. Examples of this are the sensing of carbon monoxide in air [5] and the use of nanoparticles at a liquid-liquid interface for SERS-based sensing of mercury ions in water [6].

- [1] Wilton-Ely et al, *Inorg. Chem.* **2008**, 47, 9642;
- [2] Wilton-Ely et al, *Inorg. Chem.* **2009**, 48, 3866;
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- [4] Wilton-Ely et al, *Inorg. Chem.* **2014**, 53, 1989;
- [5] Wilton-Ely, Martínez-Máñez et al, *J. Am. Chem. Soc.* **2014**, 136, 11930;
- [6] Wilton-Ely, Edel et al, *Adv. Optical Mater.* **2014**, 2, 966.

EPR and DFT insight into interaction between *o*-semiquinone radicals and metal ions

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Semiquinones are organic radical anions being the intermediate form in the redox equilibrium between quinones and hydroquinones. These radicals are present in all life forms as they act as electron-transfer agents in the mitochondrial respiratory chain and in the reaction centres of bacterial and plant photosynthesis. *o*-Semiquinones are known to possess chelating ability towards metal ions, which is particularly important for the activation of electron transfer through interaction with cations acting as Lewis acids. In this work EPR spectroscopy and density functional theory (DFT) were used to elucidate the interaction between *o*-semiquinone radicals and various diamagnetic metal ions: Mg^{2+} , Ca^{2+} , Hg^{2+} and Pb^{2+} . The effect of complexation on the molecular and electronic structures of the radicals were established and correlated with the *g* tensor. The relative stability of the complexes were also investigated.

References: Witwicki, M. et al., **(a)** *J. Phys. Chem. A* 2009, 113, 14115. **(b)** *J. Phys. Chem. B* 2011, 115, 3172. **(c)** *Theor. Chem. Acc.* 2013, 132, 1383. **(d)** *Chemosphere* 2015, 119, 479.

LIST OF AUTHORS

- | | |
|---|----------------------------------|
| Abe M. <u>19</u> | Burdukov A. <u>35</u> , 119, 133 |
| Ahmedova A. <u>20</u> | Burg A. 115 |
| Albertin G. 32 | Bushmeleva A. S. <u>36</u> |
| Al'bov D. V. 22, 36 | Buyukliev R. 24 |
| Aldoshin S. M. <u>21</u> | Čechová D. <u>37</u> |
| Alikberova L. Yu. <u>22</u> , 36 | Černák J. 121 |
| Antonov L. 103 | Chang Y.-L. 61 |
| Arsenijevic N. 43, 44, 107 | Chen H.-Y. 61 |
| Asaka M. N. 25, 26, 53 | Chorazy S. <u>38</u> |
| Augustín P. <u>23</u> | Christensen H. E. M. 26 |
| Babiak M. 65 | Chuang W.-J. 61 |
| Bakalova A. <u>24</u> , 97 | Clarke Z. H. 27 |
| Bal W. 25 | Čomić L. R. 43, 44 |
| Bali K. 41 | Coulaud J. 118 |
| Bálint H. <u>25</u> | Csipak B. 25 |
| Balogh R. K. <u>26</u> | Czene A. 25, 53 |
| Baran P. <u>27</u> | Daniele S. 32 |
| Baranová Z. 27 | Darkwa J. <u>39</u> |
| Battistel D. 32 | Davydova G. A. 112, 120 |
| Belaid S. <u>28</u> | Day P. <u>40</u> |
| Belczyk A. 25 | Derco J. 70 |
| Benali-Baitich O. 28 | Dömötör O. <u>41</u> |
| Benmerad B. 28 | Drábik M. <u>42</u> |
| Bertová P. <u>29</u> , 87, 117 | Drweesh S. A. <u>43</u> , 44 |
| Bieńko A. <u>30</u> | Đurčeková M. 64 |
| Bieńko D. <u>30</u> | Dušek M. 121 |
| Billik P. 42 | Dvořák Z. 57, 62 |
| Boča R. 23, 30, <u>31</u> , 75, 102, 110, 114,
121, 129, 132 | Dzeikala A. 80 |
| Boguslavskii E. 35 | ElFeki H. 96 |
| Bortoluzzi M. <u>32</u> , 116 | Eltsov I. 35, 119, 133 |
| Boudia S. 45 | Enomoto M. 69 |
| Bouet G. 28 | Enrichi F. 32 |
| Brabec V. <u>33</u> , 67 | Enyedy É. A. 41 |
| Breza M. <u>34</u> , 109 | Faletrov Y. A. 105 |
| Brumas V. 118 | Farkasová V. <u>44</u> , 107 |
| Bučinský L. 76 | Fernane F. 45 |
| | Fiallo M. <u>45</u> , 96, 118 |

Flaniken C. 55
 Forgácsová A. 46
 Fuhr O. 114
 Fujimori R. 89
 Gál M. 47, 74
 Gall M. 34, 48
 Gambino D. 49
 Gaona D. 50
 Gatto M. 116
 Gelalcha F. G. 50
 Gembický M. 83
 Gibson D. 33
 Golovach N. G. 80
 Gozzi M. 51
 Grohmann A. 52
 Gülzow J. 52
 Guo H.-F. 82
 Gyepes R. 72
 Gyurcsik B. 25, 26, 53, 103
 Hackl C. M. 41
 Haga M. 54, 94
 Hahn C. 50, 55
 Halaška J. 56, 93
 Hamagawa M. 89
 Handa M. 89
 Hanousková L. 57
 Hao X.-Y. 82
 Harbatsevich H. I. 105
 Harmatová Z. 58
 Hauser A. 59, 104
 Havránek E. 46, 71
 Hey-Hawkins E. 51
 Hisaeda Y. 19, 60
 Híveš J. 47, 74
 Hori S. 89
 Hošek J. 131
 Hsu S. C. N. 61
 Husáriková L. 85
 Hutyra J. 62
 Immadi S. S. 55

Imrich J. 79
 Inatomi A. 19
 Inui T. 63
 Ivanov D. 24, 97
 Jancsó A. 26
 Janík R. 64
 Janíková V. 64
 Jeremias L. 65
 Jerzykiewicz M. 136
 Jezierska J. 136
 Jomová K. 66
 Jóna E. 58, 64
 Jorík V. 84, 88
 Kakuta Y. 63
 Kandioller W. 41
 Kasparkova J. 33, 67
 Kato K. 26
 Kaval'chuk T. V. 105
 Keppler B. K. 41
 Kerekeš K. 74
 Kibaľnikov P. S. 22
 Klemens T. 68, 126
 Kojima N. 69
 Koman M. 70, 81, 93
 Kopel P. 30
 Kožíšek J. 76, 84
 Kozlevčar B. 93
 Krajčiová D. 71
 Křikavová R. 62
 Krivosudský L. 72
 Kruszyński R. 30, 126
 Krzystek J. 73
 Kubiňáková E. 47, 74
 Kuchtanin V. 29, 75, 87, 117
 Kucková L. 76, 84
 Kuriyama T. 89, 99
 Kuznetsov S. A. 77
 Lajdová Ľ. 58
 Landreau A. 28
 Lawson Daku L. M. 104

Lenčeš Z. 48
 Levitsky I. 115
 Li X. 82
 Lider E. V. 78
 Litecká M. 79
 Lodyga-Chruscinska E. 80
 Loginova N. V. 105
 Lukačovičová Z. 81
 Ma D.-Y. 82
 Machura B. 68, 126
 Mackuľak T. 47
 Marek J. 131
 Masárová P. 83
 Mašlejová A. 84
 Massarwa A. 115
 Masuda N. 63
 Matelková K. 84
 Mazur M. 85, 124
 Medvecká J. 58
 Melník M. 46, 71, 86, 90
 Mészáros J. P. 41
 Mihalčiak J. 87, 117
 Miklovič J. 88, 102
 Mikuriya M. 63, 89, 99
 Mikuš P. 46, 71, 86, 90
 Milaeva E. R. 98
 Minato S. 63
 Mironova E. A. 112, 120
 Missana A. 104
 Mizokawa T. 91
 Mohr F. 92, 134
 Momekov G. 20, 24, 97
 Momekova D. 20
 Moncol' J. 29, 37, 56, 70, 75, 81, 83,
 84, 87, 93, 101, 130
 Motoyama D. 94
 Motswainyana W. M. 100
 Nagashima T. 54
 Nagata K. 25, 26, 53
 Nakabayashi K. 38
 Nakajima K. 95
 Nasri K. 96
 Nawrot I. 126
 Nazarov A. A. 98
 Nedzhib A. 103
 Nemec I. 23, 83
 Németh E. 53
 Nikolova-Mladenova B. 24, 97
 Nitek W. 38
 Nogaš W. 38
 Nordlander E. 100
 Nosova Y. N. 98
 Novohradsky V. 33, 67
 Novosad J. 65
 Ohkoshi S.-I. 38
 Omote M. 99
 Onani M. O. 100
 Ondrejkočová I. 81
 Ondrejovič G. 101
 Ondrušová D. 64
 Oostenbrink C. 53
 Osipovich N. P. 105
 Owaga B. O. 100
 Ozarowski A. 136
 Ozawa H. 54, 94
 Packová A. 102
 Pantcheva I. 103
 Pavlik J. 104
 Pavlík V. 58, 64
 Pervukhina N. 35, 119, 133
 Petrasheuskaya T. V. 105
 Pintauer T. 106
 Podgajny R. 38
 Potočník I. 43, 44, 107
 Puchoňová M. 108, 130
 Puškárová I. 109
 Radebe M. P. 100
 Radojević I. D. 43, 44, 107
 Rajnák C. 110
 Rams M. 38

Raptis R. G. 27
 Repická Z. 130
 Rhodes C. J. 111
 Ruben M. 114
 Rukk N. S. 112, 120
 Rumonato R. 32
 Sadler P. J. 67
 Saghatforoush L. 113
 Šajgalík P. 48
 Sakiyama H. 89
 Šalitroš I. 83, 114
 Sanina N. A. 21
 Saphier M. 115
 Saphier O. 115
 Schwendt P. 72
 Scrivanti A. 116
 Segl'a P. 29, 75, 87, 88, 117
 Selektor S. 35, 119
 Sharrock P. 45, 96, 118
 Shokurov A. 35, 119
 Shutkov I. A. 98
 Siegert U. 125
 Sieklucka B. 38
 Šípoš R. 35, 119
 Skryabina A. Yu. 112, 120
 Smolentsev A. I. 78
 Smolko L. 121
 Snizhko M. I. 22
 Sobota P. 122
 Sopúchová V. 88
 Sparavier A. 25
 Stanek J. 38
 Štarha P. 57
 Strauch P. 123
 Strigáč J. 42
 Švorc L. 108
 Švorec J. 29, 108, 124
 Swarts J. C. 125
 Świtlicka-Olszewska A. 68, 126
 Sykula A. 80
 Symonowicz M. 80
 Tacke M. 127
 Taniguchi N. 19
 Thomas J. A. 128
 Titiš J. 30, 102, 129, 132
 Tomioka N. 89
 Tomoda M. 19
 Trávníček Z. 57, 62, 131
 Uhrecký R. 70
 Valigura D. 58, 85, 108, 130
 Valko M. 37, 85, 124
 Vančo J. 62, 131
 Varga F. 132
 Vargová Z. 79
 Vershinin M. 35, 119, 133
 Vilková M. 79
 Volarevic V. 43, 44, 107
 Voloshin Y. 35, 133
 Vorontsova E. V. 78
 Vranec P. 107
 Watanabe I. 69
 Werner S. 134
 Wilton-Ely J. D. E. T. 135
 Witwicki M. 136
 Yamashina M. 20
 Yoshikawa K. 94
 Yoshioka D. 63, 89
 Yoshizawa M. 20
 Zavodnik I. B. 80
 Zirnstein B. 52

50th Anniversary of the ICCBIC

The international conferences on coordination chemistry organized by the Slovak Chemical Society, Slovak Technical University and Comenius University in Bratislava, the capital of Slovakia, are held biannually as a rule at the beginning of June. They are the only scientific events in the field of coordination chemistry which are held regularly every two years at the same place (Smolenice Castle). In order to keep the tradition, from the very beginning the Conferences were focused on up-to-date problems of coordination, inorganic and bioinorganic chemistry. They have never been specialized on particular fields or techniques, nevertheless, each of the four working days of the Conferences was devoted to a main topic which was covered by plenary and section lectures, and sometimes by posters as well.

The Conferences have their characteristic atmosphere. The Castle itself and the surrounding nature create preconditions for fruitful discussions based on well and in advance prepared conference materials. Those are the Proceedings of the Conferences (abstracts only) and since 1993 a monograph – a book/CD/USB-key containing reviewed and selected papers of the participants in full extent. The monograph series are internationally recognized and registered.

Social programs of the Conferences at Smolenice helped to strengthen the friendship between participants and give them possibility to learn more about Slovakia, its folk and customs.

For those who are interested in the Conferences at Smolenice, below some details about all Conferences are given.

1st Conference on Coordination Chemistry – 1964 (Symposium on the Structure and Properties of Coordination Compounds)

The Conferences on Coordination Chemistry held regularly in Smolenice Castle started in fact by Symposium on the Structure and Properties of Coordination Compounds (with foreign participation) that was held in the new building of the Slovak Technical University in Bratislava (Gottwald square 2) and in the House of Scientific Workers of the Slovak Academy of Sciences at Smolenice (Smolenice Castle) on September 2 – 4, 1964 in connection with the 8th International Conference on Coordination Chemistry (ICCC) in Vienna (Sept., 7 – 11). This symposium is considered as the 1st Conference on Coordination Chemistry held in Bratislava and Smolenice Castle. The Symposium was organized by the Czechoslovak Chemical Society – Slovak Division in Bratislava, Institute of Inorganic Chemistry of the Slovak Academy of Sciences, Bratislava, Department of Inorganic Chemistry of the Slovak Technical University, Bratislava and J. Heyrovský Institute of Polarography of the Czechoslovak Academy of Sciences, Prague.

The symposium was attended approximately by 180 scientists and research workers from 18 countries: Australia 1, Austria 2, Czechoslovakia 100, Denmark 2, England 6, German Democratic Republic 15, German Federal Republic 10, Hungary 10, Ireland 1, Italy 2, New Zealand 1, Poland 7, Romania 6, USSR 4, Sweden 1, Switzerland 1, USA 9, Yugoslavia 1.

The role of Symposium in Bratislava was to complement scientific program of 8th ICCC in Vienna, namely in the field of the structure and properties of some coordination compounds.

The program of the symposium was divided into three sections:

- i/ Crystallochemistry of coordination compounds
- ii/ Structure of coordination compounds
- iii/ Theory and chemistry of coordination compounds.

Three plenary lectures and 76 section lectures were delivered at the Symposium. Plenary lectures were delivered by

J. C. Bailar, Jr. (USA): The Walden Inversion in the Reactions of Cobalt Complexes,

R. S. Nyholm (England): Advances in Complex Chemistry of the Early Transition Elements,

M. A. Poraj-Košic (USSR): Some New X-Ray Structural Investigations of Complex Compounds.

Among lecturers were well known scientist in the field of the coordination chemistry from all over the world. From among many others, we can name such section lecturers as *V. Gutmann* (Austria), *J. Bjerrum* (Denmark), *C. Schäffer* (Denmark), *R. Taube*, *E. Uhlig* (GDR), *E. O. Fischer* (GFR), *M. Tobe*, *M. A. Bennett* (England), *D. A. Brown* (Ireland), *B. Jezowska-Trzebiatowska*, *A. Swinarski* (Poland), *G. Schwarzenbach* (Switzerland), *S. Kirschner*, *A. D. Liehr* (USA), *I. B. Bersuker*, *B. J. Peshchevitskii* (USSR), *M. B. Celap* (Yugoslavia) were presented.

Fifty-three abstracts of the contributions are published in Bulletin of the Symposium on the Structure and Properties of Coordination Compounds, Bratislava September 2 – 4, 1964 (editor M. Zikmund, Edition of Chemical Literature, Institute of Inorganic Chemistry of the Slovak Academy of Sciences, Bratislava, 1964, 83 pp.).

The merits of Professor *Ján Gažo*, who passed away in 1983 should be mentioned here since he was the initiator of the international conferences on coordination chemistry in Slovakia. J. Gažo started his investigation of coordination compounds at the Department of Inorganic Chemistry, Slovak Technical University before year 1956, when he published two works in the journal *Chemical zvesti* on the formation and properties of chlorocopper(II) complexes in acetone. Subsequently, he became a pioneer and founder of the institutional research of coordination compounds not only at Slovak Technical University but also in Slovakia. His effort to get Slovak coordination chemistry closer to world trends led him to his “diplomatic offensive” to organize with colleagues from chemical societies and academies of sciences, especially from Slovakia, Symposium on the Structure and Properties of Coordination Compounds on Sept. 2 – 4, 1964 in connection with the 8th ICCS in Vienna (Sept. 7 – 11, 1964). In the next period, Ján Gažo organized Conferences on Coordination Chemistry with international participation regularly held in Slovakia. The 2nd Conference on Coordination Chemistry was held on December 1 – 5, 1969 in Smolenice Castle.

(See also article (including photos), Zikmund, M.: Sympóziom o štruktúre a vlastnostiach koordinačných zlúčenín v Bratislave. *Chem. zvesti* 19, 243–248 (1965) and International Conferences on Coordination Chemistry at Smolenice (Edited by Organizing Committee in Proceedings of the 10th Conference on Coordination Chemistry, June 4 – 7, 1985, 13 pp.).

2nd Conference on Coordination Chemistry – 1969

The 2nd Conference on Coordination Chemistry organized by the Slovak Chemical Society, Slovak Technical University, Komenský University, and the Slovak Academy of Sciences in Bratislava was held on December 1 – 5, 1969 at Smolenice in the House of Scientific Workers of the Slovak Academy of Sciences at Smolenice (Smolenice Castle). Chairman of the Organizing Committee: J. Gažo.

The conference was attended by 80 participants from 11 countries: Austria 3, Bulgaria 1, Czechoslovakia 45, Denmark 3, German Democratic Republic 1, Hungary 2, Italy 6, Poland 11, USSR 4, Switzerland 2, Yugoslavia 2.

The professional contents of the Conference were before all the problems of the relation of structure, properties and reactivity of the coordination compounds.

Eleven plenary lectures and 45 section lectures were presented at the conference.

The plenary lectures were presented by *B. Ježowska-Trzebiatowska* (Poland): Structure and bonding of beta-diketone complexes.

L. Cattalini (Italy): Some aspects of ligand substitutions at planar transition metal complexes.
 U. Belluco (Italy): Platinum – olefin complexes.
 A. V. Ablov (USSR): Binuclear copper compounds.
 C. Furlani and T. Tarantelli (Italy): Some developments of the coordination chemistry of thioureas and related ligands.
 E. M. Šustorovič (USSR): Fixation of molecular oxygen and nitrogen by complex compounds.
 V. Gutmann (Austria): Solute-solvent interactions.
 A. A. Vlček (Czechoslovakia): Redox interactions of coordination compounds.
 M. A. Poraj-Košic (USSR): Crystal chemistry of lanthanide complexes.
 C. Schäffer (Denmark): The angular overlap model of the ligand field.
 J. Klikorka, I. Pavlík, H. Windemannová and K. Handlir (Czechoslovakia): Reactions of the ferrocene and its derivatives with some inorganic acceptors.
 Some section lecturers from abroad: P. R. Bontchev (Bulgaria), S. E. Rasmussen (Denmark), D. Tille (GDR), M. T. Beck, K. Burger (Hungary), C. Panattoni (Italy), A. Samotus, Z. Stasicka (Poland), J. J. Daly, G. Geier (Switzerland), Yu. N. Kukushkin (USSR), M. B. Celap (Yugoslavia).
 Fifty-one papers are published in the *Proceedings of the 2nd Conference on Coordination Chemistry* 1969, 301 pp.
 (See also Jóna, E: IInd Conference on Coordination Chemistry in Smolenice. *Chem. zvesti* 23, 946–948 (1969)).

3rd Conference on Coordination Chemistry – 1971

The 3rd Conference on Coordination Chemistry organized by the Slovak Chemical Society, Slovak Technical University, Komenský University, and the Slovak Academy of Sciences in Bratislava was held on December 6 – 10, 1971 at Smolenice in the House of Scientific Workers of the Slovak Academy of Sciences at Smolenice (Smolenice Castle). Chairman of the Organizing Committee: J. Gažo.

The conference was attended by 72 participants from 11 countries: Austria 1, Bulgaria 1, Czechoslovakia 36, Denmark 2, German Democratic Republic 4, Hungary 6, Italy 1, Poland 15, USSR 4, USA 1, Yugoslavia 1.

During the conference 10 plenary lectures and 48 communications in sections were presented. The plenary lectures were presented by

M. T. Beck (Hungary): Kinetics and catalysis of chromium(III) complex formation.

J. Bjerrum (Denmark): On bridged thiocyanate complex formation.

V. Gutmann (Austria): The role of coordination chemistry in a unified approach to chemical interactions.

K. B. Jacimirskij (USSR): The application of graph method to coordination chemistry.

L. Kolditz (German Democratic Republic): On fluorine-oxygen complexes.

E. C. Lingafelter (USA): Structure of some complexes of some polyamine ligands.

G. Sartori (Italy): Luminiscence of coordination compounds.

E. M. Šustorovič (USSR): On the mutual influence of ligands in complexes containing multiple bonds metal-ligand.

M. E. Vol'pin (USSR): Reactions of carbon dioxide with complexes of transition metals.

I. A. Zacharova (USSR): Application of X-ray spectroscopy to coordination compounds.

Among those who attended the 3rd Conference on Coordination Chemistry can be mentioned:

F. Woldbye (Denmark), E. Hoyer (GDR), K. Burger, G. Liptay (Hungary), U. Belluco (Italy), A. Bartecki, R. Grobelny, B. Jezowska-Trzebiatowska, A. Samotus, Z. Stasicka (Poland), M. B. Celap (Yugoslavia).

Sixty papers are published in the *Proceedings of the IIIrd Conference on Coordination Chemistry* (Edited by Organizing Committee, 1971, 385 pp).

An exceptional event of the conference was the ceremonial bestowal of the honorary degree Doctor of Chemical Sciences and of the silver medal of the Slovak Technical University to Professor B. Jeřowska-Trzebiatowska, the head of the Institute of Chemistry at the University of Wrocław (Poland). This act was a manifestation of the friendly relations and contacts between Slovak and Polish coordination chemists as well as a culmination of a period in the history of very productive cooperation extending over many years between the Slovak Technical University and the University in Wrocław.

(See also Sirota, A., Jóna, E: The IIIrd Conference on Coordination Chemistry in Smolenice. *Chem. zvesti* 26, 478–479 (1972).

4th Conference on Coordination Chemistry – 1973

The 4th Conference on Coordination Chemistry organized by the Slovak Chemical Society, Slovak Technical University, Komenský University, and the Slovak Academy of Sciences in Bratislava was held on December 13 – 18, 1973 at Smolenice in the House of Scientific Workers of the Slovak Academy of Sciences at Smolenice (Smolenice Castle). Chairman of the Organizing Committee: J. Gažo.

The conference was at the same time the *Second Seminar on Crystallochemistry of Coordination and Organometallic Compounds*.

The conference was attended by 57 participants from 7 countries: Czechoslovakia 20, German Democratic Republic 5, Hungary 3, Poland 3, USSR 22, USA 1, Yugoslavia 3.

Twenty-nine plenary lectures were focused to topical problems of the structure of coordination and organometallic compounds, for example:

Distortion isomerism of copper(II) compounds (*J. Gažo*, Czechoslovakia).

Stereochemistry of some transitional metals carboxylates (*M. A. Porai-Koshits*, USSR).

Crystal structures of some organometallic complexes of tin and mercury (*N. G. Bokii*, USSR).

X-ray electron-spectroscopic investigation of transition metal complexes (*V. I. Nefedov*, USSR).

The latest achievements in the structural chemistry of organometallic compounds (*J. T. Struchkov*, USSR).

Stereochemistry of metallocycles and intermolecular interactions in crystals of inner-complex compounds of copper and nickel. (*P. M. Zorkii*, USSR).

Crystal structure of binuclear transition metal complexes with oxygen bridge (*B. Jeřowska-Trzebiatowska*, Poland).

Structural manifestations of Jahn-Teller effect (*I. B. Bersuker*, USSR).

Twenty-nine papers are published in the *Proceedings of the 4th Conference on Coordination Chemistry*, 1973, 177 pp.

5th Conference on Coordination Chemistry – 1974

The 5th Conference on Coordination Chemistry organized by Slovak Chemical Society, Slovak Technical University, Slovak Academy of Sciences in Bratislava, and Heyrovsky Institute of Physical Chemistry and Electrochemistry in Prague was held on June 24 – 28, 1974, in the House of Scientific Workers of the Slovak Academy of Sciences at Smolenice (Smolenice Castle). Chairman of the Organizing Committee: J. Gažo.

Eighty participants from 8 countries presented their papers, from: Austria 1, Czechoslovakia 49, GDR 4, GFR 3, Hungary 7, Poland 11, USSR 4, Yugoslavia 1.

In order to save time for discussion the Organizing Committee decided to allow the spoken presentation in full extent of only a few papers at the plenary sessions. The rest of papers was supposed to be discussed in sections. From fifty-eight active participants, 49 participants were able to deliver in time their papers for publication in the proceedings.

Twelve plenary lectures (40 min) were presented:

Influence of π -acceptor properties of ligands on acid-basic and redox properties of platinum complexes (*Yu. N. Kukushkin*, USSR).

Elementenkomplexe als Katalysatoren der stereospezifischen Dienpolymerisation (*E. Uhlig*, GDR).

Coordination compounds of molybdenum(V) in aqueous solutions (*I. N. Marov*, USSR).

On the applicability of the coordination model to aqueous solutions (*W. Libus*, Poland).

Zur Komplexxatalysierten Olefinmetathese (*R. Taube*, GDR).

Catalytic oxidation of gas molecules (*B. Jeřowska-Trzebiatowska*, Poland).

Infrared studies of acid-basic properties of decationized NaHY synthetic zeolites (*A. Bielański*, Poland).

Solvent effects on the thermodynamics and kinetics of substitution reactions (*V. Gutman*, Austria).

The use of high pressure in the elucidation of reaction mechanism of coordination compounds in solution (*H. Kelm*, GFR).

Inertness revisited (*M. T. Beck*, Hungary).

On some problems of complex formation of polymers as ligands (*S. L. Davydova*, USSR).

Reactions and coordination chemistry of unsaturated 1,1- and 1,2-sulfur and selenium donor atom ligands (*E. Hoyer*, GDR).

Some section lecturers: *L. Kolditz* (GDR), *K. Burger* (Hungary), *A. Samotus*, *Z. Stasicka*, *J. J. Ziolkowski* (Poland), *M. B. Čelap* (Yugoslavia), *J. Krätzmár-Šmogrovič*, *J. Gažo* (Czechoslovakia).

Forty-nine papers are published in the *Proceedings of the 5th Conference on Coordination Chemistry* (Edited by Organizing Committee, 1974, 294 pp.).

6th Conference on Coordination Chemistry – 1976

The 6th Conference on Coordination Chemistry organized by the Slovak Chemical Society, Slovak Technical University, Komenský University, and the Slovak Academy of Sciences in Bratislava was held on September 14 – 17, 1976, in the House of Scientific Workers of the Slovak Academy of Sciences at Smolenice (Smolenice Castle). Chairman of the Organizing Committee: *J. Gažo*.

Seventy-five participants from 12 countries: Austria 1, Czechoslovakia 42, Denmark 1, GDR 6, Hungary 3, Italy 3, Japan 1, Poland 9, Sweden 2, USA 1, USSR 4, Yugoslavia 2.

Ten plenary lectures (40 min) were presented:

The application of preferential solvent extraction for the resolution of a racemic inner complex (*S. Kirschner*, USA).

New aspects of the stereochemistry of Cu(II) complexes (*J. Gažo*, Czechoslovakia).

A mechanism for redox substitutions and related reactions in Pt(IV)/Pt(II)-systems (*L. I. Elding*, Sweden).

Solid state and interface coordination chemistry (*V. Gutman*, Austria).

On activation of hexafluorosilicates for exchange reactions in solid state (*L. Kolditz*, GDR).

Structure and bonding in 3d metal complexes of tripod ligands (*L. Sacconi*, Italy).

Stereochemistry of Co(III) complexes containing optically active aminoalcohols (*K. Saito*, Japan).

Progress in chemistry of σ -organyl transition metal compounds (*R. Taube*, GDR).

Coordination polymers containing dimeric fragments – new type of compounds with normal magnetism (*Yu. V. Yablokov*, USSR)

Steric and electronic influences on the structure of nickel(II) and copper(II) complexes (*E. Uhlig*, GDR).

Shorter plenary lectures were presented by: V. Zelentsov (USSR), A. A. Fotiev (USSR), A. Samotus (Poland), A. Vlček (Czechoslovakia), Z. Stasicka (Poland), J. Ziolkowski (Poland), E. N. Yurchenko (USSR), E. Hoyer (GDR).

A number of well known coordination chemists presented their scientific results at the conference: K. Burger (Hungary), M. B. Čelap (Yugoslavia), F. Dietze (GDR), Ya. A. Dorfman (USSR), L. I. Elding (Sweden), L. Kolditz (GDR), B. J. Krátsmár-Šmogrovič and J. Gažo (Czechoslovakia), J. Nagy (Hungary), O. Traverso (Italy), and

Fifty-five papers are published in the *Proceedings of the 6th Conference on Coordination Chemistry* (Edited by Organizing Committee, Slovak Technical University Press, 1976, 322 pp.). ES SVŠT-374/76.

7th Conference on Coordination Chemistry – 1978

The 7th Conference on Coordination Chemistry organized by the Slovak Chemical Society, Slovak Technical University, Komenský University, and the Slovak Academy of Sciences in Bratislava was held on September 11 – 14, 1978, in the House of Scientific Workers of the Slovak Academy of Sciences at Smolenice (Smolenice Castle). Chairman of the Organizing Committee: J. Gažo.

Eighty-six participants from 9 countries: Czechoslovakia 52, German Democratic Republic 4, Hungary 1, India 1, Italy 6, Poland 7, USA 1, USSR 11, Yugoslavia 3.

Fourteen plenary lectures (40 min) were presented:

Polynuclear 3d metal complexes with tertiary phosphines (*L. Sacconi*, Italy).

Structure and reactivity of organocobalt(IV) chelates (*M. E. Volpin*, USSR).

The dynamic stereochemistry of eight-coordinate inert metal chelates; nonrigid or rigid? (*R. D. Archer*, USA).

Dynamics of Jahn-Teller centres and the structure of crystals (*Yu. V. Yablokov*, USSR).

Investigation of the structure of lanthanide chloride by ultrasonic measurements for low concentration solutions (*B. Jeżowska-Trzebiatowska*, Poland).

Metal coordination in metal substituted carbonic anhydrates (*I. Bertini*, Italy).

Bioligands and complex formation with metal ions (*L. S. Davydova*, USSR).

Coordination at catalyst-surfaces and mechanism of heterogeneous halogene exchange (*L. Kolditz*, GDR).

The Jahn-Teller effect and vibronic influence on structure and reactivity of coordination compounds (*I. B. Bersuker*, USSR).

Mechanism of ligand substitution reactions of complexes of Co(III), Cr(III) and Rh(III) (*D. Banerjee*, India).

Ultraviolet photoelectron spectroscopy in the study of electronic structure of coordination compounds (*C. Furlani*, Italy).

Inhibition of biological systems by platinum and palladium complexes (*I. A. Zakharova*, USSR).

Structure and reactivity correlations of transition metal complexes in homogeneous catalysis (*J. Ziolkowski*, Poland).

Coordination of vanadium in solid oxides and its influence on the compounds properties (*A. A. Fotiev*, USSR).

Influence parameters – a quantitative characteristic on the ligand capacity to influence other bonds in compounds (*V. I. Nefedov*, USSR).

Fifty-five papers are published in the *Proceedings of the 7th Conference on Coordination Chemistry* (Edited by Organizing Committee, Slovak Technical University Press, 1978, 311 pp.). ES SVŠT-475/78.

8th Conference on Coordination Chemistry – 1980

The 8th Conference on Coordination Chemistry organized by the Slovak Chemical Society, Slovak Technical University, Komenský University, and the Slovak Academy of Sciences in Bratislava was held on December 8 – 11, 1980, in the House of Scientific Workers of the Slovak Academy of Sciences at Smolenice (Smolenice Castle). Chairman of the Organizing Committee: J. Gažo.

The conference was attended by 80 participants from 9 countries: Czechoslovakia 55, German Democratic Republic 4, German Federal Republic 1, Hungary 5, Italy 2, Poland 9, Switzerland 1, USSR 2, Yugoslavia 1.

Due to the increasing number of contributed papers it was no more possible to introduce and discuss all papers in the section sessions. And thus, for the first time, poster sessions were involved into the program of the conference.

Nine plenary lectures (40 min) and thirteen section lectures (20 min) were delivered, and sixty-eight posters were presented at the conference.

Plenary lectures:

Some contemporary aspects of the mutual influence of ligands in complexes (*J. Gažo*, Czechoslovakia).

Electronic lability in coordination compounds (*J. H. Ammeter*, Switzerland).

EPR of exchange clusters containing three and four magnetic ions (*Yu. V. Yablokov*, USSR).

The coordination chemistry of non-linear pseudohalide ligands (*H. Köhler*, GDR).

The problem of disorder and reactivity in solid coordination compounds (*L. Kolditz*, GDR).

Redox series (*A. A. Vlček*, Czechoslovakia).

Kinetics of ligand substitution in 4- and 6-coordinate chelate complexes in organic media (*H. Elias*, GFR).

Structure and dynamic properties of electron deficient d^N-metallocenes (*I. Pavlík*, Czechoslovakia).

Coordination chemical equilibria of macromolecular polyfunctional ligands (*K. Burger*, Hungary).

Thirteen section lectures (20 min) were presented in two sections, and moreover, 68 posters.

Some section lecturers from abroad: *E. Brücher* (Hungary), *H. Kozłowski*, *J. Mrozinski*, *P. Sobota*, *Z. Stasicka* (Poland).

Eighty-five papers are published in the *Proceedings of the 8th Conference on Coordination Chemistry* (Edited by Organizing Committee, Slovak Technical University Press, 1980, 487 pp.). ES SVŠT - 577/80.

(See also Kohútová, M.: VIIIth Conference on Coordination Chemistry. *Chem. zvesti* 35(6), 856 (1981)).

9th Conference on Coordination Chemistry – 1983

The 9th Conference on Coordination Chemistry organized by the Slovak Chemical Society, Slovak Technical University, Komenský University, and the Slovak Academy of Sciences in Bratislava was held from May 31 to June 3 1983, in the House of Scientific Workers of the Slovak Academy of Sciences at Smolenice (Smolenice Castle). Chairmen of the Organizing Committee: J. Gažo and M. Zikmund.

The conference was attended by 83 participants from 10 countries: Bulgaria 1, Canada 2, Czechoslovakia, 45, German Democratic Republic 6, German Federal Republic 1, Ireland 1, Poland 11, Romania 2, USSR 13, and Yugoslavia 1.

The conference was devoted to topical problems of coordination compounds, especially the relationship between their structure and chemical reactivity, questions of crystal chemistry, stereochemistry and the mutual influence of ligands in the coordination sphere of complexes,

problems of biocoordination chemistry in relation to macrocyclic ligands and to oxygen coordination, questions of photochemistry and photocatalysis of coordination compounds, problems of redox and substitution reactions, quantum chemical calculation of oxygen and nitrogen activation in complexes, equatorial-axial interactions of ligands and the specific properties of halogeno and pseudohalogeno complexes of copper.

Twelve plenary lectures (40 min) and 15 section lectures (20 min) were delivered and 70 posters were presented at the conference.

The plenary lectures presented:

Physical chemistry of tetraazamacrocyclic complexes (*K. B. Yatsimirskii*, USSR).

Factors determining redox energies in phthalocyanines and porphyrins (*A. B. P. Lever*, Canada).

The nature of metal-metal bond in binuclear coordination compounds (*V. I. Nefedov*, USSR).

On thiofluorophosphates (*L. Kolditz*, GDR).

Copper(II) stereochemistry – does spectroscopy tell the truth? (*B. J. Hathaway*, Ireland).

Metal extraction by chelating ligands (*E. Uhlig*, GDR).

Some new aspects of the nature of the magnetic centres in the crystals of the coordination compounds (*Yu. V. Yablokov*, USSR).

Homogeneous photocatalysis – a new field in coordination chemistry (*H. Hennig*, GDR).

Ligand substitution in planar platinum(II), palladium(II) complexes: the role of the substrate (*H. Elias*, GFR).

Synthesis, structure and reactions of rhodium(I) complexes (*J. Ziolkowski*, Poland).

Ligand properties of the thiocyanate group and relations to practical uses of thiocyanates (*H. Böhlend*, GDR).

The pseudochalconide – concept, principles and applications in inorganic chemistry (*H. Köhler*, GDR).

Section lecturers from abroad: *P. R. Bontchev* (Bulgaria), *U. Calov*, *E. G. Jäger* (GDR), *J. Moziński*, *A. Samotus*, *Z. Stasicka* (Poand), *I. A. Zacharova* (USSR).

Ninety-one papers are published in the *Proceedings of the IXth Conference on Coordination Chemistry* (Edited by Organizing Committee, Slovak Technical University Press, 1983, 514 pp.). ES SVŠT-81/1983.

The course of the 9th CCCS was overshadowed by the death of Professor J. Gažo, the permanent chairman of the Organizing Committee who passed away suddenly on February 15, 1983, at the age of 53 years, three months before the opening of the conference. After him, Dr. M. Zikmund, a corresponding member of the Slovak Academy of Sciences was appointed the chairman of the 9th CCCS.

Professor J. Gažo initiated the Conferences on Coordination Chemistry held at Smolenice since 1964 and contributed to a great extent to their success. All participants spoke of the merits of Professor J. Gažo concerning the organizing of the CCCS and express their conviction about the usefulness of such conferences for the development of coordination chemistry not only in Czechoslovakia. Finally they expressed their requests to the Organizing Committee to continue in the tradition of the Conferences on Coordination Chemistry.

(See also Ondrejovič, G: IXth Conference on Coordination Chemistry. *Chem. zvesti* 37(6), 855–856 (1983) and Zikmund, M.: Memorial for Professor Ján Gažo, DrSc, Corresponding Member of the Czerchoslovak Academy of Sciences and of the Slovak Academy of Sciences. *Chem. zvesti* 37(4), 573–574 (1983)).

10th Conference on Coordination Chemistry – 1985

The jubilee 10th Conference on Coordination Chemistry organized by the Slovak Chemical Society, Slovak Technical University, Komenský University, and the Slovak Academy of Sciences in Bratislava was held on June 4 – 7, 1985, in the House of Scientific Workers

of the Slovak Academy of Sciences at Smolenice (Smolenice Castle). Chairman of the Organizing Committee: G. Ondrejovič.

The conference was attended by 96 participants from 9 countries: Bulgaria 4, Czechoslovakia 61, German Democratic Republic 8, German Federal Republic 4, Hungary 4, Italy 1, Poland 9, USSR 4, Yugoslavia 1.

The conference was devoted to topical problems and various fields of contemporary coordination chemistry, especially to the relationship between the structure of coordination compounds and their chemical reactivity mainly in substitution, redox and catalytic reactions, to the problems of kinetics and mechanisms, photochemistry and photocatalysis of coordination compounds and studies of coordination compounds by means of quantum chemical calculation, X-ray, magnetic, EPR, ESCA, Mössbauer and other spectroscopic methods.

Thirteen plenary lectures (40 min) and fourteen section lectures (20 min) were delivered and seventy posters were presented at the conference.

The plenary lectures were presented by:

D. Reinen (GFR): Cu^{2+} and Ni^{2+} in tetrahedral coordination – experimental evidence for Jahn-Teller distortions?

Yu. V. Yablokov (USSR): Cooperative effects in crystals with Jahn-Teller centres.

E. Uhlig (GDR): Selective complex formation with sulfonamide substituted thioligands.

C. Friebe (GFR): Coordination chemical studies on copper(II) complexes of N-nicotinoyl amino acids.

O. Traverso (Italy): Photogeneration of reactive low-valent transition metal complexes.

D. Rehorek (GDR): Spin trapping of radicals in reactions of inorganic and coordination compounds.

H. Elias (GFR): Kinetics and mechanism of ligand substitution in four-coordinate nickel(II) chelate complexes: a study on the reactivities of planar and tetrahedral configurational isomers and octahedral adducts.

J. Ziolkowski (Poland): Homogeneous metal complex catalyst design.

H. Köhler (GDR): Actual developments of pseudoelement concepts and their application in coordination chemistry.

H. Böhlend (GDR): Influences of thiocyanate bond types in mixed ligand coordination compounds on their biochemical behaviour.

D. Steinborn (GDR): On the electronic influence of carbanions in metal complexes.

K. Burger (Hungary): Capillary Mössbauer spectroscopy – a new method in solution chemistry.

V. I. Nefedov (USSR): ESCA investigation of copper complexes.

Ninety-seven papers are published in the *Proceedings of the Xth Conference on Coordination Chemistry* (Edited by Organizing Committee, Slovak Technical University Press, 1985, 532 pp.), ES SVŠT - 87/85.

The pleasant milieu of the Smolenice Castle contributed to a good atmosphere at the conference which offered many possibilities for informal social contacts, discussions and exchange of inspiring ideas and opinions. The scientific and social program of the conference was positively affected by its jubilee character. The Slovak Technical University and Komenský University in Bratislava awarded the medals of honour to sixteen prominent chemists from all over the world for their contribution to the development of coordination chemistry and to the highest scientific level of the Conferences on Coordination Chemistry held in Smolenice.

(See also Ondrejovič, G: Xth Conference on Coordination Chemistry. *Chem. zvesti* 39(5), 719–720 (1985)).

11th Conference on Coordination Chemistry – 1987

The 11th Conference on Coordination Chemistry organized by the Slovak Chemical Society, Slovak Technical University, Komenský University, and the Slovak Academy of Sciences in Bratislava was held on June 2 – 5, 1987, in the House of Scientific Workers of the Slovak Academy of Sciences at Smolenice (Smolenice Castle). Chairman of the Organizing Committee: G. Ondrejovič.

The conference was held in the year when Slovak Technical University celebrated 50th anniversary of its foundation.

The conference was attended by 100 participants from 12 countries: Belgium 2, Bulgaria 4, Czechoslovakia 61, Denmark 1, German Democratic Republic 5, German Federal Republic 3, Hungary 4, Italy 1, Poland 11, USSR 4, USA 2, Yugoslavia 2.

The conference was devoted to topical problems and various fields of contemporary coordination chemistry, especially to the structure and bonding, synthesis and structures of new complexes, crystal structures and stereochemistry, reactivity, photochemistry and catalysis, theoretical aspects, thermal reactions, solid state chemistry and biological aspects of coordination compounds.

Thirteen plenary lectures (40 min) and seventeen section lectures (20 min) were delivered and sixty-eight posters were presented at the conference.

The plenary lectures were presented by:

D. Reinen (GFR): Structure and bonding of Mn(V), Mn(VI) and Cr(V) in the tetrahedral sites of oxidic solids.

S. V. Larionov (USSR): New groups of volatile coordination compounds.

L. Kolditz (GDR): Mechanism of solid state reactions and coordination chemistry.

R. D. Archer (USA): Kinetics and bonding considerations – a new guide to new coordination polymer structures with examples using cobalt and zirconium.

U. Belluco (Italy): Reactivity of platinum – group organometallic compounds.

Z. Stasicka (Poland): Photoredox reactions in some mixed cyanide.

I. Bertini (Italy): Metal dimers in metalloproteins.

P. R. Bontchev (Bulgaria): New platinum and palladium complexes with creatinine.

C. Friebe (GFR): EPR spectroscopic studies on tridentate Schiff base copper(II) complexes with additional monodentate donor ligands.

L. Nagy (Hungary): Electrochemical and spectroscopic studies of manganese complexes formed with sugar type ligands.

H. Elias (GFR): Preparation and application of sterically hindered pyridine bases.

M. T. Beck (Hungary): Importance of weak complexes in agricultural chemistry.

D. Steinborn (GDR). On the complex catalysis of hydrogenation of olefines.

Section lecturers: *M. Döring* (GDR), *F. N. Galsbol* (Denmark), *A. Jegorov* (Czechoslovakia), *D. Valigura* (Czechoslovakia), *J. Mroziński* (Poland), *M. Hvastijová* (Czechoslovakia), *S. Hoste* (Belgium), *B. Vlčková* (Czechoslovakia), *A. Samotus* (Poland), *A. Vlček, Jr.* (Czechoslovakia), *J. Šima* (Czechoslovakia), *A. M. Trzeciak* (Poland), *F. Joó* (Hungary), *G. P. Van der Kelen* (Belgium), *R. Boča* (Czechoslovakia), *M. Melník* (Czechoslovakia), *K. Andrä* (GDR)

Ninety-five papers are published in the *Proceedings of the XIth Conference on Coordination Chemistry* (Edited by Organizing Committee 1987, 480 pp.).

(See also Ondrejovič, G.: XIth Conference on Coordination Chemistry. *Chem. Papers* 42(1), 118 (1988)).

12th Conference on Coordination Chemistry – 1989

The 12th Conference on Coordination Chemistry organized by the Slovak Chemical Society, Slovak Technical University, Comenius University, and the Slovak Academy of Sciences in Bratislava was held on June 6 – 9, 1989, in the House of Scientific Workers of the Slovak Academy of Sciences at Smolenice (Smolenice Castle). Chairman of the Organizing Committee: G. Ondrejovič. The conference participated on celebrations of 70. anniversary of the Comenius University in Bratislava.

The conference was attended by 92 participants from 11 countries: Belgium 1, Bulgaria 3, Czechoslovakia 60, France 1, German Democratic Republic 7, German Federal Republic 2, Hungary 2, India 2, Poland 7, USSR 5, Yugoslavia 2.

The conference was devoted to topical problems and various fields of contemporary coordination chemistry, especially to the structure and bonding, formation and reactivity, theoretical aspects, thermal reactions, and biological aspects of coordination compounds.

Fourteen plenary lectures (40 min) and sixteen section lectures (20 min) were delivered and fifty-eight posters were presented at the conference.

The plenary lectures were presented by:

E. Uhlig (GDR): Displacement of bidentate oxygen ligands from the coordination sphere of their late 3d-element chalcates.

G. P. Van der Kelen (Belgium): Ceramic high T_c superconductors – survey on actual chemistry and future development.

Yu. V. Yablokov (USSR): Magnetic resonance in high temperature superconductors.

D. Benerjea (India): Thermodynamics, kinetics and mechanism of formation and dissociation of ternary complexes.

H. Elias (GFR): Preparation and kinetic investigation of model complexes for hemocyanin.

S. Ašperger (Yugoslavia): Substitution reactions of cobalt porphyrins.

E. G. Jäger (GDR): Investigations on the axial ligation of iron(III) in a hemine-like macrocyclic N₄-environment.

D. Steinborn (GDR): On synthesis, stability and reactivity of heteroatom substituted alkyl metal compounds.

V. A. Logvinenko (USSR): Thermal dissociation of coordination compounds as the ligands substitution process (thermodynamic and kinetic aspects).

M. Verdaguer (France): X-ray absorption spectroscopy in coordination chemistry.

R. Boča (Czechoslovakia): From molecular (spin) orbitals in metal complexes to band in clusters and solid-state compounds.

J. Mrozinski (Poland): Intra- and intermolecular magnetic interactions in copper(II) complexes.

M. Melník (Czechoslovakia): Relationship between the chemical and biological behaviours of copper(II) carboxylates.

C. Friebe (GFR): Chameleon-like behaviour of N-salicylidene-glycinato copper(II) complexes modified by additional monodentate donor ligands and water of crystallization.

Section lecturers: *P. Bontchev* (Bulgaria), *M. Mitewa* (Bulgaria), *M. Strašák* (Czechoslovakia), *V. V. Pavlishchuk* (USSR), *G. Stochel* (Poland), *F. Hartl* (Czechoslovakia), *B. Vlčková* (Czechoslovakia), *F. Pavelčík* (Czechoslovakia), *W. Dietzsch* (GDR), *R. Meier* (GDR), *P. Sipos* (Hungary), *L. I. Kuznetsova* (USSR), *M. B. Celap* (Yugoslavia), *H. Langfelderová* (Czechoslovakia), *P. Schwendt* (Czechoslovakia), *E. Jóna* (Czechoslovakia).

Eighty-five papers are published in the *Proceedings of the XIIth Conference on Coordination Chemistry* (Edited by Organizing Committee, 1989, 460 pp.).

(See also Ondrejovič, G.: XIIth Conference on Coordination Chemistry. *Chem. Papers* 44(3), 429 (1990)).

13th Conference on Coordination Chemistry – 1991

The 13th Conference on Coordination Chemistry organized by the Slovak Chemical Society, Slovak Technical University, Comenius University, and the Slovak Academy of Sciences in Bratislava was held from June 11 to June 14, 1991, in the House of Scientific Workers of the Slovak Academy of Sciences at Smolenice (Smolenice Castle). Chairman of the Organizing Committee: G. Ondrejovič.

The conference was attended by 70 participants from 12 countries: Austria 1, Belgium 3, Bulgaria 2, Czechoslovakia 39, Denmark 1, Germany 7, France 2, Hungary 1, Italy 1, Poland 6, USSR 4, Yugoslavia 3.

Sixteen plenary lectures (40 min) and twenty section lectures (20 min) were delivered and thirty-seven posters were presented at the conference.

The plenary lectures dealt with the following topics:

Molecular System Organization in Certain Complexes (*V. Gutmann*, Austria),

Recent Results of the Investigation of the Influence of Transition Metal Complexes Composition and Structure on Their Chromatographic Behaviour (*M. B. Čelap*, Yugoslavia),

EPR Spectroscopic Insight into the Architecture of Molecular Crystals of Copper(II) Complexes with Organic Ligands (*C. Friebe*, Germany), Application of High-Pressure Techniques in Mechanistic Studies of Bioinorganic Systems (*R. van Eldik*, Germany),

Recent Advances in Chemistry and Applications of Metal Thiocyanate Complexes (*H. Böhland*, Germany),

The Redox Behaviour of Copper(II) Complexes with Polythia Ligands (*V. Pavlishchuk*, USSR), Structure and Magnetism of Copper(II) and Nickel(II) Macrocyclic Compounds (*J. Mrozinski*, Poland),

Kinetics and Mechanism of Complex Formation: Metal vs. Ligand Control (*H. Elias*, Germany),

Multiple Mechanistic Pathways of the Oxidation of Organic Substrates by Peroxometal Complexes (*F. Di Furia*, Italy),

Oxygen Atom Transfer in Molybdenum and Tungsten Complexes (*H. Arzoumanian*, France),

Effect of Modifying Ligands (P(Ph)_3 , PPh_3 , dppe, and $\text{cp}_2\text{Zr}(\text{CH}_2\text{PPh}_2)$) on Hex-1-ene Hydroformylation Catalyzed by $[\text{HRh}\{\text{P(Ph)}_3\}_3]$ and $[\text{HRh(CO)}\{\text{P(Ph)}_3\}_3]$ (*J. J. Ziolkowski*, Poland),

On the Complex Catalyzed Addition of Alcohols to Acetylenes (*D. Steinborn*, Germany),

Ferro and/or Ferrimagnetism: How to Design Molecular-Based Magnets (*M. Verdaguer*, France),

Copper Complexes with Antihypertension Drugs Captopril and Propranolol (*P. R. Bontchev*, Bulgaria),

Molecular Orbital Study of Semiconductors and Superconductor Clusters (*R. Boča*, Czechoslovakia),

Layered Structures and the Modeling of Properties of HTSC (*Yu. V. Yablokov*, USSR).

Section lectures were delivered by *G. P. Van der Kelen* (Belgium), *H. Langfelderová* (Czechoslovakia), *G. M. Nord* (Denmark), *A. M. Trzeciak* (Poland), *S. Ašperger* (Yugoslavia), *M. Melník* (Czechoslovakia), *M. Mitewa* (Bulgaria), *M. Strašák* (Czechoslovakia), *J. Labuda* (Czechoslovakia), *J. Šima* (Czechoslovakia), *G. G. Herman* (Belgium), *A. M. Goeminne* (Belgium), *L. J. Csányi* (Hungary), *P. Schwendt* (Czechoslovakia), *M. Sivák* (Czechoslovakia), *I. N. Marov* (USSR), *I. Kováčik* (Czechoslovakia), *G. N. Vučković* (Yugoslavia), *E. Jóna* (Czechoslovakia), *F. Valach* (Czechoslovakia).

The essential parts of contributions are published in the *Proceedings of the XIIIth Conference on Coordination Chemistry* (Edited by Organizing Committee, 1991, 74 papers, 380 pp.).

(See also Ondrejovič, G.: XIIIth Conference on Coordination Chemistry. *Chem. Papers* 46(2), 144 (1992)).

14th Conference on Coordination Chemistry – 1993

The 14th Conference on Coordination Chemistry organized by the Slovak Chemical Society, Slovak Technical University, Comenius University, and the Slovak Academy of Sciences in Bratislava was held in Smolenice Castle on June 7–11, 1993 and was entitled "**Contributions to the Development of Coordination Chemistry**". Chairman of the Organizing Committee: G. Ondrejovič.

The Conference was attended by 92 participants from 16 countries: Austria 4, Belgium 3, Bulgaria 2, Czech Republic 2, France 1, Germany 13, Italy 4, Peru 1, Poland 12, Slovakia 40, South Africa 1, Spain 1, Switzerland 1, UK 3, USA 3 and Yugoslavia 1.

Participants covered in their contributions a wide range of problems of nowadays coordination chemistry reflected by eight topics:

Conceptions in coordination chemistry.

Synthesis and properties of new coordination compounds.

Coordination mode of ligands reflected in the structure of coordination compounds.

Structural correlations.

Complex formation in solutions.

Reactivity of coordination compounds.

Photochemical reactions of coordination compounds.

Biologically active complexes and ligands.

Twenty-one plenary lectures (35 min) and twenty-three section lectures (15 min) were delivered and forty-five posters were presented at the conference.

The plenary lectures were presented by V. Gutmann (Austria), H. B. Bürgi (Switzerland), P. Pallavicini (Italy), M. Verdaguer (France), C. Kutal (USA), H. Hennig (Germany), B. M. Rode (Austria), W. Linert (Austria), R. E. P. Winpenny (UK), J. Mrozinski (Poland), F. Di Furia (Italy), R. C. Thompson (USA), G. La Monica (Italy), M. D. Grillone (Italy), A. Vogler (Germany), D. M. Wagnerová (Czech Republic), B. Sieklucka (Poland), M. Mitewa (Bulgaria), O. P. Anderson (USA), H. Elias (Germany), P. R. Bontchev (Bulgaria).

Section lecturers: M. B. Celap (Yugoslavia), P. Pelikán (Slovakia), G. P. Van der Kelen (Belgium), R. Boča (Slovakia), M. Ludwig (Germany), A. Sieker (UK), V. Holba (Slovakia), A. M. Goeminne (Belgium), D. Bustin (Slovakia), S. Lis (Poland), J. Sýkora (Slovakia), J. Šima (Slovakia), G. Ondrejovič (Slovakia), M. Melník (Slovakia), L. Ballester (Spain), F. Valach (Slovakia), M. Andruh (Germany), E. Jóna (Slovakia), S. Lotz (South Africa), D. Valigura (Slovakia), P. Strauch (Germany), J. Kožíšek (Slovakia), L. Jäger (Germany).

Ninety-two reviewed papers as six-page articles are published in the monograph *Contributions to Development of Coordination Chemistry* (Editors G. Ondrejovič and A. Sirota, Slovak Technical University Press, Bratislava, 1993, 494 pp.). ISBN 80-227-0556-X.

(See also Ondrejovič, G.: XIVth Conference on Coordination Chemistry. *Chem. Papers* 47(5), 337 (1993)).

15th Conference on Coordination Chemistry – 1995

The 15th Conference on Coordination Chemistry organized by the Slovak Chemical Society, Slovak Technical University, Comenius University, and the Slovak Academy of Sciences in Bratislava was held on June 5–9, 1995 under the title "**Current Trends in Coordination Chemistry**". Chairman of the Organizing Committee: G. Ondrejovič.

The conference was attended by 92 participants from 21 countries: Austria 5, Bulgaria 2, Canada 2, Croatia 1, Czech Republic 1, France 2, Germany 9, Great Britain 1, Greece 1, Israel 1, Italy 2, The Netherlands 1, Poland 6, Russia 1, Slovakia 42, Slovenia 3, South Africa 1, Spain 1, Switzerland 3, Ukraine 4, and USA 3.

The scientific program of the conference has been aimed at four main fields:

- A. Solid state chemistry – synthesis, structure and applications,
- B. Solution chemistry – catalysis, photochemistry, and mechanisms,
- C. Molecular materials – magnetic, optical, and electrical properties,
- D. Complexes in biological systems, human medicine, and environment.

The particular fields were introduced by main plenary lectures (each 60 min) delivered by distinguished scientists: *E. Constable* (University of Basel, Switzerland), *H. Hennig* (University of Leipzig, Germany), *D. Gatteschi* (University of Florence, Italy) and *J. Reedijk* (University of Leiden, The Netherlands).

Twenty three plenary lectures (each 35 min) and fifty six section lectures (each 15 min) were presented at the conference.

The plenary lectures were delivered by *E. Uhlig* (Jena, Germany), *K. R. Koch* (Cape Town, South Africa), *H. Böhlend* (Erfurt/Mühlhausen, Germany), *L. Ballester* (Madrid, Spain), *P. Šegedin* (Ljubljana, Slovenia), *C. Kutal* (Athens, Georgia, USA), *M. Sarakha* (Aubiere, Cedex, France), *D. Meyerstein* (Beer-Sheva, Israel), *D. Steinborn* (Halle-Wittenberg, Germany), *L. McElwee-White* (Gainesville, Florida, USA), *M. Herberhold* (Bayreuth, Germany), *B. M. Rode* (Innsbruck, Austria), *Y. D. Lampeka* (Kiev, Ukraine), *M. Verdaguer* (Paris, Cedex, France), *R. Boča* (Bratislava, Slovakia), *M. Melník* (Bratislava, Slovakia), *J. Mrozinski* (Wroclaw, Poland), *O. Knop* (Halifax, Canada), *V. Gutmann* (Vienna, Austria), *H. Sigel* (Basel, Switzerland), *P. R. Bontchev* (Sofia, Bulgaria), *D. M. Roundhill* (New Orleans, Louisiana, USA), *W. Linert* (Vienna, Austria).

Seventy-seven reviewed papers as six-page articles are published in the monograph *Current Trends in Coordination Chemistry* (Editors G. Ondrejovič and A. Sirota, Slovak Technical University Press, Bratislava, 1995, 460 pp.). ISBN 80-227-0769-4.

(See also Ondrejovič, G.: XVth Conference on Coordination Chemistry. *Chem. Papers* 49(3), 164 (1995)).

16th Conference on Coordination Chemistry – 1997

The 16th Conference on Coordination Chemistry ("**Progress in Coordination and Organometallic Chemistry**") was organized by the Slovak Chemical Society, Slovak University of Technology, and Comenius University in Bratislava on June 9 – 13, 1997 in Congress Centre of the Slovak Academy of Sciences in Smolenice Castle. Chairman of the Organizing Committee: G. Ondrejovič.

At the conference participated 81 scientists from 22 countries: Algeria 1, Australia 1, Belarus 1, Bulgaria 1, Canada 3, Finland 1, France 1, Germany 6, India 1, Ireland 1, Italy 3, Japan 1, Poland 8, Portugal 1, Russia 2., Slovakia 37, Slovenia 5, Spain 2, Switzerland 2, Ukraine 1, USA 1, and Yugoslavia 1.

The scientific program of the conference was divided into four main fields:

- A. Synthesis, structure, and properties of coordination and organometallic compounds.
- B. Reactivity and stability of coordination and organometallic compounds.
- C. Complexes in biological systems and human medicine.
- D. Applied and environmental inorganic and coordination chemistry.

The particular fields were introduced by main plenary lectures (each 45 min) presented by established scientists: *P. Braunstein* (L. Pasteur University of Strasbourg, France), *J. J. Ziolkowski* (University of Wroclaw, Poland), *I. Bertini* (University of Florence, Italy), and *M. Grätzel* (École Polytechnique Fédérale, Lausanne, Switzerland).

Twenty-two plenary lectures (each 30 min) and 43 section lectures (each 15 min) were presented at the conference. In the group of plenary lecturers presented their lectures *A. Storr* (Vancouver, Canada), *M. R. Sundberg* (Helsinki, Finland), *S. V. Larionov* (Novosibirsk, Russia), *D. J. Radanovič* (Kragujevac, Yugoslavia), *P. Strauch* (Leipzig, Germany),

E. Szlyk (Torun, Poland), C. Zucchi (Modena, Italy), A. J. L. Pombeiro (Lisboa, Portugal), C. Kutal (Athens, Georgia, USA), L. Jäger (Halle/Saale, Germany), P. Sedlák (Saskatoon, Canada), M. Melník (Bratislava, Slovakia), K. B. Pandeya (Rewa, India), P. R. Bontchev (Sofia, Bulgaria), K. B. Nolan (Dublin, Ireland), L. Lomozik (Poznan, Poland), I. Turel (Ljubljana, Slovenia), H. Elias (Darmstadt, Germany), R. C. Thompson (Vancouver, Canada), R. Boča (Bratislava, Slovakia), Y. Fukuda (Tokyo, Japan), P. Pelikán (Bratislava, Slovakia), F. S. Decurtins (Zürich, Switzerland).

Fifty contributions are published as standard six-page reviewed papers in the monograph *Progress in Coordination and Organometallic Chemistry* (Editors G. Ondrejovič and A. Sirota, Slovak Technical University Press, Bratislava, 1997, 335 pp.). ISBN 80-227-0948-4.

(See also Ondrejovič, G: XVIth Conference on Coordination Chemistry. *Chem. Pap.* 52(1), 67 (1998)).

17th Conference on Coordination Chemistry – 1999

The 17th Conference on Coordination Chemistry organized by the Slovak Chemical Society, Slovak University of Technology, and Comenius University in Bratislava was held on June 7 – 11, 1999 in the Congress Centre of the Slovak Academy of Sciences in Smolenice Castle. Chairman of the Organizing Committee: G. Ondrejovič.

The scope of the Conference corresponded to title "**Coordination Chemistry at the Turn of the Century**". The conference dealt with up-to-date current problems of coordination and organometallic chemistry and with the progress achieved in these fields on the turn of both century and millenium. *Georg B. Kauffman* (California State University, Fresno), kindly met the wishes of the organizers and presented his introductory lecture of the conference on the development of coordination chemistry during the 20th century.

At the conference participated 97 scientists from 16 countries: Belgium 2, Bulgaria 1, Denmark 1, France 4, Germany 6, Greece 1, India 1, Italy 2, Japan 10, Poland 7, Portugal 1, Romania 3, Russia 1, Slovakia 49, UK 4, and USA 4.

The scientific program was divided into four main fields:

- A. Structure and reactivity of coordination and organometallic compounds (synthesis, structure, stability, kinetics, photochemistry, catalysis).
- B. Supramolecular coordination chemistry (solid state systems, host-guest chemistry, self assembling complexes, dendrimers, inorganic superstructures, molecular modeling).
- C. Complexes in biological systems, human medicine and environment (natural and model biocomplexes, relationship between structure and function of therapeutic agents and enzymes, catalyzed destruction of pollutants),.
- D. Applied inorganic chemistry (supramolecular devices, magnetic materials, superconductors, magnetic, electrical, and optical properties of inorganic and coordination compounds, application of inorganic catalysts) .

The invited plenary lecturers (*G. Kauffman* from California State University of Fresno, *J. Gladysz* from University of Utah, Salt Lake City, *M. Andruh* from University of Bucharest, *P. R. Bontchev* from University of Sofia, and *M. Verdaguer* from Université Pierre et Marie Curie, Paris) opened the main sessions of the Conference and presented their plenary lectures (each 45 minutes).

Moreover, 24 plenary lectures (each 30 minutes) were delivered by *J. L. Wardell* (UK), *B. Sieklucka* (Poland), *K. Sakai* (Japan), *K. Okamoto* (Japan), *J. Glerup* (Denmark), *M. Melník* (Slovakia), *M. Mikuryia* (Japan), *A. Maldotti* (Italy), *Ch. Kutal* (USA), *M. Lalia-Kantouri* (Greece), *K. Hegetschweiler* (Germany), *D. B. Leznoff* (Canada), *P. Hubberstey* (UK), *R. Raptis* (USA), *V. Fusi* (Italy), *K. B. Pandeya* (India), *J. Szklarzewicz* (Poland), *M. A. Santos* (Portugal), *G. Simonneaux* (France), *J. Mrozinski* (Poland), *R. Boča* (Slovakia), *J. Telser* (USA), *M. Elbanowski* (Poland), *P. Strauch* (Germany).

Thirty-eight section lectures (each 15 minutes), 11 section lectures (each 10 minutes), and 15 posters were presented at the Conference.

Sixty-eight contributions have been published as at least six-page reviewed papers in the monograph *Coordination Chemistry at the Turn of the Century* Volume 4, Monograph series of the International Conferences on Coordination Chemistry held periodically at Smolenice, Slovakia (Editors G. Ondrejovič and A. Sirota, Slovak Technical University Press, Bratislava, 1999, 473 pp.). ISBN 80-227-1225-6, ISSN 1335-308X.

The 17th Conference on Coordination Chemistry was the suitable occasion to recollect the 70th birthday of Ján Gažo (1929 – 1983) who initiated the Conferences on Coordination Chemistry organized periodically in Smolenice Castle. Ján Gažo was a very clever manager and organizer. His research projects and visions attracted many people, in particular young chemists. He deeply influenced coordination chemistry in Slovakia for a long period of time. The First Conference on Coordination Chemistry was organized at Smolenice Castle in 1964 and for next eight Conferences, until his death, he acted as a chairman of the Organizing Committee. The Conferences have been accepted for their scientific and social levels by coordination chemists from all over the world. Outstanding chemists such as S. Ašperger, D. Banerjee, M. T. Beck, U. Belluco, I. B. Bersuker, J. Bjerrum, K. Burger, M. B. Celap, E. O. Fischer, V. Gutmann, B. J. Hathaway, B. Jezowska-Trzebiatowska, S. Kirschner, E. C. Lingafelter, R. S. Nyholm, M. A. Poraj-Koshits, J. Reedijk, L. Sacconi, K. Saito, C. Schäffer, G. Schwarzenbach, J. T. Struchkov, E. Uhlig, G. Van der Kelen, A. A. Vlček, M. E. Volpin, K. B. Yatsimirskii and many other prominent coordination chemists took part in Smolenice Conferences.

(See also Ondrejovič, G.: XVIIth Conference on Coordination Chemistry. *Chem. Papers* 53(5),346 (1999)).

18th International Conference on Coordination and Bioinorganic Chemistry – 2001

The 18th International Conference on Coordination and Bioinorganic Chemistry organized by the Slovak Chemical Society, Slovak Technical University, Comenius University, and the Slovak Academy of Sciences in Bratislava was held in Smolenice Castle on June 4 – 8, 2001. Chairman of the Organizing Committee: M. Melník.

The Conference entitled "**Challenges for Coordination Chemistry in the New Century**" was a very interesting meeting of 93 participants from 19 countries (Australia 1, Bangladesh 1, Belgium 2, Finland 1, France 1, Germany 8, Hungary 2, India 2, Japan 7, Portugal 1, Poland 6, Romania 2, Russia 1, Slovakia 51, Slovenia 1, Taiwan 1, Turkey 1, UK 1, USA 3).

Topics of the scientific program:

Opening lecture: Coordination chemistry – origin, development and outlook (M. Melník, 30 min).

A. Complexes in biological systems, human medicine and environment.

B. Structure, charge density and reactivity of coordination and bioinorganic compounds.

C. Thermal analysis of inorganic and coordination compounds. Inorganic materials.

D. Applied inorganic chemistry. Magnetic, electrical and optical properties of inorganic and coordination compounds.

The invited lecturers (45 minute lectures): D. Rehder (University of Hamburg, topic A), Yu. Wang (National Taiwan University in Taipei, topic B), B. Chowdhury (Matech Associates in Scanton, USA, topic C), and J. Mrozinski (University in Wroclaw, topic D) opened the main plenary sessions

Nineteen lectures each lasting 30 minutes, were delivered by M. Melník (Slovakia), in topic A by G. Stochel (Poland), M. Humar (Slovenia), M. Nakamura (Japan), P. Balgavý (Slovakia), R. V. Singh (India), in topic B by M. R. Sundberg (Finland), J. Szklarewicz (Poland), M. Kojima (Japan), A. B. Burdukov (Russia), M. Mikuriya (Japan), P. Baran (Slovakia),

H. Hennig (Germany), G. Speier (Hungary), G. Simonneaux (France), in topic C by P. S. Thomas (Australia), and in topic D by R. Boča (Slovakia), P. Strauch (Germany) and E. Farkas (Hungary).

Moreover, participants presented 53 section lectures (each 15 minutes) and 13 shorter lectures (10 minutes) in the young scientists section. No posters were presented this time.

The reviewed contributions are published in the monograph *Challenges for Coordination Chemistry in the New Century* Volume 5, Monograph series of ICCBIC Smolenice, Slovakia (Editors M. Melník and A. Sirota, Slovak Technical University Press, Bratislava, 2001, 461 pp.). ISBN 80-227-1539-5, ISSN 1335-308X.

19th International Conference on Coordination and Bioinorganic Chemistry – 2003

The 19th International Conference on Coordination and Bioinorganic Chemistry organized by the Slovak Chemical Society, Slovak Technical University, Comenius University, and the Slovak Academy of Sciences in Bratislava was held in Smolenice Castle on June 2 – 6, 2003 and was entitled "**Progress in Coordination and Bioinorganic Chemistry**". Chairman of the Organizing Committee: M. Melník.

As usually, it represented a very interesting meeting of 96 participants. Ninety-two active participants from 18 countries presented their scientific results from Belgium 1, Canada 2, Czech Republic 3, Egypt 2, Finland 1, France 1, Germany 6, Hungary 9, Italy 1, Japan 11, Poland 6, Romania 5, Russia 1, Slovakia 39, Spain 1, Switzerland 1, UK 1, USA 1.

The scientific program was focused on following topics:

A. Complexes in biological systems, human medicine and environment.

B. Structure and reactivity of coordination and bioinorganic compounds.

C. New materials in inorganic and bioinorganic chemistry.

D. Applied coordination, bioinorganic and inorganic chemistry: electrochemistry and magnetic properties.

The main plenary lectures were delivered by the invited lecturers D. Steinborn (Martin-Luther-University Halle, Germany (topic A), A. von Zelewsky from Fribourg University, Switzerland (topic B), P. Strauch from Postdam University, Germany (topic C), and A. B. P. Lever from York University, Canada, topic D.

Twenty-five contributions were presented as 30 minute plenary lectures: in topic A by A. Llobet (Girona, Spain), Y. N. Butt (Norwich, UK), B. Lippert (Dortmund, Germany), M. Mikuriya (Sanda, Japan), in topic B by T. Ito (Sendai, Japan), W. Mori (Kanagawa, Japan), L. J. Simandi (Budapest, Hungary), M. R. Sundberg (Helsinki, Finland), K. Hegetschweiler (Saarbrücken, Germany), A. B. Burdakov (Novosibirsk, Russia), C. Kutal (Georgia, USA), J. Šima (Bratislava, Slovakia), T. Shibahara (Okayama, Japan), J. Szklarzewicz (Krakow, Poland), M. Kojima (Okayama, Japan), C. Arena (Parma, Italy), N. Kojima (Osaka, Japan), V. Stynes (Toronto, Canada), M. Handa (Matsue, Japan), , in topic C by G. Simonneaux (Rennes, France), M. Yamashita (Tokyo, Japan), E. Szlyk (Toruń, Poland), in topic D by T. Szabó-Plánka (Szeged, Hungary), R. Boča (Bratislava, Slovakia), and J. Mroziński (Wrocław, Poland).

Participants read 42 section lectures (each 15 minutes). As a matter of good tradition, young participants were given an opportunity to present their results in the form of 11 shorter (10 minutes) lectures in the young scientists section. Within the poster section 10 contributions were presented.

Sixty-eight reviewed papers are published in the monograph *Progress in Coordination and Bioinorganic Chemistry* Volume 6, Monograph series of ICCBIC Smolenice, Slovakia (Editors M. Melník, and A. Sirota, Slovak Technical University Press, Bratislava, 2003, 433 pp.). ISBN 80-227-1891-2. ISSN 1335-308X.

20th International Conference on Coordination and Bioinorganic Chemistry – 2005

The 20th International Conference on Coordination and Bioinorganic Chemistry organized by the Slovak Chemical Society, Slovak Technical University, Comenius University, and the Slovak Academy of Sciences in Bratislava was held in Smolenice Castle on June 5 – 10, 2005 and was entitled "**Advances in Coordination, Bioinorganic and Inorganic Chemistry**". Chairman of the Organizing Committee: M. Melník.

It was a scientific event of very high level. A number of active participants reached 114, covering 23 countries (Australia 1, Croatia 1, Czech Republic 4, France 1, Germany 8, Hungary 9, Iran 3, Ireland 1, Japan 18, Moldova 1, New Zealand 1, Poland 7, Portugal 3, Romania 2, Russia 3, Slovakia 38, Slovenia 2, Spain 3, Switzerland 2, Thailand 1, Turkey 1, USA 3).

Topics of the scientific program:

A. Electron, molecular and crystal structures.

B. Solution and solid state reactivity.

C. Applied inorganic and coordination chemistry.

D. Complexes in biological systems, human medicine and environment.

The main plenary lectures (45 min) were delivered by invited lecturers *M. R. Sundberg* (Helsinki, Finland, topic A), *G. Simonneaux* (Rennes, France, topic B), *M. Yamashita* (Sendai, Japan, topic C), and *H. Sigel* (Basel, Switzerland, topic D).

Twenty-two plenary lectures (30 min) were delivered, in topic A by *A. Mueller* (Bielefeld, Germany), *R. N. Bose* (DeKalb, USA), *M. Melník* (Bratislava, Slovakia), *P. Strauch* (Potsdam, Germany), *J. Šima* (Bratislava, Slovakia), in topic B by *D. Steinborn* (Halle, Germany), *Y. Sasaki* (Sapporo, Japan), *K. Hegetschweiler* (Saarbrücken, Germany), *T. Ito* (Sendai, Japan), *J. Mrozinski* (Wrocław, Poland), *S. Takeda* (Sapporo, Japan), *M. Julve* (Valencia, Spain), in topic C by *M. Mikuriya* (Sanda, Japan), *M. Nakamura* (Tokyo, Japan), *W. Mori* (Kanagawa, Japan), *E. Szlyk* (Torun, Poland), *B. Sieklucka* (Krakow, Poland), *J. Krzystek* (Tallahassee, USA), in topic D by *J. Sóvágó* (Debrecen, Hungary), *B. Zümreoglu-Karan* (Ankara, Turkey), *M. Koman* (Bratislava, Slovakia), *J. Kaizer* (Veszprém, Hungary).

The results obtained by the participants were presented in 26 plenary lectures, 59 section lectures, and 13 contributions were presented in the poster section. Based on appreciation received at previous ICCBIC, also at this conference 15 young participants, considered as future of coordination chemistry, were given an opportunity to present their results in the form of oral presentation as 10 minute lectures within Young Scientists Section.

Abstracts of contributions are published in the Book of Abstracts and reviewed full papers in CD-monograph *Advances in Coordination, Bioinorganic and Inorganic Chemistry* Volume 7, Monograph series of ICCBIC Smolenice, Slovakia (Editors M. Melník, J. Šima, and M. Tatarko, Slovak Technical University Press, Bratislava 2005, 440 pp.). CD-monograph. ISBN 80-227-2226X, ISSN 1335-308X.

21st International Conference on Coordination and Bioinorganic Chemistry – 2007

The 21st International Conference on Coordination and Bioinorganic Chemistry organized by the Slovak Chemical Society, Slovak Technical University in Bratislava, Comenius University in Bratislava, the Slovak Academy of Sciences, Alexander Dubček University in Trenčín and Pavol Jozef Šafárik University in Košice was held in Smolenice Castle on June 3 – 8, 2007 and was entitled "**Achievements in Coordination, Bioinorganic and Applied Inorganic Chemistry**". Chairman of the Organizing Committee: M. Melník.

Eighty-six active participants from 16 countries (Australia 1, Austria 1, Czech Republic 6, Egypt 2, France 4, Germany 8, Hungary 7, India 2, Ireland 2, Japan 7, Poland 5, Romania 1, Russia 4, Serbia 1, Slovakia 33, USA 2) presented their scientific results in the program of the conference.

Topics of the scientific program:

A. Electron, molecular and crystal structures.

B. Solution and solid state reactivity.

C. Applied inorganic and coordination chemistry.

D. Complexes in the human medicine and in the environment.

The main plenary lectures (45 min) were delivered by invited lecturers *M. Mikuriya* (Sanda, Japan, topic A), *R. Slade* (University of Surrey, UK, topic B), *P. Day* (Royal Institution of Great Britain, UK, topic C), and *T. Szabó-Plánka* (Szeged, Hungary, topic D),

Twenty-two plenary lectures (30 min) were delivered, in topic A by *H. Fuess* (Darmstadt, Germany), *J. Kaizer* (Veszprém, Hungary), *S. D. Zarič* (Belgrade, Serbia), *A. Ozarowski* (USA), *B. Creaven* (Dublin, Ireland), in topic B by *A. K. Powell* (Karlsruhe, Germany), *P. Comba* (Heidelberg, Germany), *J. Mroziński* (Wrocław, Poland), *R. Boča* (Bratislava, Slovakia), *N. V. Belkova* (Moscow, Russia), *M. Ferbinteanu* (Bucharest, Romania), *I. Hoskovicová* (Prague, Czech Republic), in topic C by *F. L. Lindoy* (Sydney, Australia), *N. Avarvari* (Angers, France), *T. Azais* (Paris, France), *M. Breza* (Bratislava, Slovakia), *P. Štěpnička* (Prague, Czech Republic), and *R. Podgajny* (Krakow, Poland), in topic D by *M. Melník* (Trenčín, Slovakia), *R. N. Patel* (Rewa, India), *J. Krzystek* (Florida, USA), *K. Hegetschweiler* (Saarbrücken Germany).

Thirty-four section lectures (15 min) were presented and 12 contributions were presented by posters. Young scientists presented 18 lectures (10 min) in young scientists session.

Abstracts of contributions are published in the Book of Abstracts and reviewed full papers in CD-monograph *Achievements in Coordination, Bioinorganic and Applied Inorganic Chemistry*, Volume 8, Monograph series of ICCBIC Smolenice, Slovakia (Editors M. Melník, J. Šima, and M. Tatarko, Slovak Technical University Press, Bratislava 2007, 370 pp.). CD-monograph. ISBN 978-80-227-2647-4, ISSN 1335-308X.

22nd International Conference on Coordination and Bioinorganic Chemistry – 2009

The 22nd International Conference on Coordination and Bioinorganic Chemistry organized by the Slovak Chemical Society, Slovak Technical University in Bratislava, Comenius University in Bratislava, Alexander Dubček University in Trenčín, and Slovak Academy of Sciences was held in Smolenice Castle on June 7 – 2, 2009 and was entitled "**Insights into Coordination, Bioinorganic and Applied Inorganic Chemistry**". Chairman of the Organizing Committee: M. Melník.

The Conference was a successful meeting of 110 active participants from 26 countries: Argentina 1, Austria 1, Brazil 2, Bulgaria, Czech Republic 1, Croatia 2, Finland 1, France 4, Germany 4, Greece 1, Hungary 8, India 3, Ireland 2, Italy 1, Japan 10, Moldavia 1, Netherlands 1, Poland 11, Russia 4, Slovakia 39, Slovenia 4, South Africa 2, Switzerland 1, Spain 1, Sweden 1, USA 2.

Topics of the scientific program:

A. Electron, molecular and crystal structures.

B. Solution and solid state reactivity.

C. Applied inorganic and coordination chemistry.

D. Complexes in the human medicine and in the environment.

The main plenary lectures (45 min) were delivered by invited lecturers *M. Yamashita* (Sendai, Japan, topic A), *B. Sieklucka* (Kraków, Poland, topic B), *M. R. Sundberg* (Helsinki, Finland, topic C), *M. Nakamura* (Funabashi, Japan, topic D).

Eighteen plenary lectures (30 min) were presented in topic A by *K. Hegetschweiler* (Saarbrücken, Germany), *M. Melník* (Bratislava, Slovakia), *J. B. Baruah* (Guwahati, India), *M. Meuwly* (Basel, Switzerland), in topic B by *W. Ziemkowska* (Warsaw, Poland), *T. Szabó-Plánka* (Szeged, Hungary), *H. Nakazawa* (Osaka, Japan), *M. Mikuriya* (Sanda, Japan),

J. Kaizer (Veszprém, Hungary), A. K. Boudalis (Aghia Paraskevi Attikis, Greece), in topic C by R. Boča (Bratislava, Slovakia), R. Réau (Rennes Cedex, France), R. Murugavel (Mumbai, India), in topic D by M. Tacke (Dublin, Ireland), T. Shimizu (Sendai, Japan), B. Gyurcsik (Szeged, Hungary), J. Darkwa (Johannesburg, South Africa), D. C. Crans (Colorado, USA).

Fifty section lectures (15 min) were presented and 16 contributions were presented by posters. Young scientists presented 22 lectures (10 min) in young scientists session.

Abstracts of papers are published in the Book of Abstracts. Reviewed full papers are published in CD-monograph *Insights into Coordination, Bioinorganic, and Applied Inorganic Chemistry* (Editors M. Melník, J. Šima, and M. Tatarko, Press of Slovak University of Technology, Bratislava 2009, 451 pp.). CD-monograph. ISBN 978-80-227-3085-3, ISSN 1335-308X.

23rd International Conference on Coordination and Bioinorganic Chemistry – 2011

The 23rd International Conference on Coordination and Bioinorganic Chemistry organized by the Slovak Chemical Society, Slovak Academy of Sciences, Slovak University of Technology in Bratislava, and Alexander Dubček University in Trenčín was held in Smolenice Castle on June 5 – 10, 2011 and was entitled "**New Trends in Coordination, Bioinorganic, and Applied Inorganic Chemistry**". Chairman of the Organizing Committee: M. Melník.

The conference was attended by 101 participants from abroad, 46 from Slovakia, from 29 countries, first time including China and Singapore.

The conference was attended by 145 active participants from 33 countries: Argentina 1, Australia 1, Belarus 2, Bulgaria 1, Czech Republic 4, Denmark 1, Egypt 1, Finland 1, France 6, Germany 9, Greece 2, Hong Kong 1, Hungary 13, India 2, Indonesia 2, Ireland 1, Italy 3, Japan 10, Palestine 1, Poland 15, Portugal 1, Russia 4, Slovakia 42, South Africa 2, Spain 2, Switzerland 2, Taiwan 2, The Netherlands 1, Turkey 3, UK 1, Ukraine 2, Uruguay 2, USA 4.

Scientific program was focused on topics:

A. Electron, molecular and crystal structure (guaranteed by D. Reinen, Germany).

B. Reactivity in solution and in solid state (guaranteed by J. Mroziński, Poland).

C. Applied inorganic and coordination chemistry (guaranteed E. C. Constable, Switzerland).

D. Complexes in the human medicine and in the environment (guaranteed by J. Reedijk, Netherlands).

The main plenary lectures (45 min) were delivered by invited lecturers D. Reinen (Germany), J. Mroziński (Poland), E. C. Constable (Switzerland), and J. Reedijk (Netherlands).

Twenty plenary lectures (30 min) were presented in topic A by M. Nakamura (Japan), and M. R. Sundberg (Finland), in topic B by F. Mohr (Germany), K. Hegetschweiler (Germany), R. Boča (Slovakia), N. V. Nagy (Hungary), I. Hoskovicová (Czech Republic), J. Kaizer (Hungary), in topic C by M. Knorr (France), B. Zümreoglu-Karan (Turkey), N. Gerasimchuk (USA), L. Spiccia (Australia), F. Nief (France), J. Darkwa (South Africa), in topic D by S. I. Chan (Taiwan), M. Tacke (Ireland), B. Therrien (Switzerland), L. Mishra (India), S. Dasgupta (India), W. K. Wong (Hong Kong). Fifty-four section lectures (15 min) were presented and 22 contributions were presented by posters. Young scientists presented 41 lectures (10 min) in young scientists session.

The abstracts are published in the Book of Abstracts and reviewed papers in the CD-monograph *New Trends in Coordination, Bioinorganic, and Applied Inorganic Chemistry* (Editors M. Melník P. Segl'a and M. Tatarko, Slovak University of Technology Press, Bratislava 2011, 614 pp.). CD-monograph. ISBN 978-80-227-3509-4, ISSN 1335-308X.

(See also Melník, M., Segl'a, P.: Medzinárodná konferencia o koordinačnej a bioanorganickej chémii. *ChemZi* 7/13, 21 (2011)).

24th International Conference on Coordination and Bioinorganic Chemistry – 2013

The 24th International Conference on Coordination and Bioinorganic Chemistry (ICCBIC) organized by the Slovak Chemical Society, Slovak Technical University, Slovak Academy of Sciences in Bratislava and Alexander Dubček University in Trenčín was held in Smolenice Castle on June 2 – 7, 2013 and was entitled "**Recent Developments in Coordination, Bioinorganic, and Applied Inorganic Chemistry**". Chairman of the Organizing Committee: M. Melník.

The conference was attended, until now, by the highest number of participants – 173 scientists from 28 countries: Argentina 2, Belarus 1, Bulgaria 3, China 3, Czech Republic 4, Denmark 1, Egypt 1, France 4, Germany 5, Greece 2, Hungary 17, India 2, Iran 1, Israel 2, Japan 11, Poland 27, Romania 3, Russia 15, Saudi Arabia 1, Singapore 1, Slovakia 43, South Africa 3, Tunisia 3, Turkey 4, UK 1, Ukraine 2, Uruguay 1, USA 10.

Scientific program was focused on following topics:

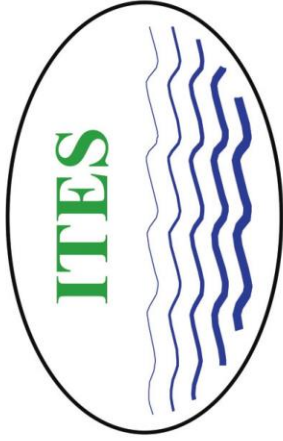
- A. Electron, molecular and crystal structure (guaranteed by N. Kojima, Japan).
- B. Reactivity in solution and in solid state (guaranteed by A. Ozarowski, USA).
- C. Applied inorganic and coordination chemistry (guaranteed by L. Brammer, UK).
- D. Complexes in the human medicine and in the environment (guaranteed by E. Solomon, USA).

The main plenary lectures were delivered by invited lecturers *N. Kojima* (Japan, 45 min), *A. Ozarowski* (USA, 45 min), *L. Brammer* (UK, 45 min) and *E. I. Solomon* (USA, 60 min).

Twenty-one plenary lectures lasting 30 minutes were presented in topic A by *C. E. Schäffer* (Denmark), *C. Train* (France), *B. Tsukerblat* (Israel), *M. Verdaguer* (France), in topic B by *O. Kovalchukova* (Russia), *E. Lodyga-Chruścińska* (Poland), *M. Mikuriya* (Japan), *M. Saphier* (Israel), *E. M. Glebov* (Russia), in topic C by *W. Mori* (Japan), *H. Lang* (Germany), *W. Ziemkowska* (Poland), *M. Abe* (Japan), in topic D by *R. Boča* (Slovakia), *M. J. Maroney* (USA), *F. Mohr* (Germany), *M. O. Onani* (South Africa), *H. Ishida* (Japan), *S. M. Aldoshin* (Russia), *D. Chatterjee* (India), and *L. Rulišek* (Czech Republic). The results obtained by the participants were presented also in 59 section lectures (15 min) and 43 contributions were presented by posters. In Young Scientists Session 49 young scientists presented their results in 10 min. lectures.

The contributions are published in the Book of Abstracts and the USB-key monograph *Recent Developments in Coordination, Bioinorganic, and Applied Inorganic Chemistry*, Volume 11, Monograph series of ICCBIC Smolenice, Slovakia (Editors M. Melník P. Segl'a and M. Tatarko, Press of Slovak University of Technology, Bratislava, 2013, 502 pp.). USB-key monograph. ISBN 978-80-227-3918-4, ISSN 1335-308X.

(See also, Drábik, M.: Slovakia: From bioinorganic to solid state chemistry. *EuCheMS Newsletter*, November 2013, 4)



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