

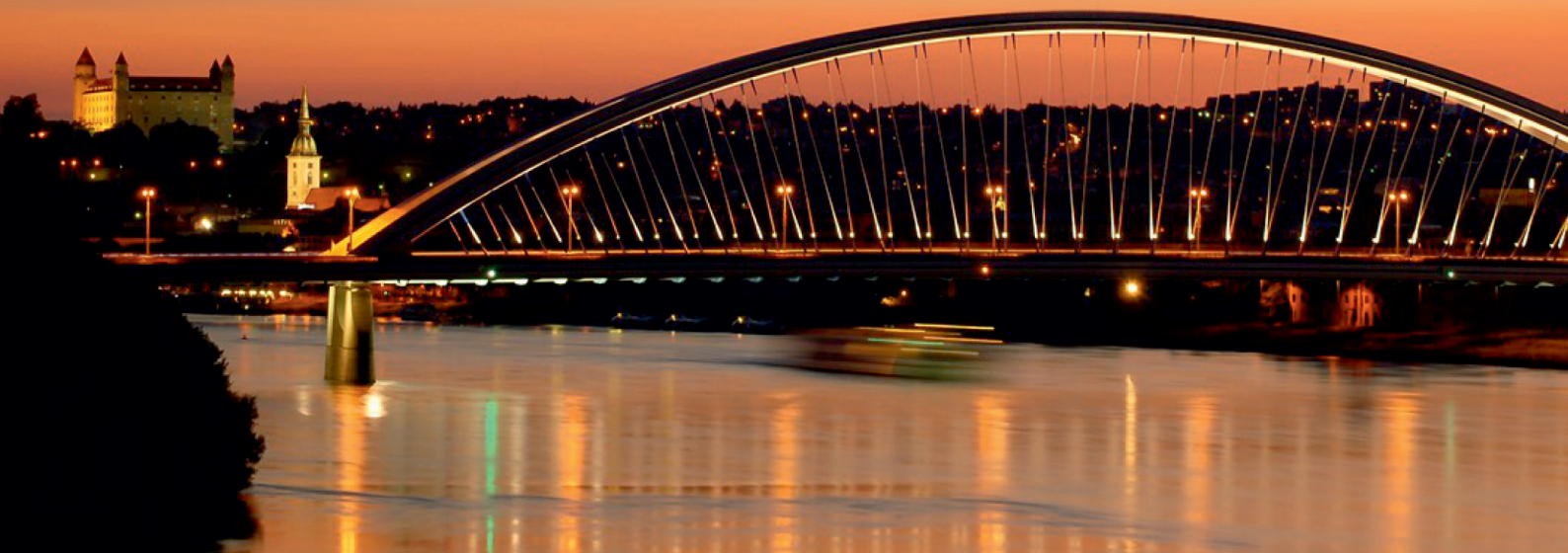


EuCOMC XXI

XXI EuCheMS
International Conference
on Organometallic Chemistry

July 5–9, 2015
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Book of Abstracts



Comenius University in Bratislava



Czech and Slovak Chemical Societies



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Click on a title to view an abstract of the oral presentation or of the poster.

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DETAILED PROGRAMME

SUNDAY JULY 5, 2015

Room: CH1 **Chairs: Martin Putala, Jan Čermák**
17:50–18:10 **Opening**

18:10–19:00 **Chair: Petr Štěpnička**
PL1: Catalytic Transformations of Alkynes
Alois Fürstner, Max-Planck-Institut für Kohlenforschung, Mülheim a. d. Ruhr, Germany

Foyer of room B1
19:00–21:30 **Welcome mixer**

MONDAY JULY 5, 2015

Room: CH1 **Chair: Manfred Bochmann**
09:00–09:50 **PL2: The functionalization of C–H bonds**
Maria Christina White, University of Illinois at Urbana-Champaign, USA

09:50–10:30 **YP1: Hydrogen Bond in Chemistry of Transition Metal Hydrides**
Oleg Filippov, Nesmeyanov Institute of Organoelement Compounds, Moscow, Russian Federation

10:30–11:00 **Coffee break**

Room: CH1 **Chair: Jun Okuda**
11:00–11:30 **KL1: TM[tzNHC] and Cobalt[Triphos] for hydrogenation of acids and esters**
Cornelis J. Elsevier, University of Amsterdam, the Netherlands

11:30–11:50 **OP01: Unsymmetrical Diborane(4) Derivatives (pinB–B((NR)₂C₆H₄)) as Versatile Precursors for Diaminoboryl Ligands**
Christian Kleeberg, Technische Universität Braunschweig, Germany

11:50–12:10 **OP03: Small molecule activation, hydrogenation and de-hydrogenation via a new mode of long-range metal ligand cooperation in novel iron PCP-pincer complexes**
Alexander Dauth, The Weizmann Institute of Science, Rehovot, Israel

12:10–12:30 **OP05: Stable N-Heterocyclic Carbenes with a 1,1'-Ferrocenediyl Backbone and Their Heavier Homologues**
Ulrich Siemeling, University of Kassel, Germany

12:30–12:50 **OP07: Compounds of Group 14 elements containing element – element bond: synthesis, structure, properties**
Kirill Zaitsev, Moscow State University, Russia

Room: B1 **Chair: Franziska Schoenebeck**
11:00–11:30 **KL 2: Frustrated Lewis Pair Chemistry with and without Metals**
Gerhard Erker, Westfäl Wilhelms University of Münster, Germany

11:30–11:50 **OP02: Density functional theory computations of the distinct mechanisms of the 1,4-shift reaction for Rh(I) and Rh(III)**
Eric A. B. Kantchev, Hefei University of Technology, China

11:50–12:10 **OP04: Structure, Bonding and Mechanism in Iron-Catalyzed Cross-Coupling**
Michael Neidig, University of Rochester, USA

12:10–12:30 **OP06: Understanding the mechanism of novel ruthenium-mediated C-H functionalization and C-F bond formation reactions**
Lucy Milner, The University of York, York, UK

12:30–12:50 **OP08: Influence of the metal center on chiroptical and photophysical properties in systems with helicene ligands – quantum-chemical perspective**
Monika Srebro, Jagiellonian University, Krakow, Poland

12:50–14:30 **Lunch**

- Room: CH1** **Chair: Maria Helena Garcia**
 14:30–15:00 **KL3: Oxidative addition of robust sigma bonds to Al(I)**
 Georgii I. Nikonov, Brock University, St. Catharines, Ontario, Canada
 15:00–15:20 **OP09: Catalysis-Relevant Au(III) Chemistry: From Au-O to Au-H, Au-R and Au-CO**
 Manfred Bochmann, University of East Anglia, Norwich, UK
 15:20–15:40 **OP11: Trapping CO₂ with Gold Complexes**
 Alba Collado-Martinez, University of St Andrews, UK
 15:40–16:00 **OP13: Cooperative Metal-Ligand Hydroamination Catalysis**
 Luis Alves, Universidade de Lisboa, Portugal
- Room: B1** **Chair: Miquel S. Costas**
 14:30–15:00 **KL4: Recent advances in selective isomerizations**
 Clément Mazet, University of Geneva, Switzerland
 15:00–15:20 **OP10: New pathway for heterocycles synthesis: combining carbonylation and nucleophilic substitution**
 Xiao-Feng Wu, Leibniz-Institut für Katalyse e. V., Rostock, Germany
 15:20–15:40 **OP12: Gold(I) catalysed asymmetric hydroamination of alkenes: effects of silver, anion and solvent on the catalyst**
 Christophe Michon, CNRS–University of Lille Nord de France, Villeneuve d'Ascq, France
 15:40–16:00 **OP14: Transition-metal catalyzed reactions that form bonds to phosphorous**
 Rory Waterman, University of Vermont, Burlington, USA
- 16:00–16:30 **Coffee break**
- Room: CH1** **Chair: Elena Shubina**
 16:30–16:50 **OP15: Two-Coordinated First-Row Transition Metal(I) Complexes [M(N(SiMe₃)₂)₂]⁻**
 C. Gunnar Werncke, CNRS Institute Laboratoire de Chimie de Coordination, Toulouse, France
 16:50–17:10 **OP17: Dialkylgallium and indium alkoxides and aryloxides with N-heterocyclic carbenes – from fundamental aspects of M–CNHC bond to stereoselective catalysts for the polymerization of rac-lactide**
 Paweł Horeglad, University of Warsaw, Warsaw, Poland
 17:10–17:30 **OP19: Reactive metal-carbon bonds in three-coordinate iron NHC complexes**
 Thomas Pugh, University of Manchester, UK
 17:30–17:50 **OP21: Aluminium-nitrogen-based active Lewis-pairs and the catalytic oligomerisation of cyanamides**
 Werner Uhl, Universität Münster, Germany
 17:50–18:10 **OP23: New reactivity patterns of gold complexes: On the importance of ligand design**
 Abderrahmane Amgoune, University Paul Sabatier-CNRS, Toulouse, France
- Room: B1** **Chair: Vladimir Dimitrov**
 16:30–16:50 **OP16: Activation of SCF₃ and SF₅ Aromatics at Rhodium Complexes**
 Thomas Braun, Humboldt University Berlin, Germany
 16:50–17:10 **OP18: Cobalt complexes as catalysts in biomass, hydrocarbon and water oxidations**
 Anthony Masters, The University of Sydney, Sydney, Australia
 17:10–17:30 **OP20: Towards room-temperature H₂ generation from C₁-molecules and H₂O**
 Martin H. G. Precht, University of Cologne, Germany
 17:30–17:50 **OP22: Coordination chemistry and catalysis inside well-defined polymeric nanoreactors**
 Rinaldo Poli, CNRS, Toulouse, France
 17:50–18:10 **OP24: Titanium catalyzed ethylene trimerization: insights on critical parameters responsible for selectivity**
 Hugo Audouin, IFP Energies nouvelles, Solaize, France
- Foyer of room B1**
 18:10–18:40 **Light refreshment**
 18:40–20:30 **Poster session 1 & beer**

TUESDAY JULY 7, 2015

- Room: CH1** **Chair: Peter Fristrup**
 09:00–09:50 **PL3: Water-soluble organometallics: dinuclear arene ruthenium complexes with anticancer properties**
 Georg Süss-Fink, Université de Neuchâtel, Switzerland
- 09:50–10:30 **YP2: Understanding and Design of Organometallic Reactivity with Experimental and Computational Tools**
 Franziska Schoenebeck, RWTH Aachen University, Germany
- 10:30–11:00 **Coffee break**
- Room: CH1** **Chair: Uwe Monkowius**
 11:00–11:30 **KL5: Ferrocene-Functionalized Rotaxane Crystals**
 Kohtaro Osakada, Tokyo Institute of Technology, Yokohama, Japan
- 11:30–11:50 **OP25: The stabilisation of highly reactive s-block complexes using sterically demanding amide ligands**
 Deborah Kays, University of Nottingham, UK
- 11:50–12:10 **OP27: Coordination Chemistry and Reactivity of Donor Functionalised Pentadienylsilanes**
 Benjamin Day, University of Manchester, UK
- 12:10–12:30 **OP29: Facile synthesis and versatile reactivity of cyclometalated Rh(I) and Ni(II) pincer complexes**
 Linda Jongbloed, University of Amsterdam, The Netherlands
- 12:30–12:50 **OP31: Dinuclear gold(I) diNHC complexes: insights on the halogen oxidative addition reaction**
 Cristina Tubaro, Università degli Studi di Padova, Italy
- Room: B1** **Chair: Rinaldo Poli**
 11:00–11:30 **KL6: Amino Triphenolates as Privileged Ligands in Catalysis**
 Giulia Licini, University of Padova, Italy
- 11:30–11:50 **OP26: C–H Activation/Functionalization Catalyzed by Simple, Well-Defined Low-Valent Cobalt Complexes**
 Brendan Fallon, Institut Parisien de Chimie Moléculaire, CNRS, Paris, France
- 11:50–12:10 **OP28: Iron and nickel complexes containing N-heterocyclic carbenes: synthesis and catalysis**
 Beatriz Royo, Universidade Nova de Lisboa, Oeiras, Portugal
- 12:10–12:30 **OP30: Backbone-decoration of imidazol-2-ylidenes by amino groups as a powerful strategy towards highly efficient NHC-catalysts**
 Vincent César, Laboratoire de Chimie de Coordination du CNRS, Toulouse, France
- 12:30–12:50 **OP32: Hydroamination Catalysis using Diolate Rare Earth Metal and Phenoxyamine Magnesium Catalysts**
 Kai Hultsch, University of Vienna, Austria
- 12:50–14:30 **Lunch**
- 14:30–21:00 **Excursions**

WEDNESDAY JULY 8, 2015

- Room: CH1** **Chair: Thibault Cantat**
09:00–09:50 **PL4: Functional Metallocenes based on Metallocenes of Iron, Cobalt and Nickel**
Ian Manners, University of Bristol, UK
- 09:50–10:30 **YP3: Development of the molybdenum-catalyzed deoxydehydration**
Peter Fristrup, Technical University of Denmark, Lyngby, Denmark
- 10:30–11:00 **Coffee break**
- Room: CH1** **Chair: Janusz Lewinski**
11:00–11:30 **KL7: Computational and experimental studies on Rh- and Ru-catalysed heterocycle formation and direct arylation**
Stuart A. MacGregor, Heriot-Watt University, Edinburgh, UK
- 11:30–11:50 **OP33: Understanding the nature of anagostic and agostic interactions – a synthesis by computation approach**
Alastair Nielson, Massey University at Auckland, New Zealand
- 11:50–12:10 **OP35: Modeling amorphous silica grafted schrock olefin metathesis catalysts**
Christophe Raynaud, Université de Montpellier, France
- 12:10–12:30 **OP37: Excited state properties of a [FeFe] hydrogenase active site models. The Time-Dependent Density Functional Theory theoretical picture**
Luca Bertini, University of Milano-Bicocca, Milan, Italy
- 12:30–12:50 **OP39: Experimental and theoretical investigations on the conditions and the mechanism of the COD-isomerization at bis(NHC) Ir(I) complexes**
Doris Kunz, Eberhard Karls Universität Tübingen, Germany
- Room: B1** **Chair: Helena Grennberg**
11:00–11:30 **KL8: Lanthanide Organometallics as Molecular Nanomagnets: Soft Ligands and Hard Magnets**
Richard A. Layfield, University of Manchester, UK
- 11:30–11:50 **OP34: Unraveling in situ the chemical structures of polyoxomolybdate based amphiphilic nano-hybrids in aqueous solutions combining ³¹P DOSY NMR and Molecular Mechanics as powerful tools**
Rudolph Willem, Vrije Universiteit Brussel, Belgium
- 11:50–12:10 **OP36: Luminescent Di- and Trinuclear Boron Complexes Based on Aromatic Iminopyrrolyl Spacer Ligands: Application in OLEDs**
Clara Gomes, Universidade de Lisboa, Lisboa, Portugal
- 12:10–12:30 **OP38: Rhodium Catalyzed P-P and P-C bond formation**
Cristina Tejel, CSIC, Zaragoza, Spain
- 12:30–12:50 **OP40: Recent Progress in Pd-SPRIX Catalyzed Enantioselective Reactions**
Hiroaki Sasai, ISIR, Osaka University, Ibaraki-shi, Japan
- 12:50–14:30 **Lunch**
- Room: CH1** **Chair: Georg Süss-Fink**
14:30–15:00 **KL9: Towards organometallic antischistosomal drug candidates**
Gilles Gasser, University of Zürich, Switzerland
- 15:00–15:20 **OP41: Metallocene β -lactam antibiotic conjugates: synthesis, antibacterial activity and mechanism of action**
Konrad Kowalski, University of Łódź, Poland
- 15:20–15:40 **OP43: Cyclopentadienyl ruthenium label for aromatic amino acids and peptides**
Dmitry Perekalin, Nesmeyanov Institute of Organoelement Compounds, Moscow, Russian Federation
- 15:40–16:00 **OP45: A new generation of antitumor organometallic compounds derived from the ferrocifen family furnishes an unprecedented class of key quinone methide metabolites**
Gérard Jaouen, Chimie ParisTech, Paris, France
- Room: B1** **Chair: Valerio Zanotti**
14:30–15:00 **KL10: Selective oxidation reactions with bioinspired catalysts**
Miquel S. Costas, University of Girona, Spain
- 15:00–15:20 **OP42: Structure-Reactivity Relationship in Bimetallic Hafnium Pyridyl-Amido Olefin Polymerization Catalysts**
Cristiano Zuccaccia, University of Perugia, Italy
- 15:20–15:40 **OP44: Stereoselective domino conjugate additions followed by reaction with carbenium ions and activated alkenes**
Radovan Šebesta, Comenius University in Bratislava, Slovakia
- 15:40–16:00 **OP46: Oxidation of Phosphasalen complexes**
Audrey Auffrant, CNRS-Ecole Polytechnique, Palaiseau, France
- Foyer of room B1**
16:00–17:30 **Poster session 2 & coffee**
- 19:00–23:00 **Conference dinner**

THURSDAY JULY 9, 2015

Room: CH1 **Chair: Clément Mazet**
09:00–09:50 **PL5: Recent progress in cooperative asymmetric catalysis**
Masakatsu Shibasaki, University of Tokyo, Tokyo, Japan

The lecture YP4 is supported by

NJC
New Journal of Chemistry

09:50–10:30 **YP4: CO₂ Conversion Using Organometallic and Organic Molecular Catalysts**
Thibault Cantat, Saclay Institute of Matter and Radiation, Iramis, CEA, Saclay, France

10:30–11:00 **Coffee break**

Room: CH1 **Chair: Jan Čermák**
11:00–11:40 **YP5: Metal-ligand synergies in early organometallics and organolanthanides for polymerization and hydroamination catalysis**

Giuliano Giambastiani, Institute of Chemistry of Organometallic Compounds, CNR, Florence, Italy

11:40–12:30 **European Prize for Organometallic Chemistry Lecture**
The occurrence of three-centre two-electron bonds in organotransition metal compounds
Malcolm L. H. Green, Oxford University, UK

12:30–13:00 **Chairs: Martin Putala, Jan Čermák, Kees Elsevier**
Awards & Closing

POSTER SESSIONS

TOPIC 1: Fundamental organometallic chemistry: synthesis, structure and reactivity

PO01: Unravelling the Mysteries of the Palladium Cluster Phase

Kate Appleby, University of York, York, UK

PO02: Synthesis of m³-Silyl Complexes of Ruthenium and Group 9 Metals and Its Transformation into m³-Silylene Complex

Masahiro Nagaoka, Graduate School of Science and Engineering, Tokyo Institute of Technology, Japan

PO03: Silylcyanocuprates: Potential Reactive Intermediates in Silylboration Reactions

Jacqueline Plotzitzka, Technische Universität Braunschweig, Germany

PO04: Photochemically Induced Activation of Tetrabutylammonium Cation by Chloroplatinate Anions

Imelda Silalahi, University of York, UK

PO05: Reactivity Studies on a Stable Dimetalloxycarbene

Albert Paparo, RWTH Aachen University, Germany

PO06: Activation of Carbon-Fluorine bonds in $[\text{Os}(\text{SC}_6\text{F}_5)_4(\text{P}(\text{C}_6\text{H}_4\text{X})_3)]$ (X = CH₃, H, F) complexes by reactions with NaSH or CH₂=CH-CH=CHOLi

Maribel Arroyo, Benemérita Universidad Autónoma de Puebla, Mexico

PO07: A comparative study on the reactivity of $[\text{RuCl}_2(\text{eta}^4\text{-}1,5\text{-C}_8\text{H}_{12})(\text{CH}_3\text{CN})_2]$ with *N,N*-diethyldithiocarbamate and *O*-ethylthiocarbonate salts

Armando Ramírez-Monroy, Benemérita Universidad Autónoma de Puebla, Mexico

PO08: Laser pump-NMR probe: a new fast reaction method for hyperpolarized metal hydrides

Barbara Procacci, University of York, UK

PO09: Synthesis of carbamoyl chiral iron complexes by nucleophilic attack of primary amines

Jose Rosas-Galicia, Universidad Autónoma de Puebla, Mexico

PO10: Intriguing reactivity of a linear tetranuclear gold(I) complex

Ekaterina Smirnova, ICIQ, Tarragona, Spain

PO11: Complexation reactions with N- and P-containing ligands as a way to high cluster cage Cu(II)-silsesquioxanes. Active media principle.

Alexey Bilyachenko, A. N. Nesmeyanov Institute of Organoelement Compounds, Rus. Acad. Sci., Moscow, Russian Federation

PO12: 3a,6a-Diaza-1,4-diphosphapentalene – unique heteroaromatic system and ligand of a new type demonstrating $\kappa(\text{P})\text{-}\pi$ complexation with metals

Alexander Kornev, G.A. Razuvaev Institute of Organometallic Chemistry, Rus. Acad. Sci., Nizhny Novgorod, Russian Federation

PO13: Outer Sphere Electrophilic Fluorination of Organometallic Fragments

John Slattery, University of York, UK

PO14: New nido-carborane derivatives and their metallocplexes

Vladimir Bregadze, A. N. Nesmeyanov Institute of Organoelement Compounds, Rus. Acad. Sci., Moscow, Russian Federation

PO15: Intramolecular hydrosilylation in 2-iminopyrrole derivatives

Marc-Etienne Moret, Utrecht University, Netherlands

PO16: Insertion and Coupling Processes in the Reactions of the Electron-Deficient Hydride $[\text{W}_2\text{Cp}_2(\text{H})(\mu\text{-PCy}_2)(\text{CO})_2]$ with Unsaturated Organic Molecules

Daniel Garcia-Vivo, Universidad de Oviedo, Spain

PO17: C–H functionalization of fluoroaromatics at palladium

Jessica Milani, University of York, UK

PO18: Dinuclear organometallic Pd(II) complexes with iminopyridines: the importance of methyl groups

Barbara Milani, University of Trieste, Italy

PO19: Multinuclear Calcium Complexes of Schiff-Base Calixpyrroles

Emma Connolly, University of Edinburgh, UK

PO20: Small Molecule Activation Chemistry Using Low-Coordinate Transition Metal Terphenyl Complexes

Deborah Kays, University of Nottingham, UK

PO21: Molecular ions of difficult reactive samples instantly confirming the synthesis

Mathias Linden, Linden CMS GmbH, Weyhe, Germany

PO22: The road less travelled? How solvents are involved during methyl migration in rhodium(III) cupferrate complexes

Johan Venter, University of the Free State, Bloemfontein, South Africa

PO23: Synthesis, Reactivity and Characterization of the Novel Stannaboroxines with SnB₂O₃ Core Containing N,C,N or C,N ligand

Barbora Mairychova, University of Pardubice, Czech Republic

PO24: Oxidative addition between [Ir(cod)(sacac)] and CH₃I: A mechanistic study

Walter Purcell, University of the Free State, Bloemfontein, South Africa

PO25: Silver, Mercury and Ruthenium Complexes of N-Heterocyclic Carbenes: Synthesis, Structure, and antibacterial studies

Rosenani A. Haque, University Sains Malaysia, Minden, Malaysia

PO26: Organofullerene metallic complexes from fullerene C₆₀

Adriana Hernández Calva, Universidad Autónoma de Puebla, Mexico

PO27: Synthesis and Reactivity of Heterometallic Complexes with Mo-Mn Bonds.

Estefania Huergo Iglesias, University of Oviedo, Spain

PO28: Reactivity of a nucleophilic pyramidal phosphinidene complex with organic azides

Isabel Gonzalez Albuérne, University of Oviedo, Spain

PO29: Iridium complexes with PCP pincer ligand: reactivity toward acids and bases

Ekaterina Kozinets, A. N. Nesmeyanov Institute of Organoelement Compounds, Rus. Acad. Sci., Moscow, Russian Federation

PO30: Platinum-Silicon Triple Bonds: The Tetrahedral Platinum Silylidyne Complex Cation [(PMe₃)₃Pt=Si(Tbb)]⁺

Ioannis Papazoglou, University of Bonn, Germany

PO31: Ruthenaphosphaalkenyls: Synthesis, structures and their conversion to η²-phosphaalkene complexes

Victoria Greenacre, University of Sussex, Brighton, UK

PO32: Low-valent derivatives of the Group 14 elements based on polydentate ligands

Badma Mankaev, Lomonosov Moscow State University, Russian Federation

PO33: New polymorph of [RuCl(PPh₃)₂(η⁵-C₅H₅)] complex – synthesis, X-ray crystal structure and electrochemical properties

Elena Gorbachuk, Kazan Federal University, Russian Federation

PO34: Synthesis of an Iridium Tetrafluoropyridyl Peroxido Complex and its Reactivity towards Brønsted Acids

Hanna Baumgarth, Humboldt-Universität zu Berlin, Germany

PO35: Base metal complexes of a diphosphine-ketone ligand: toward new bifunctional catalysts

Dide Verhoeven, Utrecht University, Netherlands

PO36: Thiazole containing amidopyridinate organolanthanides: synthesis and catalytic activity in the intramolecular hydroamination and isoprene polymerization

Lapo Luconi, ICCOM-CNR, Sesto Fiorentino, Italy

PO37: Huge temperature dependence of the metal-metal distances in cationic coinage metal complexes bearing N-heterocyclic carbenes

Uwe Monkowius, Johannes Kepler University Linz, Austria

PO38: Coinage metal complexes of a hybrid phosphine-phosphine oxide ligand

Thuy Minh Dau, University of Eastern Finland, Joensuu, Finland

PO39: Organometallic syntheses by computation: Si-H⋯M and C-H⋯M interactions

Alastair Nielson, Massey University at Auckland, New Zealand

PO40: Highly strained small phosphorus containing rings

Martha Höhne, Leibniz Institut für Katalyse, Rostock, Germany

PO41: Mixed amido-cyclopentadienyl group 4 metal complexes

Michal Horáček, J. Heyrovský Institute of Physical Chemistry, Czech Acad. Sci., Prague, Czech Republic

PO42: Redox promoted cyclometalation reactions of platinum(0) complexes

Thibault Troadec, University of Warwick, Coventry, UK

PO43: Metal Organic Frameworks (MOFs) composite materials with polymer or ceramic base

Bozena Sartowska, Institute of Nuclear Chemistry and Technology, Warsaw, Poland

PO44: B-H activation reactions of Titanium compounds

Simona Mellino, University of Oxford, UK

PO45: Solid-Phase Activation of the X–H bond (X = C, N, O): Simple and Efficient Route to Pincer-Type and Related Metal Complexes

Diana Aleksanyan, A. N. Nesmeyanov Institute of Organoelement Compounds, Rus. Acad. Sci., Moscow, Russian Federation

PO46: Synthesis and catalytic activity of new ethynylsubstituted silsesquioxanes

Beata Dudziec, A. Mickiewicz University in Poznan, Poland

PO47: Consideration of time-resolved infrared absorption spectrum observed in the coordination of small molecules on coordinatively unsaturated transition metal carbonyls in the gas phase with DFT calculation

Yo-ichi Ishikawa, Kyoto Institute of Technology, Japan

PO48: Hexaorganotin(IV) Compounds

Ireen Schrader, Leipzig University, Germany

PO49: Low-coordinate transition metal complexes with anionic bidentate NHC ligands: structure and reactivity

Mikko Hänninen, University of Jyväskylä, Finland

PO50: Metallocene Complexes with Pendant Imine Moieties: Coordination and Functional-Group Transformations

Martin Lamač, J. Heyrovský Institute of Physical Chemistry, Czech Acad. Sci., Prague, Czech Republic

PO51: Optimization in the Synthesis and Synthesis of new Bisimidazolium Salt Ligands

A.-Theresa Schmidt, University Tübingen, Institut of Inorganic Chemistry, Tübingen, Germany

PO52: eNHChanting new chemistry with Cu and Zn

Lee Collins, University of Bath, UK

PO53: Synthesis and Characterization of Novel Aluminium and Silicon Complexes Utilizing a Phosphatriafulvene Ligand

Shuhei Ozaki, Institut für Chemie, Technische Universität Berlin, Germany

PO54: Assessing the redox non-innocent character of 4,5-bis(dimethylamino)imidazol-2-ylidene ligand

Mirko Ruamps, Laboratoire de chimie de coordination CNRS, Toulouse, France

PO55: Synthesis, Computational and Application Studies of Group VI and VII Multimetal Carbene Complexes

Roan Fraser, University of Petoria, South Africa

PO56: Synthesis, Characterization, and Electrochemical properties of novel Ni(II) and other metal-NHC complexes

Frederick Malan, University of Petoria, South Africa

PO57: Oxidative addition of HCl to dinuclear gold(I) diNHC complexes

Marco Baron, Università degli Studi di Padova, Italy

PO58: Structure and Vibrational Circular Dichroism (VCD) of luminescent chiral Ir(III) complexes

Marco Fusè, Università di Milano, Italy

PO59: Synthesis and Reactivity of the Unsaturated Dinitrosyl Hydride Complex $[W_2Cp_2(m-H)(m-PPh_2)(NO)_2]$

Adrián Toyos Martín, Universidad de Oviedo, Spain

PO60: New multidentate macrocyclic ligands containing Se/S/N donor atoms and their late d-metal complexes

Alexandra Pop, Babes-Bolyai University, Cluj Napoca, Romania

PO61: New organoselenium(II) compounds with potential biological activity

Roxana Popa, Babes-Bolyai University, Cluj-Napoca, Romania

PO62: Neutral and cationic aluminium alkyl and hydride complexes supported by an *N,N,N,N*-type macrocyclic ligand: synthesis, characterization and reactivity

Debabrata Mukherjee, RWTH University, Aachen, Germany

PO63: Hydrogen Bonding to Transition Elements: A Tale of Two (Isoelectronic) Metal Fragments

Miguel Baya, Universidad de Zaragoza, Spain

TOPIC 2: Computational and mechanistic studies on organometallic compounds and their transformations**PO64: Enantioselective Arylation of N-Tosyl-Imines by Phenylboronic Acid Catalyzed by a Rhodium/Diene Complex: Reaction Mechanism from Density Functional Theory**

Nicolas Sieffert, Université Grenoble Alpes, CNRS, France

PO65: Intra- vs intermolecular metal-ligand interactions determining structure and reactivity of PC(sp³)P pincer iridium hydride complexes

Natalia Belkova, A.N.Nesmeyanov Institute of Organoelement Compounds, Rus. Acad. Sci., Moscow, Russian Federation

PO66: Hydrogen bonding to transition metal coordinated boron hydrides and amine boranes – a way of deeper E-H bond activation

Elena Shubina, A.N. Nesmeyanov Institute of Organoelement Compounds, Rus. Acad. Sci., Moscow, Russian Federation

PO67: DFT Investigations and Improvements of Methyl Methacrylate Formation with Homogenous Pd(P,N) Complexes

Luke Crawford, University of St. Andrews, UK

PO68: Mechanistic studies of Heck-Matsuda reaction of 3-cyclopenten-1-ol: origins of the 4-arylcyclopentanone byproduct

Juliana Manso de Oliveira Silva, State University of Campinas, Brazil

PO69: Bimetallic Chromium Catalyst with Flexible Bridging Ligand for Ethylene Tetramerization: Density Functional Theory Study

Minserk Cheong, Kyung Hee University, Seoul, Korea

PO70: A Synthesis, Catalytic Application and Theoretical Investigation into N·CN, SCN and PCN Pincer Palladacycles

Gavin Roffe, University of Sussex, Brighton, UK

PO71: Broadening the scope in the characterization of N-heterocyclic copper (I) complexes

Ricky Payen, Université Catholique de Louvain, Louvain-la-Neuve, Belgium

PO72: Salient Role of AlEt₃ in the Allene Carboxylation Reaction - A DFT Study

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