

CulturChem 406

2015-2016

September

Wednesday Sept 2nd
Auditorium Herpin 15h

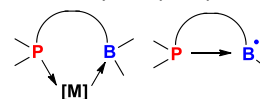


01

Dr. **Ghenwa Bouhadir** (LHFA, Université Paul Sabatier, Toulouse)
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From unusual ligands to stabilization of highly reactive species

Abstract. A quick overview of coordination chemistry of phosphine boranes (PB) will be presented. The behaviour of PB as bifunctional organo-catalysts will be briefly discussed. Finally the preparation, structure and reactivity of "stabilized highly reactive molecules" derived from PB will be discussed.



Monday Sept. 14th
Auditorium Astier 11h



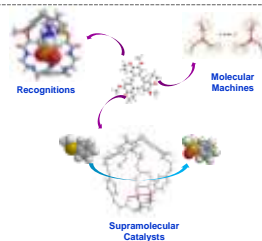
02

Prof. **Alexandre Martinez** (iSm2, Aix-Marseille Université)
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New Aspects of the Chemistry of Hemicryptophanes : From Molecular Recognitions to Supramolecular Catalysis

Abstract. Hemicryptophanes are host molecules combining a CTV (cyclotrimeratrylene) unit and another unit of C_3 symmetry. Although the first hemicryptophane was synthesized in 1982 by André Collet et Jean-Marie Lehn,¹ this cage molecule has received little attention during the twenty years following this first promising result. Nevertheless, since 2005 new aspects of their chemistry are developed as their use as (i) molecular receptors of carbohydrates or neurotransmitters,² (ii) molecular machines³ and (iii) supramolecular catalyst.⁴

[1] Canceill, J. et al. *Helv. Chim. Acta* **1982**, *65*, 1894-1897. [2] *Angew. Chem. Int. Ed.* **2012**, *51*, 504-508. [3] *J. Am. Chem. Soc.*, **2010**, *132*, 16733-16734. [4] A. Martinez *Chem. Comm.* **2013**, *49*, 1288-1290.



Monday Sept 21st
Auditorium Astier 11h



03

Prof. **Peter Zhang** (Boston College)

peter.zhang@bc.edu

Metalloradical Catalysis for Homolytic Radical Chemistry

Abstract. Organic synthesis has been dominated by chemical reactions that are based on two-electron ionic processes, either stoichiometrically or in catalytic fashion. While one-electron radical chemistry is equally rich, its application in organic synthesis has been hampered by several enduring challenges. Over the past decade, we have been in the process of formulating "Metalloradical Catalysis" (MRC) as a general concept to develop fundamentally new approaches for controlling both reactivity and stereoselectivity of radical reactions as well as for catalytic generation of carbon-, and nitrogen-based radicals from common organic precursors. For achieving enantioselective radical reactions via MRC, we have developed a family of unique chiral metalloradical catalysts based on structurally well-defined Co(II) complexes of D_2 -symmetric chiral porphyrins with tunable electronic, steric, and chiral environments.

Friday Sept 25nd
24-34, salle 307, 11h



04

Pr **Clémence Corminboeuf** (Ecole Polytechnique Fédérale de Lausanne)

<http://lcmd.epfl.ch>

Putting Forward Replica Exchange Molecular Dynamics and Volcano Plots as New Tools for Computational Homogenous Catalysis

Abstract. In computational organic chemistry, reaction profiles are generally cartooned as a series of static geometries representing the reactants, intermediates, and products, as well as their associated transition states. Fast electronic structure approaches that allow exploration of reactions beyond a static picture will first be explored. Afterwards, the usefulness of volcano plots for identifying attractive homogeneous catalysis and providing a more general picture of catalyst performance using the Suzuki reaction as a proof-of-principle example will be shown.

Monday Sept 28th
Auditorium Astier 11h



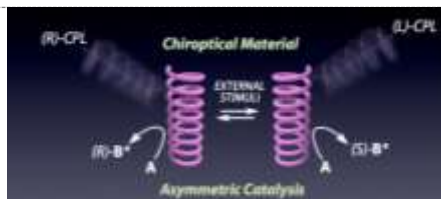
05

Prof. **Michinori Suginome** (Kyoto University, Japan)

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New Catalytic Borylations

Abstract. Transition-metal-catalyzed and organocatalytic asymmetric reactions proceeded with high enantioselectivities using polymer-based chiral catalysts whose chiral reaction environment relies on the single-handed helical structure of poly(quinoxaline-2,3-diyl)s. The enantioselection of the reactions is switched by inverting the helical sense of the ligands by external stimuli such as solvent effect and temperature change. A possibility of further applications of the screw-sense-switchable polyquinoxalines in chiroptical materials shall also be discussed.



October

Monday Oct 5th
Auditorium Astier 11h



06

Prof. Luca Banfi (Genova University)

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Coupling biocatalysis and organocatalysis with isocyanide-based multicomponent reactions

Abstract. Isocyanide-based multicomponent reactions (e.g. Ugi and Passerini reactions) represent a very useful tool for the fast generation of libraries of drug-like substances. However, stereochemical control is still an important and mostly unsolved issue. In this lecture I will describe an approach based on the biocatalytic or organocatalytic generation of chiral inputs and on their use in diastereoselective multicomponent reactions with isocyanides.

Monday Oct 12th
Auditorium Astier 11h



07

Prof. Nils Metzler-Nolte (Ruhr University Bochum, Germany)

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Biorganometallic Chemistry: Synthetic Strategies and Biomedical Applications for Metal-Peptide Bioconjugates

Abstract. In this presentation, I will highlight various synthetic strategies to obtain bioactive metal-peptide bioconjugates that have been developed in our group, and I will present some exemplary biomedical applications of such metal-peptide conjugates. Potent novel anticancer agents based on a number of different metals such as Fe, Ru, Re, and Au were developed, characterized and tested for their antiproliferative activity. I will also present novel organometallic-peptide conjugates with very potent antibacterial activities that even surpass that of a last-resort antibiotic, vancomycin. As a promising outlook towards clinical applications, these conjugates can be optimized to have little toxicity against human cells and low hemolytic potential.

Monday Oct 19th

Presentation platforms IPCM

Monday Oct 26th
Auditorium Astier 11h



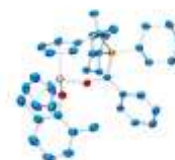
08

Dr. Pierre Le Gendre (ICMUB, Université de Bourgogne)

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Titane, zirconium et phosphore: de la catalyse aux Paires de Lewis Frustrées organométalliques (omFLPs)

Abstract. La catalyse d'hydrophosphination de diènes par des complexes de titane de basse valence sera présentée. Nous verrons que les titanocényles phosphines sont des précurseurs de catalyseur particulièrement efficaces. Ces phosphines organométalliques nous ont également permis de développer de nouvelles voies d'accès à des Paires de Lewis Frustrées Organométalliques (omFLPs). Nous présenterons la réactivité de ces omFLPs vis-à-vis de substrats modèles et nous montrerons leur potentiel en catalyse.



Novembre

Monday Nov 2nd
Auditorium Astier 11h



09

Prof. Dr. **Martin Oestreich** (Technische Universität Berlin)
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Synthetic Chemistry with Unconventional Silicon Compounds

Abstract. This talk tells how our work on tamed silicon cations led us to introduce the new concept of transfer hydrosilylation, even with monosilane! $B(C_6F_5)_3$ catalyzes the release of hydrosilanes from cyclohexa-2,5-dien-1-yl-substituted silanes. The same catalyst will then activate the Si-H bond for the reaction with representative π - and σ -donating substrates. The net transformation is a transfer hydrosilylation. The same approach is also applicable to cyclohexa-1,4-dienes, thereby enabling the Lewis acid-catalyzed transfer hydrogenation of the aforementioned unsaturated substrates. The catalytic generation of silicenium and borenium ions by cooperative Si-H and B-H bond activation will also be presented, including a mechanistic analysis of the heterolytic Si-H bond cleavage. The new catalytic entry into these main-group electrophiles is of broad synthetic utility as highlighted by electrophilic C-H bond silylation and borylation reactions as well as partial heterocycle reduction.

Friday Nov 6th
Auditorium F2 10h



10

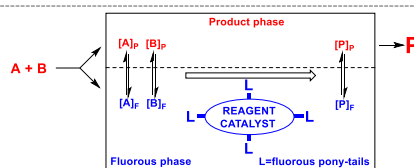
CulturChem Special Edition: Symposium on "Green Chemistry

Prof. **István T. Horváth** (City University of Hong Kong)

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Designer Fluorous Ponytails for Sustainable Fluorous Chemistry

Abstract. Fluorous chemistry was based on the attachment of fluorous ponytails to reagents and catalysts in appropriate size and numbers. The preferred size was in the range of C_6 - C_{12} perfluoroalkyl-chains to achieve efficient reagent or catalyst recycling. Compounds with C_6 - C_{12} fluorous ponytails could form C_6 - C_{12} perfluoroalkyl acids in the environment, which are persistent, toxic, and have long half-lives in humans. The combination of C_1 - C_4 -perfluoroalkyl-groups could limit accumulation and ensure facile separation. We have used perfluoro-*t*-butyl, perfluoro-*n*-butyl, and perfluoro-*n*-propyl groups to synthesize novel fluorous solvents, ligands and catalysts.



Auditorium F2 11h



11

Prof. **Chulbom Lee** (Seoul National University)

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Catalytic Use of Alkynes and Organohalides in Organic Synthesis

Abstract. Our lab has been interested in C-C and C-heteroatom bond formations based on the catalytic mechanisms involving transition metal vinylidene and radical species. While an array of methods have been developed that functionalize alkynes through cycloisomerization, addition-cyclization, alkylative cyclization, and oxidative addition reactions, studies on visible light photoredox catalysis have also led to the discovery of efficient C-C and C-N bond-forming reactions. Described in this talk will be the design, implementation and mechanistic studies of these catalytic processes and how these methods are applied to complex organic synthesis.

Monday Nov 9th
Auditorium Astier 11h



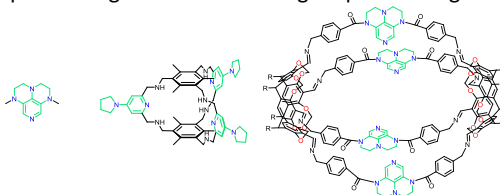
12

Dr. Olivier DAVID (Université de Versailles SQY)

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Super-Nucléophiles en Organocatalyse

Abstract. L'activation par les bases de Lewis pour déclencher des processus catalytiques sera présentée, en détaillant les aspects de chimie-physique. L'organocatalyse par des cages moléculaires organiques sera également abordée.



Monday Nov 16th
Auditorium Astier 11h



13

Michael Smietana (Université de Montpellier)

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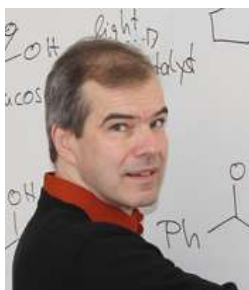
Boron-Based Nucleic Acids: From Self-Assembly to Single Point Mutations Detection

Abstract. Synthetic nucleic acids containing a backbone-, a base- or a sugar modification are very attractive for therapeutic, diagnostic or prebiotic applications. In the laboratory, we developed a new templated system allowing the reversible formation of boronate internucleosidic linkages in enzyme-free and activator-free conditions. The concept was applied to DNA- and RNA-templated ligation and oligomerization systems and proved to be capable of being active by external stimuli (T, pH, anions). To fully exploit the biological potential of boron-based nucleic acids we recently evaluated their resistance to nuclease degradation. This study eventually led us to develop a new label-free enzyme assisted fluorescence-based method for single nucleotide polymorphism detection. We will present the results of our efforts.

Monday Nov 23rd

Off

Monday Nov 30th
Auditorium Astier 11h



14

Prof. Oliver Reiser (University of Regensburg, Germany)

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Visible light photoredox catalyzed processes for carbon-carbon bond forming reactions

Abstract. New carbon-carbon bond forming processes mediated by visible light photoredox catalysis will be presented, aiming at the sustainable synthesis of natural products and analogs. A special focus will be put on copper(I)-photocatalyst, which offer unique features beyond acting as electron transfer reagents.

Leading references: D. B. Bagal, G. Kachkovskiy, M. Knorn, T. Rawnner, B. M. Bhanage, O. Reiser, *Angew. Chem. Int. Ed.* **2015**, *54*, 6999; M. Knorn, T. Rawnner, R. Czerwieniec, O. Reiser, *ACS Catal.* **2015**, *5*, 5186; D. Rackl, P. Kreitmeier, O. Reiser, *Green Chem.* **2015**, Early View; doi: 10.1039/C5GC01792K

Decembre

Monday Dec 7th
Auditorium Astier 11h



Dr. **Corinne Gosmini** (LCM - Ecole Polytechnique- Palaiseau)
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Cobalt catalyzed alkylation and arylation

Abstract. Various cobalt-catalyzed coupling of aryl or alkyl compounds with different organic compounds will be presented. This metal, which is cheap and eco-compatible, is booming since it represents an excellent alternative to other metals frequently used. These couplings are achieved under mild reaction conditions via a stoichiometric organozinc or via a catalytic organocobalt species. This more original last recent method precludes the generation of an organometallic reagent. Then, these two different processes allow the synthesis of a broad functionalized substrate scope in good yields.

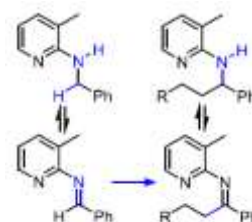
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Monday Dec 14th
Auditorium Astier 11h



Prof. **Michael Schnürch** (TU Wien)
michael.schnuerch@tuwien.ac.at
Mechanistic Investigations and Kinetic Modelling of the Direct Alkylation of Benzylic Amines

Abstract. A Rh(I)-catalyzed direct C-H alkylation of benzylic amines with alkenes co-catalyzed by K_2CO_3 was studied as a benchmark reaction to gain insight into the main kinetic influence factors associated with heterogeneous bases in metal-catalyzed reactions and to elucidate one of the associated underlying reaction mechanisms. Even though formally an $C(sp^3)$ -H activation, this reaction actually proceeds via imine intermediates and, hence, via $C(sp^2)$ -H activation.



16

Janvier

Monday Jan 18th
Auditorium Herpin 11h



Dr Vincent Coeffard (Institut Lavoisier Versailles)

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*L'Aminocatalyse au Service de la Synthèse Asymétrique
d'Architectures Cycliques Fonctionnalisées*

Abstract. L'aminocatalyse asymétrique a connu un essor considérable au cours des quinze dernières années et est devenue une méthode incontournable pour la fonctionnalisation de composés carbonyles grâce à l'émergence de divers modes d'activation. A travers quelques exemples, nous illustrerons le potentiel synthétique offert par l'aminocatalyse pour accéder à des architectures polycycliques carbonées et des hétérocycles azotés. Les séquences monotopes présentées au cours de ce séminaire montreront également la possibilité de combiner l'aminocatalyse avec d'autres types de catalyse (métallocatalyse ou photocatalyse).

17

Monday Jan 25th
Auditorium Herpin 11h



Jeroen Codée - Leiden University

jcodee@chem.leidenuniv.nl

*Stereoselective synthesis of bacterial oligosaccharides: from
mechanistic curiosity to biosynthesis probes*

Abstract. Bacterial polysaccharides often contain rare monosaccharide constituents, featuring an unorthodox substitution pattern and uncommon functional groups. As a result the synthesis of these oligosaccharides, required to study their role in biology and immunology, is full of surprises. This lecture will present our work on the *Pseudomonas aeruginosa* exo-polysaccharide alginate. The total synthesis of well-defined oligosaccharide structures of this polysaccharide, with all surprises encountered, will be described, as well as the use of these molecules to understand the bacterial biosynthesis machinery.

18

Février

Monday Feb. 1st
Auditorium Herpin 11h



Prof. J. A. Gareth WILLIAMS (Durham University, U.K.)

j.a.g.williams@durham.ac.uk

*The Luminescent Metal Complexes with N[^]C[^]N-coordinating Ligands:
From Organic LEDs to the Inside of the Living Cell*

Abstract. This multidisciplinary lecture will describe our work on the optimisation of the luminescence properties of platinum(II), iridium(III) and rhodium(III) complexes. The use of tridentate ligands may offer advantages over more commonly used bidentate analogues, owing to greater rigidity reducing excited-state distortion. Strategies for the synthesis of the ligands using metal-catalysed reactions will be described, together with methods of complex formation. The performance of the complexes as phosphors in OLEDs and as time-resolvable bio-imaging agents will be discussed.

19

Feb 8-9, Journées Bibliographiques de l'Ecole Doctorale,

Main speakers : Peter Chen (ETH Zürich), Stéphane Vincent (Univ. Namur), Frédéric Coutrot (Univ. Montpellier), Olivier Maury (ENS Lyon)

Monday Feb. 15th
Auditorium Herpin 11h



Prof. Derek A. Pratt (University of Ottawa)

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*Radical-Trapping Antioxidant Chemistry:
New Molecules & New Mechanisms*

Abstract. Hydrocarbon autoxidation continues to challenge the longevity of living organisms and petroleum-derived products. The most important strategy in slowing this process is via the intervention of radical-trapping antioxidants,¹ which are abundant in Nature and included as additives to almost every petroleum-derived product and many other commercial products. Over the years our group has investigated the mechanisms of action of many purported antioxidants,² and have used what we have learned to develop novel compounds with increased reactivity for applications in both biological and industrial contexts.³ This presentation will describe the rationale, implementation and exciting biological and industrial implications of our most recent results.

20

Monday Feb. 22nd
Auditorium Herpin 11h



Prof. Christian Limberg (Humboldt-Universität zu Berlin)

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*The Activation of O₂ and Carbon Oxides at Metal Complexes
inspired by Enzymes and Surface*

Abstract. The talk will describe some of our recent activities in the area of small molecule activation, exemplarily for the substrates O₂, CO and CO₂. The first part will deal with O₂ activation at surface-inspired chromium(II) siloxide complexes. The second part shows an example demonstrating how O₂ activation may also be inspired by nature: the synthesis and investigation of a low-molecular weight analogue for the active site of the non-heme iron enzyme, cysteine dioxygenase, is reported. Finally, biomimetic CO activation at nickel complexes is presented, which provides valuable insights into the mechanism of the acetyl-co-enzyme A synthase, and analogous to CO-dehydrogenases nickel(0) species were also found capable of reducing CO₂ to CO.

21

Monday Feb 29th
 Auditorium Herpin 11h



Prof. Kilian Muñoz (Institute for Chemical Research of Catalonia)
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Enantioselective and Light-Induced Catalysis with Iodine(III)

Abstract. Hypervalent iodine(III) reagents of the general type ArIXY represent common synthetic tools for organic transformations. This seminar discusses recent conceptual progress addressing the quest for novel *catalytic* applications of these reagents. Specific topics include the design of asymmetric homogeneous iodine(III) catalysts for intermolecular enantioselective reaction control and their structural elucidation, and the development of conceptually novel monomeric iodine catalysis for the light-initiated functionalization of hydrocarbon sites including the investigation of the underlying mechanistic details.

22

March

Monday March 7th
Auditorium Herpin 11h



23

Maurizio Fagnoni (PhotoGreen Lab, University of Pavia, Italy)

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Photocatalytic C-H Activation by Hydrogen-Atom Transfer in Synthesis

Abstract. Various recent advancements in the field of photocatalytic hydrogen-atom transfer (HAT) processes for C-H bond functionalization will be presented. The direct HAT process promoted from the excited state of a photocatalyst is limited to the classes of polyoxometalates and aromatic ketones, but alternative photocatalytic strategies have recently been devised to alleviate this shortcoming, making use of indirect HAT reactions. The seminar will mainly focus on the use of a decatungstate based photocatalyst for the formation of C-C and C-N bonds.



Monday March 14th
Auditorium Herpin 11h



24

Paul G. Williard (Brown University, Rhode Island, USA)

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Steric Hindrance Matters

Abstract. A progression of solvation and aggregation states from trisolvated monomers through hexasolvated hexamers represented formulaically as: $(M_1A_1S_3) \leftrightarrow (M_2A_2S_2) \leftrightarrow (M_2A_2S_3) \leftrightarrow (M_2A_2S_4) \leftrightarrow (M_4A_4S_3) \leftrightarrow (M_6A_4A'_2S_4) \rightarrow (M_6A_6S_6)$ M is a group 1A metal cation such as Li, Na or K. A is an enolate or 2^o amide anion such as diisopropyl amide or hexmethylidisilazide. S is a Lewis base such as an ether, 3^o amine or phosphoramidate. These structures have been characterized in solution and by x-ray diffraction analysis in my lab. Comparison of the structural features of a sequence of homologous compounds in which the size of chemically similar substituents, A and/or S, systemically increase in size will be presented with the aim of demonstrating that the steric bulk of the components is responsible for the dominant solvation state and aggregation state of the major complex formed. A priori predictability of these latter two features for new compounds seems attainable; hence size matters.

Monday March 21st
Auditorium Herpin 11h



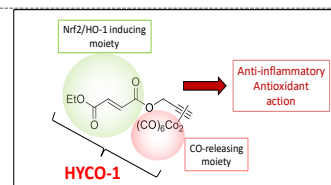
25

Roberto Motterlini (Equipe 12, INSERM U955, University Paris-Est Creteil)

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Small Molecules Targeting the Heme Oxygenase-1/Carbon Monoxide Pathway for Therapeutic Applications

Abstract. Heme oxygenase-1 (HO-1), which degrades heme to carbon monoxide (CO) and biliverdin, is an inducible cytoprotective enzyme that affords significant protection against oxidative stress and cellular injury. At molecular level, the expression of HO-1 is regulated by the redox-sensitive transcription factor Nrf2, which can be highly activated by a plethora of natural and synthetic compounds. Different strategies on how to exploit the Nrf2/HO-1 axis as a target for the development of novel anti-inflammatory and anti-ischemic agents will be presented.



Monday March 28th

Off

April

Monday April 4th
Auditorium Herpin 11h



26

Fabrice Pointillart (Institut des Sciences Chimiques de Rennes)

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Magnetism and Luminescence in Tetrathiafulvalene-Based Complexes of Lanthanides

Abstract. Lanthanide-based complexes have greatly contributed to the development of molecular magnetism in the last decade and more particularly in the branch of single molecule magnets (SMMs). In this presentation we will focus on the specific magnetic and luminescence properties of Tetrathiafulvalene(TTF)-based lanthanide complexes in which the TTF plays the roles of an antenna to sensitize the metal centred luminescence and structural agent to control the 3D assembling of the molecules. Our investigations cover the fine tune of the SMMs behaviour, luminescent SMMs and the intimate relation between magnetism and luminescence.

Monday April 11th
Auditorium Herpin 11h



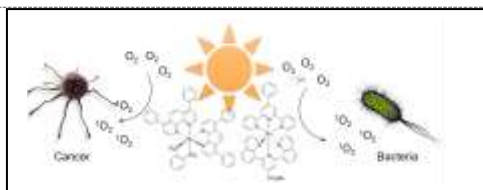
27

Gilles Gasser (University of Zurich, Switzerland)

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New Insights in the Use of Metal Complexes in Medicinal Chemistry

Abstract. Metal Complexes are currently playing a tremendous role in medicine. For instance, the Pt(II) complexes cisplatin, oxaliplatin and carboplatin are used in more than 50% of chemotherapeutic treatments.



Over the recent years, our group in Zurich has been investigating the use of Fe(II), Ru(II), Cr(0) and Re(I) complexes as drug candidates against cancer and the parasitic disease schistosomiasis. Our latest results will be presented during this talk.

Monday April 18th

Off

Monday April 25th

Off

May

Monday, May 2nd
Auditorium Astier 11h



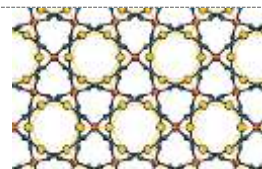
28

Daniel B. Leznoff (Simon Fraser University, Vancouver, Canada)

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Ancient Metals in Advanced Materials: Cyanoaurate-based Coordination Polymers

Abstract. My group uses non-octahedral cyanometallates to target coordination polymers with magnetic, vapochromic, birefringent, luminescent, negative-thermal expansion and other properties. In particular, neglected linear d^{10} $[\text{Au}(\text{CN})_2]^-$ units harness attractive aurophilic interactions to increase structural dimensionality. Several property-based vignettes will be presented: simple "mineral-like" $\text{M}[\text{Au}(\text{CN})_2]_2(\text{H}_2\text{O})_x$ with unusual vapochromic properties; luminescent $\text{Zn}[\text{Au}(\text{CN})_2]_2$ -based ammonia sensors and methods to prepare thin-films via rare reductive elimination of halogen from $[\text{Au}(\text{CN})_2\text{X}_2]$; and white-light emitting materials using Ln/Au and Cu/Au systems.



Monday, May 9th
Auditorium Astier 11h



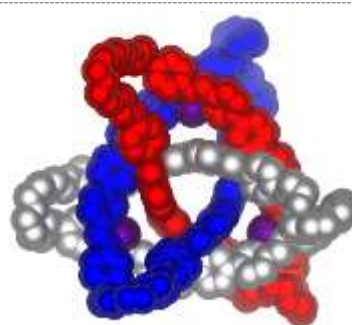
29

Jonathan R. Nitschke (University of Cambridge, UK)

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Transformative Cages and Luminous Chains: Functional Chemical Systems through Subcomponent Self-assembly

Abstract. The materials that we depend on rely upon ever-increasing structural complexity for their function. The use of chemical self-assembly as a synthetic technique can simplify materials preparation by shifting intellectual effort away from designing molecules, and towards the design of *chemical systems* that are capable of self-assembling in such a way as to express desired properties and functions. Recent examples of such systems developed in the Nitschke group will be presented, such as the [3]catenane shown at right.



Monday & Tuesday
May 23rd-24th
Auditorium Herpin

16^{ème} Journées de l'École Doctorale de Chimie Moléculaire (ED406)

Maurizio Prato
(University of Trieste, Italy)
Prix Franco-Italien SCF 2015

William Motherwell
(University College London, UK)
Prix Franco-Britannique SCF 2015

Michel Etienne
(LCC Toulouse)

Marc Robert
(Université Paris Diderot - Paris 7)

For more information, please contact: **Dr Cyril Ollivier**, UPMC, Bâtiment F, 2^{ème} étage, case 229, 4 place Jussieu, 75005 Paris. ☎ 01 44 27 38 50. 📠 01 44 27 73 60. e-mail : cyril.ollivier@upmc.fr

Monday, May 30th
 Auditorium Astier 11h



Marco Terreni (Drug Sciences Department, University of Pavia, Italy)
marco.terreni@unipv.it
Regioselective enzymatic hydrolysis of acetylated sugars, a new approach towards the semi-synthesis of neo-glycoproteins vaccines

Abstract. The results obtained in the use of immobilized lipases in the chemo-enzymatic synthesis of different oligosaccharides will be presented, including the reparation of products bearing at the anomeric position a thiocyno methyl group, required for the chemical glycosylation of proteins by selective reaction with lysines. This approach has been utilised for the preparation of several semi-synthetic neoglycoproteins. Accordingly, glycosylation of antigenic proteins from *Mycobacterium tuberculosis* (including the native protein and rationally designed mutants) has been investigated for the development of new potential glyco-conjugated vaccine products active against tuberculosis.

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June

Monday June 6th
Auditorium Astier 11h

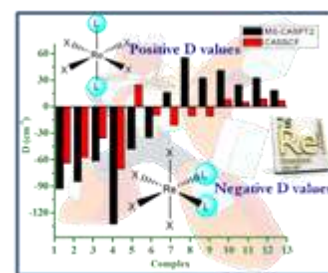
Gopalan Rajaraman (IIT Bombay, Mumbai, India)

rajaraman@chem.iitb.ac.in

Role of Molecular Modelling in the Design of Novel Magnetic Materials



Abstract. Molecular Magnets have wide spread applications ranging from magnetic storage to spintronics, Q-bits in quantum computing to refrigerative coolants. Single-molecule magnets (SMMs) are molecules which show slow relaxation of magnetization below the critical temperature and exhibit hysteresis loop similar to classical magnets. They offer key advantage over classical magnets due to their light weight, solubility and multifunctional character. Theoretical tools are indispensable in this



area for understanding the observed magnetic properties. The strength of these methods are not only limited to explain the observed magnetic properties but can also be utilized to predict novel molecules possessing superior magnetic properties. In this presentation, I will summarize the research efforts undertaken in our group towards achieving this goal.

Monday June 13th
Auditorium Astier 10h

Darren J. Dixon (Department of Chemistry, University of Oxford, UK)

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Catalytic Approaches to Simplifying Synthesis



Abstract. Catalysts that provide new reactivity and stereocontrol in efficient bond-forming reactions, are essential tools for converting low cost starting materials into high value, structurally complex, stereochemically defined product materials. In this presentation, new families of metal-free and metal-rich cooperative catalysts and their use in highly regioselective addition/coupling reactions, will be described. Further application of selected methodologies as pivotal carbon-carbon bond forming steps in the total synthesis of some complex natural products will also be presented.

Monday June 20th
Auditorium Astier 11h

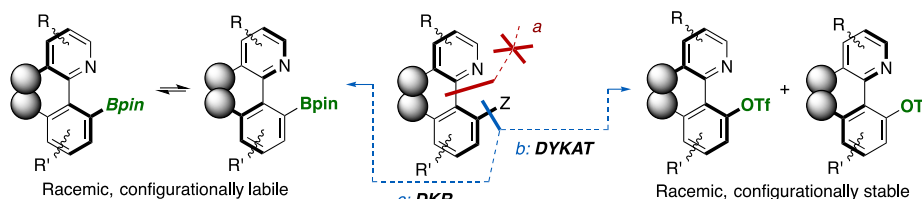
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DKR Strategies for the Asymmetric Synthesis of Axially Chiral Heterobiaryls



Abstract. The enantioselective synthesis of axially chiral heterobiaryls (e.g. 2-arylpiperidines/isoquinolines) remains as one of the major synthetic challenges in the field of asymmetric C(sp²)-C(sp²) cross-coupling reactions. In this seminar, the development of novel strategies based on dynamic kinetic resolution techniques (DKR and DYKAT) will be discussed.



Monday June 27th
Auditorium Astier 11h



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Hydrazones as Key Reagents and Ligands for Novel Applications in Asymmetric Catalysis

Abstract. The asymmetric 1,2 addition of formyl anion equivalents to carbonyl compounds is a powerful synthetic tool that provides a direct access to functionalized carbinols. In this context, we have exploited the aza-enamine character of formaldehyde *N,N*-dialkyl-hydrazones, but the development of a catalytic enantioselective version remained elusive. However, the use of *N*-*tert*-butylamino hydrazones enables a dual activation by bifunctional H-bonding organocatalysts to perform highly enantioselective additions to different activated carbonyl compounds. On the other hand, hydrazones appear as an interesting class of useful ligands in diverse contexts. The use of *C*₂-symmetric pyrrolidines as terminal dialkylamino groups, is a key design element that enabled a high enantiocontrol in a variety of reactions. The use of bis-hydrazones, phosphino-hydrazones, and pyridino-hydrazones in a variety of asymmetric catalytic transformations will be discussed.

July

Monday July 11th
Auditorium Astier 11h

Nicolas Moitessier (McGill University, Canada)

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Combining Software Development, advanced organic synthesis and biophysical methods for efficient drug discovery



Abstract. Molecular discovery is often a long, iterative, cost-inefficient and environmentally unfriendly process. More specifically, discovering asymmetric catalysts for chiral drug synthesis of novel therapeutics takes years and efforts to improve this process must be made. Our approach combines software development (ie, covalent drug docking), computational chemistry (quantum and molecular mechanics), synthetic methodology development (novel methods for synthesis and drug synthesis), biochemistry and biophysical approaches (calorimetry and NMR) to develop novel active inhibitors and asymmetric catalysts and develop methods for mechanistic studies of covalent inhibition. As an example, application of this combined approach to the discovery of asymmetric organocatalysts and potent enzyme inhibitors will be presented. Along the way, this integrated approach led to the development of drug discovery programs, to the discovery of a number of novel potent chemical series and novel asymmetric catalysts, to novel synthetic methodologies and a better understanding of the covalent inhibition.
