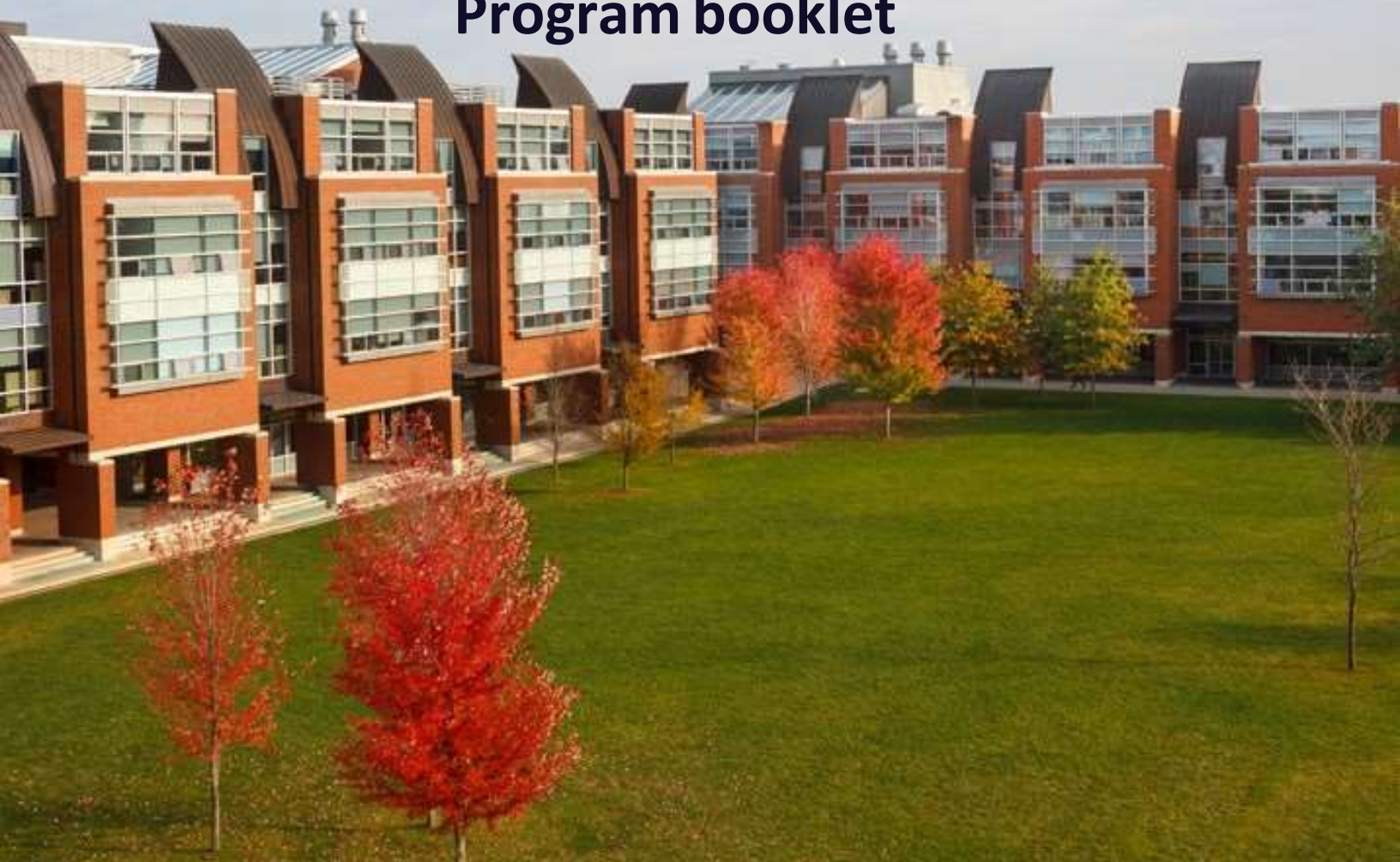


52nd Inorganic Discussion Weekend

November 8-10, 2019

Oshawa, Ontario

Program booklet



NOVEMBER 8-10

University of Ontario Institute of Technology
Oshawa, Ontario

IDW 2019



 **OntarioTech**
UNIVERSITY



Organization

Olena V. Zenkina

Associate Professor

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Conference Web page support

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Arda Celik, Arda.Celik@uoit.ca

**For further information on the Inorganic Discussion Weekends,
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Inorganic Discussion Weekend Conference

The Inorganic Discussion Weekend (IDW) has been bringing together researchers from across Ontario and Quebec for over 50 years. The conference was initiated in 1968 by Dr. Barry Lever, now a Professor Emeritus at York University, as a means to facilitate discussions with fellow Inorganic Chemists. IDW has since grown to become a perennial celebration of the scientific contributions of graduate students and postdoctoral fellows who are active in the field of inorganic chemistry. This meeting boasts strong attendance records, regularly attracting over 150 attendees from across Ontario and Quebec.

IDW2019 will feature three high profile scientists as keynote speakers:

Prof. Cathleen Crudden of Queen's University is a Canada Research Chair in Metal-Organic Chemistry and Past President of the Canadian Chemical Society. She pioneered research on the functionalization of metal surfaces by N-Heterocyclic Carbenes. In addition to her main group at Queen's, Prof. Crudden runs a satellite group in the Institute of Transformative Bio-Molecules in Nagoya, Japan. She is an active player in the areas of transition metal- and boron-based catalysis.

Prof. Milko Erik van der Boom of Weizmann Institute of Science, Israel, is a holder of the Bruce A. Pearlman Professional Chair in Synthetic Organic Chemistry. Being the head of the Department of Organic Chemistry, Prof. van der Boom is a world-recognized expert in organometallic chemistry and has an influential voice in the area of transition metal-based functional materials, molecular electronics, self-assembly, and nanoscience.

Prof. Christopher M. Kozak of Memorial University of Newfoundland, Canada, is known in the areas of synthetic organometallic & coordination chemistry, catalysis and green chemistry. His recent research is mainly focused at ligand design, the formation of new chromium complexes, small molecule activation, and catalysis, specifically carbon dioxide fixation and polycarbonate synthesis.

Keynote Speaker

Saturday, Nov.9, 9am-10am

Milko E. van der Boom,
Professor

Head of the Organic Chemistry Department
The Bruce A. Pearlman Professional Chair in
Synthetic Organic Chemistry.

Weizmann Institute of Science, Israel

<https://sites.google.com/site/milkovanderboomslab/>



Milko E. van der Boom received his B.Sc. degree (1992) from the Amsterdam University of Applied Sciences, The Netherlands, and a M.Sc. degree (1994) in Inorganic Chemistry at the University of Amsterdam (with Prof. Kees Elsevier). He earned his Ph.D. degree with distinction in 1999 from the Weizmann Institute of Science in Israel (with Prof. David Milstein). After 3 years of postdoctoral research with Prof. Tobin J. Marks at Northwestern University in the United States, he became a Faculty member in the Weizmann Institute's Department of Organic Chemistry.

His interdisciplinary materials chemistry research focuses on metalloorganic-oriented synthetic and mechanistic studies. His main interests spanning around various aspects of Molecular Assemblies aiming at a priori design of molecule-based materials with a set of predetermined properties and/or functions. He is the author of > 160 publications with more than 4000 citations.

Prof. van der Boom's prizes and honors include Adama Prize for Technological Innovation by the Israel Chemical Society; Alon Fellowship from the Israel Council for Higher Education, the Henri Gutwirth Prize from the Technion, and the Israel Chemistry Society's Prize for Excellent Young Chemists. He is the first incumbent and current holder of the Bruce A. Pearlman Professional Chair in Synthetic Organic Chemistry.

K-1**Keynote Lecture: Colorful Thin Films and Crystals Made in Israel****Milko van der Boom**

*Department of Organic Chemistry, Weizmann Institute of Science, Rehovot, Israel,
email: milko.vanderboom@weizmann.ac.il*

Coordination-based polymers and metal-organic frameworks have been explored since their serendipity discovery by a Berlin color-maker named Diesbach at the beginning of the 18th century. These intriguing materials combine metal-coordination chemistry with the complex formation of large supramolecular structures. Such materials are currently generated by the dozens in a gold-rush-type search for unique properties mainly related to the storage and release of energy (e.g., hydrocarbons, dihydrogen) at ambient temperatures and pressures. How the molecular components, metal salts and experimental conditions control the dimensions, shapes and homogeneity of these coordination-based materials is barely known. We demonstrated the controlled generation of various uniform crystals.^{1,2} Using a versatile ligand system that binds late-transition metals in a defined manner, we address various challenging issues related to the mechanism underlying the formation of such homogeneous structures at the (sub)-microscale. Coating of conductive surfaces with nanoscale layers of redox-active coordination-based polymers have been used by us to generate series of new materials. Our composite coatings can pass electrons selectively in directions that are determined by the positioning of redox-active metal complexes and the distances between them. These electron-transfer processes can be made dominantly uni- or bidirectional. We control the electrochemical communication between interfaces by the deposition sequence of the components and the length of organic spacers, and therefore we are able to program the bulk properties of the assemblies. The electrochromic properties and devices of these thin films will be discussed as well.³⁻⁴



1. di Gregorio, M. C.; Ranjan, P.; Houben, L.; Shimon, L.; Rehav, K.; Lahav, M.; van der Boom, M. E. *J. Am. Chem. Soc.* **2018**, *140*, 9132-9139.
2. Shankar, S.; Balgley, R.; Lahav, M.; Popovitz-Biro, R.; Cohen, S. R.; van der Boom, M. E. *J. Am. Chem. Soc.* **2015**, *137*, 4050-4053.
3. Balgley, R.; Algavi, Y.; Elolov, N.; Lahav, M.; van der Boom, M. E. *Angew. Chem., Int. Ed.* **2018**, *57*, 1-7.
4. Lahav, M.; van der Boom, M. E. *Adv. Mater.* **2018**, 1706641.

Keynote Speaker

Saturday, Nov.9, 1pm-2pm

Cathleen M. Crudden

Canada Research Chair, Tier 1
Professor and Killam Research Fellow
Queen's University, Canada

<http://www.cruddengroup.com>

Institute of Transformative Bio-Molecules (WPI-ITbM),

Nagoya University, Japan

<http://www.itbm.nagoya-u.ac.jp/>



Cathleen Crudden obtained her B.Sc. (1989) and M.Sc. (1990) from the University of Toronto with Dr. Mark Lautens. She completed her Ph.D. with Dr. Howard Alper at the University of Ottawa in 1995. After completing her Ph.D., Cathleen was awarded an NSERC PDF with Scott Denmark at the University of Illinois at Urbana Champaign. After one year as a postdoctoral fellow, she became an Assistant Professor at the University of New Brunswick. Prof Crudden has joined Queens University at 2006 as a Queen's National Scholar. From 2011-13, she was Vice President, President and Past President of the Canadian Society for Chemistry.

Prof. Crudden's research is centered on Asymmetric Synthesis and Catalysis, Organometallic and Organoboron Chemistry as well as on Materials Chemistry and Surface Science. She is a world-known expert on N-Heterocyclic Carbenes (NHC) and Chiral and Mesoporous Catalytic materials. She pioneered the concept of NHC-based ultra-robust monolayers on metal surfaces as a fundamentally new methodology for surface functionalization and protection. She is the author of >140 publications with over 3700 citations.

Prof. Crudden's scientific impact is highlighted by a long list of national and international awards. Most recent include the 2019 Montréal Medal; 2019 ACS A.C. Cope Scholar Awards; 2018 International Precious Metals Institute Carol Tyler award, 2018 Catalysis Award of the Chemical Institute of Canada; Synlett Best paper of 2017, etc. Prof. Crudden currently holds a Canada Research Chair in Metal-Organic Chemistry. Prof Crudden is an associate editor of ACS Catalysis one of the most recognized journals for research on heterogeneous, homogeneous, and biocatalysis with an impact factor of 11.384

K-2

Keynote Lecture: Catalytic preparation of chiral bio-molecules and the chemistry of carbon-based monolayers.

Cathleen M. Crudden*

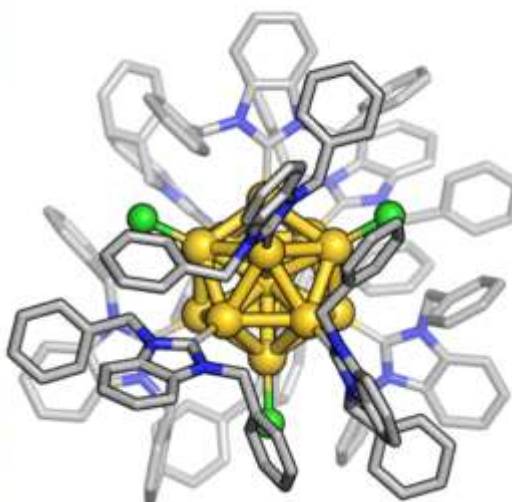
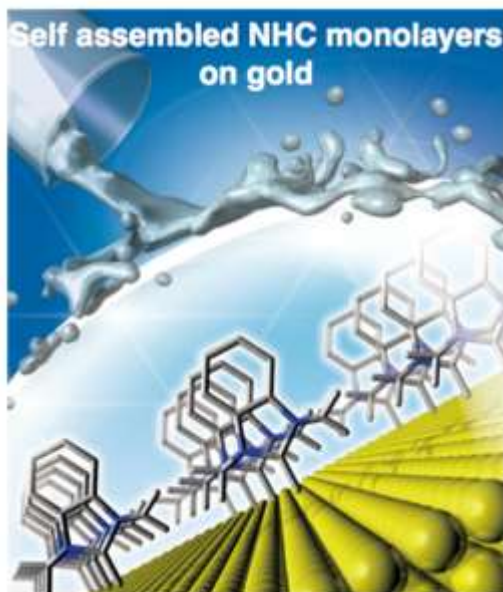
Department of Chemistry, Queen's University, Chernoff Hall, Kingston, Ontario, Canada, K7L 3N6, cruddenc@chem.queensu.ca

Abstract:

The use of N-heterocyclic carbenes to modify homogeneous metal catalysts is widespread since the high metal–NHC bond strength renders high oxidative and chemical stability to NHC–ligated metal complexes. Despite this fact, the use of NHCs to modify metal *surfaces* is virtually unprecedented.

We will describe the first example of the synthesis of gold surfaces, including Au(111), Au nanoparticles and Au nanoclusters. Films prepared by the deposition of NHCs show molecular ordering on the surface and remarkable stability. They show no decomposition upon heating for 24 hrs in THF, in boiling in water for 24hrs or upon treatment with acid (pH 2) or base (pH 12). Incredibly, they even survive largely after 24 hr exposure to hydrogen peroxide. This remarkable increase in stability relative to thiol-based SAMs will greatly increase the number of reagents and conditions to which the SAMs can be exposed.

We will also describe advances in organo boron chemistry that have dramatically broadened the applicability of this versatile element. In particular, we will describe its application in the preparation of complex chiral molecules of interest to the pharmaceutical industry and the ability to cross-couple seemingly identical boron substituents with different aryl iodides. The development of novel electrophiles for Suzuki-Miyaura cross coupling chemistry in the preparation of bioactive molecules will also be presented as will our developments in the use of sulfones as electrophiles for cross-coupling reactions.



Keynote Speaker

Sunday, Nov.10, 12pm-1pm

Christopher M. Kozak

Professor

Department of Chemistry

Green Chemistry and Catalysis Group

Memorial University of Newfoundland, Canada

<https://www.faculty.mun.ca/ckozak/>



Dr. Kozak obtained his B.Sc. Hons degree (Biological Chemistry) at McMaster University in Hamilton, Ontario. Then he obtained his Ph.D. degree at the University of British Columbia under the supervision of Dr. Mike Fryzuk. During his postdoctoral studies, he worked at the University of York (UK) with Dr. Simon Duckett; conducted his NSERC funded postdoctoral research with Dr. Philip Mountford at Oxford University (UK) and a Junior Research Fellowship at Wolfson College, Oxford. He moved back to Canada in 2004 and took up a position as Assistant Professor at Concordia University in Montreal. In 2005 he moved to his current position at Memorial University. In 2012 Dr. Kozak received the prestigious Terra Nova Young Innovator Award, sponsored by Suncor Energy. That same year he was a Honorary Visiting Researcher at Imperial College London in the group of Dr. George Britovsek.

Prof. Kozak's research focuses on synthetic organometallic and coordination chemistry, catalysis and green chemistry. He has played an integral role in the development of many homogenous non-precious metal catalysts for carbon-carbon cross-coupling, oxidation catalysis and biodegradable polymer synthesis from renewable feedstocks. Recently, a significant part of his research is focused on small molecule activation and catalysis (specifically carbon dioxide fixation and polycarbonate synthesis), carbon-carbon and carbon-heteroatom bond-forming reactions, and ligand design for organometallic and coordination chemistry.

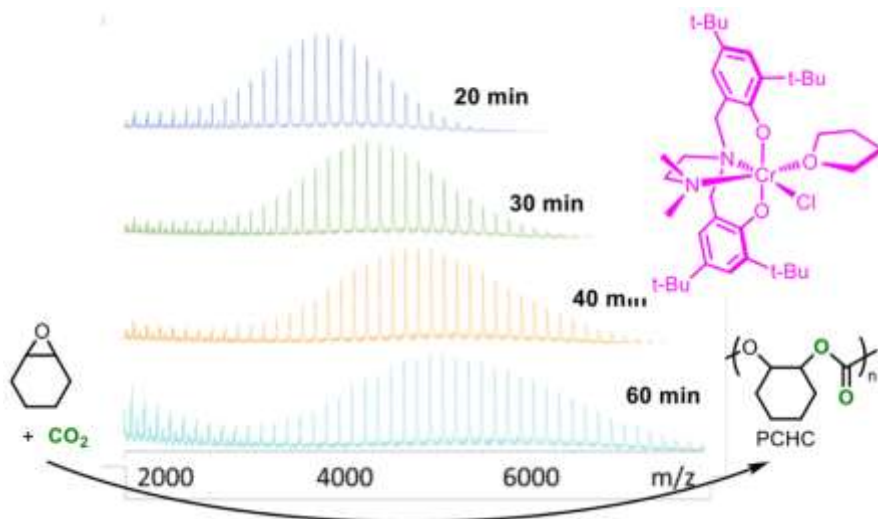
K-3

Keynote Lecture: What can we do about CO₂? Catalytic reactions of epoxides and carbon dioxideChristopher M. Kozak*

Department of Chemistry, Memorial University of Newfoundland, St. John's, Newfoundland, Canada, A1B 3X7, *ckozak@mun.ca

Abstract:

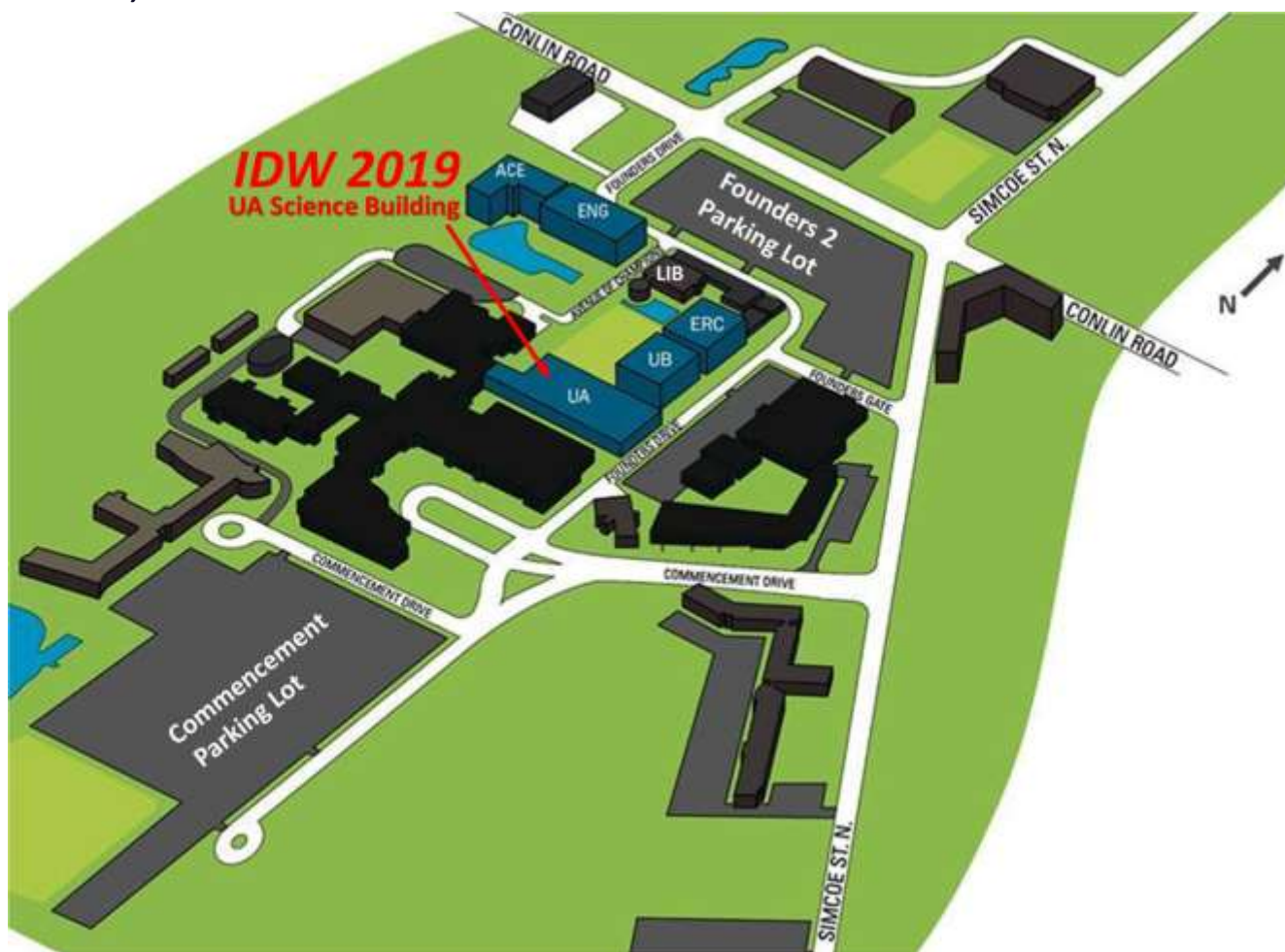
The reaction of CO₂ and epoxides to give cyclic carbonates or polycarbonates is a promising method of utilizing CO₂ as a C-1 feedstock. We developed new chromium, iron, cobalt and zinc complexes of tripodal amino-bis(phenolate) ligands as effective catalysts for the coupling of CO₂ and epoxides such as cyclohexene oxide and propylene oxide to form cyclic or poly(carbonates). Selectivity for either cyclic carbonate or polycarbonate formation can be controlled by careful tuning of reaction conditions. Mechanistic studies of the process by *in-situ* IR spectroscopy and gas phase characterization of possible intermediates by MALDI-TOF and electrospray ionization MS showed the importance of the steric and electron-donor properties of the pendent neutral donor arm of the ligand. The ability of the ligand to hinder formation of six-coordinate chromium(III) intermediates favors higher catalyst activity and modifications of the pendent donor appear more influential than modifications of the phenolate donors. The catalytic activities of cobalt and iron complexes are also highly sensitive to their geometric and electronic environments and these properties can be used to direct selectivity toward the cyclic or polycarbonate products. The epoxide reagents themselves can generate side reactions, including a previously unreported deoxygenation reaction and epoxide ring-opening polymerization giving polyethers. These reactions must be suppressed for effective carbon dioxide incorporation. Zinc complexes, for example, can be tuned to give polyethers, polycarbonates and terpolymers of CO₂ with mixtures of epoxides such as cyclohexene oxide and limonene oxide. Our recent successes and frustrations of working towards easily synthesized yet highly active catalysts for CO₂/epoxide copolymerization will be presented.



Location and Venue

Symposia will take place in the **University Science Building** at the **University of Ontario Institute of Technology**. (North campus Ontario Tech.)

Faculty of Science
Science Building UA,
University of Ontario Institute of Technology (UOIT)
2000 Simcoe Street North,
Oshawa, Canada ON L1H 7K4



Please see a detailed map at: <https://uoit.ca/maps/>



Figure was adapted from: <https://dsai.ca/services/master-planning-urban-design/>.

A 150-seat lecture auditorium UA1120 is reserved for plenary lectures. Two concurrent symposia will run in lecture halls UA 1220 and UA 1240 located near each other so it would be easy for attendees to enter and leave the room in order to see the presentation of interest. Two smaller rooms will be available for attendees to have a rest, form small discussion groups, prepare for the talk and check presentation slides.

A large atrium close to the lecture halls will serve as the venue for exhibitor tables for our Silver, Gold and Platinum sponsors, coffee breaks, and a poster session.

The conference banquet will take place in Oshawa Italian Recreation Club at the downtown Oshawa (245 Simcoe St S, Oshawa, ON L1H 4H3). We will present a traditional Italian kitchen and bar service. Exhibitor tables for Platinum sponsors will be set up at the front of the main hall to display companies' logos, provide space for the company visual materials, and to ensure representatives of the Platinum sponsor companies have an opportunity to talk with potential customers in a calm friendly atmosphere.

Bus transportation will be provided on Saturday Nov. 9 and Sunday Nov. 10 to the conference venues, banquet and then back to main hotels in downtown Oshawa and/or to Go Train/ Via Rail Oshawa station for people that commute home this day. Please see bus schedule page (see below) for details.

Schedule

Friday, Nov 8.

Downtown Campus, 2nd Floor Atrium, 61 Charles St. Oshawa, ON L1H 4X8

7:00 pm - 12:00 am conference mixer

Saturday, Nov.9

North Campus, UA building, 2000 Simcoe Street North, Oshawa, ON L1H 7K4

8:00 am - 9:00 am registration and light breakfast

9:00 am- 10:00 am UA1120 Keynote lecture

Prof. Milko E. van der Boom, Weizmann Institute of Science, Rehovot, Israel.

Colorful Thin Films and Crystals Made in Israel

10:00 - 10:15 coffee break

10:15 - 11:45 Oral sessions

am	UA1220 <i>Chair: Prof. Hocine Merazig</i>	UA1240 <i>Chair: Prof. Andrew Vreugdenhil</i>
10.15-10.35	O1 <u>A.Vasanthakumar</u> , D.J. H. Emslie* Synthesis of Cationic and Neutral Dialkyl Group 3 Complexes of Rigid Cyclometallation-Resistant NON and NNN-Donor Ligands	O7 <u>H.M.Fruehwald</u> , I. I. Ebravidze, O.V. Zenkina, E. B. Easton* <i>Iron-Terpyridine functionalized carbons as a multi-functional electrode for clean electrochemical energy systems</i>
10.35-10.55	O25 I. Gorgees, Z. Shen, J-P. Desaulniers* <i>Free-Base Corrole Ligands as Photosensitizer and Dyes in Oligonucleotides</i>	O3 <u>P.A.Lummis</u> , K.Stamplecoskie,* K. Kovnir,* T.Tsukuda,* H. Häkkinen,* C. M.Crudden* <i>NHC-protected Gold Nanoclusters – synthesis, properties and electronic structure</i>
10.55-11.15	O2 <u>A.Worrell</u> , C. Lampropoulos, M. Pilkington, Th.C. Stamatatos* <i>Oximate-Based Ligands in 3d/4f-Metal Cluster Chemistry: A Family of “Propeller”-like {Cu₃L_n} Complexes with Single-Molecule Magnetic Behavior</i>	O10 <u>Y.Liu</u> , R. Smith* <i>Identifying structural defects in hematite photoanodes by Raman spectroscopy</i>
11.15-11.35	O4 <u>N.J.Wolford</u> , D.C. Sergentu, W. W. Brennessel, J. Autschbach, M. L. Neidig <i>Homoleptic Aryl Complexes of Uranium (IV)</i>	O9 <u>A.J.Veinot</u> , J. H. Horton,* and C.M. Crudden* <i>Concurrent Reduction and Functionalization of Oxidized Copper Surfaces by N-Heterocyclic Carbenes</i>

11:45 am - 1:00 pm on-site lunch

1:00 pm - 2:00 pm UA1120 Keynote lecture

Prof. Cathleen M. Crudden, Queen's University, Kingston, Canada

Catalytic preparation of chiral bio-molecules and the chemistry of carbon-based monolayers.

2:15 - 2:30 pm coffee break

2:30 pm – 3:30 pm sessions

pm	UA1220 Chair: Prof. Marcus Drover	UA1240 Chair: Prof. Deborah Durbin
2:30- 2:50	O31 <u>M.Segizbayev</u>, K. A. Gudun, G. I. Nikonov, A. Y. Khalimon* <i>Synthesis of novel POCN pincer complexes of Nickel (II) and their use as hydrosilylation and hydroboration catalysts</i>	O11 <u>N.P.Dogantzis</u>, G. K. Hodgson, and S.Impellizzeri* <i>Optical Patterning with Photoactivated and Nanoparticle-Enhanced Fluorescence</i>
2:50- 3:10	O6 <u>C.Daneluik</u>, A. Escuerb, M. Pilkington*, Th. C. Stamatatos* <i>Facile preparation of a generic family of $\{CuL_2L_n\}$ (L_n = lanthanide) linear compounds with rare Ln coordination geometries and SMM behavior using the "metal complexes as ligands" synthetic approach</i>	O12 <u>T.Al-Faouri</u>, B. Koivisto* <i>PolyEDOT Device Architectures for Enhanced Dye Regeneration in Dye-Sensitized Solar Cells</i>
3:10- 3:30	O19 <u>K.L.May</u>, A. J. Lough , R. A. Gossage *, S.A. Westcott* <i>Investigations into Potentially Biologically Active Chelated Boron Complexes</i>	O13 <u>D.Riel</u>, A.Jones, L. Trevani* <i>Revisiting Nitrogen- and Oxygen-Doped Carbon Gels as Catalyst Supports for Energy Storage and Conversion</i>

INORGANIC DISCUSSION WEEKEND 2019

3:30 - 5:00 sessions

pm	UA1220 <i>Chair: Jean-Paul Desaulniers</i>	UA1240 <i>Chair Prof. Nisha Agarwal</i>
3:30-3:50	O-20 G.DelleMonache, Th. Stamatatos*, M. Pilkington* <i>Exploration of bhpH₂ for the Synthesis and Study of Heterometallic 3d/4f Single Molecule Magnets</i>	O-14 N.O.Laschuk, I. I. Ebralidze, E. B. Easton, O. V. Zenkina <i>Bond Conjugation Effect for Ultra Durable Electrochromic Materials</i>
3:50-4:10	O21 T.Levchenko, P.A. Lummis, ... C. M Crudden* <i>Bimetallic metal nanoclusters stabilized with N-heterocyclic carbene ligands: challenges and opportunities</i>	O15 E.P.Alsac, A. Whittingham, Y. Liu, R. D.L. Smith* <i>The Effect of Geometric Strains on Heterogeneous Electrocatalysis</i>
4:10-4:30	O27 JJimenez-Santiago, D. Song* <i>Synthesis of Iron NHC compounds towards catalytic applications</i>	O16 I.I.Ebralidze and O.V. Zenkina* <i>X-ray photoelectron spectroscopy for heavy metal detection</i>
4:30-4:50	O-23 H.Bhattacharjee, J. Zhu, J.Müller* <i>Sterically Protected Bora[1]ferrocenophanes: Enantiopure Monomers for Chiral Metallopolymers</i>	O-30 R.AlipourMoghadamEsfahani, E. B. Easton* <i>Highly stable and corrosion resistance electrocatalyst support; dual doped titanium suboxide</i>

5:00 pm- 7:00 pm poster session, UA Atrium.

Posters should be ready before 5:00.pm

7 :20 – 11.00. pm banquet (Italian Club in Oshawa)

Sunday, Nov.10

8:30 - 9:30 light breakfast

9:40 - 10:20 sessions

<i>am</i>	UA1220 <i>Chair: Prof. Kevin Coulter</i>	UA1240 <i>Chair: Prof. Bryan Koivisto</i>
9:40-10:00	O-22 Y. Maekawa, M. Nambo, C.M. Crudden* <i>gem-Difluoroolefination of Alkyl Triflones</i>	O33 K.Scotland, A. Vreugdenhil* <i>Curable Hybrid Materials For Corrosion Protection of Steel: Development & Application of UV Cured 3-Methacryloxypropyltrimethoxysilane Derived Coating</i>
10:00-10:20	O-28 A.Y.Goudreault, A.G. Botti, ...D.E. Fogg* <i>Examining the Impact of Water on Phosphine - Free Ruthenium Olefin Metathesis Catalysts</i>	O18 G.D'Amaral, M. Ranne, ... D. Foucher* <i>A Library of Flexible Asymmetric Hypercoordinate Tin Polymers</i>

10:30 - 10:45 coffee break

10:50 - 11:50 sessions

<i>am</i>	UA1220 <i>Chair: Prof. Chris Kozak</i>	UA1240 <i>Chair: Chair Prof. Sanela Martic</i>
10:50-11:10	O-29 A.Dmitrienko*, G. Nikonov* <i>Diverse reactivity of $NacNacAl(I)$ to N-heterocycles</i>	O-24 M. Affan, A. Sarkar, ... I. J.Scott,* <i>Self-Assembly of 2-Dimensional Coordination Polymers of 2x2 Square Cu Grids using Iminodiacetate Scaffolds</i>
11:10-11:30	O5 M.V.Gradiski, A. Nemati, A.J. Lough and R. H. Morris <i>Tri and tetradentate PN donor ligands and their iron and cobalt complexes. Synthesis, reactivity, and preliminary catalytic activity in base-free ester hydrogenation</i>	O-17 J.J.Clarke, C. M. Crudden* <i>Borocation-Catalyzed Dearomative Hydrosilylation/Hydrogenation of N-Heterocycle</i>
11:30-11:50	O-32 M.M.H.Sung, Sofia Jdanova, D. E Prokopchuk, R. H. Morris* <i>Ligand Design by additive Ligand</i>	O-26 Q.Liang, D. Song* <i>Iron complexes with redox active o-phenylenediamide ligands</i>

12:00 pm - 1:00 pm UA1120 keynote lecture

Prof. Christopher M. Kozak, Memorial University of Newfoundland, Canada
What can we do about CO₂? Catalytic reactions of epoxides and carbon dioxide

1:00 pm – 1:05pm. Awards announcement

1:05 pm – 4:00 pm. Workshops (need to sign in during the registration, spaces are limited).

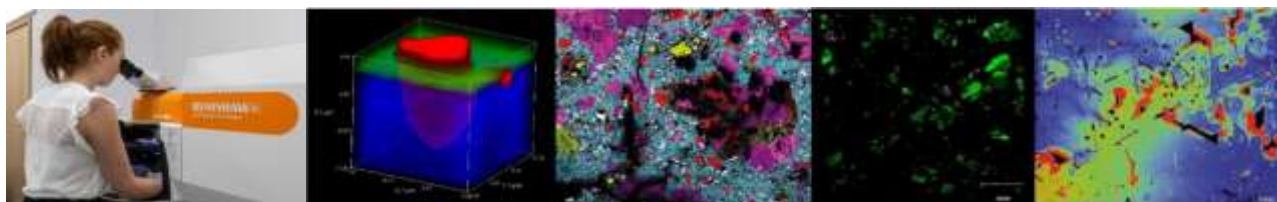
Workshops:

If you are interested to participate in the workshop please register at the registration table to secure the spot. We will apply first-asked first-served policy.

ProSpect Scientific Inc.
Canada's Raman Spectroscopy Experts

RENISHAW. 
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WORKSHOP: Raman spectroscopy for chemical & material identification

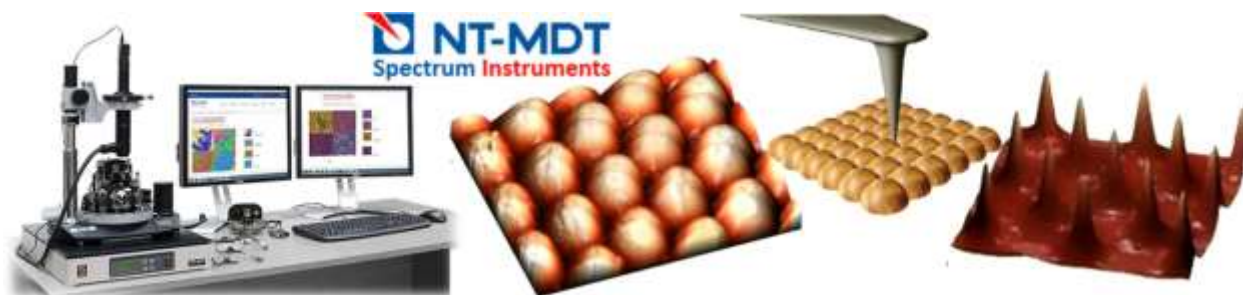


ABSTRACT: Raman imaging supports several “fast” chemical and topographical contrast methods that can greatly simplify area chemical composition and distribution analysis. The use of Raman microscopy in industrial and academic research settings has dramatically increased in the last 10 years as ease of use and wavelength options have increased. In a research environment we see the need for material and chemical analyses of samples that may vary in size from the very large to the sub-micron and nanometre domains.

Renishaw's Raman workshop will review the theory and principles of confocal Raman spectroscopy. Following the presentation, attendees have opportunity for hands-on use of a Renishaw inVia confocal Raman microscope equipped with 532 nm laser and mapping.



WORKSHOP: Scanning Probe Microscopy



ABSTRACT: Over the last 25 years, NT-MDT has been involved in the development, production and support of research instrumentation, primarily, atomic force microscopes (AFM) and its combinations with ultrahigh resolution spectroscopy for nanotechnology and its applications. NT-MDT's pathway has been marked by the creation of a large number of devices, whose functions and capabilities cover the broad range of customer needs in different areas: material science, inorganic chemistry, biology, and others. NT-MDT pioneering efforts led to the impressive combination of scanning probe microscopy with Raman spectroscopy.

During the workshop NT-MDT team will show the unique capabilities of Atomic Force Microscopes that helps to uncover the secrets of the nanoworld, discuss different applications, including high resolution measurements, electrical measurements, nanomanipulations, and perform live measurements of different samples, including samples of workshop participants.

Schedule of Bus Transportation

Saturday Nov. 9

Transportation to Conference

Pick Up Location	Pick Up Time
Oshawa GO Station 915 Bloor ST W Oshawa, ON L1J 8M6	8:20 AM
Comfort Inn- Oshawa 605 Bloor ST W Oshawa, ON L1J 5Y6	8:25 AM
Best Western Plus Durham 559 Bloor ST W Oshawa, ON L1J 5Y6	8:25 AM
Holiday Inn-Oshawa 67 Simcoe Street North Oshawa, ON L1G 4S3	8:35 AM
Drop Off Location	
UOIT-North Campus 2000 Simcoe ST N Oshawa, ON L1H 4H3	

Transportation to Banquet

Pick up Location	Pick up Time
UOIT-North Campus 2000 Simcoe ST N Oshawa, ON L1H 4H3	7:05 PM
Drop off Location	
Oshawa Italian Rec Club 245 Simcoe St S Oshawa, ON L1H 4H3	

Transportation to Hotels/GO Station

Pick up Location	Pick up Time
Oshawa Italian Rec Club 245 Simcoe St S Oshawa, ON L1H 4H3	11:00 PM
Drop off Locations	
Holiday Inn -Oshawa, Best Western Plus Durham, Comfort Inn- Oshawa, Oshawa GO Station	

Sunday Nov. 9

Transportation to Conference

Pick Up Location	Pick Up Time
Oshawa GO Station 915 Bloor ST W Oshawa, ON L1J 8M6	8:20 AM
Comfort Inn- Oshawa 605 Bloor ST W Oshawa, ON L1J 5Y6	8:25 AM
Best Western Plus Durham 559 Bloor ST W Oshawa, ON L1J 5Y6	8:25 AM
Holiday Inn-Oshawa 67 Simcoe Street North Oshawa, ON L1G 4S3	8:35 AM
Drop Off Location	
UOIT-North Campus 2000 Simcoe ST N Oshawa, ON L1H 4H3	

Pick up Location	Pick up Time
UOIT-North Campus 2000 Simcoe ST N Oshawa, ON L1H 4H3	1:10 PM
Drop off Locations	
Holiday Inn -Oshawa, Best Western Plus Durham, Comfort Inn- Oshawa, Oshawa GO Station	

Parking Information.

Free parking on campus is granted for attendees during the IDW conference (See parking map for more details.):

Friday, November 8, 2019 - 61 Charles St. - Parking will be on the South Side of the Building. **6:00PM - 11:59PM**

Saturday, November 9, 2019 - 2000 Simcoe St. N - Parking for Delegates would be in Founders Lot 2 , South-East Gates off of Founders Gate will be Raised. **7:00AM - 11:59PM**

Sunday, November 10, 2019 - 2000 Simcoe St. N - Parking for Delegates would be in Founders Lot 2, South-East Gates off of Founders Gate will be Raised. **7:00AM - 5:00PM**

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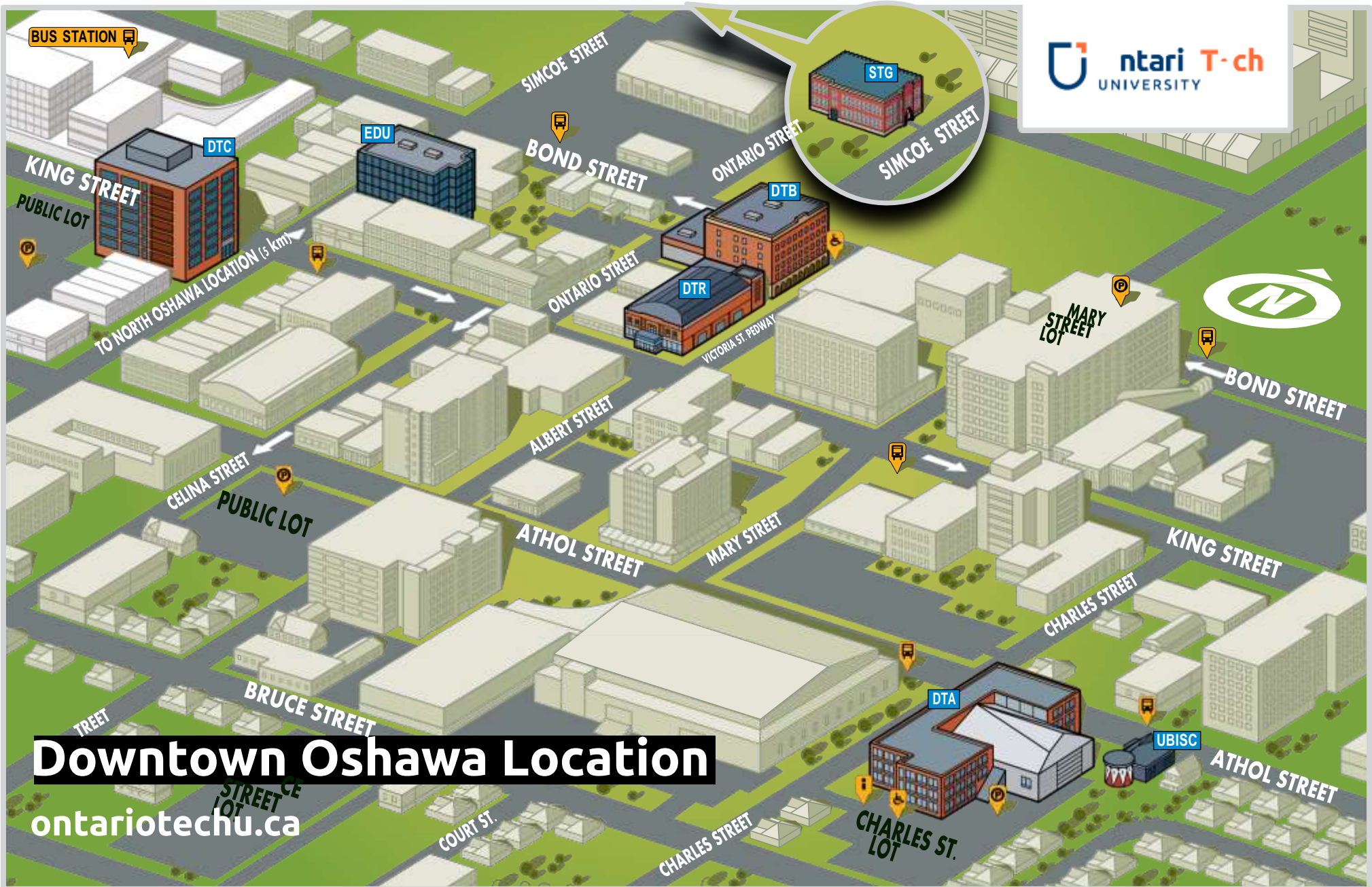
- ACE** ACE
- CC** Campus Corners
- CCE** Centre for Collaborative Education
- CERL** Clean Energy Research Lab
- CFH** Campus Fieldhouse
- CIC** Campus Ice Centre
- CRWC** Campus Recreation and Wellness Centre
- ENG** Ontario Power Generation Engineering Building

- ERC** Energy Systems and Nuclear Science Research Centre
- GWB** Gordon Willey Building
- JW** J Wing
- JSTW** Justice Wing
- LIB** Library
- RT** Residence Townhouses
- SC** Student Centre
- SIRC** Software and Informatics Research Centre
- Office of the Registrar

- SLB** Student Life Building
- SR** Simcoe Village Residence
- SSB** Student Services Building
- SVDH** South Village Dining Hall
- SVR** South Village Residence
- SW** South Wing
- UA** Science Building
- UB** Business and Information Technology Building
- UL** Classrooms
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- DTA** 61 Charles Street Building
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- DTC** Forensic Psychology Laboratory
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- DTR** Regent Theatre
50 King Street East
- EDU** Education Building
11 Simcoe Street North

- STG** Motor Behaviour and Physical
Activity Laboratory
St. Gregory's Building,
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Banquet

Oshawa is home to one of the largest Italian communities in Ontario. We invite you to explore Italian heritage and fine Italian cuisine at the Conference banquet. The Oshawa Italian club has been proudly operated by the Italian community for more than 53 years in Oshawa/Durham, providing events, services, and charitable contributions and offering a great selection of Italian food and beverages, including the best Espresso and Cappuccino in the area. The cultural wing of the club, The Italian Cultural Centre of Durham (ICCD), has been a unique partner to UOIT, establishing the first community-funded scholarships. Funds from this program have also been used to promote exchanges of students and faculty with prominent Italian universities.

The conference banquet will take place at the main banquet hall of Oshawa Italian Recreation Club, 245 Simcoe St. S. in Oshawa, ON.

Note: Open Bar service on the banquet is included into the conference fees.



O-1

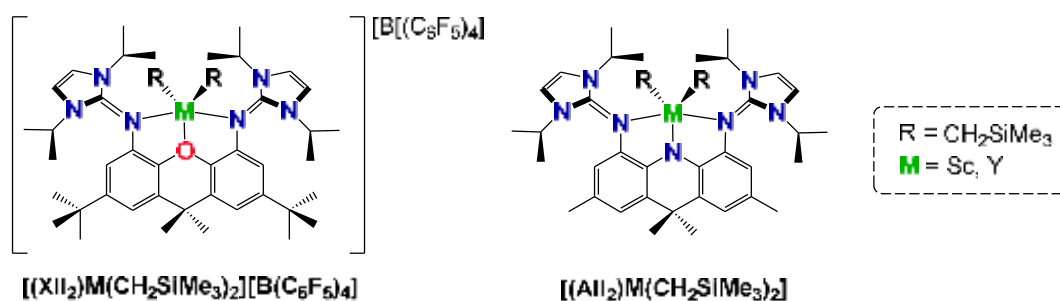
Title: Synthesis of Cationic and Neutral Dialkyl Group 3 Complexes of Rigid Cyclometallation-Resistant NON and NNN-Donor Ligands

Aathith Vasanthakumar, David J. H. Emslie*

Department of Chemistry and Chemical Biology, McMaster University, Hamilton, Ontario L8S 4M1. *emslie@mcmaster.ca

Abstract:

Cationic group 3 alkyl complexes, especially monometallic examples free from donor solvent coordination, have demonstrated high activity for catalytic processes such as intramolecular hydroamination and olefin polymerization.¹ However, the propensity for these complexes to engage in undesirable reactions such as ligand redistribution and cyclometallation have resulted in relatively few isolated examples,² and cationic group 3 hydroamination catalysts have scarcely been investigated.³ To increase the thermal stability of such complexes, design features such as carefully positioned steric bulk and ligand rigidity are beneficial. Additionally, ancillary ligands must have considerable donor ability, in order to stabilize cationic metal centers. Two new ligands, anionic AlI_2 and neutral XII_2 (see Figure), which incorporate these design features, have been prepared, and afforded stable, cyclometallation-resistant scandium and yttrium dialkyl complexes: monocationic $[(\text{XII}_2)\text{M}(\text{CH}_2\text{SiMe}_3)_2][\text{B}(\text{C}_6\text{F}_5)_4]$ and neutral $[(\text{AlI}_2)\text{M}(\text{CH}_2\text{SiMe}_3)_2]$. The alkene polymerization and hydroamination activity of the aforementioned complexes will be discussed.



1. Trifonov, A. A.; Lyubov, D. M. *Coord. Chem. Rev.* **2017**, *340*, 10.
2. a) Hayes P.G.; Piers W.E.; McDonald R. *J. Am. Chem. Soc.* **2002**, *124*, 2132. b) Arndt, S.; Spaniol, T. P.; Okuda, J. *Chem. Commun.* **2002**, *8*, 896. c) Venugopal, A.; Fegler, W.; Spaniol, T. P.; Maron, L.; Okuda, J. *J. Am. Chem. Soc.* **2011**, *133*, 17574. d) Li, T. T.; Nishiura, M.; Cheng, J. H.; Zhang, W. X.; Li, Y.; Hou, Z. M. *Organometallics* **2013**, *32*, 4142. e) Pindwal, A.; Patnaik, S.; Everett, W. C.; Ellern, A.; Windus, T. L.; Sadow, A. D. *Angew. Chem. Int. Ed.* **2017**, *56*, 628.
3. a) Lauterwasser F.; Hayes P.G.; Brase S.; Piers W.E.; Schafer L.L. *Organometallics*. **2004**, *23*, 2234. b) Bambirra, S.; Tsurugi, H.; van Leusen, D.; Hessen, B. *Dalton Trans.* **2006**, *9*, 1157. c) Ge, S. Z.; Meetsma, A.; Hessen, B. *Organometallics* **2008**, *27*, 5339.

Title: Oximato-Based Ligands in 3d/4f-Metal Cluster Chemistry: A Family of “Propeller”-like {Cu₃Ln} Complexes with Single-Molecule Magnetic Behavior

A. Worrell^a, C. Lampropoulos^b, A. Escuer^c, M. Pilkington^a and Th. C. Stamatatos^{*a}

^a Department of Chemistry, Brock University, St. Catharines, Ontario, L2S 3A1, *email addresses: mpilkington@brocku.ca and tstamatatos@brocku.ca

^b Department of Chemistry, University of North Florida, Jacksonville, Florida 32224, United States

^c Departament de Química Inorgànica i Orgànica and Institut de Nanociència i Nanotecnologia (IN²UB), Universitat de Barcelona, Martí i Franqués 1-11, 08028 Barcelona, Spain

The organic chelating/bridging ligands 9,10-phenanthrenedione-9-oxime (phenoxH) and 9,10-phenanthrenedione-9,10-dioxime (phendoxH₂) were employed for a first time in heterometallic 3d/4f-metal cluster chemistry.¹ We present a new family of {Cu₃Ln} (Ln^{III} = Gd (**1**), Tb (**2**), Dy (**3**)) complexes bearing the phenoxH ligand and possessing an oximato-bridged, “propeller”-like core. Moreover, the magnetic susceptibility data for complexes **2** and **3** were nicely fit to a Hamiltonian that accounts for parameters such as spin–orbit coupling and the axial ligand-field component around the Ln^{III} atoms. This fitting procedure is used herein for the first time to elucidate the exchange parameters for the anisotropic compounds. Complexes **1-3** are antiferromagnetically-coupled, while **2** and **3** exhibit single-molecule magnetic behavior (SMM) at low temperatures.

Figure 1. Molecular structure of the representative {Cu₃Gd} complex.

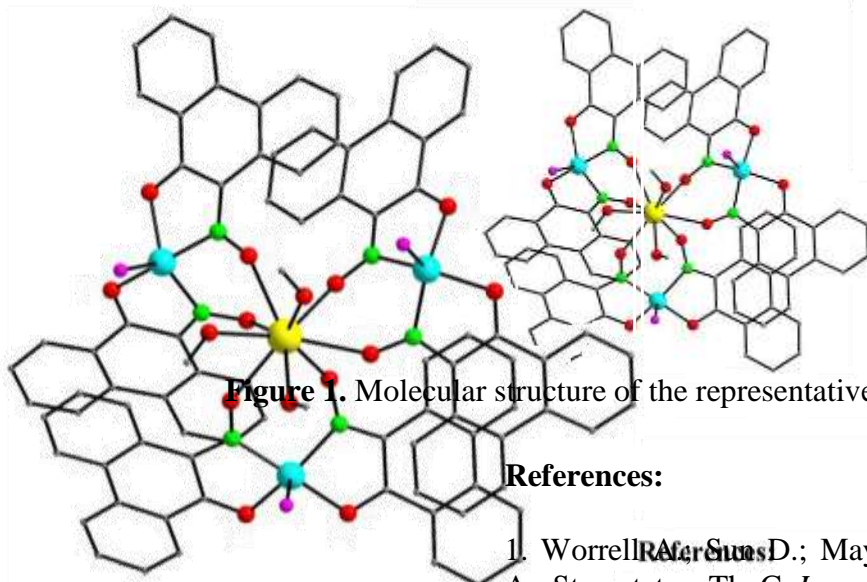


Figure 1. Molecular structure of the representative {Cu₃Gd} complex.

References:

1. Worrell A.; Sun D.; Mayans J.; Lampropoulos, C.; Escuer, A.; Stamatatos, Th. C. *Inorg. Chem.* **2018**, *21*, 13944.
1. Worrell A.; Sun D.; Mayans J.; Lampropoulos, C.; Escuer, A.; Stamatatos, Th. C. *Inorg. Chem.* **2018**, *21*, 13944.

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O-3

IDW 2019 Abstract Submission Form

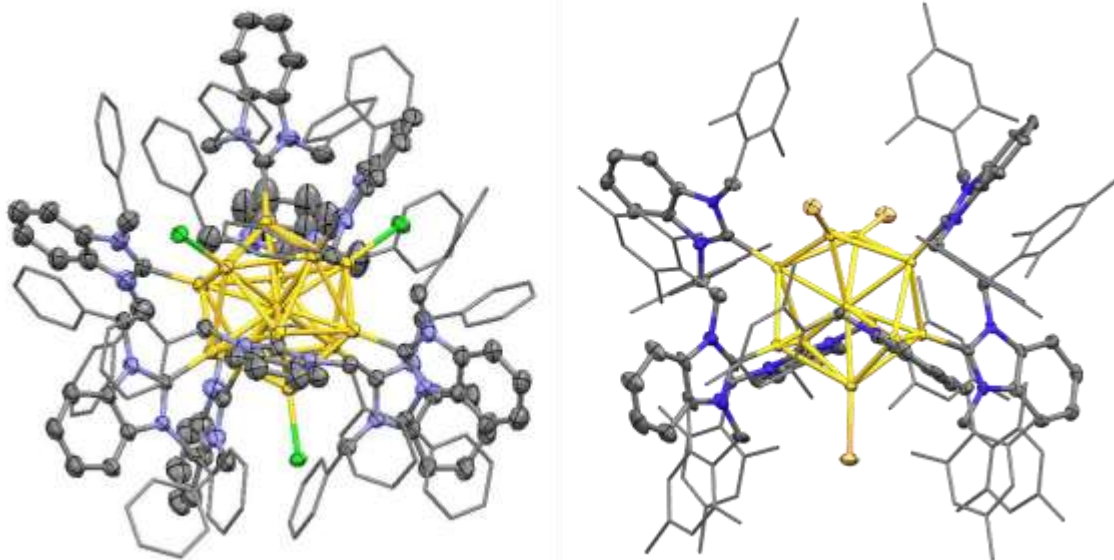
Title: NHC-protected Gold Nanoclusters – synthesis, properties and electronic structure.

Name of presenter and other authors: Paul A. Lummis, Tetyana I. Levchenko, Mina R. Narouz, Bryan Owens-Baird, Goonay Yousefalizadeh, Hannah Ramsay, Maryam Sabooni, Sami Malola, Shinjiro Takano, Kevin Stamplecoskie,* Kirill Kovnir,* Tatsuya Tsukuda,* Hannu Häkkinen,* and Cathleen M. Crudden*

*Department of Chemistry, Queen's University, Kingston, Ontario, K7L 3N6, Main
corresponding author: cruddenc@chem.queensu.ca*

Abstract: 350 words

Abstract: Gold nanoclusters are an exciting class of materials with tunable size, shape and electronic structure. The choice of co-ligand is key, and can greatly impact the overall function and stability of the cluster. In this presentation, I will describe recent progress in the Crudden lab for making these clusters, describe how different ligands can give rise to different clusters, and highlight some of the key properties of these compounds.



Presentation Preference: (check one by putting X)

Oral

Poster

References:

1. Lasr name A. B.;Smith B.C. *Journal Abbreviation*. Year,

issue, first page.

Title: Homoleptic Aryl Complexes of Uranium (IV)

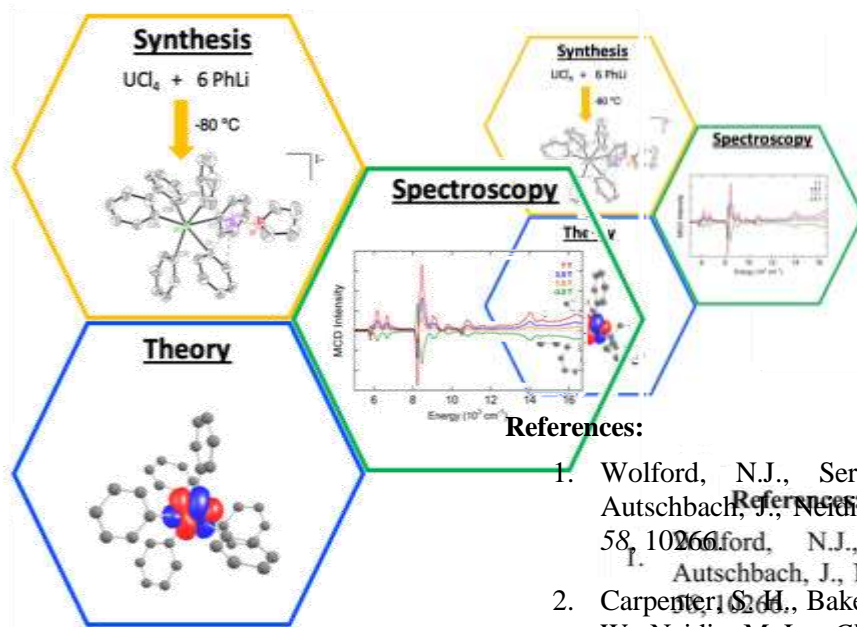
Nikki J. Wolford^a, Dumitru-Claudiu Sergentu^b, William W. Brennessel^a, Jochen Autschbach^b, and Michael L. Neidig^a.

^a Department of Chemistry, University of Rochester, nwolford@ur.rochester.edu

^b Department of Chemistry, University at Buffalo, State University of New York

Abstract: 350 words

The synthesis and characterization of sterically unencumbered homoleptic organouranium aryl complexes containing U-C σ -bonds has been of interest to the chemical community for over 70 years. Originally proposed for applications in isotope separation, the instability of the resulting products made characterization very difficult. Taking inspiration from our previous work studying unstable intermediates in iron catalysis², a series of uranium aryl species were isolated. Presented here are the first structurally characterized, sterically unencumbered homoleptic uranium (IV) aryl-ate species of the form $[\text{U}(\text{Ar})_6]^{2-}$ (Ar = Ph, *p*-tolyl, *p*-Cl-Ph). Magnetic Circular Dichroism (MCD) spectroscopy and computational studies provide insight into electronic structure and bonding interactions in the U-C σ -bond across this series of complexes. Overall, these studies solve a decades long challenge in synthetic uranium chemistry, enabling new insight into electronic structure and bonding in organouranium chemistry.



References:

1. Wolford, N.J., Sergentu, D-C, Brennessel, W.W., Autschbach, J., Neidig, M. L.; *Angew. Chem. Int. Ed.* **2019**, 58, 10266.
1. Wolford, N.J., Sergentu, D-C, Brennessel, W.W., Autschbach, J., Neidig, M. L.; *Angew. Chem. Int. Ed.* **2019**, 58, 10266.
2. Carpenter, S. H., Baker, T. M., Muñoz, S. B., Brennessel, W. W., Neidig, M. L.; *Chem. Sci.* **2018**, 9, 7931.
2. Carpenter, S. H., Baker, T. M., Muñoz, S. B., Brennessel, W. W., Neidig, M. L.; *Chem. Sci.* **2018**, 9, 7931.

Abstract should fit into one page.

O-5

IDW 2019 Abstract Submission Form

Title: Tri and tetradentate PN donor ligands and their iron and cobalt complexes. Synthesis, reactivity, and preliminary catalytic activity in base-free ester hydrogenation.

Matthew V. Gradiski, Ali Nemati, Alan J. Lough and Robert H. Morris*

Department of Chemistry, University of Toronto, Toronto, Ontario, M5S 3H6,

**robert.morris@utoronto.ca*

Recently, we reported the synthesis of various PNN' and P₂NN' ligands via a single-step reductive amination with *in situ* generated primary phosphine acetaldehydes, and their coordination chemistry with iron(II) and cobalt(II).¹ Phosphorous-nitrogen based ligands have been shown as effective scaffolds for hydrogenation catalysts. Lithiation of the PNN' ligands with *n*-BuLi and subsequent reaction with metal precursors results in a change in the coordination geometry of the ligand. This allows facile access to 4-coordinate cobalt amido and 6-coordinate iron diamido complexes, the former of which is active towards base-free ester hydrogenation. Additionally, the reactivity of select complexes with potassium graphite, carbon monoxide, carbon dioxide, as well as halide abstraction, and borohydride reagents will be discussed herein.

References:

1. Gradiski, M. V., Tsui, B. T. H., Lough, A. J., Morris, R. H. *Dalton Trans.* **2019**, 48, 2150.

Presentation Preference: (check one by putting X)

Oral X

Poster

Abstract should fit into one page.

O-6

Title: Facile preparation of a generic family of $\{Cu^{II} Ln\}$ ($Ln = \text{lanthanide}$) linear compounds with rare Ln coordination geometries and SMM behavior using the “metal complexes as ligands” synthetic approach

C. Daneluik^a, A. Escuer^b, M. Pilkington^{*,a}, Th. C. Stamatatos^{*,c}

^a Department of Chemistry, Brock University, St. Catharines, ON, L2S 3A1, cd16qd@brocku.ca

^b Department de Quimica, Universitat de Barcelona, Barcelona, Spain, 08028, albert.escuer@qi.ub.es

^c Department of Chemistry, University of Patras, Patras, Greece, 26504, thstama@upatras.gr

Abstract:

A heterocyclic, hexadentate N_3O_3 chelate ligand (H_3L ; Figure 1, left) was synthesized, and employed towards the preparation of mononuclear $[Cu^{II}L]^-$ complexes. The latter precursors were subsequently used as metalloligands for the facile synthesis of a generic family of linear $[Cu^{II}Ln^{III}Cu^{II}L_2]^+$ complexes ($Ln = \text{Gd, Tb, Dy, Er, Y}$). All metal ions are 6-coordinate with distorted octahedral (for the $3d$ -metal ions) and trigonal antiprismatic (for the $4f$ -metal ions) geometries. The trinuclear heterometallic complexes (Figure 1, right) exhibit slow relaxation of their magnetization in both the absence and presence of an external magnetic field, and their solid-state structures are retained in solution as confirmed by ESI-MS studies. The combined results demonstrate the ability of the “metal complexes as ligands” strategy to yield isoskeletal $3d/4f$ -metal clusters with diverse magnetic properties, without altering the core structures and coordination environments.

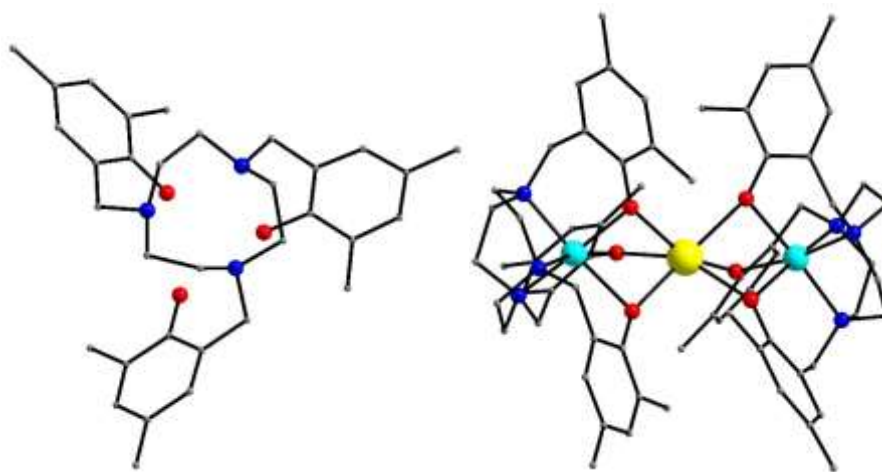


Figure 1. Structures of the chelate ligand H_3L used in the present work (left), and the cation of a representative member of the family of $[Cu_2LnL_2]^+$ complexes (right). H atoms are omitted for clarity.

References:

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²Barta, C.A., Bayly, S.R., Reed, P.W., Patrick, B.O., Thompson, R.C., Orvig, C. *Inorg. Chem.* **2008**, 47, 2280.

O-7

Title: Iron-Terpyridine functionalized carbons as a multi-functional electrode for clean electrochemical energy systems

Holly M. Fruehwald, Iraklii I. Ebralidze, Olena V. Zenkina, and E. Bradley Easton*

Faculty of Science, Ontario Tech University, Oshawa, ON, L1G 0C5,

**brad.easton@uoit.ca*

Non-precious metal catalysts for the oxygen reduction reaction (ORR) are of great interest for fuel cell technology due to their low cost and wide availability of materials. Development of these catalysts has been a constantly growing area. However, there have been very few literature reports that provide insights into the precise nature of the structure and geometry of the catalytically active sites formed in these materials. In the current literature, the most commonly proposed catalytically active site(s) for ORR corresponds to Fe-N₂₊₂/C geometry. This is typically produced through a high temperature pyrolysis step to obtain this desired configuration in the active sites^[1]. However, the pyrolysis step is very disadvantageous due to the production of a distribution of nitrogen functional groups on the surface which can negatively affect the activity of the catalyst, since only nitrogen functionalities with specified geometry are considered to be the most active for ORR^[2,3]. As well, high-temperature treatments increase the cost of production, and can be quite energy demanding. Requirement of high-temperature treatment makes it difficult to design a surface rich in a specific active sites for the desired application. The work presented here demonstrates a model system for a non-precious metal catalyst for the ORR achieved by covalently functionalizing a conventional carbon support with a nitrogen-rich ligand. The terpyridine ligand geometry allows the formation of well-defined active catalytic sites when covalently attaching an N₃/C functionality to the carbon surface, leaving exposed the most active sites for the ORR. Room temperature metal-ligand coordination with Fe results in desired Fe-N₃/C moieties on the surface. We demonstrate that this system can be prepared using mild reaction conditions and does not require high temperature treatment, in fact heat treatment to this system was detrimental to the activity. The Fe-N₃/C support was subjected to electrochemical studies in both acidic and basic aqueous media and demonstrates the potential of this system to be used as a model for an Fe-N₃/C active site for ORR and for applications in supercapacitor technology.

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- [1] M. Lefèvre, E. Proietti, F. Jaouen, J.-P. Dodelet, *Science* **2009**, 324, 71-74.
- [2] F. Charretre, F. Jaouen, S. Ruggeri, J.-P. Dodelet, *Electrochimica Acta* **2008**, 53, 2925-2938.
- [3] H. M. Fruehwald, I. I. Ebralidze, O. V. Zenkina, E. B. Easton, *ChemElectroChem* **2019**, 6, 1350.

O-9

Title: Concurrent Reduction and Functionalization of Oxidized Copper Surfaces by N-Heterocyclic Carbenes

Alex J. Veinot,^a Christian R. Larrea,^{a,b} Abrar Al-Rashed,^a J. Daniel Padmos,^a Mina R. Narouz,^a Paul A. Lummis,^a Christopher J. Baddeley,^{*b} J. Hugh Horton,^{*a} and Cathleen M. Crudden^{*a,c}

(a) Department of Chemistry, Queen's University (b) School of Chemistry, University of St. Andrews (c) Institute of Transformative Bio-Molecules (WPI-ITbM), Nagoya University
*cruddenc@chem.queensu.ca

Abstract:

While N-heterocyclic carbenes (NHCs) have been extensively studied in the context of molecular chemistry, the benefits that NHCs impart to nanomaterials have only recently been recognized. Following the initial report by Siemeling and co-workers,¹ and our determination of their stability,² self-assembled monolayers (SAMs) derived from NHCs have received significant attention from the surface science community.² Gold is the most widely employed metal in organic-on-metal type devices because of its high resistance to oxidation and ease of handling. However, more oxidation-sensitive metals such as silver and copper often have superior properties and are typically much cheaper. The interaction of NHCs with oxidized metal surfaces has received significantly less attention but is a prerequisite for applying NHC-based SAMs to more reactive metal substrates. Building upon our previous work involving NHCs on metallic surfaces,³⁻⁵ we are addressing this deficiency by studying the interactions of NHCs and their bicarbonate salts on metal oxide surfaces.

References:

1. Weidner, T.; Baio, J. E.; Mundstock, A.; Große, C.; Karthäuser, S.; Bruhn, C.; Siemeling, U., *Aust. J. Chem.* **2011**, *64* (8), 1177.
2. Smith, C. A.; Narouz, M. R.; Lummis, P. A.; Singh, I.; Nazemi, A.; Li, C.-H.; Crudden, C. M., *N-Heterocyclic Carbenes in Materials Chemistry. Chem. Rev.* **2019**, *119* (8), 4986.
3. Crudden, C. M.; Horton, J. H.; Ebraldize, I. I.; Zenkina, O. V.; McLean, A. B.; Drevniok, B.; She, Z.; Kraatz, H.-B.; Mosey, N. J.; Seki, T.; Keske, E. C.; Leake, J. D.; Rousina-Webb, A.; Wu, G., *Nat. Chem.* **2014**, *6*, 409.
4. Crudden, C. M.; Horton, J. H.; Narouz, M. R.; Li, Z.; Smith, C. A.; Munro, K.; Baddeley, C. J.; Larrea, C. R.; Drevniok, B.; Thanabalasingam, B., *Nat. Commun.* **2016**, *7*, 12654.
5. Larrea, C. R.; Baddeley, C. J.; Narouz, M. R.; Mosey, N. J.; Horton, J. H.; Crudden, C. M., *ChemPhysChem* **2017**, *18* (24), 3536.

O-10

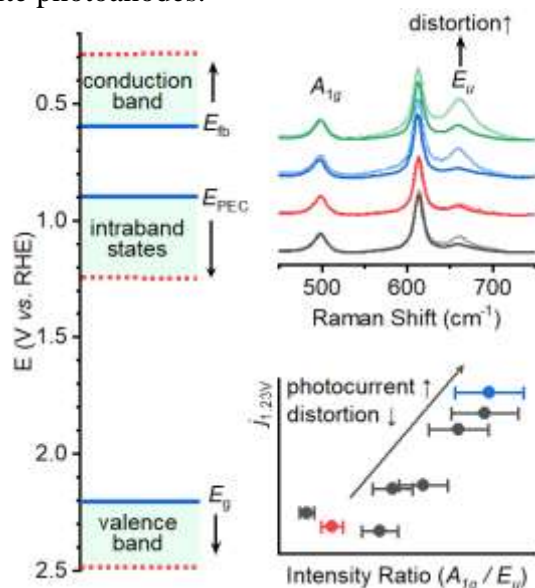
Title: Identifying structural defects in hematite photoanodes by Raman spectroscopy

Yutong Liu and Rodney Smith*

Department of Chemistry, University of Waterloo, Waterloo, ON, N2L 3G1

*rodsmith@uwaterloo.ca

Uncertainty regarding the nature of structural defects in hematite and their specific impacts on material properties and photoelectrocatalytic water oxidation inhibits their development as photoanodes. Studies on the fundamental photophysical behavior of key electron transfer processes and the effect of secondary elements have advanced our understanding, but persistently poor photoelectrocatalytic performance and high variability in reported behavior indicate missing information. We target this issue with a structure-property analysis using photoelectrochemical, X-ray diffraction, Raman and UV-visible spectroscopic data on a series of hematite photoanodes. The analysis reveals a formally Raman inactive vibrational mode in hematite films prepared by annealing lepidocrocite films whose intensity varies with annealing protocols. Correlations between the intensity of this feature in the Raman spectrum with photocurrent density, semiconductor band positions, and the location of intraband trap states signifies systematic changes in the magnitude of a crystal lattice distortion. Analysis of the nature of these key Raman vibrations, X-ray diffraction patterns, and the synthetic conditions lead us to conclude that the observed defect is iron vacancies that are induced by the trapping of protons within the crystal lattice. This finding provides a means to rapidly diagnose a specific structural defect and will aid in the optimization of fabrication protocols for hematite photoanodes.



Presentation Preference: (check one by putting X)

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Poster

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O-11

IDW 2019 Abstract Submission Form

Optical Patterning with Photoactivated and Nanoparticle-Enhanced Fluorescence

Nicholas P. Dogantzis, Gregory K. Hodgson, and Stefania Impellizzeri*

*Laboratory for nanoMaterials & Molecular Plasmonics, Department of Chemistry and Biology, Ryerson University, Toronto ON, Canada M5B 2K3, *simpellizzeri@ryerson.ca*

Acid-sensitive fluorescent dyes have been traditionally used in microlithography in the study of the mechanisms and efficiency of photoacid initiators and for delivering invaluable insights on the spatial distribution of the fabricated patterns. Furthermore, activatable fluorophores can be used for the development of lithographic features through the precise generation of functional fluorescent images. This strategy can ultimately deliver a viable, practical hybridization between imaging and lithography - patterning through fluorescence - provided that these fluorescent “inks” are (i) spatio-temporally controlled (i.e. the fluorescence is “turned-on” only in the illuminated region) and (ii) they have relatively high fluorescence outputs.

We designed a hybrid system composed of a switchable boron dipyrromethene (BODIPY) fluorophore that can be selectively activated by UVA or UVC light in the presence of a photoacid generator (PAG). The activation can be performed either in solution or in thin polymer films. Light irradiation of the PAGs encourages the release of p-toluenesulfonic, triflic, or hydrobromic acid, which promote the replacement of a catecholate chelator of the nonemissive species by two methoxide ligands, meanwhile forming a highly fluorescent species. Furthermore, the output of emission can be enhanced by plasmonic silver nanostructures. This unique and synergistic combination of photochemical, photophysical and plasmonic properties can be exploited for developing exceptional photoresponsive materials that would not otherwise be accessible through their separate organic and inorganic (metallic) components alone, and can have profound implications in patterning and information technology.

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Poster

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O-12

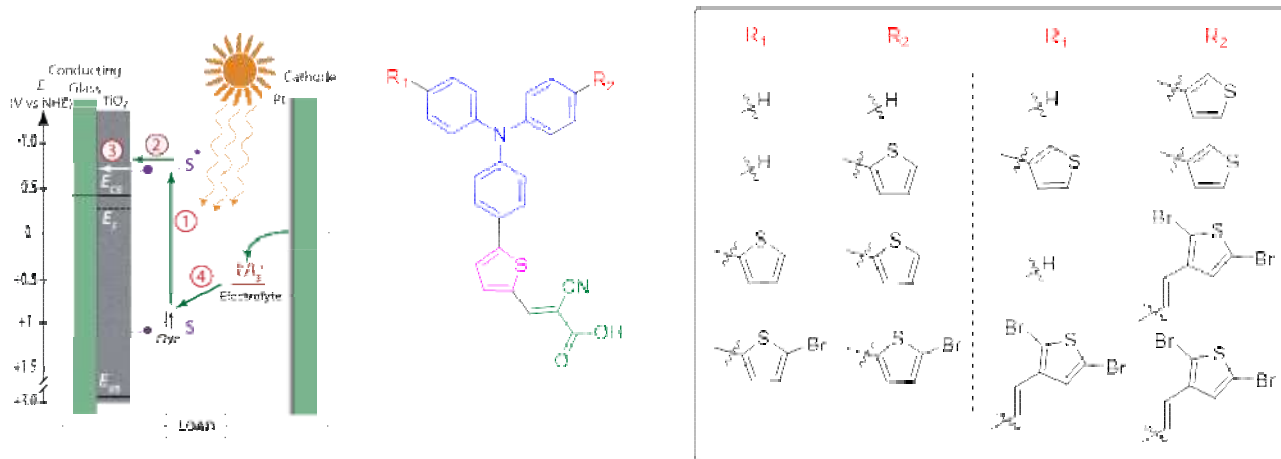
PolyEDOT Device Architectures for Enhanced Dye Regeneration in Dye-Sensitized Solar Cells

Tamara Al-Faouri, Bryan Koivisto*

Department of Chemistry and Biology, Ryerson University, Toronto, ON, M5B 2K3

*tamara.alfaouri@ryerson.ca, bryan.koivisto@ryerson.ca

Recent studies found that moving away from liquid electrolytes in dye-sensitized solar cells (DSSC), such as I^-/I_3^- , to alternative redox couples, such as $Cu^{2+/+}$, and ferrocene, and ionic liquids, to even solids state or polymer hole transport materials (HTM), such as spiro-MeOTAD and polyethylenedioxythiophene (PEDOT), to be more beneficial to DSSC performance and life-time.¹ This is because electrolytes like I^-/I_3^- tend to corrode metal contacts and electrodes, I^-/I_3^- partially absorbs visible light, photodegrade, I_2 can interact with/decompose the dye, and volatile (finite temperature for cell operation), causing the long-term stability/performance of DSSCs to drop.² In addition, solid electrolytes use hole-transport materials (HTM) to transport positive charge from the dye to the cathode to regenerate the dye, as opposed to the liquid electrolytes which shuttle electrons, in which minimizes the diffusion taking place as electrons travel back to the dye. A positive charge jumps from molecule to molecule (or polymer chain) towards the cathode, eliminating the challenges that diffusion rate imposes on the DSSCs performance.³ This work focuses on developing DSSC devices using **CB** dyes (Figure 1) with polymerizable units to facilitate internal electronic communication with PEDOT. **CB** dyes were synthesized in previous work and tested in liquid electrolytes.⁴ They consist of TPA-thiophene-cyanoacetic acid moieties, as **D- π -A**, while the R-groups on the TPA part are variations of thiophene based polymerizable units, in order to integrate with the polymer film (HTM) to increase pore filling/dye loading on TiO_2 , decrease dye-HTM interfacial capacitance, minimize recombination, and improve long term stability.



References:

1. Cai, N., *et al. Nano Lett.* **2011**, *11*, 1452.
2. Wang, M., *et al. Nat. Chem.* **2010**, *2*, 385.
3. Yanagida, S., *et al. Acc. Chem. Res.* **2009**, *42* (11), 1827.

O-13

Title: Revisiting Nitrogen- and Oxygen-Doped Carbon Gels as Catalyst Supports for Energy Storage and Conversion

Donna Riel, Allison Jones, and Liliana Trevani*

*Faculty of Science, Ontario Tech University, Oshawa, Ontario, L1G0C5,
Liliana.trevani@uoit.ca*

Abstract:

Carbon materials are extensively used in energy storage and conversion devices because of their high surface areas and electrochemical properties [1]. In recent years, a significant amount of work has been aimed to investigate new routes for the incorporation of heteroatoms such as nitrogen, sulfur, and phosphorus on carbon to enhance the catalytic activity of transition metals like iron, cobalt, and copper towards key electrochemical process. In particular, the reduction of oxygen (ORR) [2] which is of interest in the development of more efficient polymer electrolyte membrane fuel cells (PEMFCs) and lithium batteries [3], as well as the reduction of carbon dioxide (CO₂RR) to CO and liquid fuels [4].

In this study, we have revisited the synthesis of nitrogen and oxygen-doped carbon materials using sol-gel polymerization reactions and subsequent carbonization of the material [2], but using SiO₂ nanoparticles, as hard-templates to control the surface area and texture of the final carbon products [5]. Carbon products obtained by carbonization of a nitrogen-rich, melamine-formaldehyde (MF) polymer gel, resulted in high surface area mesoporous materials (~ 500 m²/g) with up to 8 N-atom% depending on the high-temperature annealing conditions (950°C or 1500°C). In the case of carbon materials obtained by combustion of a resorcinol-formaldehyde (RF) polymer, the use of both a soft- and hard-template allowed to produce carbon materials with larger surface areas (up to ~ 1000 m²/g) and oxygen contents up to 6 O-atom%.

Pt/MF-NC and Pt/RF-OC samples were prepared by an impregnation method to evaluate the stability of these catalysts under oxidizing and acidic conditions, as well as their catalytic activity toward the reduction of oxygen. The results show an improvement in the case of Pt/MF-NC when compared with Pt/RF-OC, higher Pt utilization, and stability that we attributed to the soft-template and media conditions adopted for the synthesis of the latter. Future work involves replacing Pt overall by implementing a transition metal catalyst material for key reactions in fuel cells.

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- [5] N. Zhang *et al.*, *Mater. Chem. Phys.*, vol. 232, pp. 513–519, **2019**

Title: Bond Conjugation Effect for Ultra Durable Electrochromic Materials

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Faculty of Science, Ontario Tech University, Oshawa, Ontario, L1G 0C5,

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Abstract: 350 words

Electrochromic materials (ECMs) change their color reversibly with applied voltage using redox reactions. 2,2':6',2''-terpyridine (tpy) has intense chromophoric properties with certain metal ion coordination dependent on the oxidation state of the metal center; therefore, metal-tpy complexes are suitable for ECM design. For example, two tpy ligands will coordinate iron(II) ion to form an intensely purple material. If this is oxidized to iron(III) under positive potentials, the color becomes bleached. The color returns upon additional reduction to iron(II).^{1,2}

In this study, ECMs were designed using iron(II)-tpy complexes. Three different tpy ligands were used, each differing in their 4' position conjugation. Specifically, they all had an additional pyridine group connected with an sp^3 (**s-tpy**), sp^2 (**d-tpy**), or sp (**t-tpy**) type bond (figure 1). Additionally, they were built into solid devices using conductive high surface area nanoparticles (NPs) screen printed onto conductive and transparent metal oxide glass. The change in conjugation between the ligands impacted electron transfer rates, extinction coefficients, and material coloration. The effect of the NP surface on the ECM was explored, and found to have a great effect on the overall efficiency through electrochemical impedance spectroscopy, diffuse reflectance spectroscopy, and cyclic voltammetry tests. Indium tin oxide (ITO) NPs of different surface areas were compared and contrasted, and additionally fluorine-doped tin oxide (FTO) NPs. There were a total of three iron-tpy complexes deposited onto four different substrates each, resulting in twelve systems which were fully characterized. Best materials had ultra-long term durability and impressively high coloration efficiencies.³

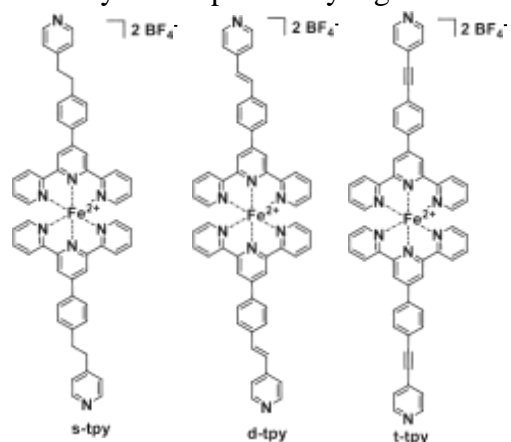


Fig. 1: Complexes deposited for ECM design.

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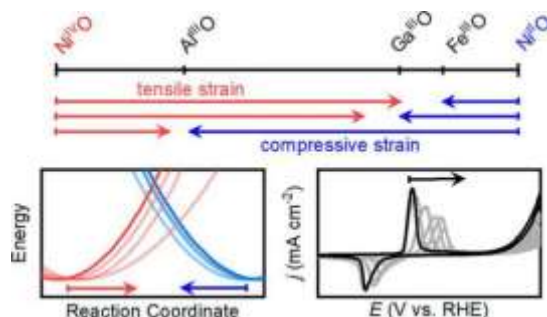
O-15

The Effect of Geometric Strains on Heterogeneous Electrocatalysis

Elif Pinar Alsac, Alex Whittingham, Yutong Liu and Rodney D.L. Smith*

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Ni(OH)₂ undergoes dramatic changes in electrochemical behavior upon doping of iron ions, transforming from one of the worst electrocatalyst to one of the best-known catalysts for the water oxidation (WO) reaction. The chemical explanation for improved Ni(OH)₂ electrocatalytic WO upon introduction of Fe ions remains a matter of debate.^[1-3] We analyzed the impact of geometric strain on the electrochemical behavior in this class of materials by systematically incorporating trivalent cations with varied ionic radii into a disordered Ni(OH)₂ lattice.⁴ Near-infrared (NIR) spectroscopy confirms that the structural lattice distorts to accommodate the additive cations. These composition series provide the first examples of Fe-free materials that mimic specific behavioral features of Fe-Ni hydroxides. DFT models suggest that secondary cations distort the potential energy surface of the oxidized and reduced forms of the materials in an asymmetric fashion, effectively decreasing the activation energy for electron transfer. The Fe (III) cation uniquely favors water oxidation, however, in its ability to significantly broaden the potential energy surface for the oxidized phase. This lowers the electron transfer coefficient (α), yielding the distinctive decrease in Tafel slope.

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O-16

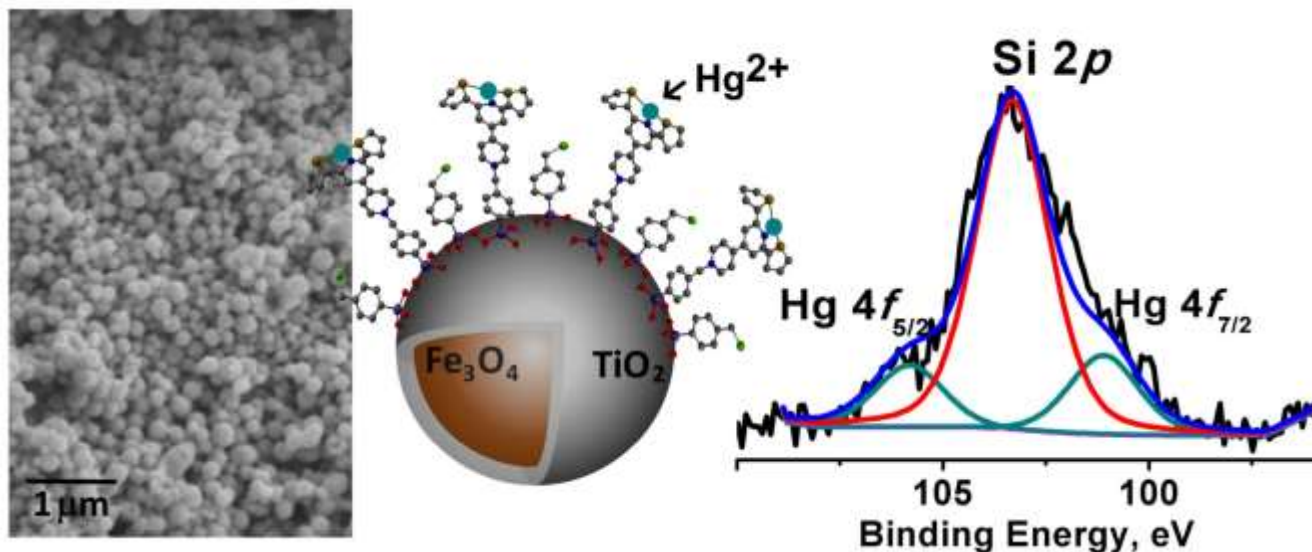
X-ray photoelectron spectroscopy for heavy metals detection

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Heavy metals impact daily well-being because the human body requires many as trace elements. However excess of heavy metals leads to various diseases. Therefore fast and reliable methods for heavy metal ions detection and removal from solutions are desirable. Most heavy-metals (except arsenic) are transition metals. Their soluble salts could be trapped by appropriate surface-anchored ligands and thus removed from the solution. X-ray photoelectron spectroscopy (XPS) is the best technique for the analysis of heavy metals on solid supports, which allows determination of the chemical composition, the oxidation state of elements and their stoichiometry.

In this talk, we will discuss basic principles of XPS and explore the role of XPS in the design of new materials for heavy metal uptake and detection. We will put a focus on materials for the detection of mercury¹ and iron².



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O-17

IDW 2019 Abstract Submission Form

Title:

Borocation-Catalyzed Dearomative Hydrosilylation/Hydrogenation of N-Heterocycles

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Abstract: 350 words

Saturated *N*-heterocycles are ubiquitous in FDA approved pharmaceuticals, with two of the most common motifs being piperidine and piperazine, derivatives of reduced pyridine and pyrazine heterocycles respectively.[1] Metal-free transfer hydrogenation of pyridines are known, using Hantzsch esters[2], silanes[3] and ammonia borane[4] with the assistance of Bronsted acids[2] or Lewis acids.[3] The use of hydrogen is more atom-economical, accomplished with Lewis-acidic boranes with incorporated fluorine atoms, either stoichiometrically[5] or catalytically[6]. In 2015 we reported the borocation-catalyzed hydrogenation of imines under very mild conditions[7]. This talk will describe our investigations into borenium-catalyzed reductions of aromatic *N*-heterocycles

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IDW 2019 Abstract Submission Form

Title: A Library of Flexible Asymmetric Hypercoordinate Tin Polymers

Gloria D' Amaral, Mohkamed Ranne, David Choi, Jeffrey Pau, Alan Lough^a and Daniel Foucher^{b*}

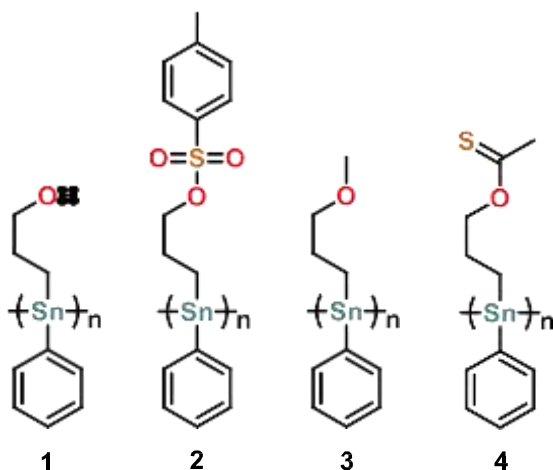
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Abstract: 350 words

Polystannanes are a unique class of polymers that consist of a backbone of covalently linked tin atoms. Unfortunately, polystannanes display an extreme sensitivity to light and moisture. Previously the Foucher group demonstrated the full synthesis and characterization of polymer **1** with evidence of hypercoordination, stability toward light and moisture, and film forming properties.¹ Using this evidence, the hypercoordinate polystannane library can be extended by substituting the alcohol group to a substitutionally labile tosyl group (**2**) that does not exhibit hypercoordination, and further functionalized pre- or post- polymerization to regain hypercoordinate properties. The functionalities to be explored include a methoxy group (**3**) and a thioester (**4**).



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Abstract should fit into one page.

O-19

Investigations into Potentially Biologically Active Chelated Boron Complexes

Kathleen L. May ^a, Alan J. Lough ^c, Robert A. Gossage ^{a*}, Stephen A. Westcott ^{b*}

^a Ryerson University, Toronto, Ontario ^b Mount Allison University, Sackville, New Brunswick

^c University of Toronto, Toronto, Ontario

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Abstract:

Prior to 2003, boron-containing compounds were mostly overlooked when considering functionality for drug design. Since the FDA approval of Bortezomib (trade name Velcade - a peptide-mimic drug) the field of medicinal boron compounds has blossomed into the synthesis and practical application of a variety of boron-containing functionality. From peptide-mimetics, BODIPY-based drugs, and more recently popularized, benzoxaboroles by the discovery of 5-fluorobenzoxaborole, boron-containing compounds have seen increased use and research interest. The boron atom has been introduced into a variety of designs for drugs, leading to the improvement of existing biologically active compounds. Boron has a particularly high affinity for oxygen, thus borates and boronic acid esters are ubiquitously found in many modern compound designs. Specifically, we are interested in N,O- and N,C-chelates of boron containing compounds. Synthesis thus far has incorporated ligand scaffolds popularized by Tohda^{1,2}, Meyers³, and Kawase^{4,5}. Using previously established methods, a boron unit (Bpin, Bcat, BF₂) was coordinated to the ligand backbone.⁶⁻⁸ Currently other ligand backbones and boron sources are being investigated. The purpose for this is to take advantage of the known biological activity of which oxazolines, oxazoles and thiazoles have and use them in tandem with those of the boron center to obtain bio-active boron compounds.

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O-20

Exploration of bhpH₂ for the Synthesis and Study of Heterometallic 3d/4f Single Molecule Magnets

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Abstract:

Two families of {Cu₂Ln₂} and {Cu₄Ln₂} clusters (Ln= Gd(III), Tb(III), Dy(III)) have been prepared from benzoate ions and the chelating/bridging ligand 2,6-bis(1-hydroxyethyl)pyridine (bhpH₂, **1**), which are the only 3d/4f clusters coordinated with bhpH₂ in the field to-date. Elucidation of their molecular structures by X-ray diffraction shows that the structural core of both sets of complexes are very similar, however magnetic susceptibility studies reveal that the Cu₂Ln₂ systems exhibit no slow relaxation of magnetization, whereas the Cu₄Ln₂ complexes are single molecule magnets (SMMs) at low temperature. The synthesis and magneto-structural studies of these two families of heterometallic clusters will be presented, highlighting how by carefully fine tuning their molecular structures, it is possible to suppress quantum tunneling mechanisms (QTM) and switch on their SMM properties.

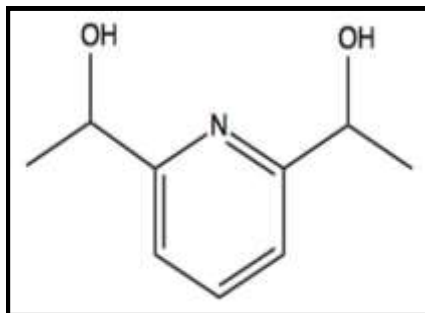


Figure 1: The molecular structure of bhpH₂ (**1**).

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Poster

Abstract should fit into one page.

Title: *gem*-Difluoroolefination of Alkyl Triflones

Yuki Maekawa, Masakazu Nambo, and Cathleen, M. Crudden*

Department of Chemistry, Queen's University, Kingston, ON, K7L 2S8

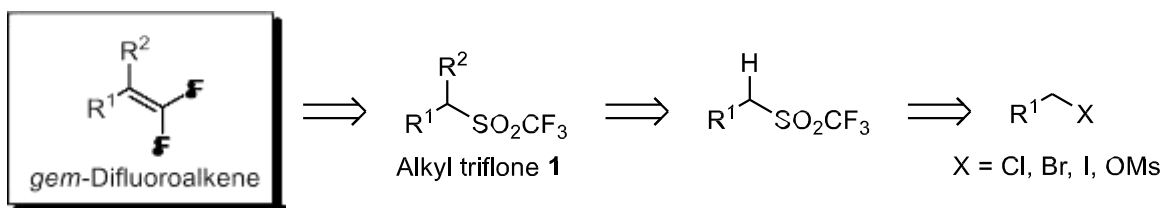
Institute of Transformative Bio-Molecules (WPI-ITbM), Nagoya University, Nagoya,

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gem-Difluoroalkenes, which represent an interesting class of fluorinated compounds, are bioisosteres of vinyl and carbonyl compounds. *gem*-Difluoroalkenes and their derivatives have been employed in pharmaceutical chemistry due to their ability to enhance and change molecular properties.¹ For example, *gem*-difluoroalkene derivatization of artemisinin displayed increased antimalarial activity.² In addition, these fluorinated compounds present versatile building blocks for synthetic applications.³

These abilities have triggered the development of synthetic methodologies to create *gem*-difluoroalkene substrates,^{3,4} the most common of which are Wittig-type reactions, and reduction-type reactions with strong reductants and photoredox catalysis. However, the dependence of these conventional methods on specific carbonyl and trifluoromethyl alkene functional groups limits the diversity of the resulting *gem*-difluoroalkenes and their practical applications.

Herein, we present an alternative synthesis that allows for facile diversification of the resulting *gem*-difluoroalkene compounds. The details of the synthetic transformation of alkyl triflones into *gem*-difluoroalkenes will be discussed.



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Poster

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O-21

Title: Bimetallic metal nanoclusters stabilized with N-heterocyclic carbene ligands: challenges and opportunities

Tetyana I. Levchenko, Paul A. Lummis, Kimberly Osten, Mina R. Narouz, Kevin G. Stamplecoskie, Tatsuya Tsukuda, Cathleen M. Crudden*

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Abstract:

Over the past decade, atomically precise metal nanoclusters remained the hot topic of research among other nanoscale materials due to fundamental importance and promising applications of metal nanoclusters in healthcare, electronics, catalysis, sensing, and light harvesting. Consistent of several to tens metal atoms (such as Au, Cu, Ag, Pt, or Pd), these ligand-stabilized nanoclusters were found to exhibit molecular-like electronic properties, including discrete, quantized energy levels and size-dependent luminescence, which positioned them aside from metal nanoparticles. Hundreds of thiolate-, phosphine- or alkyne-stabilized metal nanoclusters have been synthesized and characterized nowadays; for many of them exact structures were determined by X-ray crystallography, enabling finding correlations between structures and properties of metal nanoclusters. Recently, it was demonstrated that a different class of organic ligands—N-heterocyclic carbenes (NHCs)—can be successfully used for the preparation of gold nanoclusters, granting them remarkable stability against aggregation and unique photophysical properties.¹⁻² Finding the right synthetic strategy to prepare bimetallic nanoclusters with controlled compositions and sizes is an attractive pursuit for many applied projects because of the superior electronic, optical and catalytic properties of bimetallic nanoclusters as compared with their monometallic analogues due to the synergistic effects. Here we present the summary of our current efforts on the preparation, purification, and characterization of bimetallic NHC-stabilized metal nanoclusters.

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Title: Sterically Protected Bora[1]ferrocenophanes: Enantiopure Monomers for Chiral Metallopolymers

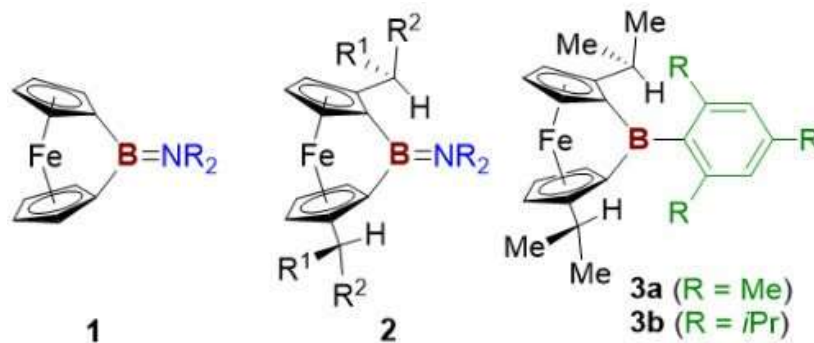
Hridaynath Bhattacharjee,[§] Jianfeng Zhu, and Jens Müller*

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Abstract: 350 words

Synthetic polymers containing metals in the main chain can impose a diverse range of different valuable properties.¹ Such polymers containing three-coordinate boron have the potential for intriguing electronic and optical properties associated with the electron deficient nature of the boron centers.² In principle, boron-containing conjugated polymers should be accessible through ring-opening polymerization (ROP) of boron-bridged [1]ferrocenophanes ([1]FCPs). However, the known boron-bridged [1]FCPs (**1** and **2**) failed to provide well defined polymers.^{3,4} We assumed, their reactivity towards ROP is hampered by π -donating R₂N groups at the bridging boron atom. In this contribution, synthesis and characterization of a new class of bora[1]ferrocenophanes (**3**) with no such electronic stabilization will be discussed. The Tip-substituted [1]FCP **3b** exhibits the most tilted Cp rings among all isolated strained sandwich compounds [$\alpha(\text{DFT}) = 33.3^\circ$] with a measured record value of the bathochromic shift ($\lambda_{\text{max}} = 516 \text{ nm}$).⁵ The Mes-substituted compound **3a** gave polymer upon attempted isolation. Circular dichroism spectroscopy and DFT calculations proved this polymer to be the first polyferrocene with a chiral secondary structure.



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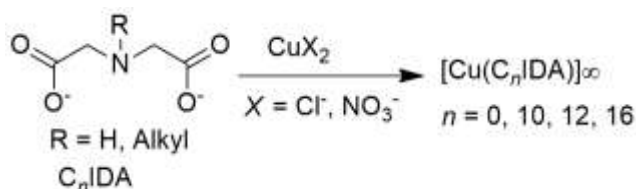
Title: Self-Assembly of 2-Dimensional Coordination Polymers of 2x2 Square Cu Grids using Iminodiacetate Scaffolds

Mohammad Affan,^a Arunima Sarkar,^a John Cull,^a Axel Richard,^a Evan Veryard,^a Emily Corcoran,^a Muralee Murugesu,^b Ilia Korobkov,^b and Jennifer Scott^{a,*}

^aDepartment of Chemistry and Chemical Engineering, Royal Military College of Canada, Kingston, ON, K7K 7B4, Canada, *Jennifer.Scott@rmc.ca, Mohammad.affan@rmc.ca

^bDepartment of Chemistry, University of Ottawa, Ottawa, ON, Canada

Abstract: Studies on self-assembled metal complexes have become an active research field in recent years. Metal-organic frameworks (MOFs) are self-assembled materials driven by suitable metal-ligand coordination, and are widely used in gas separation, the capture of nuclear waste, and magnetism. In this regard, we reported a square-lattice 2x2 Cu sheets $[\text{Cu}_4(\text{C}_1\text{IDA})_4]_\infty$ with ferromagnetic coupling between Cu atoms within the 2D sheets.¹ Herein, we describe the syntheses of other copper(II) complexes of iminodiacetates ($\text{C}_n\text{N}(\text{CH}_2\text{COO})_2 = \text{C}_n\text{IDA}$; where $n = 0, 10, 12, 16$) and characterization by X-ray diffraction, FTIR spectroscopy, elemental analysis, and magnetic susceptibility methods. Although 1D chains of $[\text{CuC}_0\text{IDA}(\text{H}_2\text{O})_2]$ have been previously published,² it can be thermally rearranged to assemble $[\text{Cu}_4(\text{C}_0\text{IDA})_4]_\infty$ as a two-dimensional lattice in which copper centers are bridged by carboxylate units in a distorted square grid. Semi-square voids are generated within the sheet, assembling channels throughout the structure. Variable temperature magnetic susceptibility measurements indicate the presence of weak intrasheet ferromagnetic exchange, as well as antiferromagnetic exchange across the layers. The long-chain $[\text{Cu}_4(\text{C}_n\text{IDA})_4]_\infty$ ($n = 10, 12, \text{ and } 16$) complexes indicate similar structures, however with different magnetic properties.



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Poster

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O-25

IDW 2019 Abstract Submission Form

Title: Free-Base Corrole Ligands as Photosensitizer and Dyes in Oligonucleotides.

Ifrodet Georgees, Zhen Shen, Jean-Paul Desaulniers*

*Department of Chemistry, University of Ontario Institute of Technology, Oshawa, Ontario, L1G 0C5, *Jean-Paul.Desaulniers@uoit.ca*

Abstract:

Simultaneous imaging and enhancement of oligonucleotides therapeutics is important in drug delivery and efficiency of the future oligonucleotide therapeutics. This project is focused on the synthesis of corrole modified oligonucleotides. Corrole ligands are relatively new. Lately, researcher's interests in using these ligands are rising in all fields of chemistry due to their great photophysical properties such as emitting and absorbing light at distinct regions of the visible wavelength spectra, high quantum yields, and high production of reactive oxygen species. Also, their ability to stabilize high oxidation state metals allows for exploration of new metal complexes for therapeutics as well as for metal sensors. The properties of corrole ligands show promising potential in various applications such as photodynamic therapy (PDT), bio-labeling, creating solar cells, organic light-emitting diode (OLED), and cancer treatment studies. In addition, oligonucleotides are being profoundly studied due to their proven therapeutic abilities to directly target specific genes that cause diseases. However, current oligonucleotides in the field show limitations such as low stability, potency, delivery, and off-target effects. In this study, we will chemically modify oligonucleotides and report a cooper-free sonogashira synthesis of a directly coupled corrole molecule by a carbon-carbon bond to the nucleobase of a dimethoxytrityl-protected 5-iodo-2'-deoxyuridine. This new construct may allow for new oligonucleotides bearing interesting biological and biophysical properties.

Presentation Preference: (check one by putting X)

Oral

Poster

O-26

Title: Iron complexes with redox active *o*-phenylenediamide ligands

QiumingLiang, and Datong Song*

Department of Chemistry, University of Toronto, Toronto, Ontario, M5S 3H6

Abstract:

Redox-active ligands have more energetically accessible levels for reduction or oxidation. Their coordination to metal centers induces radical reactivity and electron reservoir behavior, which is often utilized to develop exciting new examples of catalysis. *o*-Phenylenediamides are classic redox-active ligands that form five-membered chelate rings with a large number of transition and main-group elements. It has been established that *o*-phenylenediamides exist in three different redox forms in coordination compounds with a closed-shell dianion, and an open-shell π -radical monoanion and a closed-shell neutral form as intermediate and most oxidized forms, respectively. Herein, we present the synthesis of iron complexes bearing *o*-phenylenediamide ligands and their reactivity, including the reductive coupling of pyridines and the redox chemistry of biomimetic [2Fe2S] clusters.

O-27**IDW 2019 Abstract Submission Form****Title: Synthesis of Iron NHC compounds towards catalytic applications**Jose Jimenez-Santiago, Datong Song**Department of Chemistry, University of Toronto, Toronto, Ontario, M5S 3H6,***jose.jimenez@mail.utoronto.ca***Abstract: 350 words**

Developing catalytic systems based on iron offers a greener alternative to expensive and toxic noble metals¹. N-Heterocyclic carbenes (NHC) have been applied as ancillary ligands due to their unique donating properties to stabilize metal complexes². Our group has made study of chelating NHC ligands with a bifunctional scaffold to enhance the stability of the iron complex and potentially activate substrates by a synergic cooperation between the metal center and the ligand³. The hydrosilylation of carbonyl groups into alcohols is a powerful transformation in the laboratory and industry. Despite the recent advances in this field, the develop of catalytic systems that can activate inexpensive silanes like PMHS under mild conditions and low catalyst loadings is still a challenge⁴. Recently we reported an iron complex that was very active in the catalytic hydrosilylation of ketones using the unreactive PMHS as the hydrosilane and with a catalyst loading of 0.05%⁴. In an effort to get some insights into the reaction mechanism and increase the stability of the catalyst, a series of analogous iron complexes with the formulation FeL₂ (L = bifunctional chelating-NHC) was synthesized and their application towards the hydrosilylation of ketones is presented.

References:

1. Raya-Barón A.; Oña-Burgos P.; Fernández I. *ACS Catal.* **2019**, *9*, 5400
2. Peris E. *Chem. Rev.* **2018**, *118*, 9988.
3. Liang Q.; Janes T.; Gjergji X.; Song D.; *Dalton Trans.* **2016**, *45*, 13872.
4. Liang Q.; Liu N. J.; Song D. *Dalton Trans.* **2018**, *47*, 9889.

Presentation Preference: (check one by putting X)Oral Poster **Abstract should fit into one page.**

Title: Examining the Impact of Water on Phosphine-Free Ruthenium Olefin Metathesis Catalysts

Alexandre Y. Goudreault, Adrian G. Botti, Daniel M. Walden, Stephen Steinman, Carine Michel, Deryn, E. Fogg*

Department of Chemistry and Biomolecular Science, University of Ottawa, Ottawa, ON, K1N 6N5 *dfogg@uottawa.ca

Abstract: 350 words

With its unrivaled versatility and atom economy, olefin metathesis is arguably the most powerful catalytic methodology known for the construction of carbon-carbon bonds. When compared to Pd-catalyzed C-C coupling methodologies, however, catalyst productivity lags far behind, even for “robust” Ru metathesis catalysts. Low catalyst productivity results in part from decomposition of the Ru catalysts by impurities.¹ One such “agent of destruction” that has gone unrecognized is water, the ubiquity of which may play a more significant role in limiting catalyst performance than has been considered to date. A recent report from the Cazin group demonstrated for the first time that water is in fact highly detrimental to metathesis yields.² For PCy₃-stabilized catalysts, the Fogg group established that water, like other donors, accelerates nucleophilic attack by PCy₃ on the [Ru]=CH₂ ligand in the active species.³ For the more highly active *phosphine-free* catalysts, however, the mechanism of decomposition remains unknown. The current work surveys the impact of water on current state-of-the-art catalysts, and provides insights into the mechanism of decomposition for the important second-generation Hoveyda catalyst **HII**. Additionally, the impact of added base on H₂O-mediated decomposition is investigated in reactions involving hydroxide anion.

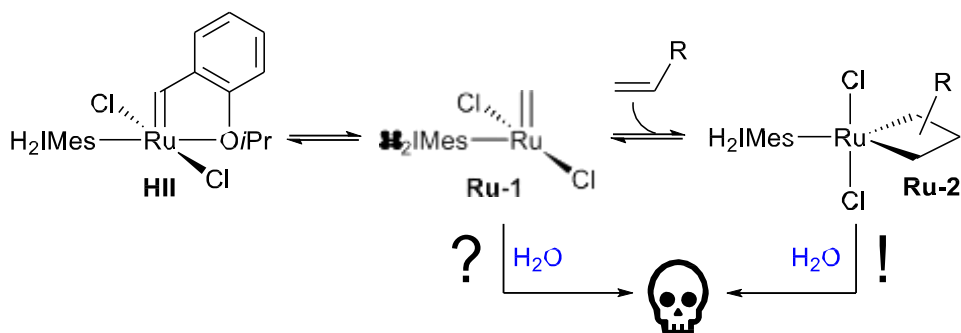


Figure 1. Decomposition of **HII** by H₂O during metathesis.

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- (1) Higman, C. S.; Lummiss, J. A. M.; Fogg, D. E., *Angew. Chem., Int. Ed.* **2016**, *55*, 3552–3565.
- (2) Guidone, S.; Songis, O.; Nahra, F.; Cazin, C. S. J., *ACS Catal.* **2015**, *5*, 2697–2701.
- (3) McClennan, W. L.; Rufh, S. A.; Lummiss, J. A. M.; Fogg, D. E., *J. Am. Chem. Soc.* **2016**, *138*, 14668–14677.

Abstract should fit into one page.

Title: Diverse reactivity of NacNacAl(I) to N-heterocycles

Anton Dmitrienko* and Georgii Nikonov

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Abstract:

Activation of C-H bonds is an atom economic way to access the whole assortment of chemical commodities with the minimal amount of waste produced. Facilitated by d-orbitals, such transformations are no longer a challenge for systems operating on transition metals, so that high yield and selectivity are ensured. On the contrary, activation of small molecules on main-group metals is less developed, as there are only *s* and *p* orbitals that can be used. A finely tuned HOMO-LUMO gap (about 30-40 kcal/mol)^[1] in NacNacAl (NacNac = [ArNC(Me)CHC(Me)NAr]⁻, Ar = 2,6-ⁱPr₂C₆H₃) enables activation of robust H-X, C-F, C-O and E-E (E = S, P) bonds as well as multiple bonds in thiourea and guanidines.^[2] Cleavage of C-H bonds though remains a challenge and requires thermal or catalytic conditions to be applied. For example, NacNacAl can add the C-H bond in Cp*H at 70°C over three days.^[3] Addition of Lewis acidic catalysts also facilitates successful transformations through pre-activation of substrates.^[4,5] Despite a wide scope of substrates screened for C-H activation, little is known about the reactivity of NacNacAl with N-heterocycles. We discovered that such a class of compounds can be eagerly involved in various transformations at room temperature in a manner of a few seconds. Herein, we report the results of selective stoichiometric reactions with 4-picoline, 3,5-lutidine, DMAP, quinoline, and phthalazine, leading to diverse coupling and CH activation products. All products were characterized by spectroscopic and diffraction techniques.

References:

1. Schoeller W.W.; Frey G.D. *Inorg. Chem.* **2016**, *55*, 10947.
2. Chu T.; Nikonov G. I. *Chem. Rev.* **2018**, *118*, 3608
3. Chu T.; Korobkov I.; Nikonov G. I. *J. Am. Chem. Soc.* **2014**, *136*, 9195.
4. Hooper T. N.; Garçon M.; White A. J. P.; Crimmin M. R. *Chem. Sci.* **2018**, *9*, 5435.
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O-30

Title: Highly stable and corrosion resistance electrocatalyst support; dual doped titanium suboxide

Reza Alipour Moghadam Esfahani*, E. Bradley Easton

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Abstract:

Proton exchange membrane fuel cells (PEMFCs) have long been considered as an attractive source of clean power in both automotive and stationary power applications. PEMFCs hold promise as highly efficient technology due to their high energy conversion efficiency, and environmental benefits. Despite the significant advances in PEMFCs technology over the past decades, the high cost of component materials and low stability of electrodes are major barriers preventing/delaying to wide commercialization of PEMFCs. Currently, PEMFC technology relies heavily on Pt-based catalysts to drive the anodic and cathodic reactions. Specially, the nature of the support materials onto which the Pt nano particles (NPs) are embedded can exert a significant influence on Pt electroactivity and durability. Carbonaceous materials have been the most common support of choice for Pt catalyst for PEMFCs applications due to its low cost and high surface area. However, the stability of carbon supported Pt catalysts is a key issue since carbon prone to corrosion under the highly acidic and oxidative operating conditions of a PEMFC. It is known that carbon oxidizes electrochemically to carbon dioxide, and carbon corrosion is detrimental to the long-term performance of a fuel cell. Furthermore, the aggregation and dissolution of Pt NPs occurs readily on carbon supports which causes a significant decay in performance.

In order to overcome the problems associated with the carbon corrosion and weak stability of Pt NPs supported on carbon, we have developed a unique, highly conductive and corrosion-resistance carbon-free support based on dual-doped TiOMoSi (TOMS). The Pt/TOMS showed considerable higher activity towards the oxygen reduction reaction (ORR) compared to the state-of-the-art Pt/C catalyst. Furthermore, the Pt/TOMS catalysts was vastly more durable than Pt/C. The extraordinary catalytic activity and stability of the Pt/TOMS is attributed to the compressive strain effect exerted by the TOMS support on Pt NPs, which is induced by reduced Pt d-bond length due to the strong metallic support interaction (SMSI). This co-functionality of TOMS support underlies the synergic effects between Ti, Mo and Si, which in addition to enhancing electronic conductivity, also enhances the stability to Pt NPs.

O-31

Title: Synthesis of novel POCN pincer complexes of Nickel (II) and their use as hydrosilylation and hydroboration catalysts

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**Chemistry Department, Nazarbayev University, Nur-Sultan, Kazakhstan, 010000,
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The chemistry of unsymmetrical pincer complexes with different side-arm donors, such as PXN, PXS, etc. ($X = C^-, N^-, N$), is known but little studied.^{1,2} Such an unsymmetrical substitution in the side-arm positions of pincer ligands allows for fine-tuning of stability vs. catalytic activity of pincer complexes, often affecting the selectivity of catalytic transformations.

A series of unsymmetrical iminophosphinite POCN pincer Ni(II) complexes, (POCN)NiMe and (POCN)NiL_n(BX₄) (L = CH₃CN, n = 0, 1; X = F, Ph, C₆F₅), have been developed and subjected to catalytic hydrosilylation of alkenes, aldehydes and ketones and catalytic hydroboration of carbonyl compounds.³ The stoichiometric reactivity of (POCN)NiMe and (POCN)Ni(BF₄) with PhSiH₃ and HBPin suggests that catalytic reactions proceed via the hydride intermediate (POCN)NiH. With regard to reactions with HBPin, efficient and mild hydroboration of a variety of carbonyl compounds, including the highly chemoselective hydroboration of benzaldehyde in the presence of other common potent reductive functional groups, such as alkenes, alkynes, esters, amides, nitriles, nitro compounds and even ketones, were demonstrated for (POCN)NiMe.³ We also report the first example of base metal catalyzed hydroboration of amides, including mild direct hydroborative reduction of primary and secondary amides to borylated amines.³

References:

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2. Choi, J., MacArthur, A. H. R., Brookhart, M., Goldman, A. S. *Chem. Rev.* **2011**, *111*, 1761.
3. Gudun, K. A., Segizbayev, M., Adamov, A., Plessow, P. N, Lyssenko, K. A., Balanay, M. P., Khalimon, A. Y. *Dalton Trans.* **2019**, *48*, 1732.

0-32

Title: Ligand Design by additive Ligand Acidity Constants

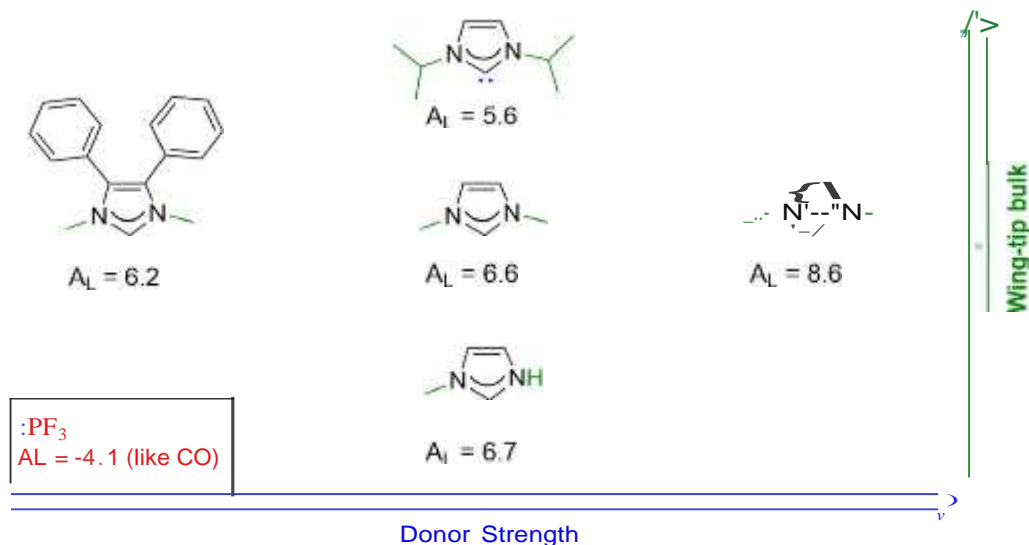
Molly M. H. Sung, Sofia Jdanova, Prof. Demyan E. Prokopchuk, and Prof. Robert H. Morris*

Department of Chemistry, University of Toronto, 80 St. George St, Toronto, Ontario M5S 3H6; molly.sung@mail.utoronto.ca

Abstract:

The acidity of metal hydrides is a key determinant of the suitability of M-H catalysts, particularly those used for hydrogenation reactions. In 2014, our group reported a simple method of predicting the acidity of metal-hydrides using additive ligand acidity constants (A_L)^{1,2} within 3 pKa units. We have subsequently shown that density functional theory can be used to support the additive method by demonstrating the linear correlation between ligands and pK_a .³ Herein, we discuss how OFT can be used to predict the A_L of additional ligands^{1,3} and how this method can be used to explain reaction mechanisms, geometry, and reactivity of Ru pincer complexes.^{1,5}

- [1] R. H. Morris, *J. Am. Chem. Soc.* **2014**, *136*, 1948-59.
- [2] R. H. Morris, *Chem. Rev.* **2016**, *116*, 8588-8654.
- [3] M. M. H. Sung, S. Jdanova, R. H. Morris, *J. Organomet. Chem.* **2019**, *880*, 15-21.
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- [5] M. M. H. Sung, D. E. Prokopchuk, R. H. Morris, *Dalton Trans.* **2019**, DOI10.1039/C9DT03143J.



O-33

Title: Curable Hybrid Materials For Corrosion Protection of Steel: Development & Application of UV Cured 3- Methacryloxypropyltrimethoxysilane Derived Coating

KevinScotland, Andrew Vreugdenhil*

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Abstract:

This work describes the synthesis and characterization of a UV crosslinked sol-gel comprised of 3-methylacryloxypropyltrimethoxysilane (MaPTMS) and tetraethoxysilane (TEOS) using isopropanol as a co-solvent and stoichiometric amounts of HNO₃ (1 M) as the acid catalyst. MaPTMS is often considered difficult to hydrolyze and keep solubilized. We have demonstrated that the use of isopropanol as the co-solvent and HNO₃ leads to rapid and complete hydrolysis of the material within 10 minutes of stirring at room temperature. Results show that the starting material is completely consumed within a few minutes compared to previously employed methods requiring up to 14 days of stirring. We also demonstrate that the use of this solvent/catalyst combination along with heating of the sol at 60 ° C for 10 minutes leads to extensive condensation and the formation of long open chain siloxane networks that can be readily crosslinked via a photo-initiated UV curing process with high efficacy. This results in a dense durable coating, that can provide corrosion protection for low carbon steel substrates for over 24 hours of immersion in dilute Harrison's solution. When crosslinked, this durable material can then be used to encapsulate corrosion inhibiting additive such as polyaniline, marking the first occasion where this material can be encapsulated in a crosslinked sol-gel material .

P-1

IDW 2019 Abstract Submission Form

Title: The Electrochemical Properties of *N*-Heterocyclic Carbene Stabilized Self-Assembled Monolayers on Gold

Dianne S. Lee, Robert M. Mayall, Christene A. Smith, Mina R. Narouz, Alexander S. Hyla, Cathleen M. Crudden, Viola I. Birss.

*Department of Chemistry, Queen's University, Kingston, Ontario, K7L 2S8, *e-mail: dianne.lee@queensu.ca*

Abstract: 350 words

Self-assembled monolayers (SAMs) have served as an inexpensive surface technology for uses in surface protection, nanoscience, and biosensing.^{1,2} The use of *N*-heterocyclic carbenes (NHCs) in place of commonly used thiols were shown to generate SAMs with excellent stability to temperature and pH extremes, and external oxidants.¹ The stability imparted by NHCs allows for the potential use of SAMs in surface technology and commercial applications. Despite their remarkable stability, it has been reported that NHC SAMs are unstable towards negative potentials beyond -0.3V.¹ I will discuss our recent investigations of the electrochemical properties and stability, to under highly reducing conditions, of NHC-based SAMS and their potential applications in the field of fuel cells, catalysis and sensing.

References:

1. Crudden, C. M. *et al. Nat. Chem.* **2014**, 6, 409–414.
2. Crudden, C. M. *et al. Nat. Commun.* **2016**, 7, 1–7.

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Oral

Poster **X**

Abstract should fit into one page.

IDW 2019 Abstract Submission Form

P-2

Title: Metal-mediated C-C Bond Formation of Organofluorine Compounds

Luana L. T. N. Porto and R. Tom Baker*

Department of Chemistry and Biomolecular Sciences and CCRI, University of Ottawa, Ottawa, Ontario, K1N 6N5 lport076@uottawa.ca

Abstract: 350 words

Fluorine's high electronegativity and small size bestows unique and advantageous physical and chemical effects on its compounds. The inclusion of fluorine and fluoroalkyl groups into organic molecules enhances the bioactivity and modulates pharmacokinetics, thus representing an important class of targets for medicinal chemistry. Organofluorine compounds have a wide range of other uses such as solvents, refrigerants and polymers. This work describes two different projects: in the first part our goal is to examine ligand effects on the formation of perfluorometallacycles from Ni(0) and chlorotrifluoroethylene (CTFE) and perfluoromethylvinyl ether (PMVE) with a view to preparing new C4 refrigerant candidates.¹ We found that the reactivity of CTFE with zerovalent Ni complexes depends on the electronics of the PX₃ ligand (where X= OⁱPr, O-o-tolyl or Ph). While phosphite ligands yielded first 3- and then 5-membered metallacycles, the phosphine example proceeded rapidly to the NiCl-perfluorovinyl complex. Moreover, regioselective metallacyclopentane formation was shown to be reversible. In contrast, regioselective metallacyclopentane stereoisomers from PMVE could be isolated with smaller P ligands, whereas PPh₃ stopped at the 3-membered metallacycle. For the second project we aim to investigate the fundamental chemistry of Cu fluoroalkyl complexes and their transfer of R^F to organic electrophiles.² We isolated three Cu fluoroalkyl complexes from Cu-H and PMVE with one NHC, two PPh₃ or three P(OEt)₃ ligands coordinated to the Cu. We were then able to transfer the R^F group from the NHC complex to organic electrophiles (Eq. 1). Currently we are working on DFT studies to help us better understand the ligand dependence on transfer efficiency of this R^F group and others to several organic electrophiles.



References

- ¹ A. J. Sicard & R. T. Baker, PCT application filed 2017; published as WO 2018/039795.
- ² N. O. Andrella, K. Liu, B. M. Gabidullin, M. Vasiliu, D. A. Dixon & R. T. Baker *Organometallics* **2018**, *37*, 422-432.

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Oral

Poster **X**

P-3

IDW 2019 Abstract Submission Form

Title: New Pathways to p-Block Adamantyls

Andrew Broomfield, Fioralba Taullaj, and Ulrich Fekl*

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**ulrich.fekl@utoronto.ca*

Abstract: 350 words

Adamantane is the simplest of the diamondoid molecules. Its lipophilicity, biocompatibility, and general chemical inertness lead it to be found in many synthetic drug targets, where incorporation of adamantyls has increased hydrophobic properties. Also, the adamantyl group has found many uses in catalyst design due to its exceptional steric bulk.

Despite many useful applications of adamantyls, methods towards making bonds between metals or metalloids and the adamantyl group are under-explored. This is often owed to the general instability of traditional adamantyl anion sources, impeding expansion into this field of work significantly.

Previous work in the group,¹ has allowed for the isolation and highly reproducible synthesis of a stable adamantyl anion source; di-adamantyl zinc. This source has allowed access to several novel adamantyl complexes of gold, bismuth, mercury, and platinum.

Building on this work, several new adamantyl compounds have been synthesized, and partially characterized. Tris(2-adamantyl)bismuth(III), indium 2-adamantyl species and di-2-adamantyl boron bromide will be presented, among others. Several of the presented species rare examples of homoleptic adamantyl metal species.

References: 1. Armstrong, D.; Taullaj, F.; Singh, K.; Mirabi, B.; Lough, A. J.; Fekl, U. *Dalton Trans.* **2017**, *46*, 6212.

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Poster X

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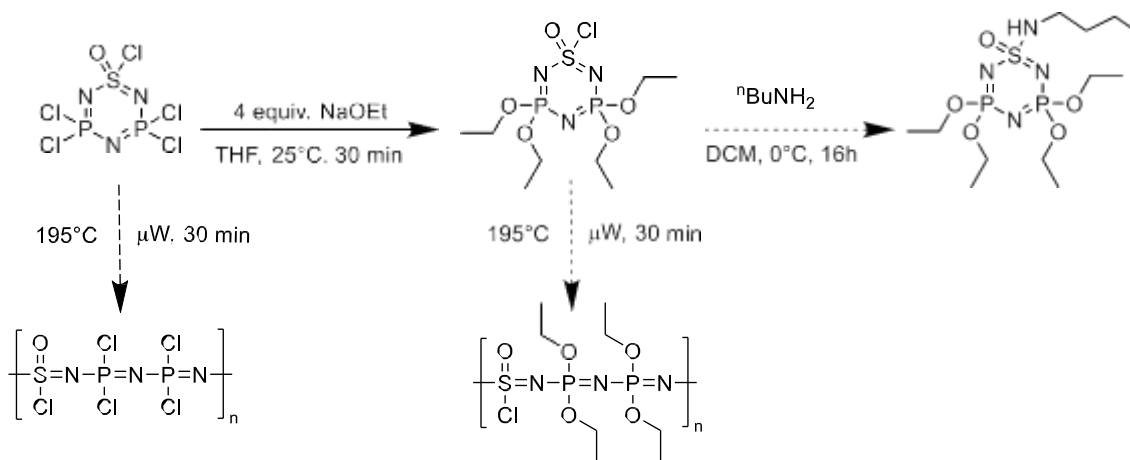
Title: Alternate Routes for Polymerization of Thionylphosphazenes

Rachele Carafa, Daniel A. Foucher* and Andrew R. McWilliams*

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daniel.foucher@ryerson.ca, amcwilli@ryerson.ca

Abstract:

One class of heterophosphazenes that has been extensively researched is the thionylphosphazene, which consists of a sulfur(VI)-nitrogen-phosphorus backbone and is a derivative of the sulfur(IV) thiophosphazene with an oxygen atom bonded to the sulfur outside of the ring skeleton.¹ The overall main goal of this study is to use poly(thionylphosphazenes) as a support for anti-bacterial side chains with a controlled loading. Ideally, leaving the sulfur-chlorine bond intact should allow for polymerization to occur post-substitution and act as an ideal quaternization site for future biological applications. To create the model compound for the desired poly(thionylphosphazene) quaternization site, the cyclic thionylphosphazene underwent an S_N2 substitution reaction with sodium ethoxide to substitute the P-Cl bonds followed by a substitution reaction with varying amounts of n-butylamine at the S-Cl site. Attempting to investigate alternate routes to polymerize thionylphosphazenes, ring-opening polymerization of both the cyclic- and tetrasubstituted thionylphosphazenes were performed using microwave irradiation.

**References**

1. Gates, D. P.; McWilliams, A. R.; Manners, I. *Macromolecules* **1998**, 9297 (31), 3494.

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X

IDW 2019 Abstract Submission Form

P-5

Title: A Reconfigurable, Dual-Output Molecular Logic Gate

Lavinia A. Trifoi, Nicholas P. Dogantzis, Gregory K. Hodgson, Stefania Impellizzeri*

*Department of Chemistry and Biology, Ryerson University, Toronto ON, Canada M5B 2K3, *simpellizzeri@ryerson.ca*

Abstract:

Boron-dipyrromethene (BODIPY) are molecular dyes known for their outstanding fluorescent properties, including their robust nature, high fluorescence quantum yield and easy modulation with ancillary residues. This project is aimed at synthesizing a probe with tunable emission for the construction of a molecular logic gate with reconfigurable single or dual output capability. The system is based on a boron-dipyrromethene (BODIPY) skeleton coupled with *p*-dimethylaminobenzaldehyde. The behaviour of the molecular logic gate can be easily investigated in solution with fluorescence spectroscopy, and the optical output (fluorescence) can be monitored in one (green) or two (green and red) channels. Remarkably, one (INHIBIT) or two (INHIBIT and IMPLY) functionally integrated logic functions are obtained, depending on the solvent of choice. Reconfiguration from single to dual output is thus expected by operating the system in acetonitrile (single output) or toluene (dual output), respectively. The same molecular system, immobilized onto a mesoporous silica film, allows for Set/Reset of the logic operator in a reversible fashion. In fact, immersion of the solid sample in acid wash, with consequent protonation and fluorescence modulation red↔green, could be easily reversed by immersing the film in a base bath, and vice versa.

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P-6

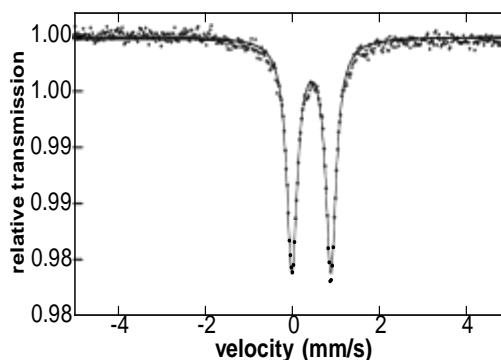
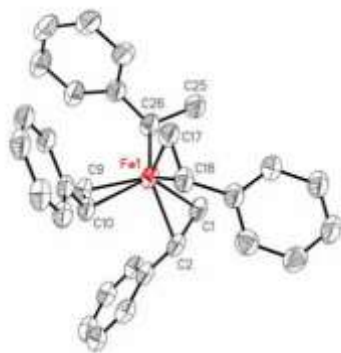
IDW 2019 Abstract Submission Form

Title: The TMEDA-Effect in Iron-Catalyzed Hydromagnesiation of Styrene Derivatives

Peter G. N. Neate, Mark D. Greenhalgh, William W. Brennessel, Stephen P. Thomas, and Michael L. Neidig*

Department of Chemistry, University of Rochester, Rochester, New York, 14627-0216,
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Iron-catalyzed hydromagnesiation of styrene derivatives offers a rapid and efficient method to generate the products of formal hydrofunctionalization, also providing an alternative to cross-coupling for C-C bond formation. Whilst iron-catalyzed methodologies exist for the hydromagnesiation of terminal alkenes, internal alkynes and styrene derivatives, the underlying mechanisms of catalysis remain largely undefined.¹⁻³ Recently, we reported the first detailed mechanistic study of this class of reactions with the bis(imino)pyridine iron-catalyzed hydromagnesiation of styrene derivatives.⁴ A follow-up to the original method demonstrated that the reaction system could be simplified, using TMEDA in place of the bis(imino)pyridine ligand.⁵ As TMEDA is widely used in a variety of iron-catalyzed reactions, as well as the same major species not being accessible, the presented work details current insights into the role TMEDA plays and the species accessible under these alternative catalytic reactions. While apparently not bound to the iron center during the reaction, TMEDA allows for the selective generation of catalytically active styrene-stabilized iron zero species. One such species has previously been identified to form during in the bis(imino)pyridine-iron-catalyzed system, resulting from displacement of the tridentate bis(imino)pyridine ligand.



References:

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2. Ilies, L.; Yoshida, T.; Nakamura, E. *J. Am. Chem. Soc.* **2012**, *134*, 16951.
3. Greenhalgh, M. D.; Thomas, S. P. *J. Am. Chem. Soc.* **2012**, *134*, 11900.
4. Peter G. N. Neate, Mark D. Greenhalgh, William W. Brennessel, Stephen P. Thomas, and Michael L. Neidig *J. Am. Chem. Soc.* **2019**, *141*, 10099.
5. Jones, A. S.; Paliga, J. F.; Greenhalgh, M. D.; Quibell, J. M.; Steven, A.; Thomas, S. P. *Org. Lett.* **2014**, *16*, 5964.

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P-7

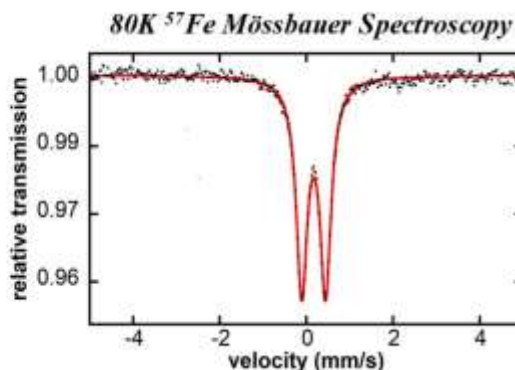
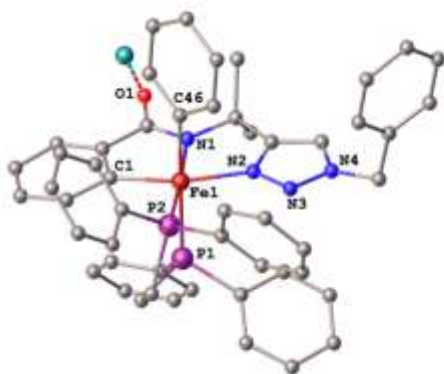
Title: Elucidation of Key Iron Intermediates in a Triazole-Directed Iron-Catalyzed C-H Allylation and Comparison to Related Systems

JoshuaDeMuth, Theresa Boddie, Stephanie Carpenter and Michael Neidig*

Department of Chemistry, University of Rochester, Rochester, New York, 14627,
jdemuth3@ur.rochester.edu

Abstract:

Recent developments in iron-catalyzed C-H functionalizations which use directing groups has led to facile organic transformations. However, the lack of fundamental understanding of the mechanisms and the key iron species involved in these catalytic transformations hinders the development of these systems. Focusing on a triazole-assisted C-H allylation system, this investigation reports the isolation and characterization of the active iron species involved using a multi-spectroscopic approach including freeze-trapped ^{57}Fe Mössbauer spectroscopy and single-crystal X-ray diffraction. These studies identify a low-spin iron(II) C-H activated intermediate which with an additional equivalent of PhMgBr generates a cyclometalated iron(II) phenyl species. Complementary reactivity studies reveal that the C-H activated complex selectively generates C-H allylated product with excess nucleophile, while the cyclometalated intermediate favors the formation of a C-H arylated product. A recently published investigation of a triazole-assisted iron-catalysis designed exclusively for C-H arylation revealed a catalytic mechanism which cycles through analogous iron intermediates. Additional reactivity studies subjecting the activated intermediates from both systems to the oxidant used in their counterparts reveals that both systems are capable of selective C-H allylation and arylation. Lastly, further extension of these studies to an iron-catalyzed C-H amination system will also be presented.



Reference:

1. Boddie, T. E.; Carpenter, S. H.; Baker, T. M.; DeMuth, J. C.; Cera, G.; Brennessel, W. W.; Ackermann, L.; Neidig, M. L., *J. Am. Chem. Soc.* **2019**, *141*, 12238.

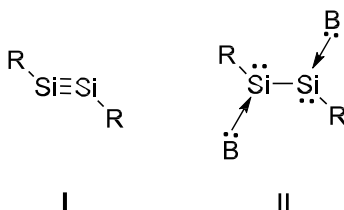
Title: New base stabilized disilylene and its chemical properties

Aliona Baradzenka, Georgii Nikonov*

Department of Chemistry, Brock University, 1812 Sir Isaac Brock Way, St. Catharines,
Ontario L2S 3A1, *gnikonov@brocku.ca

Abstract: 350 words

Silicon analogues of alkynes have drawn much interest in the last two decades¹. Shortly after the first examples of disilyne **I**²⁻³ a new Lewis base stabilized disilylene **II**⁴ was reported. The relatively low lying LUMO of disilyne **I** allows for an exothermic transformation to **II** with the addition of a donating ligand⁴. We have found an P,N platform that can stabilize the dimeric Si(I) species. As such, a novel disilylene of the general form **II** was synthesized and its reactivity will be presented herein.

**References:**

1. Guo, J.-D.; Sasamori, T., *Chem. Asian J.*, **2018**, *13*, 3800.
2. Sekiguchi, A.; Kinjo, R.; Ichinohe, M., *Science*, **2004**, *305*, 1755.
3. Wiberg, N.; Vasisht, S. K.; Fischer, G.; Mayer, P., *Z. Anorg. Allg. Chem.* **2004**, *630*, 1823.
4. Wang, Y.; Xie, Y.; Wei, P.; King, R. B.; Schaefer, H. F.; von R. Schleyer, P.; Robinson, G. H., *Science* **2008**, *321*, 1069.

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Poster **X**

Abstract should fit into one page.

P-9

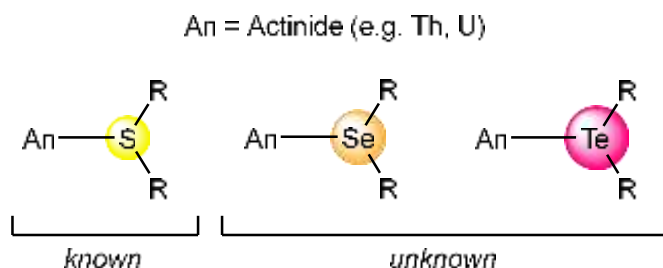
Title: Ligand Design to Promote Interactions Between Actinide Metals and Soft Neutral Chalcogen Donors

Novan A. G. Gray and David J. H. Emslie*

*Department of Chemistry and Chemical Biology, McMaster University, Hamilton, Ontario, L8S 4M1. *emslie@mcmaster.ca*

Abstract:

The actinide metals demonstrate an appreciable capacity for covalent interactions with ligands compared to the lanthanides as a result of the greater radial extension of the valence $5f$ -orbitals and therefore have a higher propensity for bonding to soft donors.¹ Actinide complexes of soft-donor ligands have been a field of interest for the past few decades and serve to broaden our understanding of f -metal–ligand covalency, in addition to holding potential implications for nuclear waste extraction and reprocessing.^{1,2} Neutral chalcogenoether interactions with actinides have been structurally characterized in the past, with a small handful of SR_2 donor complexes known.³ However, there are no known examples of heavy chalcogenoether (Se, Te) complexes for any $5f$ -element. This poster will present our recent progress towards the synthesis of actinide complexes featuring interactions with soft neutral chalcogen donors.



¹ T. Dumas et al. *Phys. Chem. Chem. Phys.* **2016**, *18*, 2887–2895.

² A. J. Gaunt, S. D. Reilly, A. E. Enriquez, B. L. Scott, J. A. Ibers, P. Sekar, K. I. M. Ingram, N. Kaltsoyannis, and M. P. Neu, *Inorg. Chem.*, **2008**, *47*, 29–41.

³ B. Vidjayacoumar, S. Ilango, M. J. Ray, T. Chu, K. B. Kolpin, N. R. Andreychuk, C. A. Cruz, D. J. H. Emslie, H. A. Jenkins, and J. F. Britten, *Dalton Trans.*, **2012**, *41*, 8175–8189, and references therein.

P-10

Title: Kagome Lattice-Type Arrangement of N-heterocyclic Carbene on Au (111)

IshwarSingh, Ryan Groome, Alex Inayeh, Alex Veinot, Cathleen M. Crudden* and Alastair McLean*

Chemistry Department, Queen's University, Kingston, ON, K7L 2S8,
**cruddenc@chem.queensu.ca*

Abstract:

Recently, *N*-heterocyclic carbenes (NHCs) have gained popularity as alternative anchors for surface modification of gold (Au) as they offer features making them an ideal choice for surface modifications. However, there has not been much research deducing the self-organization process on surfaces. This aspect has only been studied in three separate reports, where surface-assisted formation of bis-NHC-Au complexes has been observed.¹ Herein, we report formation of super-structures (Kagome lattices) with six-fold symmetry on Au(111) after reaction with NHCs. The presence/absence of these features is highly dependent on the *N,N*-substituents on the NHCs.

References:

(1) Smith, C. A.; Narouz, M. R.; Lummis, P. A.; Singh, I.; Nazemi, A.; Li, C. H.; Crudden, C. M. *N*-Heterocyclic Carbenes in Materials Chemistry. *Chem. Rev.* **2019**, *119* (8), 4986–5056.

P-11

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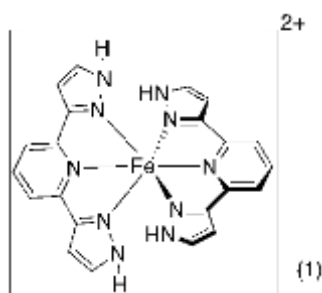
Title: The Synthesis and Study of Fe(II) Spin Crossover Complexes as a Potential Temperature Probes and PARACEST Agents for Magnetic Resonance Imaging

Paria Shahbazi and Melanie Pilkington*

*Department of Chemistry, Brock University, 1812 Sir Isaac Brock Way, St. Catharines, ON, L2S 3A1, *mpilkington@brocku.ca*

Abstract: 350 words

Spin crossover (SCO) transitions involving octahedral $3d^n$ transition metal complexes (d^4 - d^7) that switch in the solid-state from low-spin (LS) to high-spin (HS) are promising systems for attaining molecular bistability that have attracted considerable current attention in recent years [1]. In such systems, SCO is typically accomplished via the application temperature pressure or light, and is often accompanied by a change in color and magnetic properties. Furthermore, SCO properties can be optimized in a rational manner by tuning the molecular structures of the complexes, which renders them suitable for applications as thermal sensors and light switches. While the chemistry and physics of SCO materials continues to be intensively studied in the solid-state, less attention has been paid to this phenomenon in solution. Our goal is to develop encapsulated Fe^{II} complexes that undergo SCO in aqueous solution within the biological window, and to investigate their suitability as temperature probes and/or Chemical Exchange Saturation Transfer, or PARACEST agents for MRI. As the first step towards achieving these goals, the synthesis and magnetic studies of a family of Fe^{II} complexes (**1**) will be presented.



References:

1. Gimenez-Lopez M.C.; Clemente-Leon M.; M.; Gimenez-Saiz C. *Dalton Trans*, **2018**, 47, 10453.

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Abstract should fit into one page.

P-12

IDW 2019 Abstract Submission Form

Title: A Look at the First Structurally Characterized Platinum Adamantyls

Fioralba Taullaj, and Ulrich Fekl*

*Department of Chemical and Physical Sciences, University of Toronto Mississauga, Mississauga, ON, L5L 1C6. *Ulrich.Fekl@utoronto.ca*

Adamantane, the simplest diamondoid molecule, shows inherent chemical stability and structural rigidity, therefore providing a unique basis for new ligands and materials. Interest in adamantane in the organometallic community stems from its resistance to β -elimination and unique steric bulk. It is this characteristic that led to the synthesis of homoleptic adamantyl titanium¹, chromium² and iron³ complexes. Unfortunately, progress in metal adamantyl chemistry has been limited due to the difficulty of synthesis of adamantyl anions, and difficulty associated with characterization of these highly insoluble complexes. Here we present the use of our 2-Ad₂Zn precursor⁴ in the synthesis and characterization of the first adamantyl platinum complexes⁵. Starting from (COD)Pt(2-Ad)Cl, ligand substitution, transmetallation, and oxidative addition reactions have enabled the preparation of the first adamantyl platinum complexes of Pt(II), as well as now the first Pt(IV) adamantyl complexes. The adamantyl ligand has an expectedly strong electronic and steric effect in both the Pt(II) and Pt(IV) complexes, as is evident in the crystal structures presented.



References:

1. Bergman, R. G. *et al*, *JACS* **1997**, *119*, 5269.
2. Bochmann, M.; Wilkinson, G.; Young, G. B. *J. Chem. Soc., Dalton Trans.* **1980**, *10*, 1879.
3. Fürstner, A. *et al*. *Angew. Chem. Int. Ed.* **2017**, 10108.
4. Armstrong, D.; Taullaj, F.; Singh, K.; Mirabi, B.; Lough, A. J.; Fekl, U. *Dalton Trans.* **2017**, *46*, 6212.
5. Taullaj, F.; Armstrong, D.; Datta, S.; Lough, A.; Fekl, U. *Eur. J. Inorg. Chem.* **2019**, *9*, 1288.

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P-13

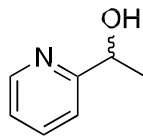
The Employment of mpmH for the Discovery of 3d Polymetallic Clusters

Parisa Abbasi, Fatma Hadi, Theocharis. C. Stamatatos* and Melanie Pilkington*

Department of Chemistry, Brock University, St. Catharines, Ontario, L2S 3A1
, * mpilkington@brocku.ca

Abstract:

Single-Molecule Magnets (SMMs) are coordination complexes of paramagnetic metal ions that display slow relaxation of magnetization below their blocking temperatures. In recent years, these compounds have been intensively researched for their potential applications as memory storage devices. The introduction of chirality into polynuclear 3d-clusters provides new opportunities for the preparation of dual-property compounds with magnetic and/or multiferroic properties. Recently, we have developed a synthetic strategy for the assembly of transition-metal clusters by employing first-row transition metals together with small potentially chiral, pyridyl alkoxide ligands such as (**1**).^{1,2} In this respect, magneto-structural studies of select cluster complexes prepared from the potentially chiral, bridging chelating ligand (**1**) together select first-row transition metals will be presented.



mpmH (**1**)

References:

1. Abbasi P.; Quinn K.; Alexandropoulos D. I.; Damjanovic M.; Wernsdorfer W.; Escuer A.; Mayans J.; Pilkington M.; and Stamatatos Th. C. *J. Am. Chem. Soc.* **2017**, *139*, 15644.
2. Pham A. T.; Abbasi P.; Delle Monache G.; Mazarakioti E. C.; Rawson J. M.; Stamatatos Th. C.; Pilkington M. *Polyhedron*, **2019**, *170*, 34.

Title: Multi-Metallic Colour-Tunable Electrochromic “Smart” Materials

RanaAhmad, Nadia O. Laschuk, Jade Poisson, E. Bradley Easton*, Olena V. Zenkina*

*Department of Chemistry, Ontario Tech University, Oshawa, Ontario, L1G 0C5,
rana.ahmad1@ontariotechu.net*

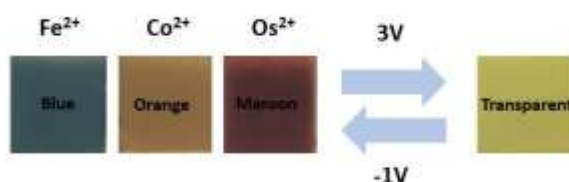
Abstract:

We present new strategies for preparing multi-metallic, multi-chromatic electrochromic materials (ECMs) that are color-tunable, display long term stability, and have very fast switching speeds.

Here we present the rational design of molecularly defined mono, bi and tri-metallic electrochromic films. X-ray Photoelectron Spectroscopy (XPS) and energy-dispersive X-ray analysis confirm homogenous distribution of molecular units within the surfaces and the chemical nature of the immobilization. The designed materials were able to switch through a variety of colours (blue, maroon, orange and transparent) depending on the applied potential. Importantly, the ability to address individual metal centers allow the unique property of sequential switching between multiple color states within one film. In-depth kinetics of the electron-transfer were studied for all materials under investigation.

These devices are produced through monolayer assembly of different transition-metal complexes on a novel high surface area indium tin oxide (ITO) nanoparticle substrate.¹ Each transition-metal complex was designed using 4'-(pyridin-4-yl)-2,2':6',2''-terpyridine ligands which were linked to the substrate covalently through a siloxane bond.² Different deposition strategies allow the user to finely tune the ratios between the metal complexes on the surface. These materials demonstrate superior coloration efficiency.

Additionally, the ECMs showed promise as energy storage materials due to their ability to achieve high energy and charge densities comparable to batteries or supercapacitors.



1. Allan, J. T. S.; Quaranta, S.; Ebralidze, I. I.; Egan, J. G.; Poisson, J.; Laschuk, N. O.; Gaspari, F.; Easton, E. B.; Zenkina, O. V., Terpyridine-Based Monolayer Electrochromic Materials. *ACS Applied Materials & Interfaces* **2017**, *9* (46), 40438-40445.

2. Laschuk, N. O.; Ebralidze, I. I.; Poisson, J.; Egan, J. G.; Quaranta, S.; Allan, J. T. S.; Cusden, H.; Gaspari, F.; Naumkin, F. Y.; Easton, E. B.; Zenkina, O. V., Ligand Impact on Monolayer Electrochromic Material Properties. *ACS Applied Materials & Interfaces* **2018**, *10* (41), 35334-35343.

P-15

Trying to Grow Crystals of Divalent Tin Compounds: Getting only Powders or Low-Dimensional Crystals

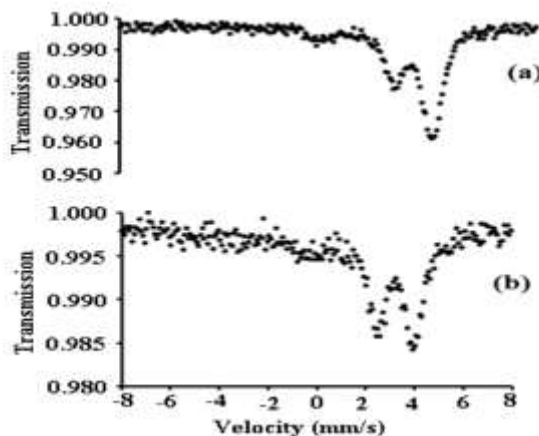
GeorgesDénès^{1,*}, Abdualhafed Muntasar¹, M. Cecilia M. Madamba¹, Abdelatif Bensegueni² and Hocine Merazig²

¹Laboratory of Solid State Chemistry and Mössbauer Spectroscopy, Department of Chemistry and Biochemistry, Concordia University, 7141 Sherbrooke Street West Montreal, Qc H4B 1R6, Canada, [*georges.denes@concordia.ca](mailto:georges.denes@concordia.ca)

²Unité de Recherche de Chimie de l'Environnement et Moléculaire Structurale CHEMS, Université des Frères Mentouri de Constantine, Constantine. Algeria.

Abstract:

Crystal growth can be very frustrating. While some species grow easily in nice three-dimensional crystals, others grow in the form of very thin plates, needles, or they stubbornly refuse to grow at all beyond the tiny size of powdery particles. A large number of divalent tin compounds have been investigated in our laboratory over several decades, with various degrees of success in growing crystals. Most of the crystals obtained are one- or two-dimensional. The lack of good quality single crystals makes it challenging to determine the crystal structure of the compounds. In such cases, the combined use of X-ray powder diffraction and Mössbauer spectroscopy has been very helpful. For example, in the case of α -PbSnF₄ that gives only large very thin brittle sheets. The variation of the asymmetry of the Mössbauer doublet with the orientation of the sheet sample in the γ -ray beam (figure) makes it possible to determine the direction of the tin lone pair in the unit-cell, and contribute to solving the crystal structure. The divalent tin doublet shows that tin is covalently bonded and has a stereoactive lone pair. This was essential in determining disordered structures such as PbSn₄F₁₀ and high temperature γ -PbSnF₄, and non-stoichiometric M_{1-x}Sn_xF₂, and also the $\mu\gamma$ -PbSnF₄ nanophase. The small peak at ca. 0 mm/s shows surface oxidation of the particles, too little to be detected by X-ray diffraction.



P-16

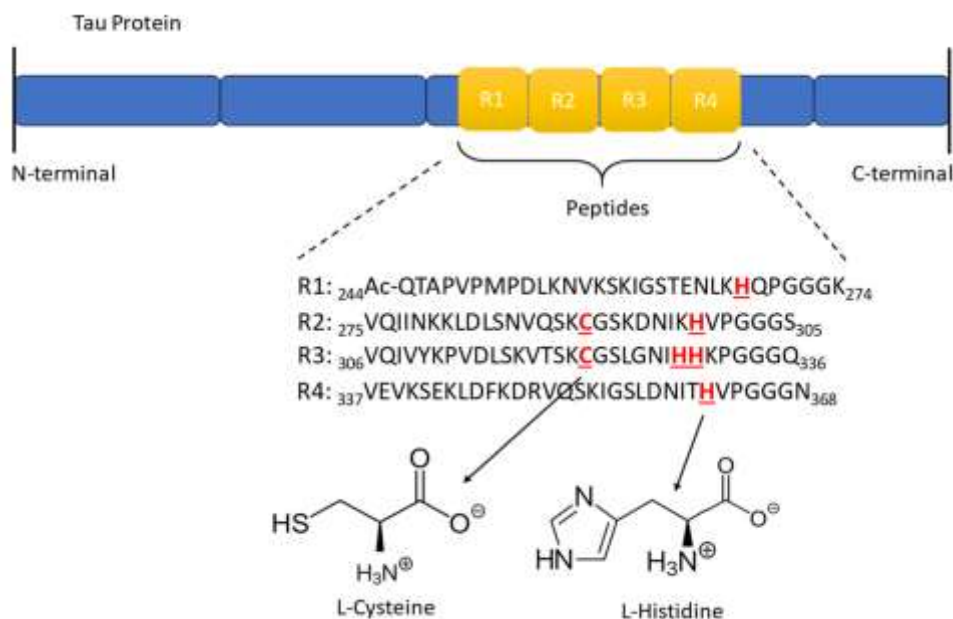
Learning About Bioinorganic Chemistry of the Brain: Cu(II) to Cu(I) Reduction and Formation of Reactive Oxygen Species

Camilla Golec,^a Shaelyn Mortensen,^a Saba Anwar,^b Sanela Martić^{a*}

^a Department of Forensic Science, Trent University, Peterborough, Ontario, Canada, K9L 0G2

^b Department of Chemistry, Oakland University, Rochester, Michigan, USA, 48309
camillagolec@trentu.ca, sanelamartic@trentu.ca

Biologically relevant metal ions contribute to normal cellular function, but metal ion dyshomeostasis may lead to diseases.¹ For example, in the presence of a biologically reducing agent, such as ascorbic acid, a metal ion-catalyzed formation of the reactive oxygen species (ROS) occurs. It is a key aspect in the Alzheimer's disease mechanism.¹ However, the mechanism of this process remains poorly identified. Herein, we evaluated the role of Cu(II)/(I) on the formation of ROS in the presence of brain related tau peptides seen below.



Several solution-based spectroscopic methods and mass spectrometry were used to study this system. Ascorbic acid UV-vis spectroscopy revealed its oxidation in the presence of Cu(II)/(I).² The Cu(II) to Cu(I) reduction was monitored by bathocuproine disulfonate (BC) ligand coordination to Cu(I), and the colourimetric Cu(I)BC₂ complex was detected by UV-vis. Fluorescence spectroscopy was used for detection of hydrogen peroxide and hydroxyl radical, both of which were formed when ascorbic acid and metal ion were present. The peptides modulated the levels of ascorbic acid oxidation, and ROS formed, which will be described.

References:

1. Faller P., Hureau C. *Chem. Eur. J.* **2012**, *18*, 15910.
2. Jiang D., Li X., Liu L., Yagnik G. B., Zhou F., Tabner B. J., Allsop D. J. *Bio. Chem.* **2014**, *289*, 12052.

P-17

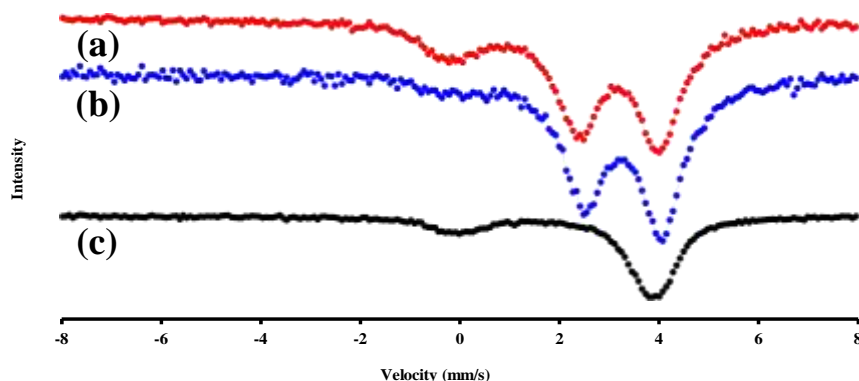
Tin Lone Pair Stereoactivity and Bonding Type in Tin(II) Chloride Fluorides

Abdualhafed Muntasar¹, Georges Dénès^{1,*}, M. Cecilia M. Madamba¹, Korzior Tam¹,
Abdelatif Bensegueni² and Hocine Merazig²

¹Laboratory of Solid State Chemistry and Mössbauer Spectroscopy, Department of Chemistry and Biochemistry, Concordia University, 7141 Sherbrooke Street West Montreal, Qc H4B 1R6, Canada, *georges.denes@concordia.ca

²Unité de Recherche de Chimie de l'Environnement et Moléculaire Structurale CHEMS, Université des Frères Mentouri de Constantine, Constantine. Algeria.

Tin(II) is known to bind to fluorine by means of covalent bonding. Bonding to chlorine is also often covalent, however bonding in SnCl_2 is ionic. In SnClF and Sn_2ClF_3 , bonding is covalent. The bonding type can be easily identified from the crystal structure when available. A full coordination with equal or near equal bond lengths shows the tin lone pair is non-stereoactive and therefore there is no orbital hybridization, hence the Sn^{2+} stannous ion is present. On the other hand, an incomplete coordination with often highly variable bond lengths is indicative of a stereoactive lone pair, therefore bonding is covalent and the tin valence orbitals are hybridized. We have studied some number of tin(II) chloride fluorides and studied the tin bonding type in them. In Ba_2SnCl_6 , the crystal structure was solved by single crystal X-Ray diffraction and bonding is fully ionic. In $\text{M}_3\text{Sn}_5\text{Cl}_3\text{F}_{10}$ ($\text{M} = \text{K}$ or NH_4), also determined by single crystal X-ray diffraction, bonding is covalent. In the doubly disordered $\text{Ba}_{1-x}\text{Sn}_x\text{Cl}_{1+y}\text{F}_{1-y}$ solid solution with the BaClF structure, there is a mixture of ionic and covalent types of bonding, depending on stoichiometry and on of the method of preparation. The bonding type and tin sublattice strength were studied by a combination of X-ray powder diffraction and ^{119}Sn Mössbauer spectroscopy.: figures (a) $\text{BaSn}_2\text{Cl}_2\text{F}_4$ and (b) BaSnClF_3 , both with covalent bonding, and (c) $\text{Ba}_{1-x}\text{Sn}_x\text{Cl}_{1+y}\text{F}_{1-y}$ with ionic bonding.



P-18

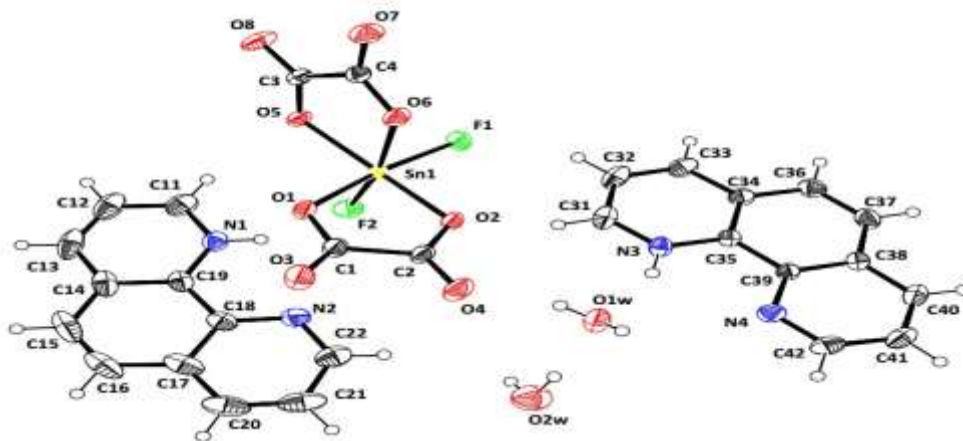
Title: New open-framework tin oxalate synthesized in the presence of organic amine.

Hocine Merazig¹, Rima Gheribi¹, Georges Dénès^{2,*}, Rochdi Ghallab¹, Tarek Benlatreche¹ and Abdelatif Bensegueni¹

¹Unité de Recherche de Chimie de l'Environnement et Moléculaire Structurale CHEMS, Université des Frères Mentouri de Constantine, Constantine. Algeria.

²Laboratory of Solid State Chemistry and Mössbauer Spectroscopy, Department of Chemistry and Biochemistry, Concordia University, 7141 Sherbrooke Street West Montreal, Qc H4B 1R6, Canada, *georges.denes@concordia.ca

One of the strategic goals in crystal engineering is to synthesize crystals with a predictable structure and valuable properties in many different fields, such as electrical and agricultural, gas storage and also biological (anti-bacterial and anti-tumor). With this in mind, our work is focused on the investigation of hybrid materials based on tin as a metal with a dicarboxylic acid and an organic amine. In the work shown here, $(C_{12}H_9N_2)_2 [Sn(C_2O_4)_2 F_2] \cdot 2H_2O$ bis 1-10phenanthroline cis-difluoro-bis-oxalate stannate(IV) dihydrate, was prepared by soft chemistry and its crystal structure solved. The unit cell is triclinic, space group P-1, with $a = 7.7863 (2) \text{ \AA}$, $b = 9.8814 (2) \text{ \AA}$, $c = 19.2398 (5) \text{ \AA}$, $\alpha = 103.196 (1)^\circ$; $\beta = 94.695 (1)^\circ$ and $\gamma = 99.723 (1)^\circ$; $Z = 2$ unit formulas/unit cell. The structure refinement resulted in final $R_{int} = 0.028$, $R_w = 0.1$ and $GOOF = 1.18$.



P-19

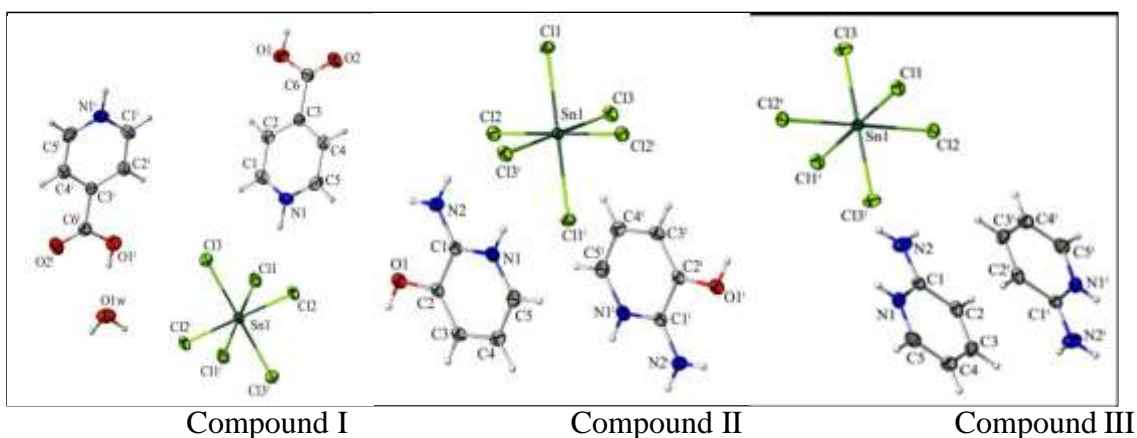
Synthesis and Structural Analysis of New Hybrid Compounds at Zero Dimension based on Tin.

Hocine Merazig¹, Rochdi Ghallab¹, Georges Dénès^{2,*}, Rima Gheribi¹, Tarek Benlatreche¹ and Abdelatif Bensegueni¹

¹Unité de Recherche de Chimie de l'Environnement et Moléculaire Structurale CHEMS, Université des Frères Mentouri de Constantine, Constantine. Algeria.

²Laboratory of Solid State Chemistry and Mössbauer Spectroscopy, Department of Chemistry and Biochemistry, Concordia University, 7141 Sherbrooke Street West Montreal, Qc H4B 1R6, Canada, *georges.denes@concordia.ca

A Zero dimension (0D) hybrid perovskites have interesting optical and structural properties. In hybrid materials, the organic part can essentially have nonlinear optical properties, while most of the physical properties come from the inorganic part, such as the semiconducting iodostannate sheets, the electronic transport properties, the optical properties (photoluminescence, photochromism, or even magnetic). This was achieved by combining the properties of organic and inorganic constituents. The flexibility of the organic part and the thermal stability and the rigidity of the inorganic part, in a single material, or by cooperative effects, can result in a synergy that is more than just the sum of the properties of each constituent. The following compounds were prepared and their crystal structure will be presented: **Compound I**: 4-carboxypyridinium hexachlorostannate(IV) monohydrate, $(\text{SnCl}_6)^{2-}[\text{C}_6\text{H}_6\text{NO}_2]^+ \cdot \text{H}_2\text{O}$ (monoclinic, $P2_1/c$), **Compound II**: aminopyridinium hexachlorostannate(IV), $(\text{SnCl}_6)^{2-}[\text{C}_5\text{H}_7\text{N}_2]^+ \cdot 2$ (triclinic, $P-1$), **Compound III**: 2-aminopyridinium-3-ol hexachlorostannate(IV), $(\text{SnCl}_6)^{2-}[\text{C}_5\text{H}_7\text{N}_2\text{O}]^{+2}$ (triclinic, $P-1$).



Synthesis of New Organotin Compounds

Hocine Merazig¹, Tarek Benlatreche¹, Georges Dénès^{2,*}, Rochdi Ghallab¹, Rima Gheribi¹, and Abdelatif Bensegueni¹

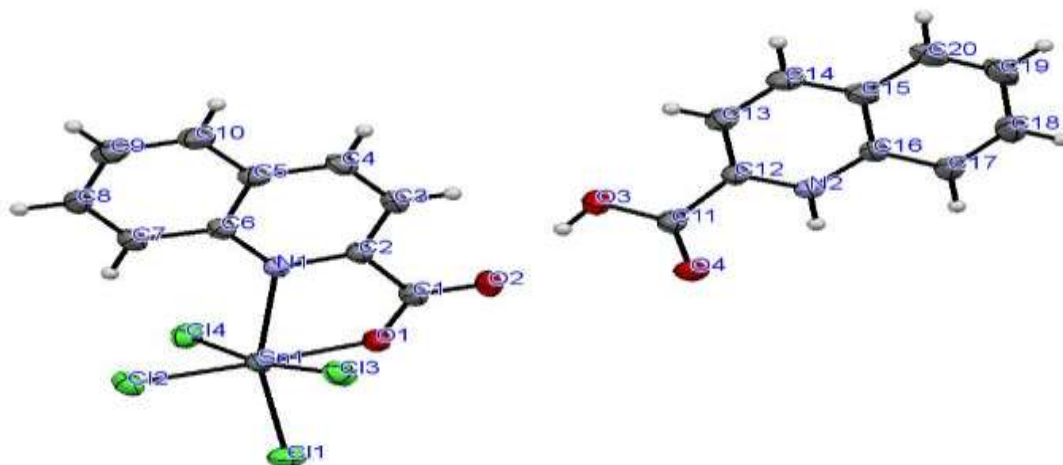
¹Unité de Recherche de Chimie de l'Environnement et Moléculaire Structurale CHEMS, Université des Frères Mentouri de Constantine, Constantine, Algeria.

²Laboratory of Solid State Chemistry and Mössbauer Spectroscopy, Department of Chemistry and Biochemistry, Concordia University, 7141 Sherbrooke Street West Montreal, Qc H4B 1R6, Canada, *georges.denes@concordia.ca

Organotin compounds show countless applications in modern technology, especially in catalysis for polymer chemistry [1]. Similarly, anticancer activity was reported by Hadjidakou and Hadjiliadis [2]. Organotin compounds such as stannoxanes have been studied for their catalytic activity in many organic processes. Several organotin compounds have shown many biological activities such as antifungal, anticancer and antiproliferative. This prompted us to prepare the following compounds and study their properties. Their crystal structure will be presented. **Compound I**: 2-(ethoxycarbonyl) quinolin-1-ium tetrachlorido(quinoline-2-carboxylato-k2N,O) stannate(IV) hydrate, **Compound II**: 2-carboxyquinolin-1-ium tetrachlorido(quinoline-2-carboxylato-k2N,O) stannate(IV). The crystal structure of compound II is shown on the figure.

[1] Davies, A. G. (2010). J. Chem. Res. 34, 181-190.

[2] Hadjekarou, S. K. & Hadjiliadis, N. (2009). Coord. Chem. Rev. 253, 235-249.



P-21

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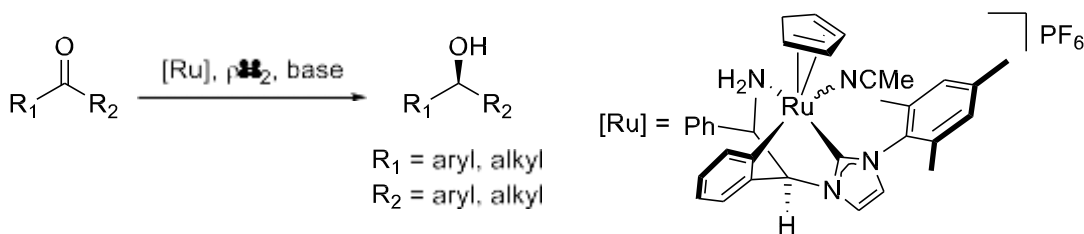
Title: Improving the enantioselectivity of ketone hydrogenation with chiral N-heterocyclic carbene ruthenium complexes by cyclometallation of the chiral backbone

Brian T. H. Tsui, Kai Y. Wan, Robert H. Morris*

*Department of Chemistry, University of Toronto, Toronto, Ontario, L4B4G4,
briantszho.tsui@mail.utoronto.ca*

Abstract: 350 words

Hydrogenation of polar unsaturated bonds to afford enantioenriched products is highly sought out in the agricultural, pharmaceutical, and fine chemical industries. Recent developments in our group have uncovered a class of homochiral bidentate N-heterocyclic carbene (NHC) ligands with a pendant amine which have seen use in extremely active ruthenium AH catalysts. Slightly modifying the parent NHC ligand affords a cyclometallated ruthenium complex via an intramolecular process. The new ketone asymmetric hydrogenation catalysts enable increased reactivity and enantioselectivity towards aliphatic ketones, a challenging class of substrates. Full characterization and optimization of the catalytic conditions are underway.



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P-22

IDW 2019 Abstract Submission Form

Title: Triazolylidene iron Complexes for the Dimerization of Terminal Alkynes

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Abstract: 350 words

Catalytic dimerization of terminal alkynes is the most ideal route to enyne synthesis, with the highest atom economy.¹ Although metal-based catalysts have been extensively established, they are mainly dominated by precious metals and f-block elements.²⁻⁴ Developing catalysts with iron is a much cheaper and potentially less toxic alternative. Our group has reported the first iron catalyst for geminal-specific homo and cross-dimerization of alkynes.⁵ NHC iron complexes are a versatile class of molecules for synthesis and catalysis. Presented here are 2 new half-sandwich iron complexes containing a 1,2,3- and 1,2,4-triazolylidene. They have been characterized and are being tested for their catalytic activity towards the dimerization of alkynes.

References:

- [1] a) B. M. Trost, *Science* 1991, 254, 1471; b) B. M. Trost, *Angew. Chem., Int. Ed.* 1995, 34, 259.
[2] *Modern Alkyne Chemistry*, Eds. B. M. Trost and C.-J. Li, Wiley, Weinheim, 2015;
[3] a) C. S. Yi, N. Liu, *Organometallics* 1996, 15, 3968; b) C. S. Yi, N. Liu, *Organometallics* 1998, 18, 3158; c) K. Ogata, A. Toyota, *J. Organomet. Chem.* 2007, 692, 4139; d) C. Conifer, C. Gunanathan, T. Rinesch, M. Hlscher, W. Leitner, *Eur. J. Inorg. Chem.* 2015, 2015, 333; e) B. Powała, C. Pietraszuk, *Catal. Lett.* 2014, 144, 413; f) A. Kawata, V. Kuninobu, K. Takai, *Chem. Lett.* 2009, 38, 836; g) M. Bassetti, C. Pasquini, A. Raneri, D. Rosato, *J. Org. Chem.* 2007, 72, 4558; h) A. Hijazi, K. Parkhomenko, J.-P. Djukic, A. Chemmi, M. Pfeffer, *Adv. Synth. Catal.* 2008, 350, 1493; i) B. M. Trost, J. T. Masters, *Chem. Soc. Rev.* 2016, 45, 2212.
[4] a) M. Nishiura, Z. Hou, Y. Wakatsuki, T. Yamaki, T. Miyamoto, *J. Am. Chem. Soc.* 2003, 125, 1184; b) K. Komeyama, T. Kawabata, K. Takehira, K. Takaki, *J. Org. Chem.* 2005, 70, 7260; c) S. Ge, V. F. Q. Norambuena, B. Hessen, *Organometallics* 2007, 26, 6508; d) R. H. Platel, L. L. Schafer, *Chem. Commun.* 2012, 48, 10609.
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Oral

Poster X

Abstract should fit into one page.

P-23

Development of Redox Active Crown Ether Macrocycles - Towards Switchable Single Molecule Magnets

Michael D'Agostino^a and Melanie Pilkington^{*a}

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Previous research within the Pilkington group has involved the use of crown ether macrocycles for the preparation of 4f SMMs due to the compatibility of oxophilic Ln(III) ions with the oxygen donors of traditional crowns. Furthermore, the versatility of crown ethers permits facile modification of the macrocyclic cavity by varying the type and number of the donor atoms as well as synthetically altering the organic framework. Exploiting crown ether macrocycles as suitable ligands for 4f ions, several families of Ln(III)-based single molecule magnets (SMMs) comprising of 15C5, benzo15C5 and dibenzo15C5 macrocycles have been structurally and magnetically characterized in recent years.^{1,2,3} To advance these studies further, our objectives are to append redox switchable moieties onto the organic framework of the crowns, in order to chemically address their magnetic properties. Following this strategy, the synthesis and characterization of two new families of ferrocene appended crown ether ligands, **1** and **2** will be reported.⁴

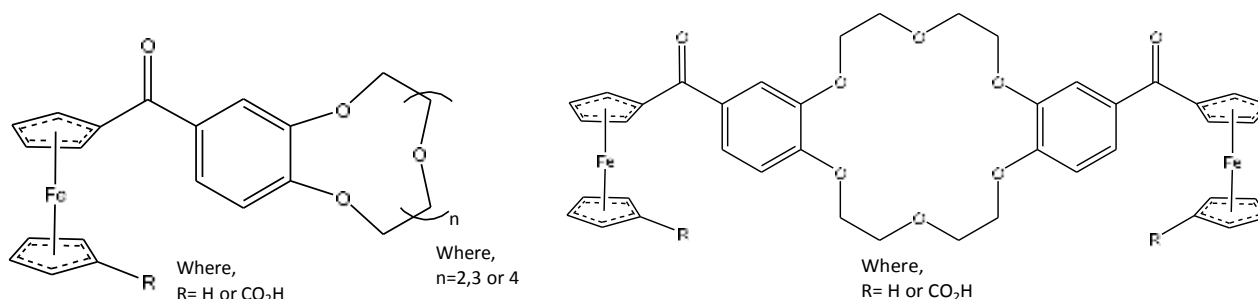


Figure 1. Molecular structures of mono and di-substituted ferrocenyl crown ethers, **1** and **2** respectively

References:

- 1) M. Al Hareri.; E. L. Gavey.; J. Regier.; Z. Ras Ali.; L. D. Carlos.; R. A. S. Ferreira.; M. Pilkington.; *Chem. Commun.*, **2016**, 52, 11335.
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- 4) U. Tunca.; *Polymer*. **1996**, 37, 3997.

P-24

Title: C-term MCD Study of U(V) O_h Complexes

Daniel J. Curran, Nikki Wolford, and Michael Neidig*

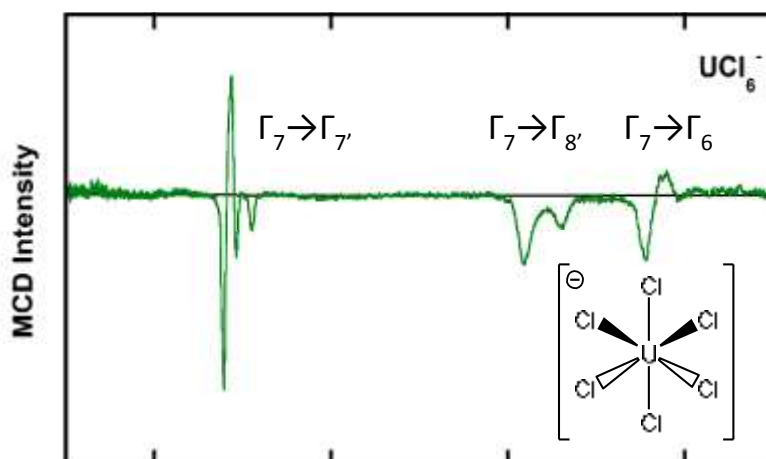
Department of Chemistry, University of Rochester, Rochester, NY, 14620,

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Abstract: 350 Words

Bonding and electronic structure in f-element complexes is of broad interest due to their role in the nuclear fuel cycle. In contrast to d-block elements, where major advances in the understanding of their bonding and electronic structure have been made using physical inorganic techniques and theory, f-elements have been neglected and with their electronic structure remaining ambiguous. To bridge this gap of knowledge, developing and applying physical-inorganic techniques for actinides is vital. C-term Magnetic Circular Dichroism (MCD) spectroscopy has the advantage of utilizing magnetization and circularly polarized light results in signed transitions that can deconvolute overlapping transitions resulting more informative spectra. A previous study in the Neidig group characterized $[UCl_6]^-$ in the UV-Vis region with C-term MCD and simulated the spectra with good agreement through theoretical calculations.¹ To continue developing this technique, this spectroscopy was extended to investigate the NIR region of octahedral complexes with a $5f^1$ electronic structure previously reported and characterized by the Hayton group. These complexes provide a well-studied series to begin understanding the effects of different ligand sets on the U(V) ion.² Theoretical calculations were also performed on the hexalide complexes to simulate their spectra. From these calculations only one transition is shown to be purely electronic demonstrating the complex nature of the electronic structure of actinide complexes. Further development is underway to make this technique useful for more conventional use to understand complexes relevant to synthetic development.

5K, 7T NIR MCD Spectrum of UCl_6^-



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P-25

IDW 2019 Abstract Submission Form

Title: Cation interactions with molecular vanadium oxide clusters: Observations of capacitive and intercalative behavior within a single complex

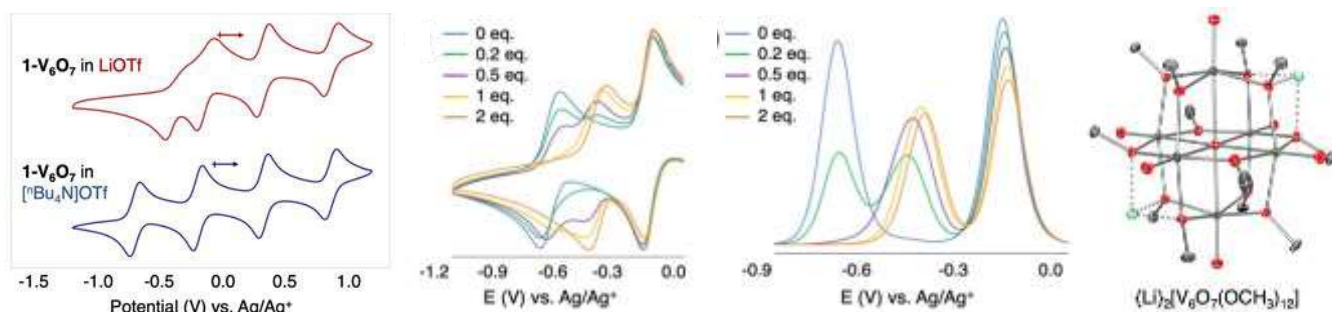
Eric Schreiber, Niamh A. Hartley, Timothy R. Cook, James R. McKone, and Ellen M. Matson*

Department of Chemistry, University of Rochester, Rochester, NY, 14620,

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Abstract: 350 words

To design materials for efficient and energy-dense energy storage, it is critical to understand the interactions between metal oxides and alkali ions. Here, we discuss the solution-phase interactions of lithium, sodium, potassium, and alkylammonium cations with Lindqvist-type polyoxovanadate-alkoxide clusters. In the presence of alkali cations, half-wave potentials of reduction events are shifted toward positive potentials relative to alkylammonium, suggesting that the observed changes in reduction potentials are the result of interactions with charge-compensating ions. Single-crystal X-ray diffraction studies indicate that two Li^+ ions undergo site-selective coordination to opposite faces of this cluster upon reduction, manifesting in sluggish re-oxidation of this ion-paired species. Our studies show that these molecular complexes demonstrate redox behaviour that spans the full range from nonspecific to highly specific cation binding, which is directly analogous to capacitive and intercalative behaviour in bulk transition metal oxides.



Abstract should fit into one page.

IDW 2019 Abstract Submission Form

Title: Synthesizing Red-Shifted Azobenzene Derivatives for Fine-Tuning Activity and Spatial Temporal Control

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Abstract: 350 words

SiRNAs are natural defense mechanisms found in the cell that are a part of the RNA interference pathway (RNAi). The cell uses the pathway as a defense mechanism against viruses or other parasites that inject dsRNA into the cells.^{1,2} Therapeutic uses of siRNAs are limited by their stability, off-target effects, poor membrane permeability and finding an effective delivery system.³ Chemical modification of the Ago2 cleavage site in the central region has shown some promiscuity with respect to both alkyl spacers⁴ and functionalized linkages and using azobenzene, should allow for a more stable siRNA that is able to be inactivated and then reactivated through the application of ultraviolet (UV) or visible light, respectively as there is a photo-isomerization from *trans* to *cis* upon UV exposure. Azobenzene as a backbone substitution is also more stable, and increases permeability through cell membranes. Azobenzene is potentially superior to photo-caged molecules because of its reversibility, allowing for tunable photo-control of the siRNA's activity. A small library of azobenzene modified siRNAs were developed with central region and 3' end azobenzene containing modifications. They were characterized bio-physically with CD, HPLC and absorbance spectra. They were then tested for activity *in vitro* and *in vivo* in HeLa cells, and the inactivation and reactivation aspects of the azobenzene modified siRNAs were evaluated. Our data shows excellent tunability and control with UV and visible light, and furthermore we have begun to explore red-shifted azo derivatives that also offer excellent control of the siRNA's activity without the use of potentially harmful UV light.

References:

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Poster **X**

Abstract should fit into one page.

P-27**IDW 2019 Abstract Submission Form****MALDI Mass Spectrometry as an Enabling Tool for Structure Elucidation in Inorganic Chemistry: Toward Benign Matrices**

Eliza-Jayne Boisvert and Deryn E. Fogg*

*Center for Catalysis Research & Innovation, and Department of Chemistry and Biomolecular Sciences, University of Ottawa, Ottawa, Ontario, K1N 6N5***dfogg@uottawa.ca*

Structural elucidation is a routine bottleneck in inorganic chemistry. A major challenge has been the difficulty in identifying the molecular constitution, owing to extensive fragmentation in standard, high-energy mass spectrometry (MS). The soft ionization methods of electrospray ionization (ESI) and matrix-assisted laser desorption-ionization (MALDI-MS) opened the door to routine analysis. MALDI-MS stands out for its unique capacity to enable analysis of *neutral* metal complexes. Use of polycyclic aromatic hydrocarbon (PAH) matrices (e.g. pyrene, anthracene) enables charge-transfer ionization: that is, one-electron oxidation to give the radical cations with minimal metal-ligand bond cleavage (Figure 1).¹ This approach enables powerful insight, not merely into identity, but mechanism.^{2,3}

A challenge, however, lies in the extreme ease with which the PAH matrices sublime and deposit throughout the instrument, creating the potential for electrical malfunction. The present work seeks to identify alternative matrices that alleviate this problem. Key criteria identified in our prior work include the absence of functional groups that can enable reaction with the analyte, and a strong electronic absorption band near the Nd/YAG laser wavelength of 355 nm,⁴ in addition to the new criterion of resistance to sublimation. A survey of alternative charge-transfer matrices will be presented, and their success in enabling observation of the intact radical cations for catalysts that serve as a benchmark MALDI-MS analysis.

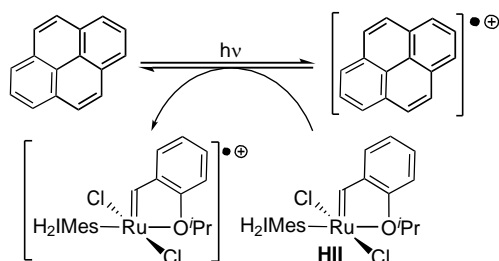


Figure 1: Anthracene-Enabled Charge-Transfer Ionization in MALDI Mass Spectrometry:

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- (4) Bailey, G. A.; Fogg, D. E. *ACS Catal.* **2016**, *6*, 4962–4971.

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Poster **X****Abstract should fit into one page.**

Novel Ruthenium Metathesis Catalysts Containing Strongly Electron-Donating Dialkyl(1,3-diarylimidazolin-2-ylidenamino)phosphines

Stephanie J. Ton, Philipp Roterig, Fabian Dielmann, and Deryn E. Fogg*

Center for Catalysis Research & Innovation, and Department of Chemistry and Biomolecular Sciences, University of Ottawa, Ottawa, Ontario, K1N 9A4

*dfogg@uottawa.ca

Abstract:

Ruthenium-catalyzed olefin metathesis offers exceptionally powerful methodologies for the construction of carbon-carbon bonds, and metathesis processes are now beginning to emerge in pharmaceutical manufacturing.¹ Ubiquitous in high-performing metathesis catalysts are strongly donating carbene ligands, typically N-heterocyclic carbenes (NHCs). With an eye to increasing the diversity of the catalyst structures available, a new class of electron-rich phosphines is explored in place of the NHCs. Dialkyl(1,3-diarylimidazolin-2-ylidenamino)phosphines (IAPs)² have been shown to be stronger σ -donors than NHCs, while the readily modified IAP backbone can be used to tune the steric environment around the ruthenium center. The synthesis of Ru-IAP metathesis catalysts is described, along with initial structure-activity relationships derived from studies of ring-closing metathesis and the cross-metathesis of electron deficient olefins.

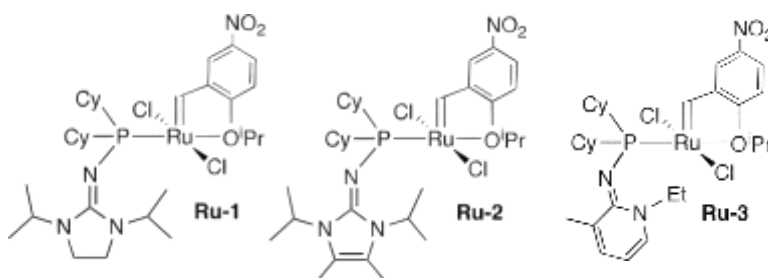


Figure 1: Exemplary ruthenium metathesis catalysts bearing IAP ligands

- (1) Higman, C. S.; Lummiss, J. A. M.; Fogg, D. E., Olefin Metathesis at the Dawn of Uptake in Pharmaceutical and Specialty Chemicals Manufacturing. *Angew. Chem., Int. Ed.* **2016**, *55*, 3552–3565.
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Title: Mass Spectrometry Evaluation of Brain-Related Metallo-peptides

Shaelyn Mortensen¹, Saba Anwar², Sanela Martic^{1,3}

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²*Chemistry, Oakland University, Rochester, MI, USA, 48309*

³*Forensic Science and Environmental and Life Sciences, Trent University, Peterborough, ON, K9L 0G2, sanelamartic@trentu.ca*

Abstract: 350 words max

Metallo-protein complexes are necessary for key biological functions, however, they can also be involved with neurodegenerative diseases, including Alzheimer's Disease (AD). For example, upon coordination to biologically relevant metal ions, such as Cu(II) and Zn(II), the brain-related tau protein undergoes structural and functional changes that have been linked to the early onset of disease. The exact nature of this coordination is currently unknown. Four repeat peptide domains (R-peptides) of the Tau protein which contain metal ion-chelating amino acid residues, His and Cys, were evaluated by mass spectrometry. The mixture of R-peptides with various metal ions, including Cu(II), Zn(II), Fe(II) and Fe(III), were characterized by matrix assisted laser desorption ionization mass spectrometry (MALDI-MS). MS spectra showed the peptide coordination to Cu(II) and Zn(II) ions, however characterization with Fe(II) and Fe(III) ions was more complex. All R-peptides formed monovalent 1:1 (peptide:Cu(II)) complexes (Fig. 1). R-peptides with Cys residues also formed peptide dimers in the absence and presence of Cu(II). The detailed results of R-peptide coordination chemistry with all metal ions will be described.

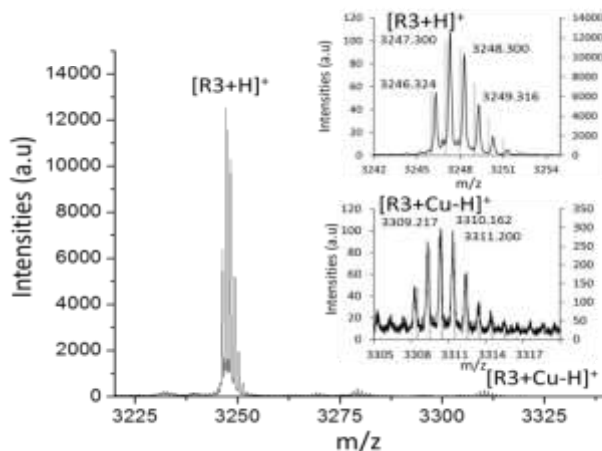


Fig.1. MS spectrum of an R-peptide coordinated with Cu(II) overlaid with comparisons to the predicted isotope patterns.

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P-30

IDW 2019 Abstract Submission Form

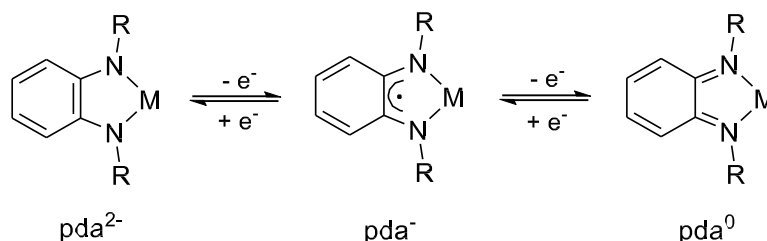
Title: Reactivity of Redox-active *o*-Phenylenediamide Complexes of Iron

Jack Lin, Qiuming Liang, and Datong Song*

Department of Chemistry, University of Toronto, Toronto, Ontario, M5S 3H6,

Abstract: 350 words

Redox-active ligands have garnered considerable attention within the last decades due to their unique electronic properties.^{1, 2} Traditional transition metal complexes bearing ancillary ligands undergo oxidation and reduction at the metal; conversely, when a redox-active ligand is present, the dominant electron source or sink can be the ligand itself. This has led to the proposal that redox-active ligands may effect 2 e⁻ transformations typical of noble metals on base metals that are more prone to 1 e⁻ oxidation state changes, which could lead to new transformations or catalytic applications.³ The coordination of non-innocent *o*-phenylenediamide (pda) ligands to iron have been reported, yielding a variety of electronic structures owing to the ligands' three accessible oxidation states: the neutral, monoanionic, and dianionic forms.⁴ As such, these complexes may exhibit diverse reactivity that is unexplored in base metal chemistry. The characterization and reactivity of a series of iron *o*-phenylenediamide complexes are presented.



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Presentation Preference: (check one by putting X)

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Poster (X)

Abstract should fit into one page.

P-31

IDW 2019 Abstract Submission Form

Title: Stereospecific Suzuki-Miyaura Cross-Coupling of Chiral Benzylic Boronic Esters and Vinyl Bromides

Nicole Dozois, Zach Ariki, Yuki Maekawa, and Cathleen Crudden*

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Abstract: 350 words

The Suzuki-Miyaura cross-coupling reaction is a powerful method for the construction of carbon-carbon bonds in academia and industry. Yet, despite extensive research in this area and the significance of the reaction, it is most often employed to prepare flat, Csp²-Csp² bonds between two aryl groups¹. Since most bioactive compounds contain several 3-D, or chiral, centers, it is more desirable to make bonds between sp²-sp³ and sp³-sp³ carbon centers¹. However, when dealing with sp³ carbons in cross-coupling chemistry, new challenges arise such as β-hydride elimination, an undesirable side reaction². In 2009, our group reported the first example of a stereospecific coupling between chiral secondary boronic esters and aryl iodides³. Herein, we report our investigations towards expanding the scope of our established Csp²-Csp³ coupling reaction with chiral boronic esters. By employing vinyl halides as electrophiles, we can stereospecifically prepare alkene-containing products—a useful handle for further functionalization. Importantly, upon hydrogenation of the alkene, we can furnish highly enantioenriched chiral hydrocarbons.

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Poster X

Abstract should fit into one page.

P-32

IDW 2019 Abstract Submission Form

Title: Iron catalysts containing monodentate NHC ligands toward *gem*-specific dimerization of terminal alkynes

Karolina Rabeda, Qiuming Liang, and Datong Song*

Department of Chemistry, University of Toronto St. George, Toronto, Ontario, M5S 3H6,

**karolina.rabeda@mail.utoronto.ca*

Abstract: 350 words

1,3-enynes are important organic precursors for the synthesis of pharmaceuticals and bioactive molecules. Alkyne dimerization is the most atom economical synthetic method to prepare them.¹ Several metal-based catalysts for terminal alkyne dimerization have been reported, predominantly using either precious metals or f-block elements. Although iron is a more abundant, less toxic and cheaper alternative to these metals, very few of these catalysts involve iron as a metal center. Moreover, not all of these catalysts can control the regioselectivity of the competing isomers- *E/Z* and *gem*.² In 2017, we reported an iron catalyst for the *gem*-specific terminal alkyne dimerization.³ In 2018, our group reported an even more efficient second-generation catalyst that was compatible with a broad scope of substrates, undergoing full conversion within half an hour at room temperature. However, this catalyst is quickly deactivated as it undergoes ligand redistribution.⁴ In an effort to enhance the robustness of the catalyst, we have synthesized several N-heterocyclic carbenes (NHCs) with various electronic properties and their corresponding Fe complexes which will be presented in this poster.

References:

- (1) Zhu, Y.; Li, T.; Qu, X.; Sun, P.; Yang, H.; Mao, J. Copper(I)-Catalyzed Synthesis of 1,3-Enynes via Coupling Between Vinyl Halides and Alkynes or Domino Coupling of Vinyl Halides. *Org. Biomol. Chem.* **2011**, *9*, 7309.
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- (3) Liang, Q; Osten, K. M.; Song, D. Iron-Catalyzed Gem-Specific Dimerization of Terminal Alkynes. *Angew. Chem. Int. Ed.* **2017**, *56*, 6317.
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Poster X

Abstract should fit into one page.

P-33

Title: Synthesis of New Group 9 and 10 Complexes using $\{\text{Me}_2\text{PCH}_2\text{AlMe}_2\}_2$

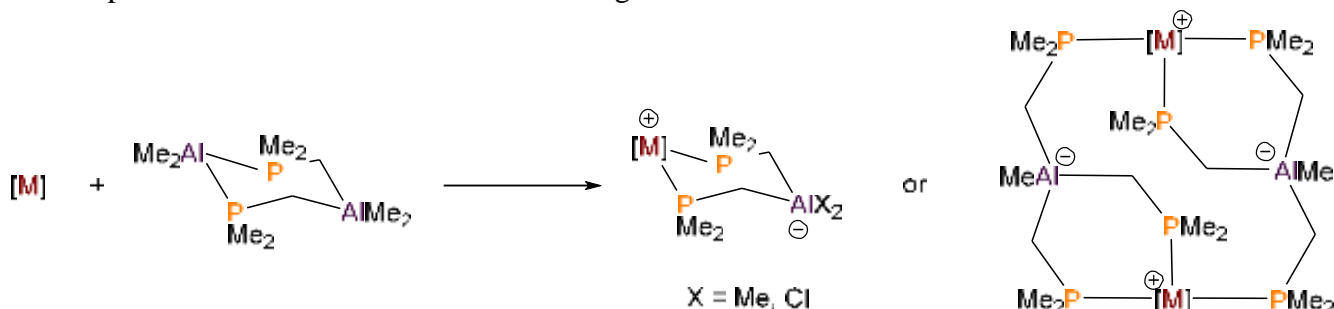
KatarinaPaskaruk, and David Emslie*

Department of Chemistry, McMaster University, Hamilton, Ontario, L8S 4M1,

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Abstract:

Ambiphilic ligands are a class of ligand that contains both conventional Lewis basic donors and Lewis acidic moieties within the same framework. These ligands are of great interest in transition metal chemistry due to their unique properties, including (i) the ability to modulate electron density of the transition metal center by direct coordination, (ii) the ability to engage in bridging interactions with co-ligands and incoming substrates, (iii) the potential to promote 1,1-insertion reactions, and (iv) the potential to activate complexes by the formation of zwitterions through the abstraction of anionic co-ligands. Previously, Zargarian¹ and Fontaine² used $\{\text{Me}_2\text{PCH}_2\text{AlMe}_2\}_2$ ($\{\text{PAI}\}_2$)³ as an ambiphilic ligand precursor in the synthesis of Ni and Rh piano-stool complexes. The current work further explores the use of $\{\text{PAI}\}_2$ as a precursor to various Rh, Ir and Pt ambiphilic ligand complexes. The PAI ligand was found to readily abstract methyl and chloride co-ligands, although it was also prone to rearrangement, forming new complexes of bi- and tri-dentate aluminate ligands.



References:

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P-34

IDW 2019 Abstract Submission Form

Proposed Synthesis of κ^2 -(N, O)-Ligands Containing an Oxazoline Group Coordinating to Platinum

Deidre Tremblay^{1E}, Matthew Hill^{1Ω}, Kathleen May^{1Y}, Robert A. Gossage^{1T}, Alan J. Lough²

¹Department of Chemistry and Biology, Ryerson University, Toronto ON.

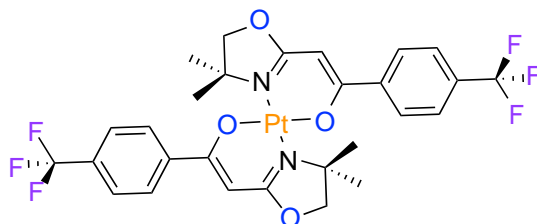
²Department of Chemistry, University of Toronto, Toronto ON

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Abstract: 350 words

Platinum complexes have seen use as drugs, cancer therapeutics, and widely as a means for chemical transformations (catalytic processes). These complexes are readily synthesized by reacting a platinum metal source with a coordinating ligand. Currently, a bidentate (N,O)-ligand system is being explored first synthesized by Tohda and colleagues. By taking advantage of the hemilability of the ligand we wish to impart increased stability of the platinum center and therefore hopefully increase its activity (biologically or catalytically). The ligand scaffold we've deemed the "Tohda ligands" are those built by reacting an oxazoline with an acyl chloride or anhydride species. This ligand scaffold has been explored by our group in which we have reported its reactivity with nickel, palladium, cobalt and copper as well as other late and early transition metals. This project aims to study the reactivity between the "Tohda ligands" and platinum, in hopes of obtaining novel platinum(N,O)-complexes. Once synthesized, the complexes will be tested in certain chemical transformations and for their potential biological activity. This poster reports the early synthetic strategies and attempts toward bis(N,O)-chelated platinum complexes.



Pt(κ^2 -N,O-L-*p*-CF₃)₂: Pt(κ^2 -N,O-(Z)-2-(4,4-dimethyl)-4,4-dimethyl-4,5-dihydrooxazol-2-yl)-1-(4-(trifluoromethyl)phenylethen-1-yl)₂: PtN₂O₄C₂₈H₂₆F₆:

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P-35

IDW 2019 Abstract Submission Form

Title: Adsorption of Naphthenic Acids from Oil Sand Process Affected Water (OSPW) Using Synthesized Activated Carbon

Elmira Nazari* and Andrew Vreugdenhil

Material Science, Trent University, Peterborough, ON, Canada, K9J 0G2,

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Abstract:

The oil sands deposits of Northern Alberta, Canada are estimated to constitute world's largest bitumen reserve, containing approximately 1.7 trillion barrels of bitumen. The bitumen extraction procedures produce large volumes of slurry wastes contaminated with naphthenic acids (NAs). Because of a "zero discharge" policy, the oil sands companies do not release any extraction wastes from their leases. The generated process-affected waters contaminated with NAs are contained onsite primarily in large settling ponds. These fluid wastes from the tailing ponds can be acutely and chronically toxic to aquatic organisms, and NAs have been associated with this toxicity. Thus, to investigate the removal of NAs from the oil sand process affected waters using adsorption method, four individual single compound naphthenic acids (2-methyl-1-cyclohexanecarboxylic acid, Diphenylacetic acid, 2-naphthoic acid and 1,4-cyclohexanedicarboxylic acid) were selected to be examined with the use of petroleum coke as a potential adsorbent for organic contaminant which was chemically activated with KOH. The kinetic of adsorption was investigated for these model naphthenic acids in order to figure out the order of adsorption capacities after 24 hours among these three NAs which is as following: Diphenylacetic acid > 2-naphthoic acid > 1,4-cyclohexanedicarboxylic acid. The removal of NAs at various pHs of 2.6, 4 and 8.6 was evaluated comparing the total organic carbon (TOC) and ElectroSpray Ionization Mass Spectroscopy (ESI-MS) of the solution before and after the adsorption process. The adsorption capacity decreased significantly with increasing pH due to its effect on both carbon surface charge and dissociation of the naphthenic acids.

References:

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Oral

Poster X

Abstract should fit into one page.

P-36

IDW 2019 Abstract Submission Form

Title: Synthesis of Azidosphingosine for biomolecular tools.

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Abstract: 350 words

Sphingolipids are a class of natural lipids comprised of a sphingoid-base backbone called sphingosine. A few examples of sphingolipids are sphingosine, ceramide and cerebroside. These compounds are important structural and functional components of the plasma membranes of eukaryotic cells. Until relatively recently, ceramides have been found to participate in a variety of cell signaling pathways.¹ For example, they have been found to have important roles in regulating proliferation, differentiation, and programmed cell death.² As such, its role has been suggested in several diseases such as cancer, diabetes, neurodegeneration, and inflammation. Another type of sphingolipid are sphingosines, sphingosines are formed by ceramides, which produce sphingosine-2-phosphate (S1P), and ultimately generate sphingolipids.³ Sphingosine kinases (SphK) catalyze the reaction of sphingosine that generate S1P, and there are two unlinked genes that encode the SphK isotypes (SphK1 and SphK2). In healthy cells the kinase regulation is controlled, however, uncontrolled activity can lead to a variety of diseases.⁴ As an example, an increased level of SphK1 activity promotes V12Ras-dependent transformation, and increases the growth and survival of cancer cells, while inhibiting apoptosis and resistance to chemotherapeutic agents. Finally, cerebroside is another type of sphingolipid that have important biological function. Sphingolipids show promising potential as therapeutics, however, they face drawbacks such as high cost and low availability. There is interest in synthesizing new cerebroside derivatives as potential lead compounds to study biological pathways. However, the synthesis of the compounds is not well established due to lack of commercially available sphingosine. There is interest in developing new methods to synthesize sphingosine derivatives as potential SphK1 or SphK2 inhibitors, and ceramide derivatives as potential anti-cancer compounds.

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Presentation Preference: (check one by putting X)

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Poster X

Abstract should fit into one page.

P-37

Title: Detection and Removal of Mercury (II) by Magnetic Core–Shell $\text{Fe}_3\text{O}_4@ \text{TiO}_2$ Nanospheres decorated by 2,6-bis(2-thienyl)pyridine.

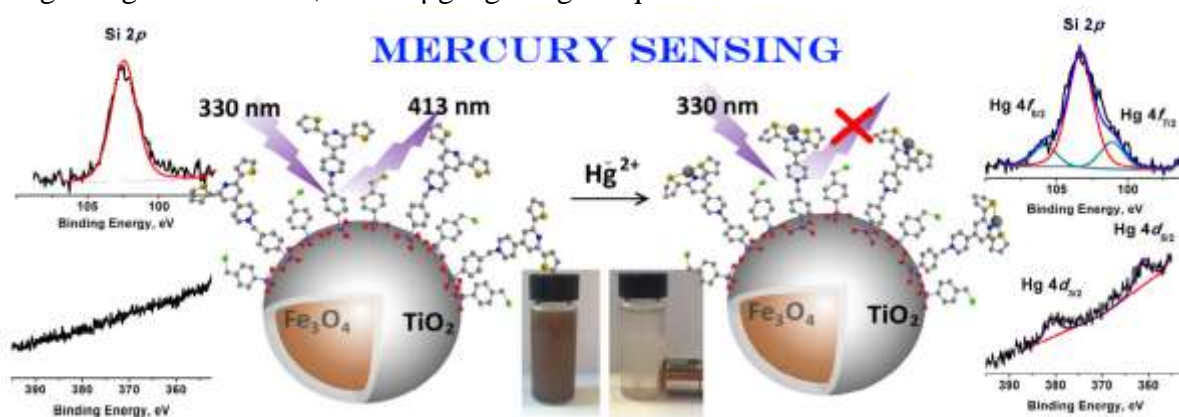
*Andrew J. Hynes, Jacquelyn G. Egan, Holly Fruehwald, Reza Alipour Moghadam Esfahani, Iraklii I. Ebralidze, Fedor Y. Naumkin, E. Bradley Easton and Olena V. Zenkina**

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Abstract:

Here we report on strong potential for Hg(II) detection and uptake demonstrated by 2,6-bis(2-thienyl)pyridine (L) molecular receptor. We confirmed S,N,S chelation as a main binding mode of the ligand with mercury metal ion based on the results of $^1\text{H-NMR}$ and Density functional theory (DFT). L showed a strong characteristics as a fluorescence sensor with a “turn-off” peak at 413nm and a “turn-on” peak at 580nm. By detailed studies at both emission wavelengths we showed ability of the ligand not only effectively detect mercury(II) ions but differentiate them from competing Zn^{2+} , Cd^{2+} , Cu^{2+} , Cr^{2+} , Ru^{2+} , Fe^{2+} ions in solution with minimum interference. Fe^{3+} was shown to be the largest interference agent, and the signals for Hg^{2+} and Fe^{3+} could be separated using electrochemical analysis. L was anchored into the surface of the coated magnetite microspheres ($\text{L-Fe}_3\text{O}_4@ \text{TiO}_2$) through a siloxane template layer and was fully characterized using thermogravimetric analysis (TGA) and X-ray photoelectron spectroscopy (XPS). The TGA showed a 2.5% weight loss of L on the surface and XPS showed the (N/N⁺) ratio of 1:1 as expected. Magnetic nanomaterial decorated by L showed promising performance as single –excitation -single emission (403/325nm) sensor for Hg^{2+} ions. The removal of this system is also easy to perform by simply applying an external magnetic field. Through the use of fluorescence and Cold-vapor atomic absorption the system was shown to remove 15 μg Hg^{2+} /mg in organic solutions, and 13 μg Hg^{2+} /mg in aqueous solutions.



P-38

IDW 2019 Abstract Submission Form

Title: A Window into the Future: Dye Sensitized Solar Cell Applications

Reeda Mahmood, Tristian Mananquil, and Bryan Koivisto*

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Abstract: 350 words

A Window into the Future: Dye Sensitized Solar Cell Applications

Dye-sensitized solar cells (DSSC) are next generation photovoltaic technology that are composed of two cathodes, electrolyte, and a dye. The advantages of DSSCs are that they are optically transparent, contain environmentally benign materials, possess a low energy payback time and their performance improves under diffuse light environments. These unique properties make them ideal candidates for use in building design and architecture; in particular, existing windows could be converted into DSSCs.

Currently, state of the art conductive electrodes used in DSSCs include fluorine-doped tin oxide (FTO) glass or Pt coated glass is used however this glass is expensive and is not found on existing windows.¹ As such, to convert existing windows into conductive panels, coatings need to be applied to substrates (glass) to meet the required conductivity. Silver and gold nanowires (AgNW and AuNW) have been used in the past to create transparent conductive substrates and have shown a lot of promise for applications in photovoltaics.

In this work, to synthesize AgNWs, the polyol method has been used whereby ethylene glycol reduces an inorganic salt in the presence of poly(vinylpyrrolidone) (PVP) as a capping agent.² Rod-coating has been used to coat various substrates, and SEM and UV-VIS are used to characterize nanowires. Future work includes testing AgNW coated substrates in DSSCs and measuring cell efficiency, lifetime, and transparency.

References:

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Poster X

Abstract should fit into one page.

IDW 2019 Abstract Submission Form

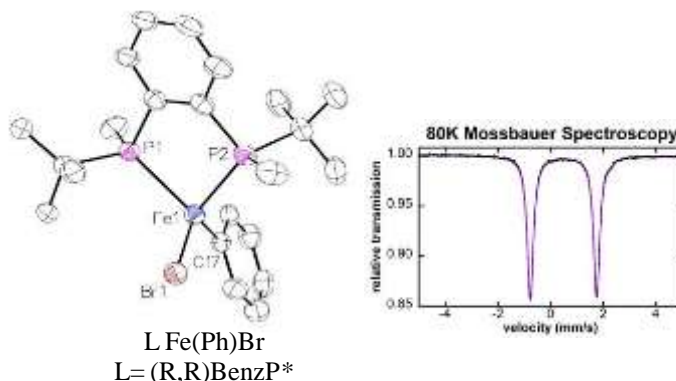
Title: Intermediates and Mechanism in Enantioselective Iron-Bisphosphine Cross-Coupling.

Maria Camila Aguilera-Cuenca and Michael L. Neidig*

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Abstract:

Iron-catalyzed cross-coupling reactions represent a great alternative for the production of industrially-relevant compounds due to iron's toxicologically benign nature, high abundance, and low cost compared to its precious metal counterparts. In addition, developments in this field have demonstrated that the use of derivatized biphosphines as precatalyst supporting ligands improve both yield and selectivity. Despite these advantages, there remains a lack of detailed mechanistic studies of iron catalyzed reactions. Recent studies from our group have established the key iron intermediates and reaction pathways in iron-ScioPP aryl-alkyl and alkynyl-alkyl cross coupling, including the critical role of iron(II) active species.¹⁻³ In 2015 Nakamura and co-workers reported the first Iron-catalyzed enantioselective cross coupling reaction using (R,R)BenzP*.⁴ Two years after, interesting DFT studies were published suggesting that the reaction may proceed via an alternative iron(II/III/II) path.⁵ To experimentally evaluate this proposal, we combine physical-inorganic spectroscopic methods to gain mechanistic insight, this work presents the analysis of iron-speciation distributions using freeze-trapped ⁵⁷Fe Mössbauer spectroscopy and the isolation and characterization of these intermediates throughout the catalytic cycle, employing single-crystal X-ray crystallography for structural determination in this reaction.

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5. Lee W.; Zhou J.; Gutierrez O. *J. Am. Chem. Soc.* **2017**, 139, 16126.

P-40

IDW 2019 Abstract Submission Form

Title: Seed layer effect onto ZnONWs electrochemically deposited

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Nowadays research is mainly focused in the use of electrodes formed by transparent and conductive oxides (TCO) for different purposes like optoelectronics and transparent devices. Within this last group, the TCO of $\text{In}_2\text{O}_3:\text{F}$ (ITO) y $\text{SnO}_2:\text{F}$ (FTO) on glass. This last one is more stable to temperature and chemical reagents. Considering the general characteristics of these substrates and considering that to choose whether to use or not to use this substrate for a certain application is mainly based in the physical properties like sheet resistance. or conductivity, other like morphology is not shown. In this work it is presented the effect of four types of FTO substrates on the morphological, structural and optical of the ZnO NWs grown electrochemically. In the present work four substrates with approximately the same sheet resistance entre 7 y 15 Ω/\square . The synthesis can be divided into two steps: i) The formation of the ZnO seed layer (SL) through spin coating, and then ii) ZnO NWs electrochemical synthesis using a -1V fixed potential. In this work three systems were used, without the use of the seed layer (OSL), with one seed layer (1SL), and two seed layer (2SL). The nanostructures obtained herein were characterized though, FE-SEM, XRD, and optical characterization techniques. The obtained materials present important differences regarding the diameter and the density of the nanowires.

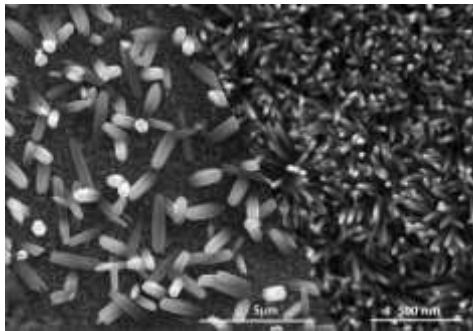


Fig 1: Micrograph with 0L and 2SL.

The diameter with 0SL is approximately 100-300 nm for the set of FTO electrodes, while 30-80 nm and 20-40 nm for 1 SL and 2 SL respectively. The texture coefficient from the diffractogram (specifically peak 0002) is higher than 1 in all cases of 1SL and 2 SL. The micrography shows the same synthesis procedure, using 0SL and 2SL. To conclude, it is important to control the morphology of the substrate

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Poster X

Abstract should fit into one page.

P-41

Title: Study of a dual electrochromic and electrofluorochromic material towards device use

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Abstract: 350 words

Electrochromism is defined as the change in color with applied potential. Typically, the color of the redox state is significantly different than its neutral state.(1) Triphenylamine (TPA) is a prime example of an electrochrome. It can be reversibly oxidized as well it undergoes a visible color change when oxidized. While TPA has interesting redox and electrochemically mediated colors changes, its intrinsic electronic donating property is also ideally suited for color enhancement. This is possible when it is coupled to electron deficient aromatics, leading to donor-acceptor type systems. This is particularly the case when TPA is conjugated with the electron withdrawing benzothiadiazole, resulting in visible colors and intense emissions. In this study, we present the electrochromic properties of a conjugated TPA-benzothiadiazole colored material. The TPA-BZT-TPA conjugated compound is also highly emissive. The combined color, fluorescence, and electroactivity make it an ideal material for a dual responsive electro- and fluorochrome material device. Towards this end, its anodically switchable properties in both solution and in a functioning device will be presented.(2)

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P-42

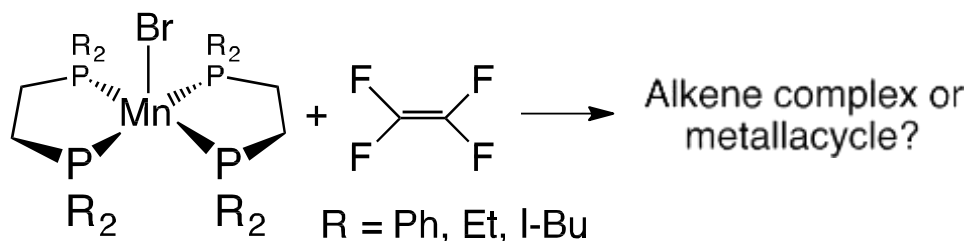
Title: Reactions of MnBr bis(phosphine) complexes with tetrafluoroethylene

BakrBarnawi and R. Tom Baker*

*Department of Chemistry and Biomolecular Sciences and CCRI, University of Ottawa, Ottawa, Ontario, K1N 6N5, *rbaker@uottawa.ca*

Abstract:

Fluoroalkenes have captured recent attention as low global warming refrigerants,¹ sources of new fluorinated fragments for pharma and agrochemicals,² and more environmentally friendly short fluorinated chains for materials applications.³ Previous work with tetrafluoroethylene (TFE) has demonstrated that low-valent metal complexes form stable alkene complexes, dinuclear products with bridging (C₂F₄)²⁻ units, or metallacyclopentanes by oxidative cyclization.⁴ Examples of the latter are currently restricted to d⁶⁻⁸ metals. In this work we describe reactions of TFE with electron-rich MnBr(P-P)₂ in an effort to prepare the first examples of d⁴ perfluorometallacyclopentanes so that we can investigate their C-F and M-C bond reactivity with a view to new catalyzed processes.



References:

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P-43

Title: Reactivity of iron complexes of picolyl N-heterocyclic carbene ligand

QiumingLiang, and Datong Song*

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Abstract: 350 words

N-Heterocyclic carbenes (NHCs) functionalized with additional donors are widely used in organometallic chemistry, where the additional donors provide enhanced stability by chelate effect. The use of picoline to generate N-picolyl-NHC ligands is known and has been applied to many transition metals. In addition to typical hemilabile property of the picolyl arms, we have also demonstrated the dearomatization-rearomatization reactivity as well as an unusual carbene rearrangement. In this poster, we present the dearomatization-rearomatization reactivity of half sandwich picolyl-NHC iron complexes towards bond activation such as H₂, silanes and diphenyldiazomethane.

P-44

Title: Modelling Lever Parameters by Repulsion-corrected Eigenvalues

PirouzKiani, Elaine S. Dodsworth, A. B. P. Lever, and William J. Pietro*

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In 1990, Lever¹ introduced the concept of the ligand electrochemical parameter, now known as Lever parameters, E_L . A ligand's Lever parameter describes the effect the ligand has on the E° of an octahedral transition metal redox couple, according to the equation **1**, where S_m and I_m are

$$E^\circ = S_m \sum_{i=1}^6 E_L(i) + I_m \quad (1)$$

parameters characteristic of the particular metal center, and $E_L(i)$ is the Lever parameter of the ligand attached to the coordination site i . The original parameterization was performed using experimental Ru(II/III) data in organic solvent, and thus $S_m=1$ and $I_m=0$ for Ru(II/III). It has been found that Lever parameters determined from ruthenium data are directly applicable to redox couples of a variety of other transition metals, requiring only a change in scaling factor S_m and offset I_m .

Understanding the differences in Lever parameters with respect to other ligands and how an individual ligand additively contributes their own characteristic voltage potential onto the metal complex can aid in advancing fields such as bioinorganic chemistry, homogenous catalyst synthesis, and photovoltaic cells. Hence, an *ab initio* approach in explaining E_L values would allow calculations to be performed on hypothetical complexes that could aid the above fields.

In this work, we analyze the effects of electron donation on E_L using density functional theory (DFT). From first principles, the redox potential of a complex should be directly related to the energy of the metal's HOMO (Koopman's theorem). From this, we predict that any ligand attached to the metal changes this energy by a proportional amount. Our research has shown that a simple Koopman's theorem was not appropriate in defining Lever parameters. We found that this is likely due to reasons in DFT formalism that propagates errors in electronic repulsion which leads to errors (self-interaction error and frozen-orbital approximation).

In this paper we introduce a correction factor, δ , for the abovementioned errors which has shown a significant improvement in theoretical calculations related to predicting Lever parameters.

Title: First Use of nanpH₂ and nacpH₂ as Bridging/Chelating Ligands in Heterometallic Mn/Ln Cluster Chemistry: Ferromagnetic Complexes and Single-Molecule Magnets

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Schiff-base ligands are a widely known family of ligands in coordination chemistry. In particular, aromatic bridging/chelating Schiff-bases have been reported to form heterometallic 3d/4f-metal clusters which possess unique topologies and interesting magnetic properties.^[1] We present herein two new families of {Mn₁₂Ln₆} clusters, where Ln^{III} = Gd (**1**) and (**2**), Dy (**3**) and (**4**), Y (**5**) and (**6**), from the employment of the organic bridging/chelating ligands N-Naphthalidene-2-amino-naphthol (nanpH₂) and N-Naphthalidene-2-amino-5-chlorophenol (nacpH₂) in heterometallic Mn/Ln cluster chemistry for the first time. Structural similarities between the employed ligands led to the resulting complexes having analogous inorganic core structures. Furthermore, the magnetic susceptibility data revealed ferromagnetic exchange interactions occurring between the Mn and Ln ions in complexes **3** and **4**, with both complexes displaying single-molecule magnetic (SMM) behavior.

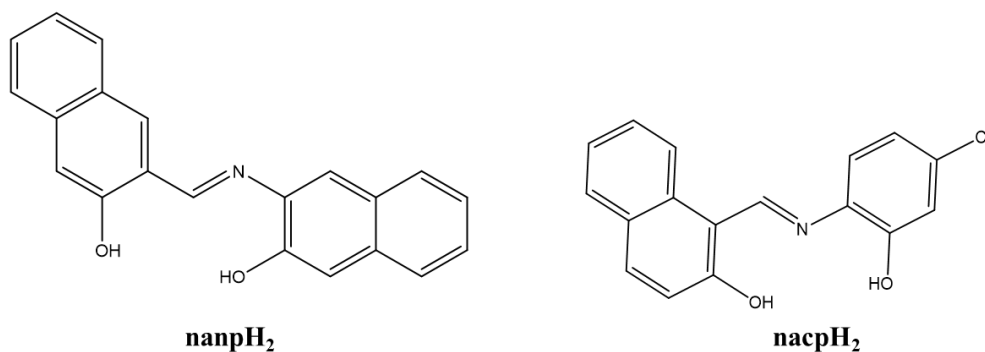


Figure 1. Molecular structures and abbreviations of the Schiff-base ligands employed.

References:

- Alexandropoulos D. I.; Nguyen Tu. N.; Cunha-Silva L.; Zafiroopoulos T. F.; Escuer, A.; Christou, G.; Stamatatos Th. C. *Inorg. Chem.* **2013**, *3*, 1179.