

Saturday AM

ROZH 103

Session 1

08:30 Introductory Remarks

08:40 0001 *Inclusion compounds of cadmium dibenzoylmethanate complexes through the design of discrete and extended host entities.* Okeke Emeka B., Soldatov Dmitriy V

09:00 0002 *Atomic Layer Deposition of oxide films on metal substrates* Gordon PG, Barry ST

09:20 0003 *Polymerisation of rac-lactide by a chiral zinc diketiminate complex* Drouin F., Oguadinma P. O., Schaper F.

09:40 0004 *Electrochemical reduction of CO₂ with novel ruthenium(II) complexes.* Chu J., Abedin T., Potvin P. G., Lever A. B. P.

10:00 0005 *Characterization of a Rhodium-Sparteine Complex, [(η^5 -Sparteine)Rh(η^4 -COD)]⁺: Crystal Structure and DFT Studies on Ligand-Rotation Dynamics* De Crisci A. G., Annibale V. T., Hamer G. K., Lough A. J., Fekli U.

10:20 Dalton Chemicals Coffee Break

This break is sponsored by Dalton Chemicals

10:40 0006 *New class of Iridium complexes containing N-nitroamides* Chua Z., Bohle S.

11:00 0007 *Functionalized Ionic Liquids as Stabilizing Ligands in the Synthesis of Transition Metal Nanoparticles.* Luska K.L., Moores A.

11:20 0008 *Development of Transition Metal Reagents for Oxygen Atom Transfer Reactions* S. Askari M., Ottenwaelder X.

11:40 0009 *Monomeric and Dimeric POCN-Type Pincer Complexes of Nickel* Spasyuk D.M., Zargarian D

12:00 Bruker Spectrospin Lunch

Lunch is being sponsored by Bruker Spectrospin

ROZH 102

Session 2

08:40 0010 *Donor Stabilization of Germlyenes* Baumeister M.T.F., Denk M.K., Rheingold A.L., Moore C., Golen J.

09:00 0011 *Coordination Study of Acyclic Imino-N-Heterocyclic Carbene Ligands to Group II Transition Metals.* Badaj A.C., Lavoie G.G.

09:20 0012 *Using Conceptual Density Functional Theory as an Alternative Approach to Modelling Inorganic Chemistry: Application to Systems with Degenerate Ground States* Johnson P. A., Ayers P. W.

09:40 0013 *Methylplatinum chemistry of Quinoline functionalized thiophene* Tan R., Song D.

10:00 0014 *Mechanistic Insights into the Role of Lewis Acidic Metal Complexes as Amine-Borane Dehydrogenation Catalysts* Rachiero G. P., Baker R. T., Kivi C.

10:20 Dalton Chemicals Coffee Break

This break is sponsored by Dalton Chemicals

10:40 0015 *Heavy Heteroatom Ferromagnets under Pressure: Structural Modifications and the Magnetic Response* Cvrkalj K., Leitch A. A., Mito M., Tse J. S., Oakley R. T.

11:00 0016 *Design and Synthesis of electroactive Tetrathiafulvalene Building Blocks: Towards Molecule-Based Magnetic and/or Electronic Materials* Acha R. T., Pilkington M

11:20 0017 *The cycloaddition and oxidative dehydrogenation reaction of SNS⁺ with 1,4-benzoquinone and 1,4-naphthoquinone leading to ring fused 1,3,2-dithiazolyl radicals* Mailman A., Passmore J

11:40 0018 *The Addition of Nitriles to Group 14 (Di)metallenes* Hardwick Julie A., Baines Kim M.

12:00 Bruker Spectrospin Lunch

This lunch is sponsored by Bruker Spectrospin

Saturday PM

ROZH 103

Session 1

13:00 0019 *Isolation, surface deposition and electrochemical activity of Ti(IV) complexes bearing non-innocent ligands for methanol oxidation in Direct Methanol Fuel Cells.* Donzelli A., Potvin P.G.

13:20 0020 *Energetics of C-H Activation Using [TpRh(CNneopentyl)]: Quantifying Resonance and Inductive Effects* Evans M. E., Jones W. D.

13:40 0021 *Photo-Splitting of Water Using a Molecular Cobalt Catalyst* McCormick T., Weinberg D., Lazarides T., Eisenberg R

14:00 0022 *Polyoxometalate-based Hybrid Platforms Presenting Remote Polydentate Coordination Sites : Toward Complexation of Transition-Metals for Novel Charge-Transfer Systems.* Santoni M.-P., Hanan G. S., Hasenknopf B., Proust A.

14:20 0023 *Synthesis, Coordination Chemistry and Applications of 2-Phosphino-1-dimethylaminoferrocenes* Van Belle L., Zaifman J., Dodge L., Metallinos C.

14:40 0024 *Design and synthesis of dyads utilizing charge-separation for use in molecular devices* Dares C., Lever A. B. P., Fournier R.

15:00 O'Zone Software Coffee Break

This break is sponsored by O'Zone Software

Plenary Lecture ROZH 103

15:20 Prof. Abdel Sayari will present the 'Catalysis Lectureship Award' plenary lecture titled 'Catalysis over Pore-Expanded Mesoporous Silica'

OCE Presentation ROZH 103

16:20 A presentation by the Ontario Centres of Excellence titled "From an idea at the bench to product on benches"

16:30 End of Session

16:30 See Poster Session Information

ROZH 102

Session 2

13:00 0025 *Ni \rightarrow B interactions in Nickel Phosphino-Alkynyl-Borane Complexes* Zhao X., Otten E., Song D., Stephan D. W.

13:20 0026 *The development of new sulfur(II) delivery reagents* Martin C. D., Ragogna P. J.

13:40 0027 *Hybrid Multifunctional Materials: An Investigation of Synergistic Interactions between Magnetic Spin and Electron Transport* Djukic B., Lemaire M.T.

14:00 0028 *Zinc Chalcogenolate Complexes as Molecular Precursors to Manganese (II) Containing Ternary Nanoclusters.* Khadka C. B., Corrigan J. F.

14:20 0029 *New Ligand Frameworks for Supporting N-Heterocyclic Phosphonium Cations* Brazeau A. L., Price J. T., Jones N. D.

14:40 0030 *Luminescence Vapochromism in Triarylboron-Pt(II) Complexes for Detection of Organic Vapours* **Hudson Z.M.**, Sun C., Wang S.

15:00 **O'Zone Software Coffee Break**

This break is sponsored by O'Zone Software

15:20 See the Prof. Abdel Sayari plenary lecture information in Session 1

16:20 See the Ontario Centres of Excellence presentation information in Session 1

16:30 End of Session

16:30 See Poster Session Information

ROZH Foyer

Poster Session

From 16:30 until 18:30

0031 *Synthesis and Reactivity Studies of Bifunctional Phosphino-Borane "Frustrated Lewis Pairs"* **Schedler M.**, Heiden Z. M., Stephan D. W.

0032 *Stabilization of low coordination numbers with polyamines* **Krause M.**, Denk M.K.

0033 *Exploring the Heterocyclic Chemistry of Group 14: Pyrrolides and Indolides* **Poisson J.**, Wharf I., Barsan M. M., Butler I. S.

0034 *Catalytic hydrosilylation by cationic ruthenium and iron complexes.* **Gutsulyak D.V.**, Nikonov G.I.

0035 *Luminescent metal organic framework (MOF) based on substituted 4,4'-stilbene dicarboxylic acid (SDA)* **Li Y.**, Song D.

0036 *Pd nanoparticles supported on cellulose nanocrystallites as active hybrid material for catalytic hydrogenation reaction* **Cirtiu C.M.**, Dunlop-Brière A., Moores A.H.

0037 *High-Yield Synthesis of ReO₃F and a Study of its Fluoride Ion Donor and Lewis Acid Properties* **Ivanova M. V.**, Hughes M. J., Mercier H. P. A., Schrobilgen G. J.

0038 *Insights On Metallation of Pincer-Type Ligands by Nickel(II)* **Vabre B.**, Zargarian D

0039 *Photo-splitting of water with a sensitized metal oxide semiconductor* **McCormick T.**, Farkas D, Eisenberg R

0040 *The Synthesis of Constrained-Geometry Tetradentate Ligands for Small Molecule Activation.* **Skrela B.C.**, Hossain D., Lavoie G.G.

0041 *Characterization of the Inclusion Capabilities of Dipeptide Leucyl-Leucine* **Brown Chris T.**, Soldatov Dmitriy V

0042 *Silver (I) Coordination Polymers Supported by Oligomeric Dinitrile Ligands Containing S- and N- Donors* **Andreychuk N.R.**, MacKinnon C.D., Parent S.L.M., Assoud A.

0043 *New Thiophene Containing Selenium and Phosphenium Cations* **Price J. T.**, Jones N. D.

0044 *Solid-State NMR of Inorganic Systems: Molecules, Networks and Nanoparticles studied via ¹⁹F, ⁴³Sc, ³⁵Cl, ⁶³Cu, ⁸⁹Y, ⁹¹Zr, ¹⁰⁹Ag, ¹¹³In, ¹¹⁹Sn, ¹⁹⁵Pt, ¹⁹⁹Hg, ²⁰⁷Pb, and ²⁰⁹Bi NMR spectroscopy.* **Harris K.J.**, Hamaed H., Lucier B.E.G., MacGregor A.W., Rossini A.J., Schurko R.W.

0045 *Ring-opening of 1,4-dioxane and trapping of sulfur dioxide with Frustrated Lewis Pairs* **Birkmann B.**, Stephan D. W.

0046 *Synthesis of a New Sterically-Hindered Dicarboxamide Ligand* **Tan L. L.**, Lee S. C.

0047 *Synthesis and properties of ferrocene-amyloid beta peptide conjugates* **Beheshti S.**, Kraatz H-B

0048 *Synthesis and Coordination Chemistry of 2,2'-Bipyridine-3,3'-(2-Pyridinecarboxamide).* **Hurley N. J.**, Wang J., Zarrabi N., Pilkington M.

0049 *Addition polymerization of a silene* **Guo J.**, Pavelka L., Baines K.

0050 *Palladium β -Diiminato Chemistry: Reactivity with Ligands, and Transmetalation Reagents* **Annibale V. A.**, Song D.

0051 *New Tetracarboxamide bis-Bipyridyl Ligands: Synthesis and Coordination Chemistry* **Zarrabi Nilofar.**, Pilkington Melanie

0052 *Shedding Light onto the Nature of Electronic Transitions in Highly Coupled Inorganic Complexes* **Dares C.**, Lever A. B. P., Fournier R.

0053 *Photoisomerisation properties of boron-functionalized platinum dimers linked by trans-1,2-bis(4-pyridyl)ethylene* **Lee K. A.**, Rao Y., Wang S.

0054 *Synthesis of phosphonium ionic liquids with a pendant aza-crown ether and its metal complexes* **Dube J.W.**, Ragogna P.J.

0055 *Transition Metal Complex-Catalyzed Dehydrogenation of Amine-Boranes in Ionic Liquids* **Wright W. R. H.**, Baker R. T., Sneddon L. G.

0056 *Thiophene-Containing N,O-Donor Ligands for Metal Complexes* **Swanick K.N.**, Price J.T., Jones N.D.

0057 *An Investigation of 1,2,3-Dithiazolyl Based Radicals as Spin-Bearing Ligands Towards the Development of Novel Magnetic Materials* **MacDonald D.J.**, Preuss K.E., Koutentis P.A.

0058 *Ferrocenyl Amidinate Complexes of Ti(IV) and Zr(IV): Synthesis, Characterization and Ethylene Polymerization Activity* **Multani K.**, Stephan D.W.

0059 *Heteroleptic Guanidinate Aluminum Hydrides for Atomic Layer Deposition of Aluminum Metal Thin Films* **Delahunt J. R.**, Barry S. T.

0060 *Transmetalation of a Primary Amino-functionalized N-Heterocyclic Carbene from Nickel(II) to Platinum Group Metal Precatalysts for Transfer and Direct Hydrogenation of Ketones.* **O W. W. N.**, Lough A. J., Morris R. H.

0061 *Phase Diagram of the System Leucyl-alanine - DMSO with 1:1 Inclusion Compound.* **Yazdani A.**, Chimanov V.V., Soldatov D.V.

0062 *Olefin Addition to Frustrated Amine/Borane Lewis Pairs* **Voss T.**, Sortais J. B., Kehr G., Fröhlich R., Erker G.

0063 *Synthesis and Characterization of a New Thiadiazolo- Fused Para-Semiquinone* **Morgan I. S.**, Preuss K. E., Jennings M., J.,

0064 *Gas-Phase Thermolysis of Copper Precursors. Unraveling the Fragmentation of Guanidates and Amidinates by Time-of-Flight Mass Spectrometry Matrix-Isolation FTIR Spectroscopy.* **Coyle J.P.**, Johnson P., DiLabio G., Mueller J., Barry S.T

0065 *New Rod-Like Dyads of Ru(II) and Terpyridyl Ligands: Effect of Bis-Pyridyl-1,3,5-Triazine in the Tuning of the Photophysical Properties.* **Santoni M.-P.**, Medlycott E., Hanan G. S., Hasenknopf B., Proust A., Nastasi F., Campagna S., Chiorboli C., Argazzi R., Scandola F.

0066 *The Halogen-Free Synthesis of Rhodium Nanoparticles for Applications in Catalysis* **Stratton S.A.**, Luska K.L., Moores A. **PAPER WITHDRAWN**

0067 *Photochromic behaviour of 4-coordinate organoboron compounds* **Murphy S.**, Baik C, Wang S

0068 *Synthesis, structure, volatility, and thermal stability of molybdenum and tungsten complexes containing nitrogen rich ligands.* **El-Kadri O. M.**, Winter C. H., Heeg M. J

0069 *A novel Schiff base complex of Co^{II} based on the N-hydroxyamidine motif: structural, spectroscopic and electrochemical properties* **Derossi S.**, Cibian M., Hanan G. S.

0070 *[Ru(η^5 -C₅H₅)(6,6'-diamino-2,2'-bipyridine)(CH₃CN)](OTf) as a Metal-ligand Bifunctional Catalyst Under Acidic Conditions.* **Di Mondo D.**, Schlaf M.

0071 *Facile synthesis of cyclic phosphonium salts for use as phosphine-aldehyde precursors in metal templating and ligand synthesis.* **Mikhailine A. A.**, Lagaditis P., Sues P., Lough A. J., Morris R. H.

0072 *Looking at Arsenicals for treatment of Acute Promyelocytic Leukemia.* **Gu Y.**, Bohle DS, Garnier N

0073 *Spin Catalysis of Azo Photoisomers* **Rosadiuk K.**, Bohle D.S.

0074 *Determining the Degradation Products of the Malaria Pigment.* **Hill A.**, Bohle D.S

0075 *Synthesis of Amine Stabilized Nanoparticles as Precursors in Ligand Exchange* **Rak M. J.**, Luska K. L., Moores A.

0076 *Synthesis and Characterization of a Bis-DTA Pyridin-4-one Neutral Radical Ligand* **Carello CE.**, Preuss KE

0077 *New POCN-Type Pincer Complexes of Nickel(II) and Nickel(III)* **Spasyuk D M.**, Zargarian D

0078 *In Situ EXAFS and NMR Study of Ultrathin Bismuth Sulfide Nanowires* **Thomson JW.**, Ozin GA

0079 *A combined ⁷³Ge solid state NMR spectroscopic and computational study of GePh₄ and GeCl₂-dioxane* **Hanson M. A.**, Sutrisno A., Rupar P. A., Huang Y., Baines K. M.

0080 *Coordination of Imino-N-Heterocyclic Carbenes to Transition Metals.* **Badaj A.C.**, **Larocque T.G.**, Lavoie G.G.

0081 *Cationic Complexes of Tin(II)* **Avery Jessica C.**, Rupar Paul A., Baines Kim M.

0082 *Late Transition Metal Complexes of η^3 -Coordinated Vinylboranes* **Kolpin K.B.**, Emslie D.J.H.

0083 *Coordination Study of Nonenolizable Bis(Imino)-N-Heterocyclic Carbene Pincer (NCN) Ligand to Transition Metals.* **Al Thagfi J.**, Lavoie G.G.

0084 *A New Dithiazolo Fused o-Quinone Potential Spin Bearing Ligand* **Smithson C. S.**, Preuss K. E., Jennings M. J.

0085 *New POCOP-Type Pincer Complexes of Nickel(II)* **Salah A.**, Zargarian D

0086 *Triarylboron complexes of Pt(II)-acetylide: synthesis, computational studies and luminescence vapochromism.* **Sun C.**, Hudson Z.M., Wang S.

0087 *Carboxymethyl-Dextran Modified Magnetic Nanoparticle Conjugated to Peptide Octreotide* **Han G.**, Kraatz H.

0088 *Evidence for the Formation of Trithiatetrazocinyl Radicals Anions* **Yu X.**, Boere R. T., Roemmele T. L

0089 *The Preparation and Characterization of a New Family of Spin-bearing Tetrathiafulvalene Donors* **Veneri S.**, Pilkington M

Sunday AM

ROZH 103

Session 1

08:40 0090 *Potential Use of Red Mud as a Catalyst for the Upgrading of Pyrolysis Bio-Oil* **Karimi E.**, Schlaf M

09:00 0091 *Template Synthesis of Iron(II) and Ruthenium(II) Complexes Containing Multidentate Ligands with Phosphorus and Nitrogen Donor Atoms* **Lagaditis P.O.**, Lough A.J., Morris R.H.

09:20 0092 *Visible-light Photocatalytic Activity of Eco-friendly TiO₂-SiO₂-Mn Aerogels in Air Purification* **Kalebaila K.**, Klabunde K.

09:40 0093 *Mechanism of carbonyl hydrosilylation catalyzed by (Cp)(ArN=)Mo(H)(PMe₃).* **Shirobokov Oleg G.**, Nikonov Georgii I

10:00 0094 *Formation of self-assembled monolayers (SAMs) on Au(111) surfaces by dithiophosphinic acids (DTPAs) with nanoscale structural control* **San Juan R.R.**, Müller J., Breen Carmichael T.

10:20 MBraun Coffee Break

This break is sponsored by MBraun

Plenary Lecture ROZH 103

10:40 Prof. Terrence J. Collins will present the plenary lecture titled 'Iron-TAML activators: highly successful mimics of peroxidase enzymes for green chemical applications'

Awards ROZH 103

11:40 Awards Ceremony

12:00 End of Session

ROZH 102

Session 2

08:40 0095 *Synthesis and Characterization of a New 1,2,3,5-Dithiadiazolyl (DTDA) Radical Ligand and Mn(II)(hfac)₂(DTDA) Complex* **Fatila E.M.**, Preuss K.E., Clerac R., Jennings M., Assoud J.

09:00 0096 *Synthesis, Reactivity and Coordination Chemistry of Novel 2,2'-Bipyridine Schiff-Base Ligands.* **Gumbau-Brisa R.**, Pilkington M.

09:20 0097 *Dicationic Selenium and Tellurium Complexes* **Dutton J.L.**, Ragogna P.J.

09:40 0098 *A Diversity of Metal-Ligand Interactions in Halide (X = I, Br, Cl, F) and Halide-Free Ambiphilic Ligand Rhodium Complexes* **Cowie B.E.**, Emslie D.J.H.

10:00 0099 *Gallium Analogs of Hemozoin: novel approaches to exploring the structure and drug-interactions of malaria pigment* **Dodd E. L.**, Bohle D. S.

10:20 MBraun Coffee Break

This break is sponsored by MBraun

10:40 See the Prof. Terrence J. Collins plenary lecture information in Session 1

11:40 See the Awards Ceremony information in Session 1

12:00 End of Session

1 08:40 Saturday ROZH 103

Inclusion compounds of cadmium dibenzoylmethane complexes through the design of discrete and extended host entities. **Emeka B. Okeke** <eokeke@uoguelph.ca> and **Dmitriy V Soldatov** <dsoldato@uoguelph.ca>, Department of Chemistry, University of Guelph, Guelph, ON, N1G 2W1.

The complexes $[M(\text{DBM})_2\text{A}_2]$ ($M = \text{metal(II)}$, $A = \text{amine}$, $\text{DBM} = \text{C}_6\text{H}_5\text{COCHOCOC}_6\text{H}_5$, dibenzoylmethane) have proven to be excellent motifs for the design and synthesis of porous materials and inclusion compounds (1). $[M(\text{DBM})_2\text{A}_2]$ complexes that are cis-configured deviate from the geometry expected for the host property and so do not form inclusion compounds (2). Strategic design of versatile supramolecular materials can be achieved by the choice of a suitable ligand A with the possibility of progression from discrete to polymeric complexes (3). $[M(\text{DBM})_2\text{Q}_2]$ (i), $[M(\text{DBM})_2\text{lq}_2]$ (ii), $[M(\text{DBM})_2(\text{na})_2]$ (iii) and $[M(\text{DBM})_2(\text{ina})_2]$ (iv) ($Q = \text{quinoline}$, $\text{lq} = \text{isoquinoline}$, $\text{na} = \text{nicotinamide}$, $\text{ina} = \text{isonicotinamide}$) were synthesized and characterized with XRD and TGA. (i) and (ii) are discrete complexes with inclusion ability. (iii) and (iv) form 1D H-bonded chains due to the amide-amide supramolecular synthon. (iii) and (iv) illustrate the concept of H-bond assisted guest inclusion observed for the cis-configured $[M(\text{DBM})_2\text{A}_2]$ complex.

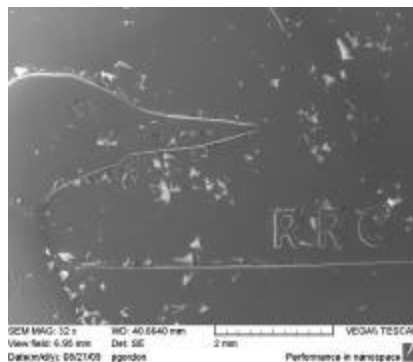
Ref. (1) D. V. Soldatov, *J. Chem. Crystallogr.* 2006, 36, 747-768. (2) D.V. Soldatov, G. D. Enright, J. A. Ripmeester, *Supramol. Chem.* 1999, 11, 35-47. (3) C. B. Aakeroy et al, *Cryst Eng Comm.* 2004, 6, 413-418.

2 09:00 Saturday ROZH 103

Atomic Layer Deposition of oxide films on metal substrates **PG Gordon** <pgordon@connect.carleton.ca> and **ST Barry** <sbarry@connect.carleton.ca>, Carleton University, 1125 Colonel By Dr., Ottawa, ON K1S 5B6.

Transparent oxide films with thicknesses ranging from 1000 to 10,000 Å were grown by atomic layer deposition (ALD) on metal alloy as well as on Si(100) substrates. Characterization of these films will be discussed with attention given to conformality, continuity, and adherence. Growth rates will also be discussed, with consideration given to the possibility that there is a chemical vapor deposition (CVD) component to the deposition.

Thickness-dependent colour changes including iridescence have been observed, particularly with respect to the metal substrates. A thickness vs. colour study will be presented. At higher thicknesses the substrate materials displayed dissimilar but characteristic delamination morphologies. Annealing studies under air and nitrogen were performed to determine the impact on film density and integrity.



3 09:20 Saturday ROZH 103

Polymerisation of rac-lactide by a chiral zinc diketiminate complex **F. Drouin** <fredric.drouin@umontreal.ca>, **P. O. Oguadinma** and **F. Schaper** <Frank.Schaper@umontreal.ca>, Université de Montréal, Montréal, QC.

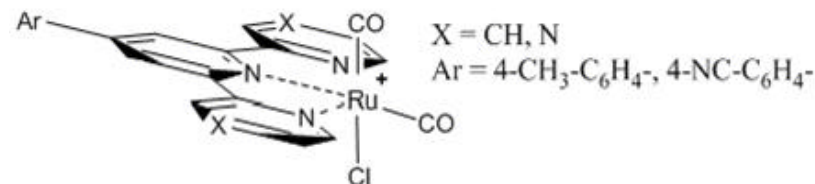
Poly(lactic acid) can be obtained from monomeric lactide by a great number of metal complexes via ring opening polymerization. Zinc isopropanolate complexes bearing -diketiminato ligands have shown to be highly active catalysts, which show high selectivity towards syndiotactic enchainment by chain-end control.

While most systems focus mainly on diketiminato zinc complexes with aromatic substituents on nitrogen, we extended this chemistry to systems with aliphatic nitrogen ligands, with the idea of introducing C_2 -symmetry or eventually even chirality. We thus prepared diketiminato zinc complexes with benzyl- and (S)-methylphenyl substituents on nitrogen and tested them in lactide polymerisation. While both catalysts were active and showed reduced preference for syndiotactic enchainment, the introduced catalytic site control seems to be weak to overcome chain end control in these systems.

4 09:40 Saturday ROZH 103

Electrochemical reduction of CO₂ with novel ruthenium(II) complexes. **J. Chu** <jason.chu@yorku.ca>, **T. Abedin** <tareque@yorku.ca>, **P. G. Potvin** <pgpotvin@yorku.ca> and **A. B. P. Lever** <blever@yorku.ca>, Department of Chemistry, York University, 4700 Keele St., Toronto, ON M3J 1P3.

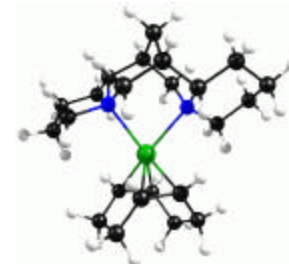
Ru^{II} dicarbonyl complexes of general formula $[\text{LRu}(\text{CO})_2\text{Cl}]^+\text{PF}_6^-$ were synthesized from various tridentate ligands L . The complexes were characterized by $^1\text{H-NMR}$, $^{13}\text{C-NMR}$, IR and UV-visible spectroscopies and by mass spectrometry. DFT calculations and cyclic voltammetric studies were also carried out. This presentation will highlight the synthetic strategies, characterization, mechanistic studies and electrochemical studies of these new complexes in the context of electrocatalytic CO_2 reduction.



5 10:00 Saturday ROZH 103

Characterization of a Rhodium-Sparteine Complex, $[(\text{-})\text{Sparteine}]\text{Rh}(\eta^4\text{-COD})]^+$: Crystal Structure and DNMR/DFT Studies on Ligand-Rotation Dynamics **A. G. De Crisci** <antonio.decrisci@utoronto.ca>, **V. T. Annibale**, **G. K. Hamer** and **U. Fekl** <ulrich.fekl@utoronto.ca>, University of Toronto Mississauga, 3359 Mississauga Rd N., Mississauga, Ontario L5L 1C6; **A. J. Lough**, University of Toronto, 80 St. George Street, Toronto, Ontario M5S 3H6.

A cationic rhodium-sparteine complex, $[(\text{-})\text{sparteine}]\text{Rh}(\eta^4\text{-COD})^+$ (1^+ : $\text{COD} = 1,5\text{-cyclooctadiene}$) was obtained, isolated as its tetrafluoroborate salt (1BF_4), and characterized using X-ray crystallography and multinuclear (^1H , ^{13}C) and multidimensional NMR spectroscopy. This is the first structurally characterized sparteine complex of rhodium. The Rh-N bonds of the chiral complex are unusually long (2.214(3) and 2.242(3) Å), apparently due to steric repulsion between COD and sparteine. ^1H NMR exchange experiments (EXSY) demonstrate 180° ligand rotation in solution (CD_2Cl_2) with a first-order rate constant of 460 s^{-1} at coalescence, 314 K, and interpolated rate of 150 s^{-1} at 298 K. DFT studies (B3LYP) suggest that the weakly bound sparteine ligand is the rotating ligand and rotation occurs through a concerted pseudo-tetrahedral transition state (shown in figure). Experimental activation barriers agree very well with DFT computed barriers.



6 10:40 Saturday ROZH 103

New class of Iridium complexes containing N-nitroamides **Z. Chua** <zhijie.chua@mail.mcgill.ca> and **S. Bohle** <scott.bohle@mcgill.ca>, Dept. of Chemistry, McGill University, 801 Sherbrooke Street W., Montreal, QC H3A 2K6.

Transition metal complexes containing coordination carboxamides as ligands are uncommon. In most cases, the carboxamide group is linked to another organic fragment through the acyl fragment. Most transition complexes often coordinate through the oxygen atom.¹ In rare cases has direct coordination to the N atom of the amide being observed.²

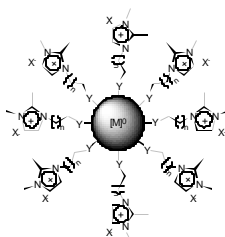
N-nitroamides³ is an interesting class of carboxamides in which the amide proton is relatively acidic. The -NO_2 group directly bonded to the amide functional group exerts an electron-withdrawing effect on the amide functionality. N-nitroamides which have the general chemical formula $\text{RC}(\text{O})\text{NHNO}_2$ ($\text{R} = \text{CH}_3, \text{C}_2\text{H}_5$) have been synthesized from the corresponding anhydrides with nitramide. The N-nitroamides are relatively stable in bases but are prone to hydrolysis to the corresponding acids and nitramide in strongly acidic media. The N-nitroamides oxidatively add to $\text{trans-Ir}(\text{PPh}_3)_2\text{Cl}(\text{N}_2)$ to give the corresponding $[\text{Ir}(\text{PPh}_3)_2(\text{H})(\text{Cl})(\eta^2\text{-RC}(\text{O})\text{NNO}_2)]$ complexes.

The reactivity of $[\text{Ir}(\text{PPh}_3)_2(\text{H})(\text{Cl})(\eta^2\text{-CH}_3\text{C}(\text{O})\text{NNO}_2)]$ was carried out with nucleophiles, CO and PMe_2Ph . Methylation using methyl trifluoromethanesulfonate resulted in the ligand being labile.

1. I. S. Kolomnikov, T. V. Lysyak, S. L. Rusakov, Y. Y. Kharitonov, *Russ. Chem. Rev.*, **1988**, 57, 406.
2. D. L. Cockriel, J. M. McClain, K. C. Patel, R. Ullom, T. R. Hasley, S. J. Archibald, T. J. Hubin, *Inorg. Chem. Comm.*, **2008**, 11, 1.
3. A. A. Lobanova, S. G. Il'yasov, N. I. Popov, R. R. Sataev, *Russ. J. Org. Chem.*, **2002**, 38, 1.

Functionalized Ionic Liquids as Stabilizing Ligands in the Synthesis of Transition Metal Nanoparticles. **K.L. Luska** <kylie.luska@mail.mcgill.ca> and **A. Moores** <audrey.moores@mcgill.ca>, Department of Chemistry, McGill University, 801 Sherbrooke St. W., Montreal, Quebec, Canada, H3A 2K6.

Functionalized ionic liquids (FILs) have been employed as NP ligands since the imidazolium moiety provides electrostatic stabilization, while a metal binding moiety (Y) attaches to the metal surface and provides covalent stabilization of the NPs.^{1,2} We have investigated the use of thiolate (Y = S) and phosphine (Y = PPh₂) FILs in the synthesis of Au and Pd NPs respectively and have shown that the properties of the NPs are dependent on the characteristics of the FIL stabilizing ligand. To this end, the NP size and surface plasmon band of thiolate stabilized Au NPs are dependent on the length of the *N*-alkyl chain (*n*) and the FIL counter-ion (X), while the NP size of phosphine stabilized Pd NPs is only influenced by the counter-ion (X). The use of phosphine stabilized Pd NPs as biphasic hydrogenation catalysts have also been studied and are active and recyclable catalyst systems.

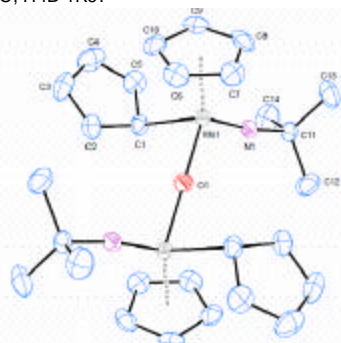


Schematic representation of FIL stabilized metal NPs (For M = Au, Pd; Y = S, PPh₂; n = 2, 5, 8; X = OTf, NTf₂).

Ref. (1) Kim, K.S., Demberelnyamba, D. and Lee, H. *Langmuir*, **2004**, *20*, 556. (2) Itoh, H.; Naka, K. and Chujo, Y. *J. Am. Chem. Soc.* **2004**, *126*, 3026.

Development of Transition Metal Reagents for Oxygen Atom Transfer Reactions **M.S. Askari** <ms.askari@gmail.com> and **X. Ottenwaelder** <xotten@alcor.concordia.ca>, The XoRG, Department of Chemistry and Biochemistry, Concordia University, 7141 Sherbrooke W., Montreal, QC, H4B 1R6.

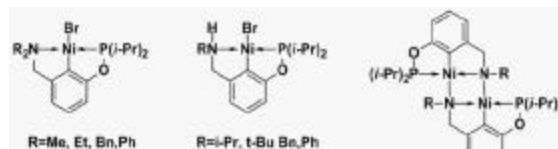
In search of strong and efficient oxygen atom transfer reagents for the synthesis of fine chemicals, we are investigating the synthesis of compounds containing a metallocaxaziridine ring. We have prepared molybdenum-imido complexes capable of receiving an oxygen atom and studied their reactivity towards oxidizing agents, which yielded in the formation of a structurally unusual molybdenum dimer which was characterized by UV-Vis, variable-temperature ¹H-NMR, and X-ray crystallography. Computational investigations using the B3LYP functional and double- ζ basis sets revealed the formation of two intermediates upon the reaction of the molybdenum-imido complex with an oxygen atom. Based on the electronic structures of the intermediates we hereby propose a mechanism for the formation of the dimer which accounts for the experimentally observed product.



Monomeric and Dimeric POCN-Type Pincer Complexes of Nickel **D.M. Spasyuk** <denis.spasyuk@umontreal.ca> and **D. Zargarian** <zargarian.davit@umontreal.ca>, Département de chimie, Université de Montréal.

Pincer complexes are now widely used in organometallic chemistry and catalysis thanks to their versatility, robustness, thermal stability and ease of preparation. The tendency of pincer ligands to stabilize unusual oxidation states of metals make pincer complexes very useful in mechanistic investigations. Therefore, many different types of pincer complexes have been reported, of which most are based on bulky, tertiary diamine or diphosphine ligands.

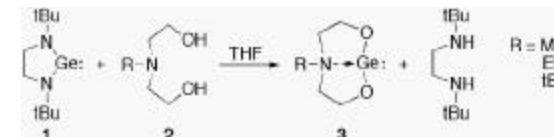
Our long-standing interest in organo-nickel complexes and the little explored chemistry of POCN-type pincer ligands prompted us to investigate the preparation and catalytic activities of POCN-Ni complexes. A recent publication has reported the chemistry of complexes based on tertiary amine moieties (Organometallics, 2009, ASAP). This presentation will describe our preliminary results on the chemistry of the complexes based on secondary amines, including the preparation and reactivities of amido-bridged dimers.



Donor Stabilization of Germynes **M.T.F. Baumeister** <mbaumeis@uoguelph.ca> and **M.K. Denk** <mdenk@uoguelph.ca>, University of Guelph; **A.L. Rheingold** <arheingold@ucsd.edu>, **C. Moore** <cmoore@ucsd.edu> and **J. Golen** <jgolen@umassd.edu>, University of California, San Diego.

Reactions of the stable germylene **1** [1,2,3] with diethanolamines **2** (R = Me[4], Et, tBu) leads to the formation of donor stabilized germynes **3**. Depending on R, the germynes exist as monomers or dimers in the solid state. Reaction of **3** with Ni(CO)₄ leads to the respective Ni(CO)₃ germylene complexes. Dimerization energies were obtained through DFT methods and post-SCF methods (CBS-4m level).

(1) Herrmann, W. A.; Denk, M. K.; Behm, J.; Scherer, W.; Klingan, F. R.; Bock, H.; Solouki, B.; Wagner, M.; *Angew. Chem. Int. Ed. Engl.* **1992**, *33*, 1485-8. (2) M. Denk, PhD thesis 1992. (3) Lehmann, J. F.; Urquhart, S. G.; Ennis, L. E.; Hitchcock, A. P.; Hatano, K.; Gupta, S.; Denk, M. K.; *Organometallics*. **1999**, *18*, 1862-72. (4) Synthesis of **3** for R = Me; Silverman, L. D.; Zeldin, M.; *Inorg. Chem.* **1980**, *19*, 272-3. Germylene was described but not fully characterized.

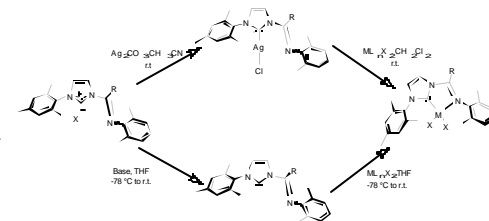


Coordination Study of Acyclic Imino-N-Heterocyclic Carbene Ligands to Group 11 Transition Metals. **A.C. Badaj** <anabad@yorku.ca> and **G.G. Lavoie** <glavoie@yorku.ca>, Department of Chemistry, York University, 4700 Keele Street, Toronto, ON M3J 1P3.

N-Heterocyclic carbene (NHC) fragments offer opportunities to tune the steric and electronic nature of the ligand, and therefore to control the reactivity of the resulting transition metal complexes.^{1,2} Organometallic complexes of heteroditopic ligands containing N-heterocyclic carbene have exhibited catalytic activities for a wide range of chemical reactions.³ Our group is interested in the coordination chemistry of bidentate ligands based on imino-N-heterocyclic carbenes. We herein report the synthesis and characterization of the first aryl-substituted acyclic imino-NHC ligand precursor, as well as coordination of the carbene to Group 11 transition metals.

Reference:

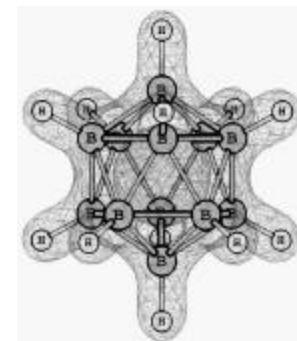
- Herrmann, W. A.; Kocher, C. *Angew. Chem. Int. Ed. Engl.* **1997**, *36*, 2162.
- Leuthäuser, S.; Schwarz, D. Plenio, H. *Chem. Eur. J.* **2007**, *13*, 7195.
- Peris, E.; Crabtree, R.H., *Coordination Chemistry Reviews* **2004**, *248*, 2239-2246.



Using Conceptual Density Functional Theory as an Alternative Approach to Modelling Inorganic Chemistry: Application to Systems with Degenerate Ground States **P. A. Johnson** <johnsopa@mcma.ster.ca> and **P. W. Ayers** <ayers@mcma.ster.ca>, Department of Chemistry, McMaster University, Hamilton, Ontario, L8S 4M1.

Frontier molecular orbital (FMO) theory based on Kohn-Sham density functional theory (DFT) is often employed to explain inorganic reactions. This is unsatisfying since it is not only based on artificial molecular orbitals but it can also predict incorrect behaviour, as in the case of M₂(hpp)₄ (M=Cr, Mo, W)¹. FMO fails when orbital relaxation effects are significant. Conceptual DFT is an alternative approach that provides a description formulated from the density, a physical observable, and is very similar in structure to classical thermodynamics. In this context, many classical chemical principles (eg., electronegativity, hardness) and previously unknown concepts (eg., local softness) can be expressed in a simple way. Systems with degenerate ground states have been studied as they provide a challenge to conceptual DFT and because they are prevalently observed in inorganic applications.

- L. J. Bartolotti and P. W. Ayers, *J. Phys. Chem. A* **109**, 1146 (2005)

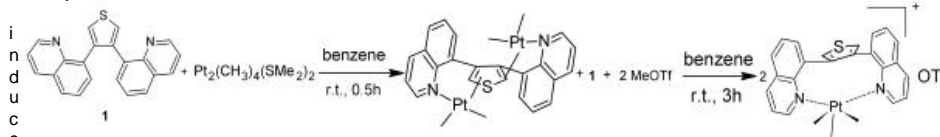


13 09:40 Saturday ROZH 102

Methylplatinum chemistry of Quinoline functionalized thiophene **R. Tan** and **D. Song**

<dsong@chem.utoronto.ca>, Davenport Chemical Research Laboratories, Department of Chemistry, University of Toronto, 80 St. George Street, Toronto, Ontario, M5S 3H6.

Transition metal complexes of thiophenes with various coordination modes have been observed and isolated. These include sulfur-bound η^1 mode with groups 6 and 7 metals, η^2 mode (π -bound via one CC double bond) with groups 8 and 11 metals, η^4 mode (π -bound via four carbon atoms) with groups 8 and 9 metals, η^5 mode with group 6 metals. However, the mechanistically very important group 10 metal complexes of η^2 -thiophene, which have been proposed as key intermediates in the platinum catalyzed hydrodesulfurization processes, have not been isolated. Here, we report the design and syntheses of a series of quinoline functionalized thiophene ligands and the isolation of the first group 10 metal complexes of μ^2 -thiophene. We tested some preliminary reactivities of these complexes and successfully isolated and characterized three novel air- and moisture- stable five-coordinate Pt(IV) complexes. Chirality



14 10:00 Saturday ROZH 102

Mechanistic Insights into the Role of Lewis Acidic Metal Complexes as Amine-Borane Dehydrogenation Catalysts **G. P. Rachiero** <grachier@uottawa.ca>, **R. T. Baker** <rbaker@uottawa.ca> and **C. Kivi** <kivichar@tbaytel.net>, Centre for Catalysis Research and Innovation, Department of Chemistry - University of Ottawa.

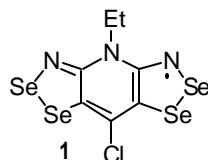
Ammonia borane (H_3NBH_3 , AB) with a very high hydrogen capacity (19.6 wt%) and low molecular weight (30.9 gmol⁻¹) represents a leading material for hydrogen storage applications. Metal complex-catalyzed dehydrogenation of AB and substituted amine-boranes enables a considerable extent of hydrogen release at affordable temperatures. Effective catalysts fall into two classes: those that provide a fast release of one equiv. of H_2 per AB and insoluble aminoborane oligomers (NH_2BH_2)_n and those that offer slower release of > 2 equiv. H_2 along with B-N cross-linked borazine (polyborazylene, BNH_x). Baker et al. recently found that carbonylmetal-based Lewis acids constitute a third class of catalysts in which predominant formation of soluble cyclotriborazane (NH_2BH_2)₃ is observed (Scheme 1). DFT studies suggest that Lewis acid activation of AB via M-H-B complexation lowers the barrier to intramolecular H_2 loss. Subsequent dehydrocyclization and chain end back-biting then afford the observed product.

Shimoi et al.¹ recently proposed an alternative pathway in which photogenerated carbonylchromium-based catalysts operate via "Cr(CO)₄" whereas Heinekey, Goldberg et al.² showed concomitant formation of Cr hydrides such as [HCr₂(CO)₁₀], suggesting hydride abstraction from AB as observed previously³ with B(C₆F₅)₃. In a study of thermally generated Lewis acid catalysts, we investigated

15 10:40 Saturday ROZH 102

Heavy Heteroatom Ferromagnets under Pressure: Structural Modifications and the Magnetic Response **K. Cvrkajli** <kcvrkajli@uwaterloo.ca>, **A. A. Leitch** and **R. T. Oakley**, University of Waterloo; **M. Mito**, Kyushu Institute of Technology; **J. S. Tse**, University of Saskatchewan.

We recently reported a selenazyl radical **1** that orders ferromagnetically with a T_c value of 17.0 K.¹ This ordering temperature is the highest ever observed for a nonmetal based ferromagnet. We have now explored the effect of *physical pressure* on the crystal structure and magnetic properties of **1** over the pressure range 0-4 GPa.² We found that the application of physical pressure to a ferromagnetic bisdiselenazyl radical leads to a decrease in π -stack slippage. Initially, this leads to an increase in the T_c , which reaches a maximum of 21 K near 1 GPa. At higher pressures, as the π -stacks become more nearly superimposed, the value of T_c diminishes. In this presentation, we compare the solid state structures to the theoretical and experimental magnetic exchange properties of this radical.



1. C. M. Robertson, et al. *J. Am. Chem. Soc.* **130**, 8414-8425 (2008).
2. M. Mito, et al. *J. Am. Chem. Soc.* **131**, 16012-16013 (2009).

16 11:00 Saturday ROZH 102

Design and Synthesis of electroactiveTetrathiafulvalene Building Blocks: Towards Molecule-Based Magnetic and/or Electronic Materials **R. T. Acha** <ra06tu@brocku.ca> and **M Pilkington** <mpilkington@brocku.ca>, Department of Chemistry, Brock University, 500 Glenridge Ave., St. Catharines, ON, L2S 3A1.

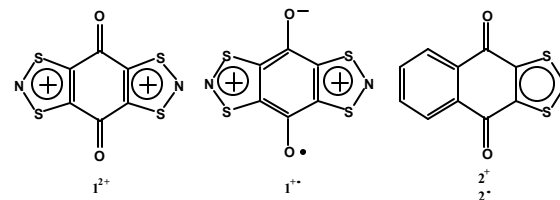
Magnetic and electronic materials permeate every aspect of modern technology. Trends toward device miniaturization have led to increased interest in combining electronic and magnetic properties into multifunctional materials, so that a single device component can perform more than one task. As materials science is moving towards the synthesis, study and processing of new materials exhibiting well-defined and complex functions, the synthesis of new multifunctional materials is one of the important challenges.[1] Research in our group focuses on the realization of novel spin-bearing tetrathiafulvalene (TTF) donors and their assembly into materials with magnetic and/or conducting properties. The design, synthesis and study of the first imine-bridged TTF-pyridine donor ligand will be presented. The crystal structure reveals that the imine N atom participates in chelation to the paramagnetic centre, thus making this ligand an attractive precursor for the assembly of -d systems.[2]

[1] E. Pardo, R. R. Garcia, J. Cano, X. Ottenwaelder, R. Lescouezac, Y. Yournaux, F. Lloret, M. Julve, Dalton, Trans., 2008, 2780.
[2] M. Chadma, N. Hassan, A. Alberola, H. S.- Evans, and M. Pilkington. *Inorg. Chem.*, 2007, 46, 3807- 3809.

17 11:20 Saturday ROZH 102

The cycloaddition and oxidative dehydrogenation reaction of SNS⁺ with 1,4-benzoquinone and 1,4-naphthoquinone leading to ring fused 1,3,2-dithiazolyl radicals **A Mailman**^{a,b} <amailman@sciborg.uwaterloo.ca> and **J Passmore** <passmore@unb.ca>, ^aUniversity of New Brunswick; ^bUniversity of Waterloo.

SNSMF₆ (M = As, Sb) reacts with 1,4-benzoquinone and 1,4-naphthoquinone in a series of cycloaddition and oxidative dehydrogenation reactions to give 1²⁺ and 2²⁺, respectively. The reduction of 2²⁺ led to the isolation and full characterization of the expected 1,3,2-dithiazolyl, 2 in SO₂ solution and the solid state. In contrast, reduction of 1²⁺ in SO₂ solution yields a unique semiquinodal-thiazyl radical cation, 1^{•+} as observed by EPR and supported by DFT calculations. These new 'one-pot' routes open up the exploration of the potentially interesting electronic and magnetic properties of a new class of fused quinone-thiazyl hybrid radicals. The site selective cycloaddition and oxidative dehydrogenation chemistry of SNSMF₆ and recent results will be discussed.



18 11:40 Saturday ROZH 102

The Addition of Nitriles to Group 14 (Di)metallenes **Julie A. Hardwick** and **Kim M. Baines** <kbaines2@uwo.ca>, Department of Chemistry, The University of Western Ontario, London, ON, N6A 5B7.

The organic functionalization of Si and Ge surfaces is of much interest in the fabrication of molecular electronic or sensing devices. The addition of nitriles to the surface is particularly intriguing given that hydrolysis of the nitrile functional group should result in the formation of a carboxylic acid derivative which could then be used in the attachment of biomolecules. To better understand the addition of nitriles to Si and Ge(100) - 2 x 1 surfaces, we have examined the addition of nitriles to Mes₂Si=SiMes₂ and Mes₂Ge=GeMes₂, the molecular analogs of the dimers on the surfaces. We have also examined the addition of nitriles to silenes (R₂Si=CR₂).

Nitriles (R₂CHCN) add to the doubly-bonded silicon compounds through the α -CH bond and to the digermene through the CN triple bond. Interestingly, CH₃CN adds to Mes₂Si=SiMes₂ through the α -CH bond or the CN triple bond depending upon the reaction conditions.



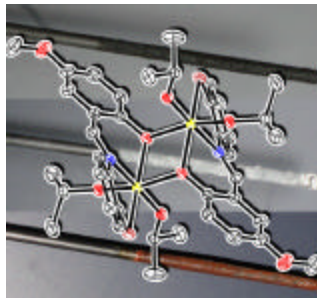
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13:00 Saturday

ROZH 103

Isolation, surface deposition and electrochemical activity of Ti(IV) complexes bearing non-innocent ligands for methanol oxidation in Direct Methanol Fuel Cells. **A. Donzelli** <donz@yorku.ca> and **P.G. Potvin** <pgpotvin@yorku.ca>, Department of Chemistry, York University, 4700 Keele St., Toronto, Ont. M3J 1P3.

Titanium complexes are widely used as catalysts in a large number of chemically useful transformations, both for preparative and industrial purposes, such as stereo-controlled oxidations of unsaturated substrates and olefin polymerization. However, the electrochemical investigation of this class of compounds, because of the high oxidation state of the metal center and its reticence to engage in active redox processes, has in most cases been neglected and, consequently, new potential applications for these complexes have not been considered. Taking advantage of several of the properties that Ti^{IV} complexes exhibit, including fast alcohol/alkoxide exchange for reactant loading and product unloading, along with the use of appropriate non-innocent ligands, we believe that Ti^{IV} complexes make excellent candidates for electrochemical catalytic oxidation of primary and secondary alcohols and, ultimately, for methanol oxidation in Direct Methanol Fuel Cells. Here we present our study of mixed alkoxide sulphur-containing Ti^{IV} complexes, including their synthesis, characterization, as well as a first investigation of their deposition on an electrode surface and their activity toward secondary alcohol oxidation.



20

13:20 Saturday

ROZH 103

Energetics of C-H Activation Using [Tp'RhL(CNneopentyl)]: Quantifying Resonance and Inductive Effects **M. E. Evans** <mevans6@mail.rochester.edu> and **W. D. Jones** <jones@chem.rochester.edu>, Department of Chemistry, University of Rochester, Rochester, NY 14627.

Several transition-metal systems have been used to establish correlations between metal-carbon and carbon-hydrogen bonds. Here, the [Tp'RhL] fragment, where Tp' = tris(3,5-dimethylpyrazolyl)borate and L = neopentyl isocyanide, is used to investigate C-H bond activation of molecules which offer unique resonance stabilization effects such as acetonitrile, acetone, 2-butyne and chloromethane. Using a combination of kinetic techniques, relative free energies can be found for the C-H activation compounds, Tp'RhL(CH₂R)H, where R = CN, COCH₃, C≡C-CH₃ and Cl. It is found that these substituents dramatically strengthen the M-C bond more than anticipated, and the stabilization gained from C-H activation adjacent to double bonds, triple bonds and chlorine is quantified. Examination of M-C vs. C-H bond strengths shows that a double bond provides ~9.0 kcal/mol, while a triple bond provides ~11.8 kcal/mol. An α-chlorine offers ~8.0 kcal/mol. Even though these molecules have weak C-H bonds, upon C-H activation they make surprisingly strong M-C bonds.

21

13:40 Saturday

ROZH 103

Photo-Splitting of Water Using a Molecular Cobalt Catalyst **T. McCormick** <tmccormi@mail.rochester.edu>, **D. Weinberg**, **T. Lazarides** and **R. Eisenberg**, Department of chemistry, University of Rochester, Rochester New York.

The photo-catalytic reduction of water to hydrogen (that can be used as a clean fuel source) classically relies on either high energy light or platinum based catalysts. The cobaloxime catalyst [Co(dmgH)pyCl] (dmgH = dimethylglyoximate, py = pyridine) that has been shown to be an electro-catalyst for hydrogen production has recently also been used as homogeneous catalyst in the photo-splitting of water, in conjunction with either Pt based dyes or halogenated organic dyes (eosin) as the visible-light chromophore and triethanolamine (TEOA) as a sacrificial reducing agent. Using eosin as the chromophore ~900 turnovers can be achieved, but the dye is not photo-stable and decomposes in ~5 h. By using a non-halogenated fluorescein based dye, bound to the cobaloxime through the pyridine, the stability of the system is greatly improved such that hydrogen production can be sustained for close to 72 hours with λ > 410 nm light, however with a very low turnover frequency. The halogenated dyes are thought to transfer electrons to the catalyst from the excited triplet state while the non-halogenated dyes transfer electrons from the singlet state; under different reaction conditions both will produce hydrogen. This talk will discuss the development of a molecular catalyst for water splitting and the insights into the mechanism of the catalyst that have been gained through the use of various chromophores.

22

14:00 Saturday

ROZH 103

Polyoxometalate-based Hybrid Platforms Presenting Remote Polydentate Coordination Sites : Toward Complexation of Transition-Metals for Novel Charge-Transfer Systems. **M.-P. Santoni**^{a,b} <marie-pierre.santoni@umontreal.ca> and **G. S. Hanan** <garry.hanan@umontreal.ca>, ^aDépartement de Chimie, Université de Montréal, Canada; **B. Hasenkopf** <berold.hasenkopf@upmc.fr> and **A. Proust**, ^bInstitut Parisien de Chimie Moléculaire, UMR7201, Université Pierre et Marie Curie, Paris, France.

Hybrid materials are advantageous in allowing the combination of the intrinsic properties of their individual components. Polyoxometalates (POM), early-transition-metal-oxide anionic clusters, are well-known electron acceptors and have been widely applied in preparing charge-transfer salts with organic cation donors for multifunctional molecular materials (electrochromism, magnetic molecular conductors, photocatalysts). We are interested in the design of Light-Harvesting Devices (LHD) to split water and use H₂ as a carbon-neutral energy source. We target covalent charge-transfer molecular hybrids (as opposed to large-spread ionic systems), involving a POM and a transition-metal complex (Ru(II), Re(I)) as photosensitizer, to achieve multi-electronic photochemical processes. Synthesis, characterization and preliminary studies of our target systems will be presented.

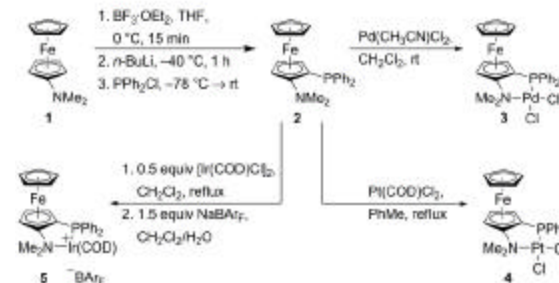
23

14:20 Saturday

ROZH 103

Synthesis, Coordination Chemistry and Applications of 2-Phosphino-1-dimethylaminoferrocenes **L. Van Belle** <lv08cp@brocku.ca>, **J. Zaifman** <jz05jo@brocku.ca>, **L. Dodge** <ld05xu@brocku.ca> and **C. Metallinos** <cmetallinos@brocku.ca>, Brock University, St.Catharines, ON, L2S 3A1.

Many axial and central chiral ligands of importance in transition metal catalysis lack planar chiral ferrocenyl analogues, especially for aminoferrocenes where nitrogen is directly attached to the cyclopentadienyl ring (e.g. 1). The lack of examples may be attributed to limitations or impracticality imposed by previous synthetic routes. In response, we have developed a direct synthesis of planar chiral aminoferrocenes using BF₃-activated lithiation (1→2). An asymmetric version of this procedure is under provisional patent protection. The talk will focus on the synthesis and coordination chemistry of rare aminophosphines such as 2 with the catalytically useful transition metals Pd(II), Pt(II) and Ir(I) (3, 4 and 5). Preliminary studies using racemic complexes of this series show that they promote a number of transformations including hydroaenation, hydroamination and aryl chloride coupling.



24

14:40 Saturday

ROZH 103

Design and synthesis of dyads utilizing charge-separation for use in molecular devices **C. Dares** <cdares@yorku.ca>, **A. B. P. Lever** <blever@yorku.ca> and **R. Fournier** <renef@yorku.ca>, York University, 4700 Keele St. W., Toronto, ON M3J 1P3.

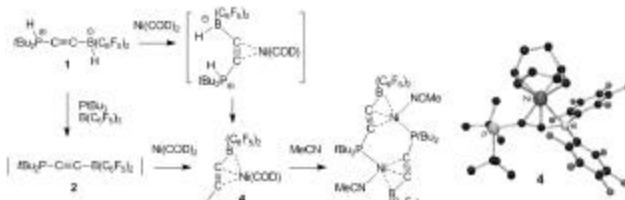
The use of charge-separation can be advantageous for use in various molecular devices. Current research in our lab has focused on the synthesis of various dyads comprised of ruthenium donors and a cobalt acceptor units, linked with an assortment of organic ligands. These dyads are designed to exploit charge-separation for use as either molecular-switches, where the charge separated species is meta-stable allowing for high-density information storage, or as catalysts for the photo-decomposition of water where the charge separated excited-state species is able to generate useful products. This presentation will focus on the synthesis, characterization, and computational results of the various components of the dyad systems, both separate, and incorporated into the dyad.

Ni→B interactions in Nickel Phosphino-Alkynyl-Borane Complexes **X. Zhao** <xzhao@chem.utoronto.ca>, **E. Otten, D. Song** and **D. W. Stephan** <dstephan@chem.utoronto.ca>, Department of Chemistry, University of Toronto, 80 St. George Street, Toronto, ON, M5S 3H6.

Several phosphino-alkynyl-boranes and their derivatives were synthesized by reacting $\text{HC}\equiv\text{CPR}'_2$ ($\text{R}' = \text{tBu}$, Mes) with $\text{R}^2\text{B}(\text{C}_6\text{F}_5)_2$ ($\text{R}^2 = \text{Cl}$, C_6F_5).

The compounds $\text{R}'_2\text{RPC}\equiv\text{CBR}(\text{C}_6\text{F}_5)_2$ (**1**: $\text{R} = \text{H}$, $\text{R}' = \text{tBu}$; **2**: $\text{R}' = \text{tBu}$; **3**: $\text{R}' = \text{Mes}$) were examined for their reactivity towards transition metal reagents.

Upon reacting **1** or **2** with $\text{Ni}(\text{COD})_2$, $(\text{COD})\text{Ni}(\text{tBu}_2\text{PCCB}(\text{C}_6\text{F}_5)_2)$ (**4**) was generated. Likewise, the reaction of **3** with $\text{Ni}(\text{COD})_2$ afforded $(\text{COD})\text{Ni}(\text{Mes}_2\text{PCCB}(\text{C}_6\text{F}_5)_2)$ (**5**). Both experimental characterization and computational analysis revealed the interaction of the borane moiety with Ni in addition to the ordinary alkyne coordination to the metal. **4** was reacted with acetonitrile to give a dimeric complex **6**, in which the Ni→B interaction is preserved. These compounds are the first examples of metal complexes containing alkynylboranes as the ligands with the novel $\eta^3\text{-}(\text{BC}\equiv\text{C})$ coordination mode.

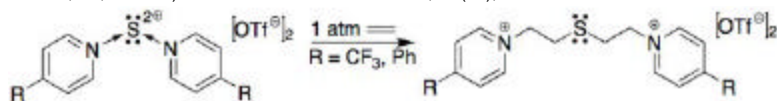


The development of new sulfur(II) delivery reagents **C. D. Martin** <cmarti95@uwo.ca> and **P. J. Ragogna** <pragogna@uwo.ca>, The University of Western Ontario.

Recently we have reported the synthesis of dicationic sulfur(II) complexes sequestered by nitrogen based tridentate and bidentate ligands.¹ While these complexes are intrinsically interesting, the challenge has been presented whether these systems will be useful in further chemistry, for example as chalcogen(II) delivery reagents.² Multidentate derivatives have proven to be too stable or unreactive for this purpose thus far. However, their monodentate counterparts can be easily synthesized and readily undergo insertion reactions with olefins. This reactivity is not restricted to C=C bonds as this insertion has also been extended to a C=N bond within carbodiimides. This represents a new mode of reactivity for dicationic main group complexes. We herein discuss the synthesis of these new reagents and their subsequent reactivity with a selection of organic molecules.

References:

1. a) C. D. Martin, M. J. Ferguson, M. C. Jennings and P. J. Ragogna. *Angew. Chem. Int. Ed.* **2009**, *48*, 2210. b) C. D. Martin, C. M. Le and P. J. Ragogna. *J. Am. Chem. Soc.* **2009**, *131*, 15126. 2. a) T. Chivers and J. Konu. *Angew. Chem. Int. Ed.* **2009**, *48*, 3025. b) S. Ritter. *C and E News.* **2009**, 87(41), 12.

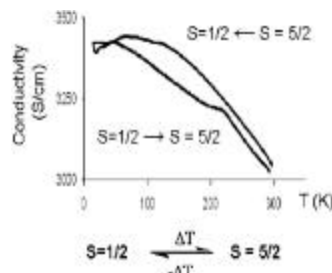


Hybrid Multifunctional Materials: An Investigation of Synergistic Interactions between Magnetic Spin and Electron Transport **B. Djukic** <brandon.djukic@brocku.ca> and **M. T. Lemaire** <mlemaire@brocku.ca>, Brock University, 500 Glenridge Avenue. St. Catharines, ON, Canada, L2S 3A1.

New materials that combine several disparate physical properties including magnetic switching from spin crossover or valence tautomer metal centres will be presented and will address our efforts in the following areas:

- 1) tailoring and controlling the magnetic switching by chemical or physical means
- 2) the effects on magnetic switching after attaching the metal centres to paramagnetic poly-thiophene "wires" used for electron transport
- 3) synergistic interactions between electron transport and magnetic switching

i) O'Sullivan, T. J.; Djukic, B.; Dube, P. A.; Lemaire, M. T. *Chem. Commun.*, 2009, 1903. ii) Djukic, B.; Dube, P. A.; Razavi, F.; Seda, T.; Jenkins, H. A.; Britten, J. F.; Lemaire, M. T. *Inorg. Chem.* **2009**, *48*, 699.



Zinc Chalcogenolate Complexes as Molecular Precursors to Manganese (II) Containing Ternary Nanoclusters. **C. B. Khadka** <ckhadka@uwo.ca> and **J. F. Corrigan** <corrigan@uwo.ca>, Department of Chemistry, The University of Western Ontario, London, Ontario, N6A 5B7, Canada.

The demonstrated ability of metal-trimethylsilylchalcogenolate complexes to act as precursors for the controlled assembly of ternary clusters¹ has prompted us to develop this general synthetic route for the assembly of semiconducting systems containing paramagnetic ions, Mn(II). The chalcogenolate complexes $(\text{N},\text{N}'\text{-tmeda})\text{Zn}(\text{ESiMe}_3)_2$ ($\text{E} = \text{S}, \text{Se}$), have been utilized as molecular precursors to isolate the ternary nanoclusters, $(\text{N},\text{N}'\text{-tmeda})_6\text{Mn}_6\text{Zn}_6\text{S}_{13}\text{Cl}_2$ (**1**) and $(\text{N},\text{N}'\text{-tmeda})_6\text{Mn}_6\text{Zn}_6\text{Se}_{13}\text{Cl}_2$ (**2**). These complexes are characterized by single-crystal X-ray diffraction and photoluminescence spectroscopy. Complexes **1** and **2** represent first examples of Mn-E-Zn nanoclusters with complete structural characterization and accurate determination of the local environment of the magnetic ions. These nanoclusters could provide a platform to investigate different phenomenon due to the influence of quantum confinement on the exchange interactions between magnetic ions, Mn(II) and a ZnE semiconductor host.² In this presentation, the optical properties of complex **1** and **2** will be described and contrasted with the isostructural binary materials, $(\text{N},\text{N}'\text{-tmeda})_6\text{Zn}_{14}\text{E}_{13}\text{Cl}_2$ ($\text{E} = \text{S}$, **3a**; $\text{E} = \text{Se}$, **3b**).

1) Degroot, M.W.; Corrigan, J. F. Z. *Anorg. Allg. Chem.* **2006**, *632*, 19-29

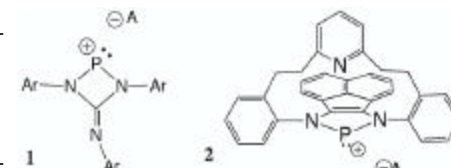
2) Raola, O.E.; Strouse, G.F. *Nano. Lett.*, **2002**, *12*, 1443-1447

New Ligand Frameworks for Supporting N-Heterocyclic Phosphenium Cations **A. L. Brazeau** <abrazeau@uwo.ca>, **J. T. Price** and **N. D. Jones** <njones26@uwo.ca>, Department of Chemistry, The University of Western Ontario, London, ON, N6A 5B7.

N-Heterocyclic phosphenium cations (NHP) are two-coordinate, formally cationic organophosphorus species that are analogous to Arduengo-type carbenes (NHC). While NHC and NHP are isostructural and isovalent, they are electronically inverse. NHP are therefore weak σ -donors and good π -acceptors. Many ligand frameworks have been used in the synthesis of NHP, including diazabutadienes, β -diketiminates, diaminonaphthalene (DAN) and bis(arylimino)acenaphthene (BIAN). We are currently investigating some new ligand frameworks to support NHP.

Although the library of NHP continues to grow, there are few examples featuring four-membered rings. We have focused our efforts on using dianionic guanidinate ligands to stabilize NHP (**1**). Also, we are investigating a framework that includes a BIAN "backbone" and a tethered pyridine ring (**2**).¹ Progress towards these new NHP frameworks will be discussed.

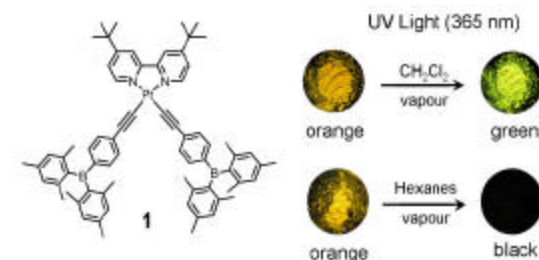
¹ Leung, D. H.; Ziller, J. W.; Guan, Z. *J. Am. Chem. Soc.* **2008**, *130*, 7538.



Luminescence Vapochromism in Triarylboron-Pt(II) Complexes for Detection of Organic Vapours **Z. M. Hudson, C. Sun** and **S. Wang** <suning.wang@chem.queensu.ca>, Department of Chemistry, Queen's University, 90 Bader Lane, Kingston, ON, K7L 3N6.

A new complex (**1**) has been synthesized based on a Pt(II)-diimine core and three-coordinate organoboron. This complex displays intense orange-yellow phosphorescence in both solution and the solid state at room temperature. Exposure of **1** to organic vapours reversibly alters the molecular packing in the solid state, shifting the MLCT energy and switching both the absorption and emission colours of the sample. While the majority of common laboratory solvents switch the emission colour from yellow-orange to green,

hydrocarbons such as hexane selectively cause the sample to turn black, with complete phosphorescent quenching.



31 16:30 Saturday ROZH Foyer

Synthesis and Reactivity Studies of Bifunctional Phosphino-Borane "Frustrated Lewis Pairs" **M. Schedler** <mschedle@chem.utoronto.ca>, J. Gutenberg-Universitaet Mainz, Duesbergweg 10-14, 55099 Mainz, Germany; **Z. M. Heiden** <zheiden@chem.utoronto.ca> and **D. W. Stephan** <dstephan@chem.utoronto.ca>, University of Toronto, 80 St. George Street, Toronto, ON, M5S 3H6, Canada.

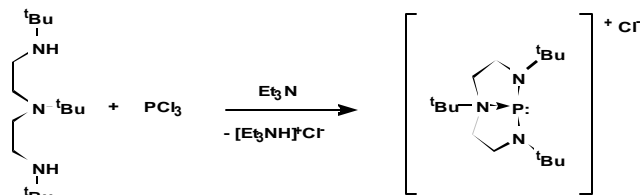
Sterically encumbered heteroatoms have been found to preclude the standard Lewis acid-base adduct, thus exhibiting unusual chemical behaviour towards the activation of dihydrogen. We have synthesized five membered heterocycles containing sterically crowded phosphorus and boron centers connected through a benzylic backbone. We have found that both the steric bulk and Lewis acidity of the boron center have a large effect on the stability of the P-B bond which is crucial for the ability to add H₂. The reactivity of these complexes towards the activation of H₂ and hydrogenation of imines was investigated both experimentally and theorectically.

32 16:30 Saturday ROZH Foyer

Stabilization of low coordination numbers with polyamines **M Krause** and **M.K. Denk** <mdenk@uoguelph.ca>, University of Guelph, Department of Chemistry, 50 Stone Road, Guelph, Ontario N1G 2W 1.

Polyamines of general type R-NH-[(CH₂CH₂)_n]-CH₂CH₂NHR can be obtained from 1,2-dibromoethane and primary amines. [1] The synthesis and characterization of the amines as well as their use for the stabilization of low coordination numbers (phosphonium cations) is described.

[1] M. Denk, M. Krause, D. Niyogi, N. Gill, *Tetrahedron* **2003**, 59, 7565-7570.



33 16:30 Saturday ROZH Foyer

Exploring the Heterocyclic Chemistry of Group 14: Pyrrolides and Indolides **J. Poisson**, I. Wharf, M. M. Barsan and I. S. Butler <ian.butler@mcgill.ca>, McGill University, Department of Chemistry, 801 Sherbrooke Street West #335, Montreal, PQ, H3A 2K6.

Pyrrole (C₄H₄N) and indole (C₈H₆N) are very important heterocyclic substituents in natural products, polymer networks and pharmaceutical agents. Their use in chemical synthesis, however, presents a particular challenge in that they polymerize easily both in light and in solution, especially in the presence of acid catalysts. When self-polymerization is avoided, combination of these heterocycles with an alkyl-lithium reagent provides a direct avenue to metallic salts containing a metal-nitrogen bond. A general synthesis of N-linked group 14 metal pyrrolides and novel analogous indolides (MPh₃X, M = Si, Ge, Sn; X = C₄H₄N, C₈H₆N) is presented. The white crystalline products formed have been characterized by ¹³C-, ²⁹Si- and ¹¹⁹Sn-NMR, EI-mass and Raman spectroscopy, and elemental analysis.

34 16:30 Saturday ROZH Foyer

Catalytic hydrosilylation by cationic ruthenium and iron complexes. **D.V. Gutsulyak** <dg06to@brocku.ca> and **G.I. Nikonov** <gnikonov@brocku.ca>, Department of Chemistry, Brock University, 500 Glenridge Ave., St. Catharines, Ont. L2S 3A1.

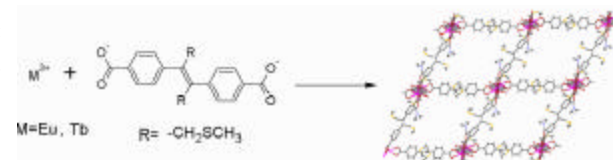
Cationic ruthenium and iron complexes of the general formula [CpM(PR₃)(CH₃CN)₂]⁺An (M= Ru (**1**) or Fe (**2**)) are found to catalyze hydrosilylation of carbonyls and dehydrogenative coupling of silanes with alcohols and amines.¹ The reactions can be performed in polar solvents or under solvent-free conditions. The catalytic activity of complexes **1** and **2** varies from being totally inactive to excellent, depending on the nature of silane and phosphine ligands. In the absence of organic substrate, the reaction of **1** with silanes yields relatively rare cationic silane σ-complexes [CpRu(PR₃)(CH₃CN)(η²-HSiR₃)]⁺BAF (**4**). Compounds **4** exhibit typical for silane σ-complexes large Si-H coupling constants (J(Si-H) > 30 Hz). The effect of substitution at silicon and donating ability of phosphine ligand on the extent of Si-H activation will be discussed.

1. D. V. Gutsulyak, G. I. Nikonov et al., *J. Am. Chem. Soc.* **2008**, 130, 3732.

35 16:30 Saturday ROZH Foyer

Luminescent metal organic framework (MOF) based on substituted 4,4'-stilbene dicarboxylic acid (SDA) **Y. Li** <yuli@chem.utoronto.ca> and **D. Song** <dsong@chem.utoronto.ca>, Davenport Chemical Research Laboratories, Department of Chemistry, University of Toronto, 80 St. George Street, Toronto, Ontario, Canada, M5S 3H6.

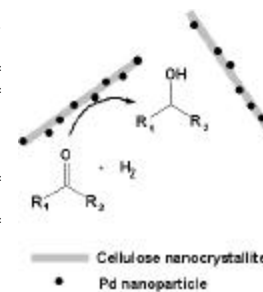
A large number of MOFs with different functionalities have been reported in the past decade. Because of their porosity and flexible ligand/metal choices, different applications have been demonstrated including gas storage and separation, sensing and heterogeneous catalysis. Among all the examples, lanthanide MOFs have attracted our interests because of their characteristic metal-based luminescence. In addition, the unique emitting mechanism involving ligand-to-metal energy transfer allows a distinct way to design sensors, i.e., instead of using analyte-metal interactions, analyte-ligand interactions can be utilized to modulate the energy transfer process, and thus causes luminescence signal modulations. The goal of our research is to build porous luminescent MOFs with different dangling functional groups that can potentially interact with guests. Here we reported the design and synthesis of luminescent MOFs based on Eu/Tb and SDA derivatives. Preliminary characterization revealed difference in porosity, luminescence and stability as a result of different functional groups and synthesis conditions.



36 16:30 Saturday ROZH Foyer

Pd nanoparticles supported on cellulose nanocrystallites as active hybrid material for catalytic hydrogenation reaction **C.M. Cirtiu** <mihai.cirtiu@mail.mcgill.ca>, **A. Dunlop-Brière** <alexandre.dunlop-briere@mail.mcgill.ca> and **A.H. Moores** <audreymoores@mcgill.ca>, McGill University, Department of Chemistry, 801 Sherbrooke St. W, Montreal, QC H3A 2K6.

In the present study, cellulose nanocrystallites (CNCs) are employed to support Pd nanoparticles (PdNPs) in order to obtain an active hybrid catalyst (Pd@CNCs) for hydrogenation reaction (figure 1). This hybrid catalyst is synthesized by subjecting a suspension of CNCs to metal precursor (PdCl₂) followed by a reduction step of the adsorbed Pd(II) ions with H₂ at 4 bars. Physico-chemical characterization of CNCs (FTIR, TEM, TGA, and zeta-potential) showed that CNCs are stable in the conditions of the palladium deposition as well as in the conditions of catalytic hydrogenation tests. Optimization of reaction allowed obtaining PdNPs (3.6 nm) with a good repartition onto the whole length of the CNCs. The catalytic activity of the obtained hybrid catalyst Pd@CNCs was tested towards phenol hydrogenation. The preliminary results indicated good catalytic activity of Pd@CNCs with 40% of phenol transformed in cyclohexanone within 4 hours of reaction in very mild conditions, namely room temperature and 4 bars of H₂.



37 16:30 Saturday ROZH Foyer

High-Yield Synthesis of ReO_3F and a Study of its Fluoride Ion Donor and Lewis Acid Properties **M. V. Ivanova** <ivanovm@mcmaster.ca>, **M. J. Hughes**, **H. P. A. Mercier** and **G. J. Schrobilgen**, Department of Chemistry, McMaster University, Hamilton, ON L8S 4M1.

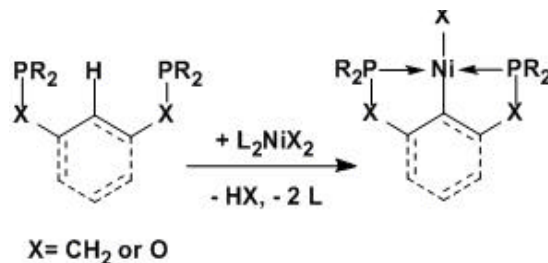
Rhenium trioxide fluoride was synthesized in high yield by the solvolysis of Re_2O_7 in anhydrous HF (aHF) in the presence of F_2 gas over a period of 48 h. A colorless crystalline material was characterized by low-temperature (-160 °C) Raman spectroscopy under aHF and was isolated as a pale yellow solid after removal of aHF under dynamic vacuum. Slow cooling to -78°C of an HF solution containing ReO_3F yielded colorless plate-like crystals which were shown to be $\text{ReO}_3\text{F}\cdot 2\text{HF}$ by single-crystal X-ray diffraction. The coordination sphere around Re(VII) is a distorted octahedron consisting of three oxygen atoms that are cis to one another, a fluorine atom, and two HF molecules that are trans to an oxygen ligand. The HF molecules cis to one another are coordinated to Re(VII) through the fluorine atom. The ReO_3^+ cation has been synthesized for the first time as its AsF_6^- salt by reaction of ReO_3F with AsF_5 in aHF. A free-flowing white solid, which is insoluble in aHF and HF/ AsF_5 solvents, was obtained after removal of aHF under dynamic vacuum and was characterized by low-temperature (-160 °C) Raman spectroscopy. When ReO_3F was dissolved in CH_3CN at -40°C, a white solid precipitated that has been characterized as $\text{ReO}_3\text{F}\cdot 2\text{CH}_3\text{CN}$ based on its Raman spectrum. Quantum-chemical calculations using B3LYP methods were used to calculate the gas-phase geometries and vibrational frequencies of ReO_3F , ReO_3^+ , $[\text{ReO}_3][\text{AsF}_6]$, and $\text{ReO}_3\text{F}\cdot 2\text{CH}_3\text{CN}$ in order to aid in the assignment of the experimental vibrational frequencies of these compounds.

38 16:30 Saturday ROZH Foyer

Insights On Metallation of Pincer-Type Ligands by Nickel(II) **B. Vabre** <boris.vabre@laposte.net> and **D. Zargarian** <zargarian.davit@umontreal.ca>, Département de chimie, Université de Montréal.

Pincer-type complexes have attracted much interest because of their remarkable activities in a wide range of catalytic processes. An attractive feature of many pincer complexes is the availability of facile coordination-metallation routes by which they can be prepared. The way in which such metallation reactions occur, whether they are more appropriately described as C-H activation, electrophilic activation, or base-assisted deprotonation, is a topic of current interest.

During our studies on the preparation and reactivities of pincer-type nickel complexes we have used both experimental studies and DFT calculations to address the question of how the nickellation of pincer ligands proceeds. The present poster will describe our results to-date



39 16:30 Saturday ROZH Foyer

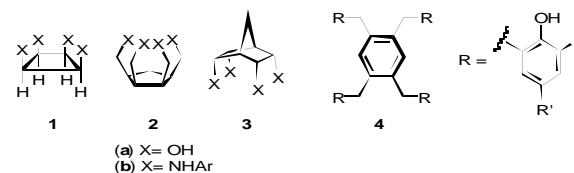
Photo-splitting of water with a sensitized metal oxide semiconductor **I. McCormick** <imccormi@mail.rochester.edu>, **D. Farkas** and **R. Eisenberg**, Department of chemistry, University of Rochester, Rochester New York.

The photo-catalytic reduction of water to hydrogen is a potential method to store solar energy that can be used as clean fuel source. Platinised (0.5%) TiO_2 has been shown to be a good catalyst and electron relay for the photo-reduction of water, under UV irradiation. By sensitizing the TiO_2 with dyes, it is possible to get hydrogen production using visible light, with triethanolamine (TEOA) as a sacrificial reducing agent. The efficiency of hydrogen production from the sensitized dyes should be proportional the efficiency of electron injection into the TiO_2 surface. The stability and efficiency of xanthenes based dyes will be discussed. The nature of the connecting group that binds the dye to the surface as well as the population of the triplet excited state both influence hydrogen production. The conduction band of TiO_2 is approximately 3.1 eV, while SrTiO_3 is approximately 0.2 eV higher. It is believed that by changing semiconductors, higher energy electrons can be created and used with a non-platinum based catalyst. This poster will discuss the study of different dyes, metal oxides and catalysts for the sensitized photo-reduction of water to hydrogen.

40 16:30 Saturday ROZH Foyer

The Synthesis of Constrained-Geometry Tetradentate Ligands for Small Molecule Activation. **B.C. Skrela** <bskrela@yorku.ca>, **D. Hossain** <hossaind@yorku.ca> and **G.G. Lavoie** <glavoie@yorku.ca>, Department of Chemistry, York University, 4700 Keele Street, Toronto, ON M3J 1P3.

This work involves the synthesis of ligands that constrain transition metal complexes to square planar geometries. From a frontier orbital perspective, these complexes are well-suited for small molecule activation, such as dinitrogen fixation. At the onset of this project, we investigated cyclobutane- (1), cyclopentane- (2), and norbornane- (3) based ligand sets. More recently, we have been evaluating the synthesis of a rigid tetradentate ligand based on the benzene scaffold (4). These ligands allow for steric and electronic tuning of the metal centre. The synthesis of these ligands is presented, along with density-functional theory calculations on the corresponding dinitrogen transition metal complexes.

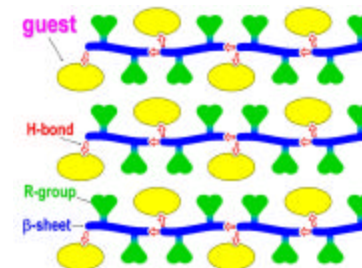


41 16:30 Saturday ROZH Foyer

Characterization of the Inclusion Capabilities of Dipeptide Leucyl-Leucine **Chris T. Brown** <cbrown01@uoguelph.ca> and **Dmitriy V Soldatov** <dsoldato@uoguelph.ca>, Department of Chemistry, University of Guelph, Guelph, ON N1G 2W1.

Peptides are prospective as biocompatible, versatile, and environmentally friendly host molecules. [1] Leucyl-Leucine dipeptide (LL) has been known to form crystalline solvates with simple alcohols and DMSO. [2,3,4] The interest of this project was to create inclusion compounds of LL with various aromatic and aliphatic molecules to investigate the inclusion ability of LL, characterize the cavity space and develop a model for the ideal guest for LL. Powder XRD and GC MS analyses of several dozen samples revealed a variety of new inclusion compounds with unique crystal structures, while thermal analysis was used to confirm dipeptide:guest ratios.

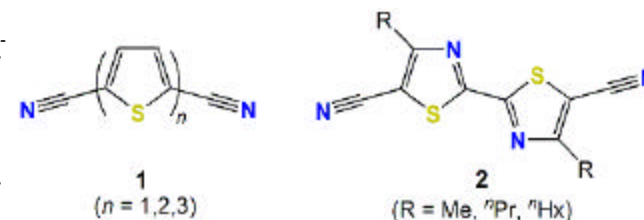
Ref. [1] D.V. Soldatov, in: Nanoporous Materials 5, 213 (2008). [2] S.N. Mitra and E. Subramanian, Biopolymers 34, 1139 (1994). [3] C.H. Görbitz, Acta Chem. Scand. 52, 1343 (1998). [4] C.H. Görbitz, Acta Crystallogr. C55, 670 (1999).



42 16:30 Saturday ROZH Foyer

Silver (I) Coordination Polymers Supported by Oligomeric Dinitrile Ligands Containing S- and N- Donors **N.R. Andreychuk** <andreyrn@mcmaster.ca>, Department of Chemistry, McMaster University, 1280 Main Street West, Hamilton ON, L8S 4L8; **C.D. MacKinnon** and **S.L.M. Parent**, Department of Chemistry, Lakehead University, Thunder Bay ON, P7B 5E1; **A. Assoud**, Department of Chemistry, University of Waterloo, Waterloo ON, N2L 3G1.

For the preparation of metal-organic framework (MOF) materials, the nitrile-Ag(I) interaction has been extensively investigated. Research in the MacKinnon group has focused on utilizing oligomeric dinitriles as bridging ligands for Ag(I), oligothiophenes 1 in particular. Ag(I) coordination polymers supported by ligands 1 form 1D ribbons with no interaction between thiophene S-donors and the Ag(I) cations. Recently, we have begun to investigate the Ag(I) chemistry of bithiazole-based dinitrile ligands 2, and have prepared 2- and 3D coordination networks. We find that the identity of R has a major impact on both the Ag(I) coordination, and crystal structure morphology.



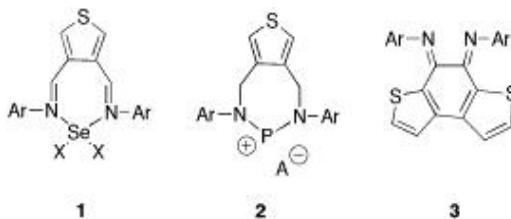
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16:30 Saturday

ROZH Foyer

New Thiophene Containing Selenium and Phosphonium Cations **J. T. Price** <jprice6@uwo.ca> and **N. D. Jones** <njones26@uwo.ca>, Department of Chemistry, University of Western Ontario, London, ON.

Thiophene-based polymers have attracted considerable attention because of their use in a wide range of devices and there is a strong push to develop new thiophene monomers with donor acceptor properties that could be easily tailored. Our approach is to incorporate Group 15 and 16 elements into thiophene monomers by way of either diimine (1) or diamine (2) substituents. This allows one to easily tune the electronic and photophysical properties of the compound e.g., by halide removal, as in the phosphonium cation (2).



Bis(aryl)acenaphthenequinonediimine (BIAN) is a commonly used ligand for the coordination of many main group atoms. A thiophene containing analogue (3) of this could have interesting photophysical properties because of the two contiguous thiophene rings. Challenges arising from, and progress towards ligands like 3 and their main group coordination chemistry will be discussed.

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16:30 Saturday

ROZH Foyer

Solid-State NMR of Inorganic Systems: Molecules, Networks and Nanoparticles studied via ^{19}F , ^{45}Sc , ^{35}Cl , ^{65}Cu , ^{89}Y , ^{91}Zr , ^{109}Ag , ^{119}In , ^{119}Sn , ^{195}Pt , ^{199}Hg , ^{207}Pb , and ^{209}Bi NMR spectroscopy. **K. J. Harris**, **H. Hamaed**, **B. E. G. Lucier**, **A. W. MacGregor**, **A. J. Rossini** and **R. W. Schurko** <rschurko@uwindsor.ca>, Department of Chemistry and Biochemistry, University of Windsor, Essex Hall, 401 Sunset Avenue, Windsor, ON Canada N9B 3P4.

Solution NMR spectroscopy has traditionally been the premier method for characterizing molecular structure and dynamics; however, solid-state NMR (SSNMR) spectroscopy has become increasingly prominent due to the wide range of solid materials requiring atomic-level characterization. Widespread adoption of SSNMR for characterizing many nuclei has been hindered by two main challenges: (i) dilution of spectral intensity over large frequency ranges, and (ii) absence of empirical NMR data for most nuclides in the periodic table. We demonstrate that recently developed SSNMR techniques allow for relatively straightforward access to chemical information from a variety of less commonly studied nuclei. Several SSNMR studies involving spin-1/2 nuclei are presented: a ^{207}Pb study of bonding trends in lead-II thiolates, a ^{109}Ag study of alkylamine absorption in silver 4-pyridinesulfonate, a ^{19}F and ^{89}Y study of core/shell differences in YF_3 nanoparticles, as well as ^{119}Sn , ^{195}Pt and ^{199}Hg studies of model inorganic compounds. Quadrupolar nuclei will also be discussed: a ^{91}Zr and ^{35}Cl study of a zirconocene olefin-polymerization catalyst (and precursors), a ^{65}Cu study of ligand hardness in copper bisphosphine fluoroacetates, as well as ^{115}In and ^{209}Bi NMR of model inorganic salts.

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16:30 Saturday

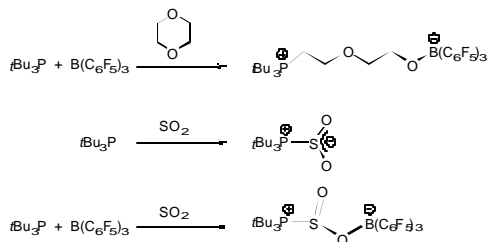
ROZH Foyer

Ring-opening of 1,4-dioxane and trapping of sulfur dioxide with Frustrated Lewis Pairs **B. Birkmann** <bbirkman@chem.utoronto.ca> and **D. W. Stephan** <dstephan@chem.utoronto.ca>, Department of Chemistry, University of Toronto, 80 St. George Street, Toronto, Ontario, M5S 3H6, Canada.

We have recently developed the concept of "Frustrated Lewis Pairs" (FLPs) in which steric congestion precludes formation of classical Lewis adducts.^[1] This has led to unique maingroup systems capable of H_2 activation, hydrogenation, and unprecedented small-molecule reactivity.^[2] $\text{B}(\text{C}_6\text{F}_5)_3$ forms an adduct with 1,4-dioxane, however, in the presence of $t\text{Bu}_3\text{P}$ at 50 °C we observe ring-opening.

SO_2 is a major component of acid rain, and is, therefore, an environmental pollutant gas. Tertiary phosphines react with SO_2 to form the P-S compound, which can be trapped with $\text{B}(\text{C}_6\text{F}_5)_3$ to form the PS(O)OB linked compound.

[1] (a) D. W. Stephan, *Org. Biomol. Chem.* **2008**, 1535; (b) D. W. Stephan, *Dalton Trans.* **2009**, 3129. [2] (a) C. M. Mömring, E. Otten, G. Kehr, R. Fröhlich, S. Grimme, D. W. Stephan, G. Erker, *Angew. Chem. Int. Ed.* **2009**, 48, 6643; (b) E. Otten, R. C. Neu, D. W. Stephan, *J. Am. Chem. Soc.* **2009**, 131, 9918.



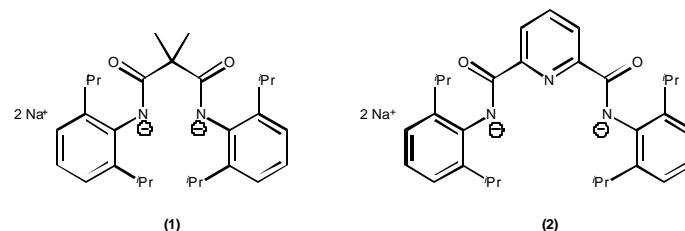
46

16:30 Saturday

ROZH Foyer

Synthesis of a New Sterically-Hindered Dicarboxamide Ligand **L. L. Tan** <lltan@uwaterloo.ca> and **S. C. Lee** <sclee@uwaterloo.ca>, Department of Chemistry, University of Waterloo, Waterloo, ON N2L 3G1.

The new bidentate ligand disodium *N,N*-bis(2,6-diisopropylphenyl)-2,2-dimethylmalonamidate (1) was synthesized through a deprotonation reaction of *N,N*-bis(2,6-diisopropylphenyl)-2,2-dimethylmalonamide with NaNH_2 . The properties of 1 and a previously reported tridentate analogue, disodium *N,N*-bis(2,6-diisopropylphenyl)-2,6-pyridinedicarboxamidate (2), and the deprotonation chemistry of the parent carboxamide precursors will be discussed. Preliminary metallation studies with FeCl_2 will also be presented.



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16:30 Saturday

ROZH Foyer

Synthesis and properties of ferrocene-amyloid beta peptide conjugates **S. Beheshti** <sbehesh@uwo.ca> and **H-B Kraatz** <hkraatz@uwo.ca>, Department of Chemistry, the University of Western Ontario, 1151 Richmond St., London, ON, Canada, N6A 5B7.

Amyloid beta peptide ($\text{A}\beta$) has 40-42 amino acids and is found in amyloid plaques in people with Alzheimer's disease.¹ It is thought that hydrogen bonding interactions between the peptide strands are responsible for the aggregation of peptides and that the presence of metal ions influence the formation of aggregates.^{2, 3} Ferrocene peptide conjugates allow us to study these two issues in details using well-behaved model systems. The use of ferrocene (Fc) achieves two goals: a) it enhances the solubility of the Fc-amyloid conjugate and b) it has an electrochemical handle to probe the systems in more details. Here, we report the synthesis and characterization of ferrocene $\text{A}\beta$ -peptide conjugates and their interaction with β -sheet breakers.

- Hardy, J.; Selkoe, D. J. *Science* 2002, 297, 353.
- Petty, S. A.; Decatur, S. M. *J. Am. Chem. Soc.* 2005, 127, 13488.
- Bush, A. I.; Pettingell, W. H.; Multhaup, G.; Paradi, M.; Vonsattel, J. P.; Gusella, J. F.; Beyreuther, K.; Masters, C. L.; Tanzi, R. E. *Science* 1994, 265, 1464.

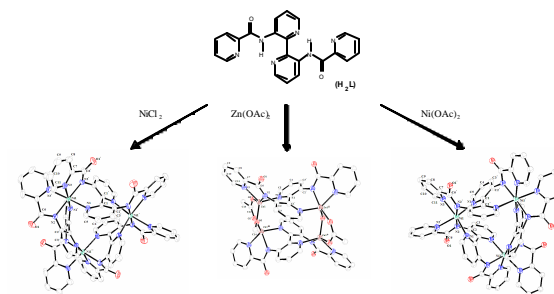
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16:30 Saturday

ROZH Foyer

Synthesis and Coordination Chemistry of 2,2'-Bipyridine-3,3'-(2-Pyridine carboxamide). **N. J. Hurley** <nh04zg@brocku.ca>, **J. Wang**, **N. Zarrabi** and **M. Pilkington** <mpilkington@brocku.ca>, Brock University, 500 Glenridge Avenue, St. Catharines, Ontario, Canada, L2S 3A1.

2,2'-Bipyridine-3,3'-(2-Pyridinecarboxamide)³ (H_2L), a bis-tridentate ligand, has been synthesized via reaction of 3,3'-diamino-2,2'-bipyridine with 2-pyridine carbonyl chloride.¹ The synthesis, characterization and coordination chemistry of the ligand will be presented.



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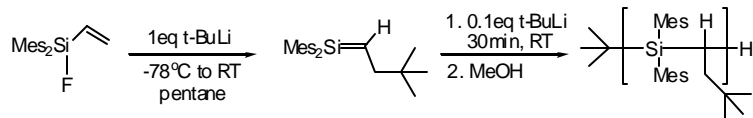
16:30 Saturday

ROZH Foyer

Addition polymerization of a silene **J. Guo**, **L. Pavelka** and **K. Baines** <kbaines2@uwo.ca>, Department of Chemistry, University of Western Ontario, 1151 Richmond St. London, Ont. N6A 5B7.

We have reported the first addition polymerization of a silene ($R_2Si=CR_2$) in pentane using t-BuLi as an initiator as a new route to polymers with a $[SiC]_n$ backbone.¹ This method successfully gives polysilene with fairly high molecular weights and in high isolated yields. Currently, we are investigating whether the polymerization can be carried out under living anionic conditions by examining different initiators and solvent systems. Alkyl lithium reagents, such as MeLi and BuLi, can initiate polymerization of the silene in ether. We have also investigated the copolymerization of the silene with a vinylic monomer, methyl methacrylate, in an attempt to afford hybrid inorganic-organic copolymers. The results of these studies will be discussed.

1. Pavelka, L. C.; Milnes, K. K.; Baines, K. M. *Chem. Mat.* **2008**, *20*, 5948.



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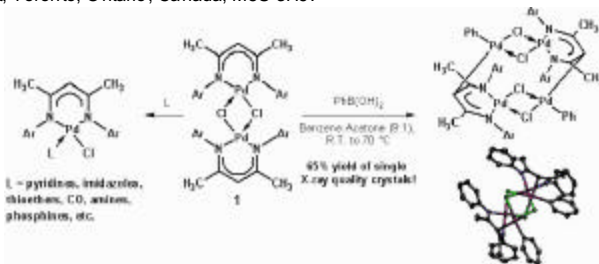
16:30 Saturday

ROZH Foyer

Palladium β -Diiminate Chemistry: Reactivity with Ligands, and Transmetalation Reagents **V. A. Annibale** and **D. Song** <dsong@chem.utoronto.ca>, Davenport Chemical Research Laboratories, Department of Chemistry, University of Toronto, 80 St. George Street, Toronto, Ontario, Canada, M5S 3H6.

The initial synthesis and observed reactivity of $[Pd(Ar_2nacnac)(\mu-Cl)]_2$ (1: a) $Ar=Ph$) by our group¹ has prompted the synthesis of other chloro-bridged Pd β -diiminate dimers with various Ar groups. These dimeric complexes can serve as versatile starting materials, and as a gateway into Pd β -diiminate chemistry which has been relatively unexplored. Here we describe the reactivity of Pd β -diiminate dimers towards ligands to generate monomeric species, and the unusual products obtained from reactions with common transmetalation reagents.

1. Hadzovic, A.; Song, D. *Organometallics* **2008**, *27*, 1290-1298.



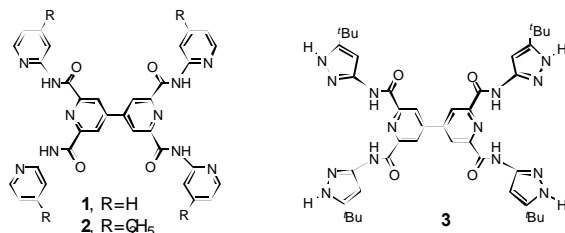
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16:30 Saturday

ROZH Foyer

New Tetracarboxamide bis-Bipyridyl Ligands: Synthesis and Coordination Chemistry **Nilofar Zarrabi** <nz07ty@brocku.ca> and **Melanie Pilkington** <mpilkington@brocku.ca>, Department of Chemistry, Brock University, St. Catharines, ON, L2S 3A1.

During recent years, pyridyl carboxamide ligands have proved to be spectacular ligands in metallosupramolecular chemistry due to their ability to direct self-assembly via coordinate bond formation (via pyridine) in conjunction with H-bonding (via amide C=O and N-H groups). They have applications in the fields of asymmetric catalysis, dendrimer synthesis, molecular receptors, as well as for the preparation of platinum complexes with antitumor properties. Although studied widely for their biological applications, these ligands have not yet been exploited as precursors to molecule-based magnetic materials. Furthermore, carboxamide ligands containing a bipyridyl moiety are much more rare and have not yet realized their full potential as versatile ligands in the field of coordination chemistry. In this respect, we have targeted the tetracarboxamide bis-bipyridyl ligands **1**, **2** and **3** and report herein their synthesis, characterization and coordination chemistry of these ligands with different transition metal ions.



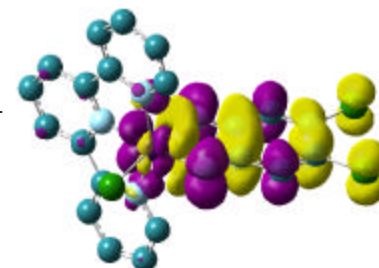
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16:30 Saturday

ROZH Foyer

Shedding Light onto the Nature of Electronic Transitions in Highly Coupled Inorganic Complexes **C. Dares** <cdares@yorku.ca>, **A. B. P. Lever** <blever@yorku.ca> and **R. Fournier** <renef@yorku.ca>, York University, 4700 Keele St. W, Toronto, ON M3J 1P3.

In classical transition metal complexes, observed electronic transitions can typically be assigned with conventional labels (e.g. - MLCT, LMCT, LLCT, d-d, etc.). These labels however have proven to be insufficient to describe many of the electronic transitions observed in transition metal complexes incorporating non-innocent ligands. This is due to the high degree of delocalization between the metal and non-innocent ligand(s). Using a series of ruthenium(II) compounds which utilize the non-innocent ligand *o*-benzoquinonediimine (bqdi), we herein describe a method for the assignment of electronic transitions derived from computational results on compounds, regardless of the amount of mixing present. We have extended our results in turn to generate a predicted spectrum, which is based on the assignment of the transitions, and typically allows for better correlation with the experimentally observed spectrum.



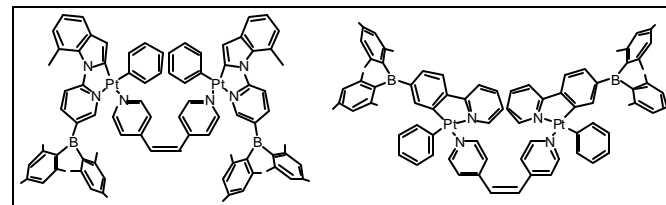
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16:30 Saturday

ROZH Foyer

Photoisomerisation properties of boron-functionalized platinum dimers linked by *trans*-1,2-bis(4-pyridyl)ethylene **K. A. Lee** <kla@queensu.ca>, **Y. Rao** <yjingli.rao@chem.queensu.ca> and **S. Wang** <swang@chem.queensu.ca>, Department of Chemistry, Queen's University, Kingston, ON, K7L 3N6.

An unprecedented isomerisation phenomenon was observed when a boron-functionalized platinum complex was linked by *trans*-1,2-bis(4-pyridyl)ethylene to create a racemic mixture of bowl-shaped *cis*-dimer with the ligands wrapped around a small cavity with C_2 symmetry. Depending on the ligand, either the *cis*-dimer was crystallized *in situ* during synthesis, or the isolated *trans*-dimer underwent isomerisation in solution. Detailed synthesis, characterisation and study of the photoisomerisation phenomenon of the dimers will be presented.



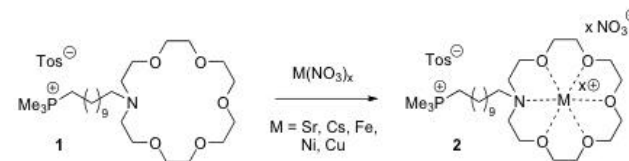
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16:30 Saturday

ROZH Foyer

Synthesis of phosphonium ionic liquids with a pendant aza-crown ether and its metal complexes **J.W. Dube** <jdube7@uwo.ca> and **P.J. Ragogna** <pragogna@uwo.ca>, The University of Western Ontario.

The use of ionic liquids as an extracting phase for liquid-liquid separations has been actively pursued over the past decade as high metal ion distribution coefficients have been observed. In this context, a task-specific phosphonium ionic liquid with a pendant aza-crown ether ligand has been targeted because the extracting ability can be tuned by changing the cavity size or the pH while the phosphonium cation will provide superior stability compared its imidazolium and ammonium relatives. The synthesis of the model compound **1** and metal complexation experiments will be presented. References: *Ionic Liquids in Synthesis*, P. Wasserscheid, T. Welton, Wiley-VCH, 2nd edition, 2008; M. L. Dietz, *Sep. Sci. Technol.*, **2006**, *41*, 2047; H. Luo, S. Dai, P. V. Bonnesen, A. C. Buchanan, *J. Alloys Compd.*, **2006**, *418*, 195.



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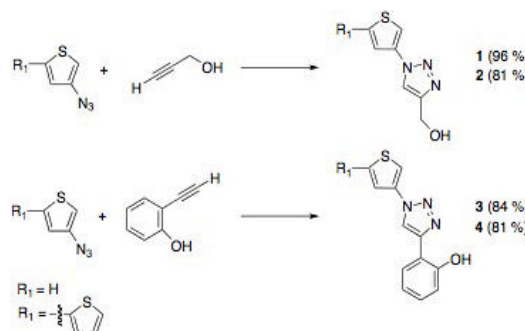
Transition Metal Complex-Catalyzed Dehydrogenation of Amine-Boranes in Ionic Liquids **W. R. H. Wright** and **R. T. Baker** <rbaker@uottawa.ca>, Department of Chemistry and Centre for Catalysis Research and Innovation, 30 Marie Curie, Ottawa, ON K1N 6N5; **L. G. Sneddon**, Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104-6323 USA.

Due in part to their high hydrogen content amine-boranes have been identified as promising candidates for chemical hydrogen storage. Although partial release of hydrogen from amine-boranes can be thermally induced, further methodologies are needed to enable controlled hydrogen release under mild reaction conditions. One promising approach is the utilization of ionic liquids (ILs), which have been shown to promote the dehydrogenation of NH_2BH_3 (**AB**).¹ This rate enhancement is thought to result from the unique solvation environment of ILs, which increases the rate of formation of the boronium salt, $[\text{BH}_2(\text{NH}_2)_2][\text{BH}_4]$, an initiator for the dehydro-oligomerization of **AB**. Furthermore, ILs typically contain anions which are capable of coordinating to a metal centre. Thus, it is likely that established **AB** dehydrogenation catalysts will have different resting states in ILs and hence may display different reactivity to that found in "conventional" solvents. In this work a range of transition metal complexes have been employed as **AB** and Me_2NHBH_3 dehydrogenation catalysts in ILs. By probing reaction mixtures using ¹¹B NMR spectroscopy, it has been found that the use of ILs does indeed alter the activity and the selectivity is shown to vary with the nature of the IL. 1) M. E. Bluhm, M. G. Bradley, R. Butterick III, U. Kusari, and L. G. Sneddon, *J. Am. Chem. Soc.*, 2006, 128, 7748-7749.

56 16:30 Saturday ROZH Foyer

Thiophene-Containing N,O-Donor Ligands for Metal Complexes **K.N. Swanick** <kswanick@uwo.ca>, **J.T. Price** and **N.D. Jones** <njones26@uwo.ca>, The University of Western Ontario, London ON, N6A 5B7.

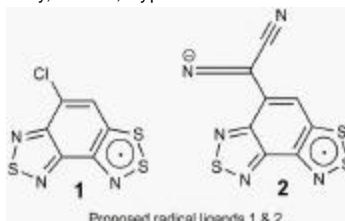
Thiophene-containing compounds are electrically conductive and have fluorescent properties that are of high interest. Applications of these compounds include organic light-emitting diodes (OLEDs), sensors and fluorescent biomarkers. Our focus has been to synthesize, using the Cu(I) azide-alkyne cycloaddition (CuAAC), thiophene-based, deep-blue fluorescent, N,O-chelating ligands for Al and Zn for possible subsequent inclusion in OLEDs. Varying the conjugation in the thiophene ring system or adding a phenol substituent to the thiophene-triazole backbone will potentially create a useful series of ligands that can be used for a variety of applications.



57 16:30 Saturday ROZH Foyer

An Investigation of 1,2,3-Dithiazolyl Based Radicals as Spin-Bearing Ligands Towards the Development of Novel Magnetic Materials **D.J. MacDonald** <dmacdo01@uoguelph.ca> and **K.E. Preuss** <kpreuss@uoguelph.ca>, University of Guelph, Department of Chemistry, Guelph, ON, Can. N1G 2W1; **P.A. Koutentis** <koutenti@ucy.ac.cy>, University of Cyprus, Department of Chemistry, Nicosia, Cyprus.

Most work in the field of spintronic research has focused on the use of Ga-As materials doped with Mn^{2+} to fold both magnetic and semi-conductive properties into the same material; however an essential understanding of how these materials work can only be elucidated from a molecular standpoint. My project focuses on a ligand design motif that promotes lateral intermolecular contacts and delocalization of the singly occupied molecular orbital (SOMO) over a significant portion of the molecular area in an attempt to inhibit the formation of diamagnetic dimers and promote the formation of pi-stacked radicals. While the precursors to radicals **1** and **2** are already known¹, there has been no investigation into the properties of their radical counterparts. EPR experiments have shown that the unpaired electron is delocalized over much of the molecular area for both species. Cyclic voltammetry experiments will also be presented, giving quantitative reduction and oxidation potentials for the radical precursors.

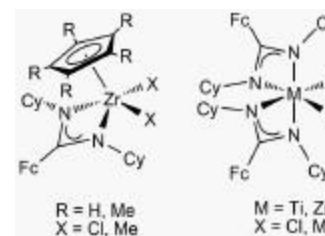


1) Koutentis, P.A.; Rees, C.W. *J. Chem. Soc., Perkin Trans. 1*, 2002, 315.

58 16:30 Saturday ROZH Foyer

Ferrocenyl Amidinate Complexes of Ti(IV) and Zr(IV): Synthesis, Characterization and Ethylene Polymerization Activity **K. Multani** <kmultani@chem.utoronto.ca> and **D.W. Stephan** <dstephan@chem.utoronto.ca>, Department of Chemistry, University of Toronto, 80 St. George St., Toronto, ON M5S 3H6.

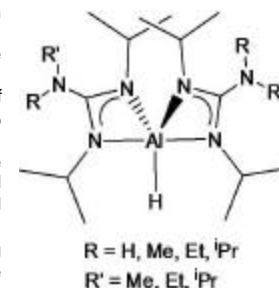
Amidates have received considerable attention as ancillary ligands for various transition metal complexes. Versatile synthesis of amidates and easy manipulation of their steric bulk and electronic properties makes them highly desirable. Sterically bulky ferrocene substituted amidates have been considered as ancillary ligands for the design of novel olefin polymerization catalysts. In group IV complexes containing ferrocenyl amidates, the close proximity of the electron rich iron center has the potential for stabilization of the cationic metal center during polymerization. In this work, bis(amidinate) and half sandwich mono(amidinate) dichloride complexes and their corresponding dialkyl complexes have been synthesized. Cyclic voltammetry studies on the metal complexes and ethylene polymerization activity after activation with MAO, $\text{B}(\text{C}_6\text{F}_5)_3$ and $[\text{Ph}_3\text{C}][\text{B}(\text{C}_6\text{F}_5)_4]$ will be detailed.



59 16:30 Saturday ROZH Foyer

Heteroleptic Guanidinate Aluminum Hydrides for Atomic Layer Deposition of Aluminum Metal Thin Films **J. R. Delahunty** <jdelahun@connect.carleton.ca> and **S. T. Barry** <sbarry@ccs.carleton.ca>, Department of Chemistry, Carleton University, 1125 Colonel By Drive, Ottawa, Ont. K1S 5B6.

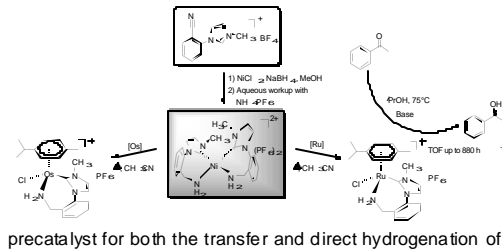
Traditional methods for the deposition of aluminum metal films in electronics, such as sputtering, are unable to deliver the high control over thickness and uniformity that is now required with the downsizing of electronic devices into the nanoscale regime. Current atomic layer deposition methods for aluminum metal thin films employ harsh reducing agents, such as H_2 plasma, which require a large excess of energy and can be detrimental to film quality. The goal of this research is to develop a process by which aluminum metal is deposited using only hydrogen gas as a reducing agent. The ability to use a milder reducing agent can be made achievable through the design of the aluminum precursor; the synthesis and thermolysis of $[\text{Me}_2\text{NC}(\text{N}^i\text{Pr})_2]_2\text{AlH}$, $[\text{Et}_2\text{NC}(\text{N}^i\text{Pr})_2]_2\text{AlH}$, $[\text{Pr}^i\text{HNC}(\text{N}^i\text{Pr})_2]_2\text{AlH}$, and $[\text{Pr}^i\text{NC}(\text{N}^i\text{Pr})_2]_2\text{AlH}$ compounds will be discussed, and their viability as precursors will be assessed. Characterization of aluminum metal deposition using $[\text{Pr}^i\text{HNC}(\text{N}^i\text{Pr})_2]_2\text{AlH}$ precursor with hydrogen gas as a reducing agent will be described and the mechanism of deposition will be explored.



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Transmetalation of a Primary Amino-functionalized N-Heterocyclic Carbene from Nickel(II) to Platinum Group Metal Precatalysts for Transfer and Direct Hydrogenation of Ketones. **W.W.N.O.** <wo@chem.utoronto.ca>, **A. J. Lough** and **R. H. Morris** <rmorris@chem.utoronto.ca>, Davenport Laboratory, Department of Chemistry, University of Toronto, 80 St. George Street, Toronto, Ontario M5S 3H6.

The first axially chiral square planar nickel(II) complex with chelating primary amino-functionalized N-heterocyclic carbene ligands (C-NH₂) was synthesized under mild conditions by the reduction of a nitrile-functionalized imidazolium salt. A novel transmetalation reaction moved this chelating C-NH₂ ligand from the nickel(II) complex to $[\text{M}(p\text{-cymene})\text{Cl}]_2$ dimers (M = Ru, Os) yielding the complexes $\text{M}(\eta^6\text{-}p\text{-cymene})(\text{C-NH}_2\text{Cl})\text{PF}_6$ (M = Ru, Os). These are the first platinum group metal complexes with such a novel chelating C-NH₂ ligand. The ruthenium(II) complex is a precatalyst for both the transfer and direct hydrogenation of acetophenone to 1-phenylethanol with a turnover frequency (TOF) of up to 880 h⁻¹ and conversion of 96%.

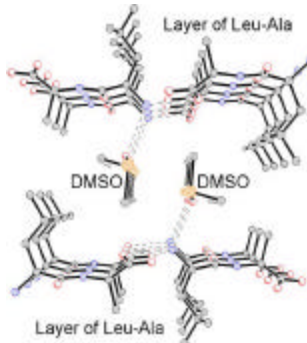


(1) O, W. W. N.; Lough, A. J.; Morris, R. H. *Organometallics* 2009, 28, 853-862. (2) O, W. W. N.; Lough, A. J.; Morris, R. H. *Organometallics* 2009, in press.

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Phase Diagram of the System Leucyl-alanine - DMSO with 1:1 Inclusion Compound. **A. Yazdani** <ayazdani@uoguelph.ca>, **V.V. Chirmanov** <vchirman@uoguelph.ca> and **D.V. Soldatov** <dsoldato@uoguelph.ca>, Department of Chemistry, University of Guelph, Guelph, ON N1G 2W1.

Inclusion compounds of simple peptides are prospective materials for pharmaceutical and other applications [1] but little is known about their stability and conditions of their formation. The leucyl-alanine (Leu-Ala) dipeptide forms an inclusion compound with dimethylsulfoxide (DMSO) [2]. Using DSC and TGA techniques, the phase diagram of the system Leu-Ala - DMSO was preliminary determined in order to investigate stability, limits of existence and modes of decomposition for the inclusion compound. The 1:1 inclusion compound Leu-Ala·DMSO is thermodynamically stable up to ~150°C at which temperature it dissociates into solid Leu-Ala and liquor (incongruent melting). The system is complicated by irreversible cyclization of the Leu-Ala molecule. [1] D.V. Soldatov, in: Nanoporous Materials 5, 213 (2008). [2] M. Akazome, A. Hirabayashi, K. Takaoka, A. Nomura and K. Ogura, Tetrahedron 61, 1107 (2005).

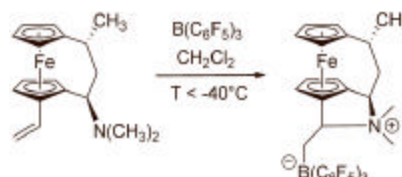


62 16:30 Saturday ROZH Foyer

Olefin Addition to Frustrated Amine/Borane Lewis Pairs **T. Vos** <tvoss@chem.utoronto.ca>, **J. B. Sortais**, **G. Kehr**, **R. Fröhlich** and **G. Erker**, Institute of Organic Chemistry, WWU Münster, Corrensstraße 40, Münster, Germany.

In many cases the combination of sterically encumbered Lewis acids and bases does not result in classical adduct formation but yields "frustrated Lewis pairs" (FLP) that show a unique reactivity. They are e. g. able to activate and/or bind small molecules like H₂, CO₂, N₂O, thf, alkynes or carbonyl compounds.[1]

Besides it was shown that frustrated phosphine/borane pairs add to alkenes inter- as well as intramolecular.[2] We now investigated whether FLPs other than P/B systems also react with olefins. For this study we chose the α -dimethylamino-*o*-vinyl[3]ferrocenophane and related systems. These indeed undergo intramolecular 1,2 N/B addition to the alkene upon reaction with B(C₆F₅)₃. [3]



[1] D. W. Stephan, Dalton Trans. 2009, 3129-3136; [2] J. S. J. McCahill, G. C. Welch, D. W. Stephan, Angew. Chem. Int. Ed. 2007, 46, 4986-4971; [3] J. B. Sortais, T. Voss, G. Kehr, R. Fröhlich, G. Erker, Chem. Commun. 2009, doi: 10.1039/b915657g

63 16:30 Saturday ROZH Foyer

Synthesis and Characterization of a New Thiadiazolo- Fused Para-Semiquinone **L.S. Morgan** <lmorgan@uoguelph.ca>, **K., E., Preuss** <kpreuss@uoguelph.ca> and **M., J., Jennings**, University of Guelph, Guelph, ON, N1G 2W1.

Ortho-quinones can behave as non-innocent ligands and therefore can act as either radical anion semiquinonates or dianion catecholates. These ligands have been studied extensively with respect to coordination to transition metal ions and some have shown interesting magnetic properties.¹ However, synthesis and coordination of 2,1,3-thiadiazolo (TDA) para-semiquinone derivatives has never been attempted throughout the literature.

Naphtho[2,3-c][1,2,5]thiadiazole-4,9-dione is a neutral 2,1,3-TDA fused para-quinone previously reported compound², however no studies to form the semiquinone radical anion, 9-oxido-4-oxonaphtho[2,3-c][1,2,5]thiadiazolo-1-(4H)-yl have been attempted. Synthesis and characterization with cobaltocenium as the counter ion has lead to an interesting 3:2 ratio respectively which demonstrates semiconductivity. Within the crystal structure there is no evident dimerization which might demonstrate fascinating magnetic behavior and therefore the material has the possibility of being a new spintronic material.

(1) C.G. Pierpont, Coord. Chem. Rev., 219-221, 2001, 415.

(2) Mayer, R., Domschke, G., Bleisch, S., Bartl, A, Zeitschrift fuer Chemie, 1981, 21. 324.

64 16:30 Saturday ROZH Foyer

Gas-Phase Thermolysis of Copper Precursors. Unraveling the Fragmentation of Guanidines and Amidinates by Time-of-Flight Mass Spectrometry Matrix-Isolation FTIR Spectroscopy. **J.P. Coyle** <jcoyle@connect.carleton.ca>, **P. Johnson**, **G. DiLabio**, **J. Mueller** and **S.T. Barry**, Carleton University.

The gas-phase thermolysis of a copper(I) guanidinate and amidinate were investigated using matrix-isolation FTIR spectroscopy and time-of-flight mass spectrometry (ToF-MS) to analyze the thermal fragments that were generated in-situ. The experiments were conducted in a unique apparatus whereby the gaseous precursor was passed through a small Al₂O₃ tube furnace (35 mm x 1mm) that was heated between 150-600 °C. Contrary to our initial report, guanidines and amidinates have similar thermolysis. ToF-MS identified the thermal fragments with masses corresponding to protonated ligand, protonated ligand-2, and dihydrogen. FTIR spectrums of the matrix isolated fragments confirmed their identity by comparison to spectrums of the synthesized fragments.

Two plausible mechanisms were conceived due to the thermolysis fragments; beta-hydride abstraction or metal ligand bond homolysis. Theoretical calculations were carried out for the copper(I) guanidinate to determine the most likely mechanism. These calculations showed beta-hydride abstraction to be more favourable than bond homolysis as well as carbodiimide deinsertion. These pathways will be discussed with respect to gas phase vs. solution phase thermolysis.

65 16:30 Saturday ROZH Foyer

New Rod-Like Dyads of Ru(II) and Terpyridyl Ligands: Effect of Bis-Pyridyl-1,3,5-Triazine in the Tuning of the Photophysical Properties. **M.-P. Santoni**^{a,b} <marie-pierre.santoni@umontreal.ca>, **E. Medlycott** and **G. S. Hanan** <garry.hanan@umontreal.ca>, ^aDépartement de Chimie, Université de Montréal, Canada; **B. Hasenknopt** <bernold.hasenknopt@upmc.fr> and **A. Proust**, ^bInstitut Parisien de Chimie Moléculaire, UMR7201, Université Pierre et Marie Curie, Paris, France; **F. Nastasi**, **S. Campagna**, **C. Chiorboli**, **R. Argazzi** and **F. Scandola**, 3Università di Messina & ISOF-CNR & Università di Ferrara, Italy.

Ru(II) polypyridyl complexes have attracted considerable attention due to their interesting photophysical properties. Good absorption of visible light, a relatively long excited-state life time of the triplet state and capacity to transfer energy and electrons, are important criteria for chromophores in building up efficient Light-Harvesting Devices (LHD). Multicomponent rod-like systems are structurally well-suited for studying intramolecular vectorial energy transfer in a LHD.

We are interested in tuning the photophysical properties of linear Ru(II) polypyridine dyads by using tridentate electron deficient ligands, such as bis-pyridyl-1,3,5-triazine. Synthesis, characterization and photophysical studies of symmetric and non-symmetric dyads will be presented.

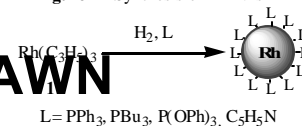


66 16:30 Saturday ROZH Foyer

The Halogen-Free Synthesis of Rhodium Nanoparticles for Applications in Catalysis **S.A. Stratton** <samantha.stratton@mail.mcgill.ca>, **K.L. Luska** <kylie.luska@mail.mcgill.ca> and **A. Moores** <audreymoores@mcgill.ca>, McGill University, Sherbrooke Street W., Montreal, QC, H3A 2K6.

Among catalysts, nanoparticles (NPs) have gained considerable popularity due to their many advantages including high reactivity, tunability and ease of recovery.¹ Frequently, NPs are synthesized from halogen-based precursors; however, the resulting NPs can have reduced catalytic activity due to halogen contamination of the metal surface. Several halogen-free precursors, such as Ru(cod)(cot)¹, have been used in the synthesis of NPs; although, this approach has not been reported for rhodium. We have applied Rh(C₃H₅)₃ (1) as a halogen-free precursor, which upon reduction with H_{2(g)} in the presence of stabilizing ligands, produces Rh NPs and propane, a non-coordinating by-product. The influence of the stabilizing ligand on the properties of the NPs, including NP size and catalytic activity, is particularly important and a series of ligands such as phosphines, phosphites and nitrogen donors will be investigated. Moreover, complex 1 has also been investigated as a precursor in the synthesis of Rh NPs embedded in imidazolium ionic liquids and are active arene hydrogenation catalysts.

Figure 1 - Synthesis of Rh NPs



Ref. 1. Migowski, P., Dupont, J., Chem.Eur.J., 2007, 13, 32.

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16:30 Saturday

ROZH Foyer

Photochromic behaviour of 4-coordinate organoboron compounds **S. Murphy, C. Baik and S. Wang** <wangs@chem.queensu.ca>, Queen's University, Kingston, ON, K7L 3N6.

A four-coordinate boron compound, (2-ph-pp)BMe₂, has recently been discovered which exhibits reversible C-C bond formation and accompanying photochromism. However, once C-C bond formation occurs, the luminescence of the compound is quenched, rendering it ineffective in opto-electronic devices such as organic light emitting diodes (OLEDs). To address this, studies have been undertaken to synthesize highly conjugated molecules containing the 4-coordinate organoboron motif, which were expected to display greater photostability. Monoboryl and polyboryl compounds have been synthesized which display different photochromic properties depending on the extent of conjugation and number of boron centres. In this poster, the synthesis, characterization, TD-DFT studies, and photochromic properties of this new class of compounds will be presented.

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16:30 Saturday

ROZH Foyer

Synthesis, structure, volatility, and thermal stability of molybdenum and tungsten complexes containing nitrogen rich ligands. **O. M. El-Kadri** <oelkadri@aus.edu>, American University of Sharjah, Sharjah, UAE; **C. H. Winter** and **M. J. Heeg**, Wayne State University, Detroit, MI, USA.

Tungsten nitride (WN_x, x = 0.5-1.0) and related carbonitride phases are promising barrier materials for copper metallization in future microelectronics devices. For device applications, barrier material films must be grown in narrow (<65 nm) and deep features with perfect conformal coverage. In addition, very thin (<10 nm), defect-free films are required. Atomic layer deposition (ALD) is an emerging layer-by-layer film growth technique, and is of great interest for microelectronics manufacturing due to the perfect conformal coverage that can be obtained and for its precise control over film thickness. Important properties of ALD metal precursors include high thermal stability on the surface of the growing film to avoid CVD-like growth and high reactivity toward a second reagent to afford the desired thin film material. These requirements create new challenges for precursor design. We will present the synthesis, structure, volatility, and thermal stability of novel molybdenum and tungsten complexes containing pyrazolate or imidinate ligands. We will also discuss the potential of the new complexes for use as precursors in thin film growth experiments.

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16:30 Saturday

ROZH Foyer

A novel Schiff base complex of Co^{II} based on the N-hydroxyamidine motif: structural, spectroscopic and electrochemical properties **S. Derossi** <sofia.derossi@umontreal.ca>, **M. Cibian** and **G. S. Hanan** <garry.hanan@umontreal.ca>, Université de Montréal, Montréal, Québec, H3C 3J7.

A new, versatile family of N,O chelating ligands, N-hydroxyamidines, was prepared through an easy route: their Co^{II} complexes resemble closely the well known Co(salen)₂ and Co(dmgl)₂ compounds, widely employed in catalytic and photocatalytic applications. The crystal structures of these novel Co^{II} complexes reveal square planar coordination, an unusual feature for d⁷ compounds of cobalt, leaving two potential sites available for supramolecular coordination. Furthermore, the redox and thus catalytic properties of the metal centre can be finely tuned by designing N-hydroxyamidines of suitable steric and electronic configurations.

The reactivity of this new class of compounds is presented, together with their electrochemical and spectroscopic properties, casting light on some fundamental aspects of these complexes.



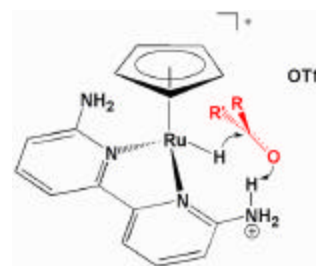
70

16:30 Saturday

ROZH Foyer

[Ru(η⁵-C₅H₅)(6,6'-diamino-2,2'-bipyridine)(CH₃CN)](OTf) as a Metal-ligand Bifunctional Catalyst Under Acidic Conditions. **D. Di Mondo** <ddimondo@uoguelph.ca> and **M. Schlaf** <mschlaf@uoguelph.ca>, Department of Chemistry, University of Guelph, 50 Stone Rd. E, Guelph, Ont., N1G 2W1.

The synthesis of the precatalyst [Ru(η⁵-C₅H₅)(dabipy)(CH₃CN)](OTf) has been achieved, where dabipy = 6,6'-diamino-2,2'-bipyridine. The amino groups present in the ortho position of the chelating ligand allow for a possible concerted hydrogenation of a substrate through a metal-ligand bifunctional mechanism. As seen in Dr. Noyori's fundamental work on the subject a catalyst operating through a metal-ligand bifunctional mechanism can be highly active. In this study we demonstrate the ability of [Ru(η⁵-C₅H₅)(dabipy)(CH₃CN)](OTf) to behave as a metal-ligand bifunctional system by comparing its activity to that of the analogous non-bifunctional system [Ru(η⁵-C₅H₅)(bipy)(CH₃CN)](OTf), using the hydrogenation of various carbonyls under acidic neat conditions as the test reaction. The catalytic behavior of both complexes will be presented.



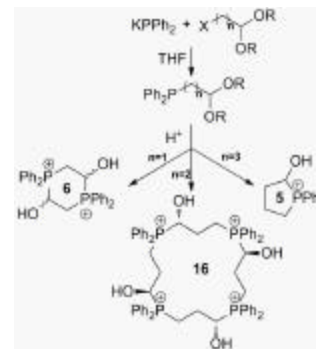
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16:30 Saturday

ROZH Foyer

Facile synthesis of cyclic phosphonium salts for use as phosphine-aldehyde precursors in metal templating and ligand synthesis. **A. A. Mikhailine, P. Lagaditis, P. Sues, A. J. Lough and R. H. Morris**, Department of Chemistry, University of Toronto, 80 St. George St., Toronto, Ont. M5S 3H6. r.morris@chem.utoronto.ca.

Phosphine-aldehydes are important building blocks in the synthesis of polydentate ligands and organometallic compounds. Conventional synthesis and utilization of these amphoteric molecules is problematic as a result of high instability and air sensitivity. In order to address this issue our group has developed a synthesis of cyclic phosphonium structures that are formed by the deprotection of unstable phosphine-acetals in acidic solution. Depending on the number of carbon spacers between the phosphorus and aldehyde functionalities, monomeric, dimeric or tetrameric species are formed. The phosphonium salts react with base to generate unstable phosphine-aldehydes in situ, which are used in the template synthesis of Fe(II) and Ni(II) PNNP complexes. The Fe(II) complexes that were formed by this method are highly active and enantioselective catalysts for transfer hydrogenation of ketones using isopropanol as the hydrogen source.



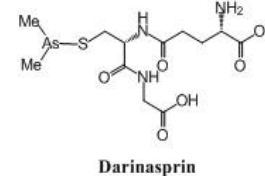
72

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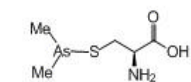
ROZH Foyer

Looking at Arsenicals for treatment of Acute Promyelocytic Leukemia. **Y. Gu** <yuxuan.gu@mail.mcgill.ca>, **DS Bohle** <scott.bohle@mcgill.ca> and **N. Garnier** <nicolas.garnier@mail.mcgill.ca>, McGill University, Montreal, Quebec, H3A 2T5.

Certain arsenic based drugs are shown to be particularly effective against Acute Promyelocytic Leukemia (APL) which constitutes roughly 5% of Leukemia cases. The organoarsenic drug, Darinasprin, which is currently in Phase I development, has improved action and lower side effects when compared to the inorganic drug arsenic trioxide (Trisenox). This project attempts to elucidate the mechanism of arsenic in the cell, and hence provide valuable insight into ways to improve the design of arsenic based anti-cancer drugs.



Dimethylarsino-cysteine was synthesized as a possible drug candidate. The stability of the molecule was tested in various media using UV spectroscopy. We have demonstrated that molecule has a half-life of 3 days in water and 1 day in serum. Dimethylarsinos acid was also synthesized and its activity was compared to that of Dimethylarsino-cysteine in NB4 cells.



Dimethylarsino-cysteine

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ROZH Foyer

Spin Catalysis of Azo Photoisomers **K. Rosadiuk** <Kristopher.Rosadiuk@mail.mcgill.ca> and **D.S. Bohle** <Scott.Bohle@mcgill.ca>, McGill University, 801 Sherbrooke St. O., Montreal, QC, H3A 2K6.

Spin catalysis has been proposed as an essential missing factor in our understanding of chemical reactivity; nitric oxide, as one of the most commonly encountered molecules with spin catalytic function, may be an overlooked participant in a variety of chemical systems. Its small size, relative stability, and radical reactivity give it a unique functionality in the transformation of other molecules. Here we investigate its influence over the thermal transformation of cis-trans photoisomers of the azo moiety, using diazenium diolate as a delivery mode. NO is found to catalyze cis-trans isomerization of azo bonds without loss due to reaction, in a manner suggestive of a reversible but durable association between the molecules.

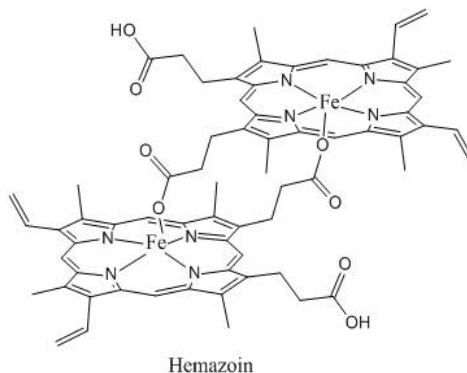
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16:30 Saturday

ROZH Foyer

Determining the Degradation Products of the Malaria Pigment. **A Hill** <andrea.hill3@mail.mcgill.ca> and **D.S Bohle** <scott.bohle@mcgill.ca>, McGill University.

The plasmodium parasite, which induces malaria, detoxifies the heme found in red blood cells by converting them into black crystals known as hemazoin. Within the phagolysosome of a macrophage, these crystals are bombarded with hydrogen peroxide, bleach and other reactive oxygen species. To examine the processes which are occurring within the macrophage, synthetic hemazoin was exposed to such oxidants. A comparison was done to determine if the degradation of hemazoin by bleach or hydrogen peroxide would produce the same products as the degradation of heme. The methylated products were compared and analyzed by HPLC, mass spectroscopy and NMR. It was determined that there was methylvinylmaleimide, hematinic acid and four types of propentidyloxy among the degradation products.



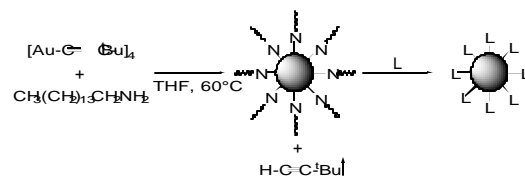
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16:30 Saturday

ROZH Foyer

Synthesis of Amine Stabilized Nanoparticles as Precursors in Ligand Exchange **M.J. Rak** <monika.rak@mail.mcgill.ca>, **K. L. Luska** and **A. Moores** <audrey.moores@mcgill.ca>, Department of Chemistry, McGill University, 801 Sherbrooke St. W., Montreal, Quebec, H3A 2K6.

Insight into the influence of stabilizing ligands on the properties of the Au NPs, independent of alterations to the NP size or shape, is required. We are therefore interested in developing a method to synthesize monodisperse Au NPs capable of undergoing complete ligand exchange while minimizing changes to the metal core. Our system involves the reaction of [Au-C≡C⁻Bu]₄ with pentadecylamine (PDA) to form



mono-dispersed Au NPs in which the amine plays the dual role of reducing agent and labile stabilizing ligand. Using a halide-free gold precursor avoids halide contamination of the Au NPs, this is desirable because halogenides can influence the growth of NPs and the subsequent ligand exchange reactions. The weakly coordinating PDA can be exchanged with a variety of stronger ligands (L = thiols, phosphines, and nitrogen donors) and should allow for a general method for ligand exchange without alterations to the size and shape of the NPs.

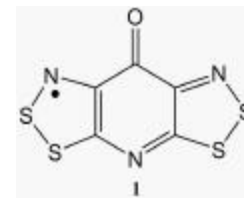
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16:30 Saturday

ROZH Foyer

Synthesis and Characterization of a Bis-DTA Pyridin-4-one Neutral Radical Ligand **CE Carello** <ccarello@uoguelph.ca> and **KE Preuss** <kpreuss@uoguelph.ca>, University of Guelph, Guelph, ON, N1G 2W1.

Molecules possessing both conductive and magnetic properties are a strong area of interest.¹ The synthesis of paramagnetic thiazyl ligands has shown promise and still remains largely untapped.² The title bis-DTA neutral radical ligand, **1**, will be synthesized in hopes of displaying excellent conductive and magnetic properties when coordinated to various metal ions.



¹ Robertson, C. M., Myles, D. J. T., Leitch, A. A., Reed, R. W., Doolley, B. M., Frank, N. L., Dube, P. A., Thompson, L. K., Oakley, R. T. *J. Am. Chem. Soc.* 2007, 129, 12688.

² Hearn, N. G. R., Fatila, E. M., Clerac, R., Jennings, M., Preuss, K. E., *Inorganic Chemistry*, 2008, 47(22), 10330.

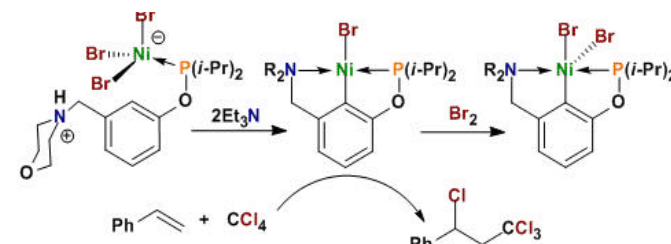
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16:30 Saturday

ROZH Foyer

New POCN-Type Pincer Complexes of Nickel(II) and Nickel(III) **D.M Spasyuk** <denis.spasyuk@umontreal.ca> and **D Zargarian** <zargarian.da.vit@umontreal.ca>, Département de chimie, Université de Montréal.

Pincer-type complexes are very versatile for fundamental studies in the context of catalytic transformations. Our group studies pincer-type nickel complexes with a view to developing catalytic reactivities of interest. A recent report described the reactivities of POCN-type complexes bearing different tertiary amines coordinated to divalent and trivalent nickel centres. (Spasyuk et al., *Organometallics*, 2009, ASAP) This poster will review some of these results and will present our latest results on the synthesis, characterization, electrochemical, thermal and EPR studies of new POCN-type complexes of Ni(II) and Ni(III).



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16:30 Saturday

ROZH Foyer

In Situ EXAFS and NMR Study of Ultrathin Bismuth Sulfide Nanowires **JW Thomson** <jthomson@chem.utoronto.ca> and **GA Ozin** <gozin@chem.utoronto.ca>, Department of Chemistry, University of Toronto.

Recently, our lab synthesized ultrathin bismuth sesquisulfide nanowires with a diameter of less than 2 nm and lengths up to microns long. These nanowires are flexible, a rare property of inorganic nanocrystals, and have an extremely high extinction coefficient on the order of 10⁸ M⁻¹ cm⁻¹. Potential applications aside, these nanowires represent a very interesting class of materials that has not been studied much to this point. Characterization of these nanocrystals has proven elusive with traditional techniques such as PXRD, due to the extremely small crystal size, and HRTEM due to sensitivity to beam damage. We decided to utilize the non-destructive techniques of Extended X-Ray Absorption Fine Structure (EXAFS) on colloidal dispersions of nanowires and 1D/2D solution NMR to provide accurate structural information of the inorganic core and organic-inorganic interface. In the case of these nanowires, surface plays a large role in determining properties and structure as the surface: volume ratio is very high for such small crystallites. To our knowledge, this is the first example of a study utilizing both solution phase EXAFS and NMR to study colloidal nanocrystals.

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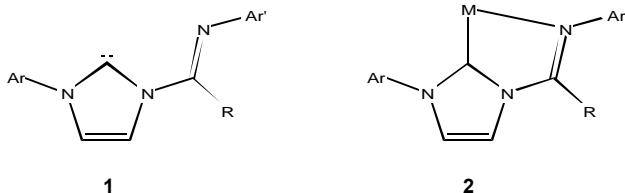
A combined ^{73}Ge solid state NMR spectroscopic and computational study of GePh_4 and GeCl_2 -dioxane **M. A. Hanson** <mhanson4@uwo.ca>, **A. Sutrino**, **P. A. Rugar**, **Y. Huang** and **K. M. Baines** <kbaines2@uwo.ca>, The University of Western Ontario, London, ON, N6A 5B7.

While most of the elements of Group 14 (ie carbon, silicon, tin and lead) possess at least one spin 1/2 isotope, germanium has only one NMR active isotope, ^{73}Ge , with a spin of 9/2 and a relatively large quadrupole moment ($Q=0.22$ barn). Furthermore, ^{73}Ge has one of the lowest gyromagnetic ratios in the periodic table ($\gamma=-0.9332\times 10^7$ rad T^{-1} s^{-1}), which leads to low sensitivity. However, the increasing availability of higher field spectrometers is making the study of challenging nuclei more feasible. Through the use of an ultra high (21.1 T) magnetic field, we were able to obtain static solid state NMR spectra for tetraphenylgermane, a compound with Ge in a highly symmetrical environment, and GeCl_2 -dioxane, a compound with Ge in a much lower symmetry environment. The experimental data are supplemented by a theoretical study.

80 16:30 Saturday ROZH Foyer

Coordination of Imino-N-Heterocyclic Carbenes to Transition Metals. **A.C. Badaj** <anabad@yorku.ca>, **I.G. Larocque** <ilarocqu@yorku.ca> and **G.G. Lavoie** <glavoie@yorku.ca>, Department of Chemistry, York University, 4700 Keele Street, Toronto, ON M3J 1P3.

Recently, there has been a great deal of new transition metal complexes with N-heterocyclic carbene (NHC) ancillary ligands reported as viable candidates for homogeneous catalysis. Our research group has developed an efficient synthetic route to iminocarbene **1**. This ligand scaffold is unique and allows for binding the metal in a bidentate fashion, through the carbene and the imino nitrogen atom. The aryl groups further offer the opportunity to tune the electronics and sterics of the complexes. We herein report our work towards coordinating **1** to transition metals.



81 16:30 Saturday ROZH Foyer

Cationic Complexes of Tin(II) **Jessica C Avery**, **Paul A. Rugar** and **Kim M. Baines** <kbaines2@uwo.ca>, Department of Chemistry, The University of Western Ontario, London, ON, N6A 5B7.

The ability of the main group metals in groups 1 and 2 to form free cations and complexes with cryptands and crown ethers has been extensively studied. Recently, our group has stabilized germanium(II) dication by entombing them within the cavity of either a cryptand¹ or crown ethers². With this advancement, we have explored the reactivity of tin(II) halides with cryptands and crown ethers. Synthesis and structural characterization of the tin(II) cryptand complexes will be discussed.

1. Rugar, P.A.; Staroverov, V.N.; Baines, K.M. *Science* **2008**, 322, 1360.
2. Rugar, P.A.; Bandyopadhyay, R.; Cooper, B.F.T.; Stinchcombe, M.R.; Ragogna, P.J.; Macdonald, C.L.B.; Baines, K.M. *Angew. Chem. Int. Ed.* **2009**, 48, 1-5.

82 16:30 Saturday ROZH Foyer

Late Transition Metal Complexes of η^3 -Coordinated Vinylboranes **K.B. Kolpin** and **D.J.H. Emslie** <emslie@mcmaster.ca>, Department of Chemistry and Chemical Biology, McMaster University, 1280 Main Street West, Hamilton, ON, L8S 4M1, Canada.

π -Ligands based on an all carbon backbone have been at the core of organometallic chemistry since its inception. However, substitution of carbon for other main group elements provides the potential for changes in metal-ligand bonding, ligand charge and overall donor ability, and metal- and/or ligand-based reactivity. Formally monoanionic boratabenzene and dianionic borole ligands, boron analogues of arene and cyclopentadienyl ligands, are now well established in d- and f-element chemistry. However, acyclic boron/carb on π -ligands are extremely rare.

In this presentation we discuss the synthesis and study of late transition metal vinylborane complexes in which the vinylborane exhibits a π -allyl-like coordination mode (Figure 1). These complexes are the first η^3 -1-borataallyl complexes, and have been studied using NMR spectroscopy, X-ray crystallography and DFT calculations.

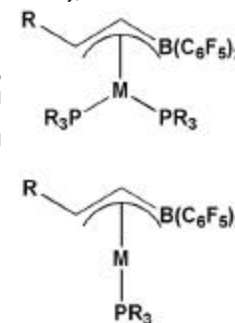
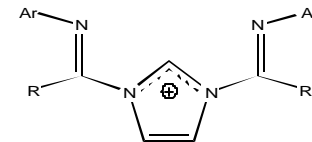


Figure 1.

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Coordination Study of Nonenolizable Bis(imino)-N-Heterocyclic Carbene Pincer (NCN) Ligand to Transition Metals. **J. Al Thagfi** <jameel1@yorku.ca> and **G.G. Lavoie** <glavoie@yorku.ca>, Department of Chemistry, York University, 4700 Keele Street, Toronto, ON M3J 1P3.

Iron and cobalt catalysts with bis(arylimino)pyridine ligand exhibit exceptional catalytic activities for ethylene polymerization.¹ However, the polymerization rates of α -olefins are very low. Furthermore, rapid decomposition of the catalysts is observed upon heating. Our group is interested in evaluating the effect N-heterocyclic carbenes (NHC) as a replacement for the pyridine moiety. NHCs are strong σ -donor and impart good thermal stability to transition metal complexes. Furthermore, sterics and electronics can be easily tuned to control the reactivity of the resulting transition metal complexes.^{2,3} 1,3-(N-Arylimino)imidazolium salts have been isolated and spectroscopic data is presented. Our attempts to coordinate the corresponding carbene to transition metals are also reported.



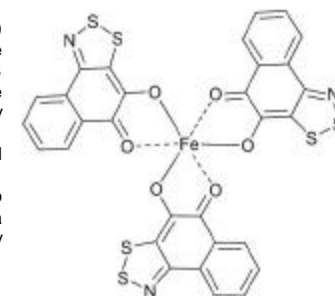
Reference:

1. Gibson, V. C.; Redshaw, C.; Solan, G. A. *Chem. Rev.* **2007**, 107, 1745.
2. Herrmann, W. A.; Kocher, C. *Angew. Chem. Int. Ed. Engl.* **1997**, 36, 2162.
3. Leuthäufner, S.; Schwarz, D. Plenio, H. *Chem. Eur. J.* **2007**, 13, 7195.

84 16:30 Saturday ROZH Foyer

A New Dithiazolo Fused o-Quinone Potential Spin Bearing Ligand **C. S. Smithson** <csmithso@uoguelph.ca>, **K. E. Preuss** <kpreuss@uoguelph.ca> and **M. J. Jennings**, University of Guelph, Guelph, Ontario, 21 G 2W 1.

The 1,2,3-dithiazolo (DTA) or ortho-naphthoquinone radical (o-DTANQ) has previously been identified[1] by EPR studies reporting the expected three line pattern for coupling to one ^{14}N , but the species has never been characterized in the solid state. Currently, I have isolated the [o-DTANQ⁺][OTf⁻] salt and performed cyclic voltametry (CV) measurements showing the reversible reduction to the radical. I have isolated the radical as an amorphous solid, as well as several metal coordination complexes of the semiquinone oxidation state. Molecular materials incorporating the 1,2,3 DTA moiety are known to exhibit activated conductivity. It is also known that coordination to a paramagnetic metal ion gives rise to magnetic coupling. By combining the potential semiconductive and magnetic properties, metal complexes of o-DTANQ may function as a spintronic material. Furthermore, there is the possibility that these complexes will be able to exist as valence tautomers.



[1] Mayer, Roland; Domschke, Guenter; Bleisch, Siegfried; Zeitschrift fuer Chemie ; (1981), 21(9), 324-5.

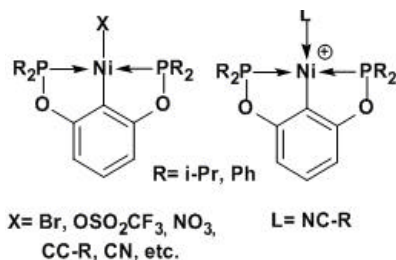
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16:30 Saturday

ROZH Foyer

New POCOP-Type Pincer Complexes of Nickel(II) **A. Salah** <salahbderrahmen@yahoo.fr> and **D Zargarian** <zargarian.davit@umontreal.ca>, Département de chimie, Université de Montréal.

Pincer-type complexes have attracted much interest because of their remarkable activities in a wide range of catalytic processes. An attractive feature of pincer complexes is the ease with which their reactivities can be modulated by variations in ligand structure. We study pincer-type nickel complexes with a view to developing catalytic reactivities. One family of ligands that has shown interesting reactivities is the so-called POCOP ligands shown here. Previous reports from our group have described the reactivities of nickel complexes featuring POCOP-type ligands bearing *i*-Pr₂P phosphinite moieties. (Chem. Comm. 2007, 978; Organometallics 2007, 26, 4321; Dalton 2008, 4756) As an extension of these studies, we have begun to examine the chemistry of POCOP-type complexes of nickel bearing Ph₂P phosphinite moieties. This poster will describe our recent results on the preparation and reactivities of various derivatives based on the ligand Ph₂PO(C₆H₃)OPPh₂.



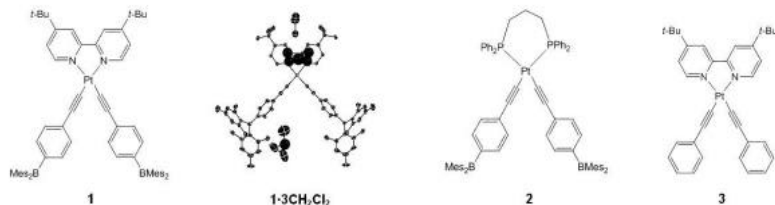
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16:30 Saturday

ROZH Foyer

Triarylboron complexes of Pt(II)-acetylide: synthesis, computational studies and luminescence vapochromism. **C. Sun, Z.M. Hudson and S. Wang** <suning.wang@chem.queensu.ca>, Department of Chemistry, Queen's University, 90 Bader Lane, Kingston, ON, K7L 3N6.

Several platinum(II) phenylacetylide complexes containing two BMe₂ acceptors and diimine or diphosphine chelates have been synthesized (**1**, **2**). The boron centre promotes metal-to-ligand charge-transfer that results in more intense ambient-temperature luminescence than in the absence of boron acceptors (**3**). In addition, solid state (**1**) displays luminescence vapochromism in presence of organic solvent vapours. Interestingly, fluorescent emission ($\lambda_{\text{exc}} = 365$ nm) is selectively quenched after exposure to hexane vapours.



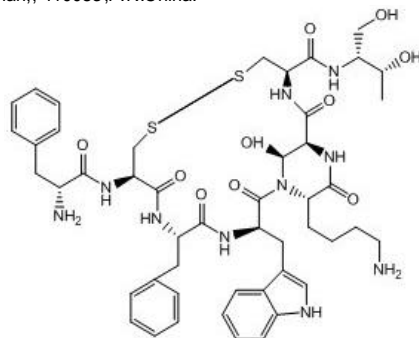
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16:30 Saturday

ROZH Foyer

Carboxymethyl-Dextran Modified Magnetic Nanoparticle Conjugated to Peptide Octreotide **G. Han**^{a,b} <ghan6@uwo.ca> and **H. Kraatz** <hkraatz@uwo.ca>, ^aUniversity of Western Ontario, 1151 Richmond St., London, ON., N6A 5B9; ^bCentral South University., Changsha., Hunan., 410083, P.R.China.

A multifunctional system of carboxymethyl-dextran modified magnetic nanoparticles (CMD-MNPs) capped by the peptide octreotide (Oc) were prepared and characterized by FT-IR, AFM, TEM and XRD. Magnetic Resonance Imaging results show that magnetite nanocapsules and the octreotide conjugate (CMDMNP/Oc) can be used as a T₂ MRI contrast agent. The internalization of the free MNPs and CMDMNP/Oc into *bc*-3 pancreatic cancer cells was investigated. Results show that CMDMNP/Oc were accumulated mostly in the cytoplasm, whereas free MNPs were mostly found in the cell nuclei and lysosome. These experimental results demonstrate that CMDMNP/Oc are an efficient delivery vehicle to transport octreotide to the cytoplasm via endocytosis.



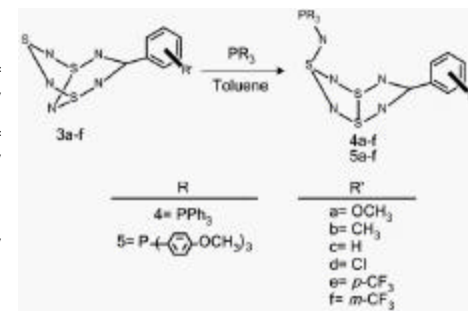
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16:30 Saturday

ROZH Foyer

Evidence for the Formation of Trithiatetrazocinyl Radicals Anions **X. Yu** <x3yu@uwaterloo.ca>, University of Waterloo, ON; **R. T. Boere** <boere@uleth.ca>, University of Lethbridge, AB; **T. L. Roemmele**, University of Calgary, AB.

The 1,3,5,2,4,6,8-trithiatetrazocine ring has been known since 1985. To our knowledge no electrochemical studies have been reported to date. In view of recent success in characterization of the unstable radical anions of 1,3,5,2,4,6,8-trithiatetrazocines, it was of interest to apply our sensitive *in situ* EPR technique to the title compound. We describe here the synthesis of 11 new compounds of this class with full characterization including X-ray crystallography, voltammetry and EPR studies. EPR evidence for the formation of the title radicals will be presented. These radicals are unstable and rapidly convert into the known 1,2,3,5-dithiadiazoles which are indefinitely stable in absence of air.



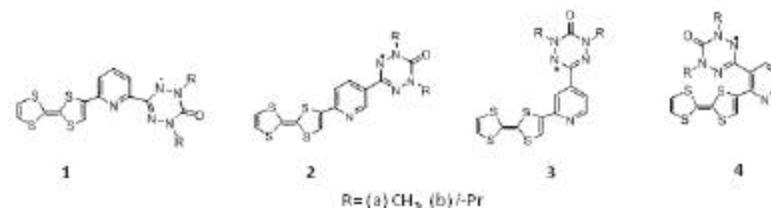
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16:30 Saturday

ROZH Foyer

The Preparation and Characterization of a New Family of Spin-bearing Tetrathiafulvalene Donors **S. Venneri** <sv040q@brocku.ca> and **M Pilkington** <mpilkington@brocku.ca>, Brock University, 500 Glenridge Ave. St. Catharines On. Canada L2S 3A1.

Working towards the realization of molecule-based ferromagnetic conductors, two families of tetrathiafulvalene (TTF) donors appended with verdazyl radicals bridged by pyridyl linkers (**1**) (**4**) have been prepared and characterized.^{[1][2]} The electronic properties of these compounds were studied by EPR, cyclic voltammetry and UV-Vis spectroscopy. The molecular structures of two of the TTF-py-diisopropylverdazyl radicals were determined by X-ray crystallography. These are the first examples of organic donors bearing verdazyl radicals to be characterized in the solid state.



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08:40 Sunday

ROZH 103

Potential Use of Red Mud as a Catalyst for the Upgrading of Pyrolysis Bio-Oil **E. Karimi** <ekarimi@uoguelph.ca> and **M. Schlaf** <mschlaif@uoguelph.ca>, Department of Chemistry, University of Guelph, Canada N1G 2W1.

Acetic and formic acid impart a high acidity on bio-oil (obtained by fast pyrolysis of ligno-cellulosic biomass) preventing its direct use as fuel. At temperatures ≥ 330 °C, Red Mud, a waste by-product of the Aluminium industry produced at > 70 million tons p.a., is an excellent catalyst for thermal decomposition of these acids. Formic acid serves as an internal source of hydrogen through the formation of syn gas and the WGSR. The C₆-C₁₀ hydrocarbon distribution in the non-polar phase, the identification of C₄-C₇ hydrocarbons and CO₂ in the gas and acetone in polar liquid phases can be rationalized through mechanisms involving ketene as the intermediate formed by acetic acid dehydration and FT chemistry. Higher hydrocarbons, mostly alkanes and alkenes, can be formed through iterative aldol condensations, hydrogenation, hydrogenolysis and deoxygenation. The chain length dependence on the amount of acetic acid feed suggests that acetic acid functions as the main carbon and formic acid acts as hydrogen source. In the absence of hydrogen or formic acid, the composition of the non-polar products tends to be unsaturated rather than saturated hydrocarbons.

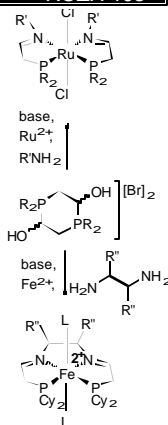
Keywords: acetic acid; formic acid; bio oil; hydrogenation; catalysis; red mud

91 09:00 Sunday

ROZH 103

Template Synthesis of Iron(II) and Ruthenium(II) Complexes Containing Multidentate Ligands with Phosphorus and Nitrogen Donor Atoms **P.O. Lagaditis, A.J. Lough** and **R.H. Morris** <rmorris@chem.utoronto.ca>, Department of Chemistry, University of Toronto, 80 St. George St., Toronto, Ontario M5S 3L1.

Metal complexes with multidentate ligands bearing both phosphorus and nitrogen donor atoms have gained much attention, as they lead to active catalysts. We have previously reported a template approach in the synthesis of novel iron(II) complexes with tetradentate PNNP ligands starting from a conveniently prepared phosphonium dimer. This template methodology led to the discovery of iron(II) precatalysts that have enzymatic-like activities and remarkable enantioselectivity for the transfer hydrogenation of prochiral ketones. These results inspired the current work to explore the scope and versatility of the use of such phosphonium dimers in the template synthesis with other metals. In this presentation, the synthesis and characterization of new phosphonium dimers and iron(II) complexes with new tetradentate PNNP ligands will be presented. Template synthesis leading to other platinum group metal complexes, in particular those of ruthenium(II) with bidentate PN ligands, were explored and tested for direct hydrogenation.



92 09:20 Sunday

ROZH 103

Visible-light Photocatalytic Activity of Eco-friendly TiO₂-SiO₂-Mn Aerogels in Air Purification

K. Kalebaila <sashi952001@yahoo.ca> and **K. Klabunde** <kenkj@ksu.edu>, Kansas State University, Chemistry Department, Manhattan, Kansas, 66506.

Titanium dioxide is widely used as a photocatalyst in environmental remediation using UV light. To improve efficiency, visible light excitation of TiO₂ in photocatalytic decomposition of water and air pollutants has attracted a lot of research interest. For instance, visible active V and Cr TiO₂-doped materials have been reported in the literature, but these metal dopants are toxic. To avoid toxicity, and to increase surface area while still preserving the anatase phase, TiO₂-SiO₂ gels doped with eco-friendly Mn were prepared.

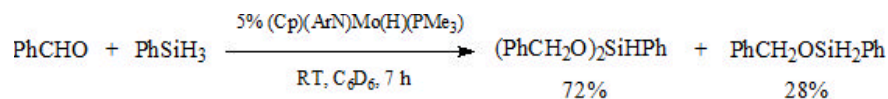
Results show that under visible light, Mn-doped samples degrade gaseous acetaldehyde (CH₃CHO, a common indoor air pollutant). The decomposition is evidenced by CO₂ production detected by GC-MS. About 50-80 % of initial CH₃CHO is decomposed while less than 10 % of CO₂ is produced (other intermediates are formed). Electron Spin Resonance (ESR) of a TiO₂-SiO₂-Mn sample before degradation of CH₃CHO suggests that Mn⁴⁺ ions are the active sites. After photocatalysis, additional peaks appear between the major sextet lines attributed to Mn²⁺ (since Mn³⁺ is ESR silent). The photoactivity of previously used TiO₂-SiO₂-Mn can be regenerated by prolonged exposure to visible light in the presence of air or by recalcination at 500 °C.

93 09:40 Sunday

ROZH 103

Mechanism of carbonyl hydrosilylation catalyzed by (Cp)(ArN)Mo(H)(PMe₃). **Oleg G. Shirobokov** <sholegg@gmail.com> and **Georgii I Nikonov** <gnikonov@brocku.ca>, Department of Chemistry, Brock University, 500 Glenridge Ave., St. Catharines, Ont. L2S 3A1.

The imido-hydride complex (Cp)(ArN)Mo(H)(PMe₃) (**1**, Ar = 2,6-ⁱPr₂C₆H₃) was found to catalyze a variety of carbonyl hydrosilylation reactions. Detailed mechanistic studies were carried out for the reaction of benzaldehyde with PhSiH₃, including kinetic studies of individual steps and determination of activation parameters. The reaction starts with associatively activated insertion of carbonyl across the Mo-H bond of **1** to give the alkoxy derivative (Cp)(ArN)Mo(OCH₂Ph)(PMe₃) followed by associatively activated reaction with PhSiH₃ to regenerate **1**. The latter reaction is characterized by the inverse isotope effect, suggesting late transition state.



94 10:00 Sunday

ROZH 103

Formation of self-assembled monolayers (SAMs) on Au(111) surfaces by dithiophosphinic acids (DTPAs) with nanoscale structural control **R.R. San Juan** <san@uwindsor.ca>, **J. Müller** and **T. Breen Carmichael** <tcarmic@uwindsor.ca>, University of Windsor, Windsor, ON, Canada.

We present the formation of new self-assembled monolayers (SAMs) on gold that feature nanoscale control of the SAM composition as well as the structure normal to the substrate. Our studies use dialkyldithiophosphinic acids (RR'P(S)SH), which spontaneously form SAMs by chelating to the gold surface. Symmetrical dialkyldithiophosphinic acids (R = R') yield SAMs that are similar to alkanethiolate SAMs: The crystallinity of the alkyl chains increases as the alkyl chain length increases. Unsymmetrical dialkyldithiophosphinic acids form SAMs with a 50:50 mixture of the R and R' groups. Tuning the relative lengths of the R and R' alkyl groups enables the formation of SAMs composed of a densely-packed layer of alkyl chains close to the gold surface covered by a layer of loosely-packed alkyl groups. Both the symmetrical and unsymmetrical dialkyldithiophosphinate SAMs were characterized using X-Ray photoelectron spectroscopy, reflection-absorption infrared spectroscopy, contact angle measurements and electrochemical impedance spectroscopy. We will discuss potential uses for these new SAMs.

95 08:40 Sunday

ROZH 102

Synthesis and Characterization of a New 1,2,3,5-Dithiadiazolyl (DTDA) Radical Ligand and Mn(II)(hfac)₂(DTDA) Complex **E.M. Fatila** <efatila@uoguelph.ca> and **K.E. Preuss** <kpreuss@uoguelph.ca>, University of Guelph, 50 Stone Rd. E., Guelph, ON, N1G 2W1; **R. Clerac** <clerac@crpp-bordeaux.cnrs.fr>, Centre de Recherche Paul Pascal, 115 Avenue Schweitzer, 33600 Pessac; **M. Jennings**, 185 Chelsea Ave., London, ON., N6J 3J5; **J. Assoud** <aasoud@uwaterloo.ca>, University of Waterloo, Waterloo, ON, N2L 3G1.

The synthesis and characterization of the benzoxazole-1,2,3,5-dithiadiazolyl (boADTDA) (**1**) radical ligand and the corresponding Mn(hfac)₂(boADTDA) (**2**) complex will be discussed. Of great interest are the crystallographic and magnetic properties of **2**. Crystallographic data and magnetometry show that complex **2** is paramagnetic in the solid state. The magnetic susceptibility data shows antiferromagnetic interactions between the Mn(II) ion and coordinated radical **1** as well as antiferromagnetic interactions between the Mn(II) centre and DTDA radical of adjacent complexes of **2** leading to pairs of **2** with an overall spin ground state of S=4. Crystallographic data shows short S(DTDA)-O(hfac) contacts lead to the association of **2** into pairs.

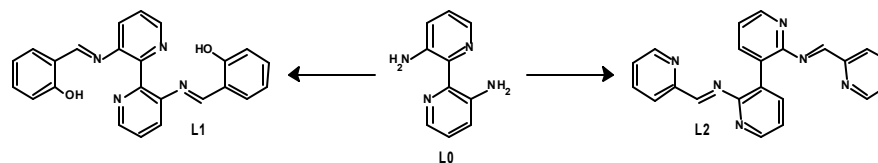


96 09:00 Sunday

ROZH 102

Synthesis, Reactivity and Coordination Chemistry of Novel 2,2'-Bipyridine Schiff-Base Ligands. **R. Gumbau-Brisa** and **M. Pilkington** <mpilkington@brocku.ca>, Brock University.

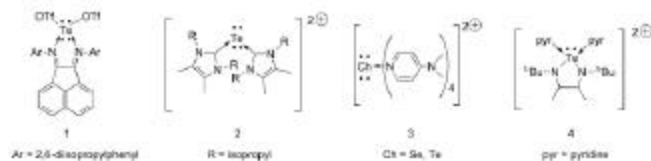
In the quest for novel molecule-based magnetic materials, we decided to target polynuclear complexes because: i) the presence of paramagnetic metal centres in close proximity promotes interactions between them, ii) chemical modification of the ligand can be used to tune these interactions, iii) they present interesting magnetic properties such as spin crossover behaviour or superparamagnetism. We chose 3,3'-diamino-2,2'-bipyridine **L0** as backbone for our systems because the amino groups can be easily converted to imines, allowing the incorporation of organic moieties with additional binding sites. The reactivity and coordination chemistry of our two first synthetic targets, **L1** and **L2**, is influenced by the electrophilicity of the imine functionality and the chelation of Lewis acidic metal ions. The intervention of these metal cations adds an extra dimension to their coordination chemistry.



Dicationic Selenium and Tellurium Complexes **J.L. Dutton** <jldutton@uwo.ca> and **P.J. Ragogna** <pragogna@uwo.ca>, The University of Western Ontario.

The synthesis and isolation of main group dicationic species is a topic of increasing interest in the chemical community. Our work has focused on group 16 dicationic species, which represent a challenge, as the electronegative chalcogen elements are generally considered to prefer an electron rich environment. However, we have

found that "naked" Se(II) and Te(II) dicationic species can be stabilized by strong donor ligands (e.g. N-heterocyclic carbenes). The key to forming these compounds is the synthesis of appropriate chalcogen(II) precursors (1), featuring ligands and anionic fragments easily displaced from the group 16 centre. The compounds generated include a dicationic analogue of the "carbodicarbene" (2), and novel square planar pinwheel complexes featuring four ligands (3). We have also recently discovered a route to base stabilized Ch(IV) dicationic species, which are isovalent and isoelectronic congeners of the ubiquitous NHC ligand (4). References: J. L. Dutton, H. M. Tuononen, P. J. Ragogna; *Angew. Chem. Int. Ed.*, **2009**, 4409; J. L. Dutton, G. J. Farrar, M. J. Sgro, T. L. Battista, P. J. Ragogna; *Chem. Eur. J.*, **2009**, 10263.



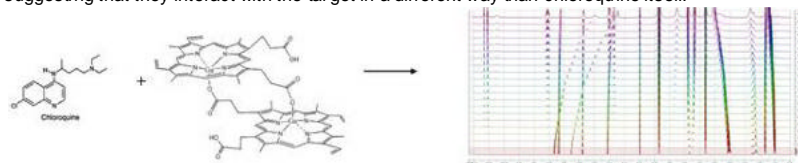
A Diversity of Metal-Ligand Interactions in Halide (X = I, Br, Cl, F) and Halide-Free Ambiphilic Ligand Rhodium Complexes **B.E. Cowie** <cowieb@mcmaster.ca> and **D.J.H. Emslie** <emslie@mcmaster.ca>, McMaster University, 1280 Main Street West, Hamilton, Ontario, L8S 4M1.

A series of ambiphilic ligand rhodium(I) halide complexes, $[\text{RhX}(\text{CO})(\text{TXPB})]$ [X = Cl (1), Br (2), I (3) and F (4); TXPB = a phosphine/thioether/borane ligand], have been prepared, as well as the halide-free cation $[\text{Rh}(\text{CO})(\text{TXPB})][\text{PF}_6]$ (5). In all complexes, the TXPB ligand binds to rhodium via the phosphine and thioether groups, and in 1 and 2, bromide and chloride adopt bridging positions between rhodium and boron. By contrast, iodide in 3 binds strongly to rhodium and interacts only weakly with the borane unit in TXPB, while fluoride in 4 binds solely to the borane, converting TXPB to an anionic fluoroborate, TXPB-F. In complexes 4 and 5, approximate square planarity at rhodium is maintained by $\eta^2\text{CC}$ -coordination of a *B*-phenyl ring in the TXPB-F ligand, or $\eta^2\text{BC}$ -coordination of the borane in TXPB, respectively.



Gallium Analogs of Hemozoin: novel approaches to exploring the structure and drug-interactions of malaria pigment **E.L. Dodd** <erin.dodd@mail.mcgill.ca> and **D. S. Bohle** <scott.bohle@mcgill.ca>, McGill University, Montreal, Quebec H3A 2T5.

In this work we explore the structural interactions between anti-malarial drug and a model heme target outside the malaria organism. This interaction is notoriously difficult to observe using iron heme due to extreme insolubility and paramagnetism. NMR titrations of the anti-malarial drug chloroquine and several other drugs from the quinoline family were performed against a structural analog of its heme target, diamagnetic gallium (III) protoporphyrin IX, in methanolic solution, giving new insight into the drug-target interaction within the malaria parasite. The data show drastic shift of proton peaks upon complexation, allowing us to map the dramatic structural rearrangements and allow determination of binding affinity. Such dramatic shifts were not observed for all members of the quinoline drug family, suggesting that they interact with the target in a different way than chloroquine itself.



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