

May 15-18, 2012

Hosted by *Cape Breton University*



37th Annual Science Atlantic/CIC Student Chemistry Conference



Program and Abstract Book



Science
Atlantic  Atlantique
connecting science education and research
le lien entre l'enseignement des science et la recherche

CAPE BRETON
UNIVERSITY

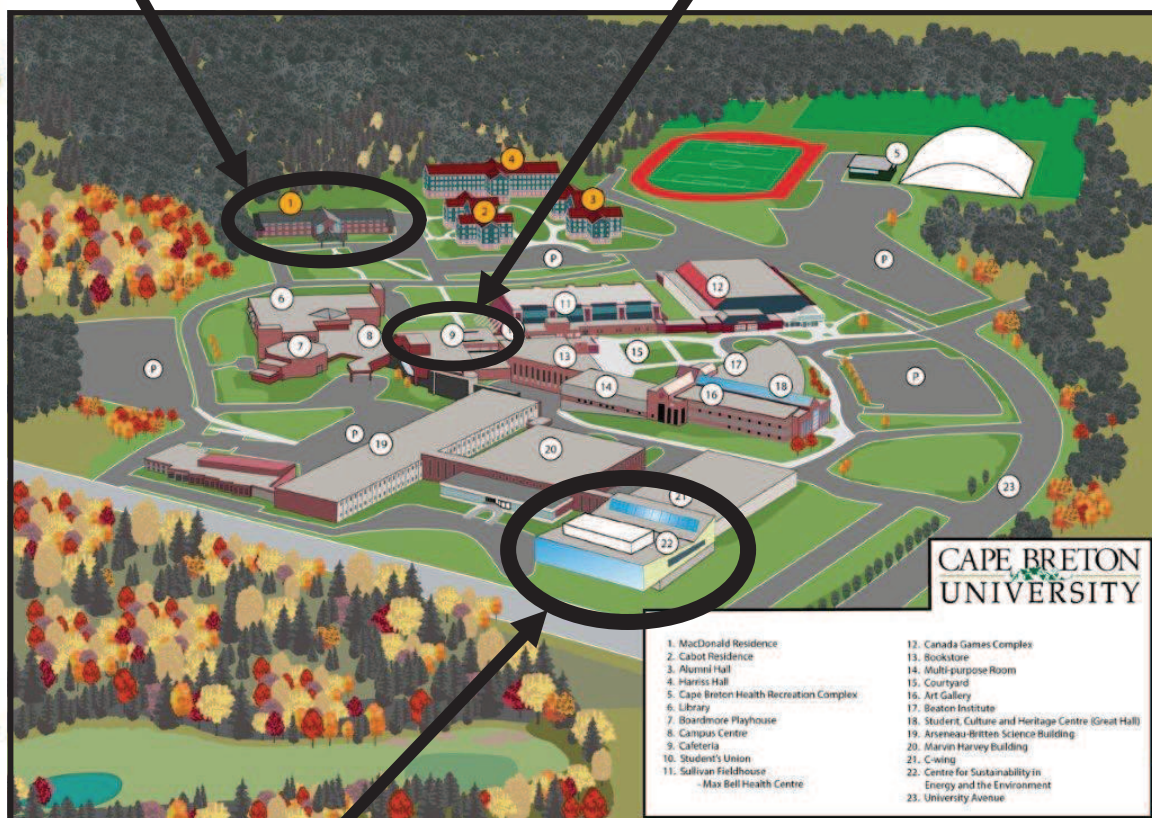
Table of Contents

Campus Map.....	3
Map of Sydney.....	4
Map to Trade & Convention Centre.....	5
Map to Sydney Legion.....	6
Restaurants.....	7
General Information.....	8
Message from the Conference Chair.....	9
Message from the Department Chair.....	10
Organizing Committee.....	11
Presenting Delegates.....	12
Keynote Speaker—Dr. Philip Jessop.....	13
Keynote Speaker—Dr. Jason Pearson.....	14
Sponsors.....	15
Awards.....	16
Schedule of Events.....	17
Presentation Schedule (May 16 th).....	18
Presentation Schedule (May 17 th).....	19
Abstracts: Oral Presentations.....	20
Abstracts: Poster Presentations.....	55

Campus Map

**MacDonald Residence
(where you'll sleep!)**

The Pit Lounge

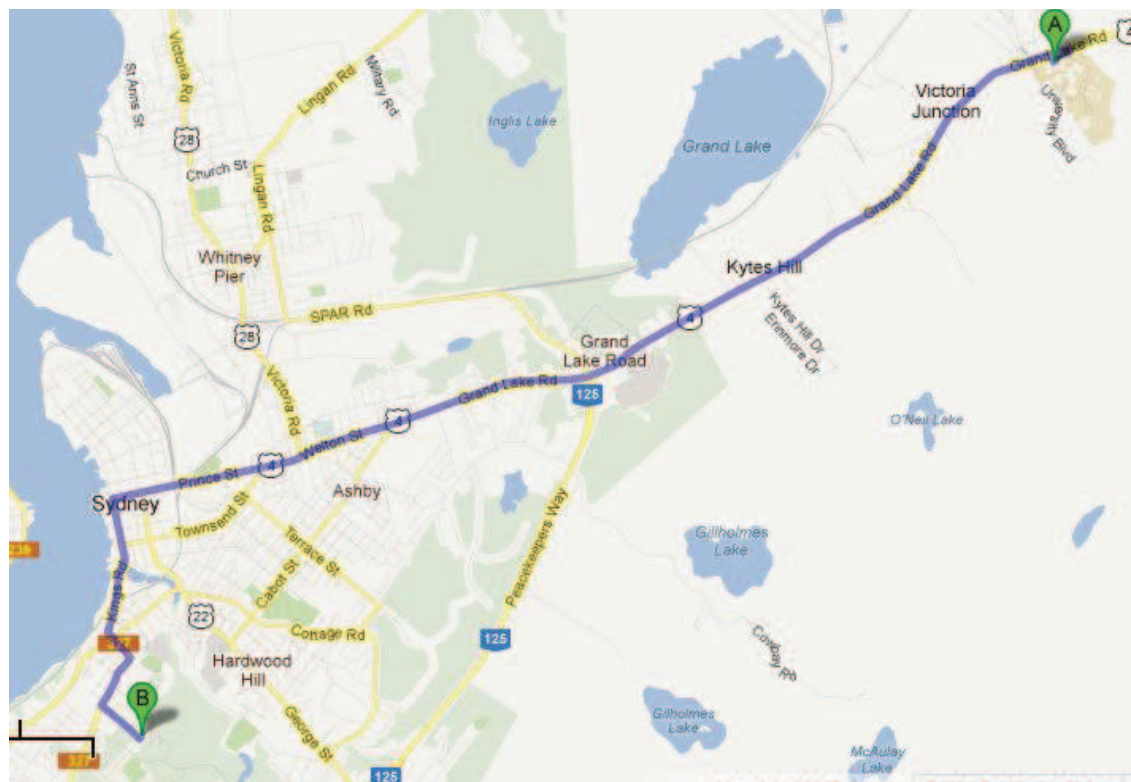


**Centre for Sustainability in Energy and the
Environment aka CSEE (where most of the
action takes place!)**

Map of Sydney



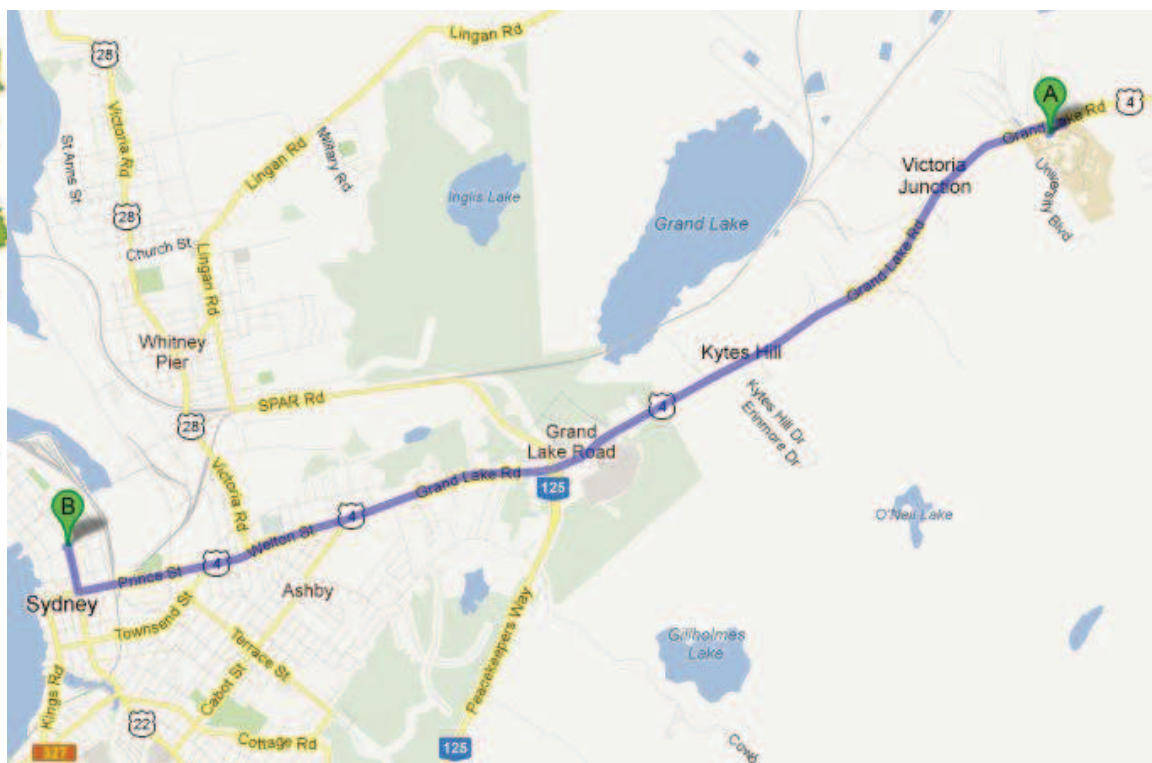
Map to Trade & Convention Centre



Directions from CBU:

- Leaving the school, turn left onto Grand Lake Road
- Continue all the way down this road until the end
- Turn left onto Esplanade (downtown Sydney)
- Turn left onto Alexandra Street and veer right at fork
- Turn left onto Towerview PI
- Turn left onto Maillard Street (should be on left)

Map to Sydney Legion



Directions from CBU:

- Leaving the school, turn left onto Grand Lake Road
- Continue down this road
- Turn right onto George Street
- Turn left onto Dorchester Street
- Legion will be on right

Restaurants

Restaurants along route to Downtown (Grand Lake Road/Welton Street/Prince Street):

- ◇ Flavor 19 (across from CBU; 562-2233)
- ◇ East Side Mario's (Mayflower Mall)
- ◇ Food court at Mayflower Mall
- ◇ Swiss Chalet
- ◇ Huang's (Chinese)
- ◇ Simeon's
- ◇ Various Tim Hortons and Robin's Donuts
- ◇ Boston Pizza
- ◇ Various Fast food (Wendy's, Burger King, McD's, Subway)
- ◇ Yassu (Greek; 453 Prince Street; 562-4000)
- ◇ Olive Tree (137 Victoria Road; 539-1553)
- ◇ Smitty's (alongside Zellars)
- ◇ Kiju's (in Membertou; 50 Maillard Street; 562-6220)

A Few Downtown Restaurants:

- ◇ Punjab Spices (Pakistan/Indian; 100 Kings road; 567-3311)
- ◇ Oka Maki (Sushi; 191 Charlotte Street; 564-9505)
- ◇ New Moon (Chinese; 78 Townsend St.; 539-4422)
- ◇ Bean Bank (Coffee)
- ◇ Wentworth Perk (Coffee)
- ◇ Allegro (222 Charlotte St.; 562-1623)
- ◇ Amedeo's (Italian; 100 Townsend St.; 270-8008)
- ◇ Flavor (16 Pitt Street; 562-8611)
- ◇ Kenny's Pizza
- ◇ Napoli Pizza
- ◇ Coldstone Creamery (Ice cream)
- ◇ Governor's Pub&Eatery (233 Esplanade St.; 562-7646)

Closest Liquor Store (NSLC):

- ◇ In *No Frills* grocery store (332 Welton Street)

General Information

PRESENTATIONS:

- ◇ All presentations will occur in the Centre for Sustainability of Energy and the Environment (CSEE). The oral presentations will be in CS104 which is the lecture theatre while the poster presentations will be in the atrium.
- ◇ For the oral presentations, all presenters have a strict 15 minute time slot. This allows for a 12 minute talk with 3 minutes for questions. Presentations must be uploaded to computer beforehand.

BARBEQUE:

- ◇ An opening day free barbeque provided by Prince Street Sobeys. Join us for food and a little bingo trivia located in the Pit Lounge on campus!

CAPE BRETON CEILIDH:

- ◇ This event is inspired by the traditional Scottish Ceilidh, which is a party involving live folk music and dancing (and refreshments). This scaled-up kitchen party will be hosted in downtown Sydney at the Royal Canadian Legion Branch No 12., with live music provided by the ECMA nominated Sprag Session (formerly the Colin Grant Band).

BIDS FOR CHEMCON 2013:

- ◇ Bids can be made for ChemCon2013 at the banquet. Computer and projector will be provided. We ask that the bids remain under 10 minutes.

**TOUR OF SYDNEY TAR PONDS AND COKE OVENS
REMEDIATION PROJECT:**

- ◇ The tour of this \$400 million project should illustrate some of the important applications of a chemistry background to careers in government and industry.

Message from the Conference Chair

On behalf of the ChemCon 2012 organizing committee, it is my pleasure to welcome you to the 37th annual Science Atlantic/CIC Chemistry Conference as well as to beautiful Cape Breton Island. The Department of Chemistry here at Cape Breton University is honoured to have the opportunity to host this conference, especially as it is the 50th Anniversary of Science Atlantic. Since CBU last hosted ChemCon in 2003, the university has seen an incredible transformation. Campus has welcomed a name change as well as many new buildings and renovations over the last nine years. I encourage you to wander the campus and check out all of the development, especially the recently opened Verschuren Centre for Sustainability in Energy & the Environment.

ChemCon is a very important conference, as it allows young researchers to share their research with delegates from all over Atlantic Canada. In this, the 50th Anniversary of Science Atlantic, we have a special opportunity to reflect on previous Science Atlantic conferences and recall many great memories and events that we have shared, some of us over the last three to four years, others over the last 10-20 years. We are thrilled to welcome two prestigious keynote speakers this year, Canada Research Chair of Green Chemistry Dr. Philip Jessop from Queen's University and CBU alumni Dr. Jason Pearson from the University of Prince Edward Island.

Only through the generosity of our sponsors could the next three days be possible. I would like to take this time to acknowledge their generosity. Also, I would like to extend my thanks to my organizing committee. They have worked very hard over the last year and their dedication is greatly appreciated!

I am very excited to share these next few days with you all and hope that you take advantage of the great events we have planned and enjoy your time on Cape Breton Island.

Sincerely,

Mary Tait
ChemCon 2012 Conference Chair



Message from the Department Chair

Welcome to ChemCon 2012

As Chair of the Department of Chemistry, it is my pleasure to extend greetings to the 37th Annual Science Atlantic/CIC Chemistry Conference. We are extremely delighted to be your host for ChemCon 2012. The conference, being held at Cape Breton University, focuses on undergraduate research in all areas of chemistry. This conference is the primary forum for our undergraduate students to come together and share their research endeavours. I have no doubts that from this meeting of young minds new responses and tangible solutions will emerge.

I would like to formally thank the organizing committee (Mary Tait in particular), keynote speakers, sponsors, and all those who tirelessly work towards the success of this conference.

Finally, I welcome you to take the opportunity to visit our research laboratories and get acquainted with our wonderful faculty members with the view for future research collaborations.

On behalf of the faculty and staff of the Department of Chemistry at Cape Breton University, I wish you an enjoyable, memorable and successful ChemCon2012.



Adango Miadonye, Ph.D
Professor & Chair, Department of Chemistry.

Organizing Committee

Chair

Mary Tait

Secretary

Jessica Prendergast

Faculty Advisor

Stephanie MacQuarrie

Volunteers

Alexander Rudiuk

Alyssa Moss

Abstract Coordinators

Margaret Gillis

Jean Gillis

Brittany MacDonald

Bruce MacDonald

Erica Campbell

Scott Cameron

Events Coordinator

Sam Lloy

Banquet Coordinator

Kelsey Aucoin

Finance Coordinator

Tiffany Wilcox

Sponsorship Coordinator

Adam Brown

Technical Coordinator

Chris MacLean

Presentations Coordinator

Preston MacQueen

Presenting Delegates

Acadia University

Alex Chase
Emily Fraser
Julie Colpitts
Kimberly Hyson
Tariq Sainuddin
Crystal Sweeney
Hannah Nickerson
Jim Ghoshdastidar
Martin Sichinga
Paul Gray
Richard Lincoln
Tin Yi-Chou

Cape Breton University

Chris Keefe
Jean Gillis
Kelsey AuCoin
Tiffany Wilcox
Preston MacQueen
Adam Brown
Mary Tait
Chris MacLean
Erica Campbell

Dalhousie University

Zack Brown
Alexander Baker
Brandon Groves
Lauren Doyle

Memorial University

Jennifer Murphy
Liam Whelan
Nicholas Randell
Lucas Stewart
Marcus Drover

Nova Scotia Agricultural College

Khushwant Bhullar

Saint Francis Xavier University

Colin Kelly
Christina LeGay
Zack O'Toole

Saint Mary's University

Andrew Long
Amber Blair
Reem Karaballi
Lauren Keyes
Arthur Hendsbee
Barb Goodall
Jane Ferguson
Scott Harroun
Kenson Ambrose
Tyler Cuthbert
Alexander McPherson
Luke Murphy
Osai Clarke
Alanna Durand

Université de Moncton

Ngocnu Maithi
Dean Ferguson
André Odjélé
Pierre Lyons
Carole Hebert

University of New Brunswick

Julien Martin

Keynote Speaker

Dr. Philip Jessop

Department of Chemistry—Queen's University



Dr. Jessop is a professor of Inorganic Chemistry as well as Canada Research Chair of Green Chemistry at Queen's University in Kingston, Ontario. The Jessop Research Group focuses on hydrogen storage, CO₂ fixation, switchable solvents and surfactants, liquid polymers, homogenous catalysis

as well as catalyst recovery methods. In addition to his work at Queen's University, Dr. Jessop is also the Technical Director of GreenCentre Canada which brings academic researchers and industry partners together with the goal of developing clean, less energy-intensive alternatives to traditional chemical products and manufacturing processes.

Outside of chemistry, Dr. Jessop enjoys wildlife photography, hiking, kayaking, and spending time with his family.

May 15th from 4:00—5:00 PM
Room CS104

Keynote Speaker

Dr. Jason Pearson

Department of Chemistry—
University of Prince Edward University



Dr. Pearson is an Assistant Professor of Chemistry at the University of Prince Edward Island in Charlottetown, PEI. His research interests are in computational chemistry and he focuses on the understanding of inter- and intra-molecular interactions as well as how such interactions affect chemical properties and reactivity. To accomplish this, the Pearson group uses and develops quantum chemical methods for electronic structure prediction and analysis. Topics that are of particular interest to the Pearson group are Intracule Functional Theory and Molecular Design.

When not at the university he enjoys spending time with his wife and son, travelling, watching movies and geocaching.

May 16th from 3:15—4:15 PM
Room CS104

Sponsors

PLATINUM

- ◇ CBU School of Science
- ◇ Sydney Tar Ponds Agency

CAPE BRETON
UNIVERSITY

Sydney
Tar Ponds
Agency

GOLD

- ◇ CBU Chemistry Society/Student's Union
- ◇ Council of Canadian University Chemistry Chairs
- ◇ Red Label kilts
- ◇ Sunovion (former Sepracor) Award
- ◇ Green Centre Canada

GreenCentre
Canada

SILVER

- ◇ Nova Scotia Lands
- ◇ Waters
- ◇ CIC
-BioMedical
- ◇ CBU Alumni Association
- ◇ NS PWR



BRONZE

- ◇ SLR
- ◇ JA Dougals McCurdy Sydney Airport Authority
- ◇ Nova Scotia Power
- ◇ J&K Scientific
- ◇ Protocase
- ◇ CIC
-Physical and Computational Chemistry
-Materials Chemistry
-Inorganic Chemistry
-Organic Chemistry
- ◇ ACEmat (former AIMMS) Award
- ◇ Science Communication Award
- ◇ NSERC Reps Award
- ◇ CBU Student's Union



- ◇ Best *Undergraduate* Oral Presentation in Physical, Theoretical, or Computational
- ◇ Best *Undergraduate* Poster in Physical, Theoretical, or Computational
- ◇ Best *Undergraduate* Oral Presentation in Biological/Medicinal
- ◇ Best *Undergraduate* Poster in Biological/Medicinal
- ◇ Best *Undergraduate* Oral Presentation in Materials Chemistry
- ◇ Best *Undergraduate* Poster in Materials Chemistry
- ◇ Best *Undergraduate* Oral Presentation in Organic Chemistry
- ◇ Best *Undergraduate* Poster in Organic Chemistry
- ◇ Best *Undergraduate* Oral Presentation in Analytical Chemistry
- ◇ Best *Undergraduate* Poster in Analytical Chemistry
- ◇ Best *Undergraduate* Oral Presentation in Inorganic Chemistry
- ◇ Best *Undergraduate* Poster in Inorganic Chemistry
- ◇ Murray Brooker Award for Best *Undergraduate* Oral or Poster Presentation in Chemical Education
- ◇ E. Gordon Young Award for Best Pedagogical *Graduate* Oral Presentation
- ◇ Best *Graduate* Oral Presentation
- ◇ Best *Graduate* Poster Presentation
- ◇ Apics Science Communication Award
- ◇ NSERC Reps Award
- ◇ ACEmat (former AIMMS) Award
- ◇ Sepracor

Schedule of Events

May 15th	12:00—3:00	Registration and Career Fair (CSEE)
	3:45—4:00	Opening Remarks
	4:00—5:00	Keynote Speaker—Dr. Philip Jessop
	5:30—bedtime	Barbeque/Ice-Breaker at The Pit Lounge
May 16th	8:00—9:00	<i>Breakfast</i>
	9:00—10:15	Oral Presentation Session 1A
	10:15—10:30	<i>Nutrition Break</i>
	10:30—11:45	Oral Presentation Session 1B
	11:45—12:30	<i>Lunch</i>
	12:00—12:25	Chalk-Talk or Industry Presentation
	12:30—1:45	Oral Presentation Session 2A
	1:45—2:00	<i>Nutrition Break</i>
	2:00—2:45	Oral Presentation Session 2B
	3:00—4:00	Keynote Speaker—Dr. Jason Pearson
	4:00—5:00	Maritimes Centre for Green Chemistry Meeting (CS101)
	4:30—6:30	Poster Presentations (CSEE Atrium)
	6:30—8:30	<i>Supper (Not included in registration fee)</i>
	8:30—11:30	Cape Breton Kitchen Party
	11:30—bedtime	Tour of Local Establishments
May 17th	8:00—9:00	<i>Breakfast</i>
	9:00—10:15	Oral Presentation Session 3A
	10:15—10:30	<i>Nutrition Break</i>
	10:30—11:30	Oral Presentation Session 3B
	11:30—12:15	<i>Lunch</i>
	12:15—1:00	Oral Presentation Session 4A
	1:15—1:30	<i>Nutrition Break</i>
	1:30—2:00	Oral Presentation Session 4B
	2:15—3:15	Judges Meeting
	3:45—5:45	APICS/CIC Meetings
	5:15	First bus leaves from CBU to Banquet
	5:30—6:30	<i>Cocktail hour at Banquet</i>
	6:30—1:00	Dinner and After Dinner Festivities
May 18th	10:00—11:30	Tour and Information session of the Tar Ponds/Coke Ovens

Presentation Schedule

May 16, 2012:

1A-1	9:00	Paul Gray, Acadia
1A-2	9:15	Alexander McPherson, SMU
1A-3	9:30	Preston MacQueen, CBU
1A-4	9:45	Luke Murphy, SMU
1A-5	10:00	Alanna Durand, SMU
	10:15	<i>Nutrition Break</i>
1B-1	10:30	Jean Gillis, CBU
1B-2	10:45	Jane Ferguson, SMU
1B-3	11:00	Lucas Stewart, MUN
1B-4	11:15	Osai Clarke, SMU
1B-5	11:30	Christina LeGay, STFX
	11:45-12:30	<i>Lunch</i>
2A-1	12:30	Chris MacLean, CBU
2A-2	12:45	Raha Omran, DAL
2A-3	1:00	Nicholas Randell, MUN
2A-4	1:15	Arthur Hendsbee, SMU
2A-5	1:30	Tyler Cuthbert, SMU
	1:45	<i>Nutrition Break</i>
2B-1	2:00	Barbara Goodall, SMU
2B-2	2:15	Mary Tait, CBU
2B-3	2:30	Lauren Keyes, SMU
2B-4	2:45	Scott Harroun, SMU
	3:00-4:00	KEYNOTE SPEAKER–Dr. Jason Pearson
	4:30-6:30	Poster Session

**All presentations will occur in CS104 which is the lecture theatre in the CSEE building. The poster session will be in the atrium in CSEE.

Presentation Schedule

May 17, 2012:

3A-1	9:00	Kenson Ambrose, SMU
3A-2	9:15	Marcus Drover, MUN
3A-3	9:30	Richard Lincoln, Acadia
3A-4	9:45	Lauren Doyle, DAL
3A-5	10:00	Adam Brown, CBU
	10:15—10:30	<i>Nutrition Break</i>
3B-1	10:30	Liam Whelan, MUN
3B-2	10:45	Tiffany Wilcox, CBU
3B-3	11:00	Hannah Nickerson, Acadia
3B-4	11:15	Kelsey Aucoin, CBU
	11:30-12:15	<i>Lunch</i>
4A-1	12:15	Tin Yi-Chou, Acadia
4A-2	12:30	Julien Martin, UNB
4A-3	12:45	Martin Sichinga, Acadia
4A-4	1:00	Crystal Sweeney, Acadia
	1:15—1:30	<i>Nutrition Break</i>
4B-1	1:30	Khushwant S. Bhullar, NSAC
4B-2	1:45	Jim Ghoshdastidar, Acadia
4B-3	2:00	Brandon Groves, DAL
	2:15-3:15	<i>Judges Meeting in CS101</i>
	3:45-5:45	Science Atlantic/CIC in CS101

**All presentations will occur in CS104 which is the lecture theatre in the CSEE building

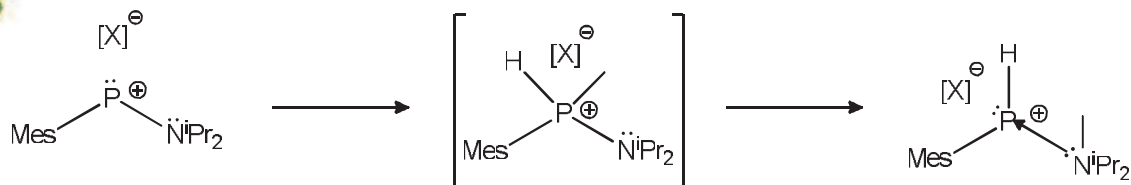
1A-1 Paul Gray, Acadia University

N,C-Bound Phosphenium Cations: Synthesis and Reactivity with Small Molecules

Paul A. Gray and Bobby D. Ellis*

Department of Chemistry, Acadia University

Several monochlorophosphines, each possessing a diisopropylamido substituent and either an alkyl (*tert*-butyl = *t*Bu) or an aryl (2,4,6-trimethylphenyl = Mes) substituent, were synthesized. Phosphenium cations were then generated from a number of these precursors through either halide abstraction with the Lewis acid Al_2Cl_6 , or through salt metathesis with AgOTf ($\text{OTf} = \text{CF}_3\text{SO}_3^-$) and characterized using ^{31}P NMR spectroscopy. H_2 gas was bubbled through a CH_2Cl_2 solution of either the phosphenium AlCl_4^- or OTf^- salts and the reaction mixture was analyzed by ^{31}P NMR spectroscopy to investigate the formation of an H_2 activation product. The AlCl_4^- derivative was also tested for NH_3 activation and the

*Notes:*

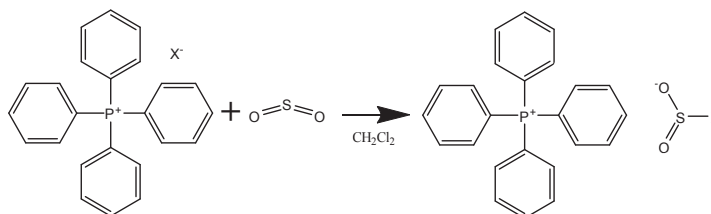
1A-2 Alexander McPherson, Saint Mary's University

Ionic liquids and the formation of halosulfites

Alex M. McPherson, Luke J. Murphy, Katherine N. Robertson and Jason A.C. Clyburne*

Department of Chemistry, Saint Mary's University

Ionic liquids (ILs), specifically phosphonium-based ILs, have proven to be effective solvents for promoting ion forming reactions. The chemistry of SO₂ with various halides has been known for many years, but is now newly relevant in IL research due to the confounding effects of acidic gases in CO₂ capture. Herein we report the reactions of dry SO₂(g) with a series of tetraphenylphosphonium halide salts [Ph₄P]X (X = Cl, Br, I) and the pseudo-halide [Ph₄P][BF₄] as well as 1,3-bis(2,4,6-trimethylphenyl)imidazolium chloride ([IMesH]Cl) in anhydrous dichloromethane to produce crystals of the resulting halosulfites. Crystals were isolated for [Ph₄P][SO₂X] (X = Cl, Br, I) and [IMesH][SO₂Cl]. The resulting crystals have been characterized using infrared spectroscopy and X-ray crystallography. The presence of sulfur oxygen bonds in these compounds is associated with new peaks observed in the region of 1200-1300cm⁻¹ in the infrared spectra of the SO₂Cl, SO₂Br and SO₂I salts. Scheme 1 illustrates the general reaction between the halide salts [Ph₄P]X and SO₂.



Scheme 1: General reaction of [Ph₄P]X with dry SO₂(g) forming crystals of [Ph₄P][SO₂X].

Notes:

1A-3 Preston MacQueen, Cape Breton University

Catalytic Activity of Newly Formed Proline-Based Periodic Mesoporous Organosilicas

Preston MacQueen, J. Prendergast, C. MacLean, S. MacQuarrie
Department of Chemistry, Cape Breton University

It is well known that proline is a versatile organic catalyst with remarkable selectivity; it is also relatively non-toxic and cheap. Surprisingly, however proline is not often used by industry and pharmaceutical processes because it suffers two major draw backs; i) proline has limited solubility in most organic solvents, therefore requiring the use of more toxic and harmful solvents and ii) very high catalyst loadings (up to 30mol %) are required to complete a reaction in a reasonable time frame (two days). In order to overcome some of these barriers and make proline a more appealing catalyst to industry and pharmaceuticals we are developing proline based periodic mesoporous organosilicas (ProPMOs). ProPMOs have uniform porosity where the proline catalyst is homogeneously distributed throughout, allowing for more access to the catalytically active microenvironments potentially leading to high enantioselection. The heterogeneous catalyst is easily reused and recycled, improving purification and labor costs. Catalytic testing of our novel monomer has begun using a simple aldol reaction between acetone to *p*-nitro-benzaldehyde and early results indicate high catalytic activity.

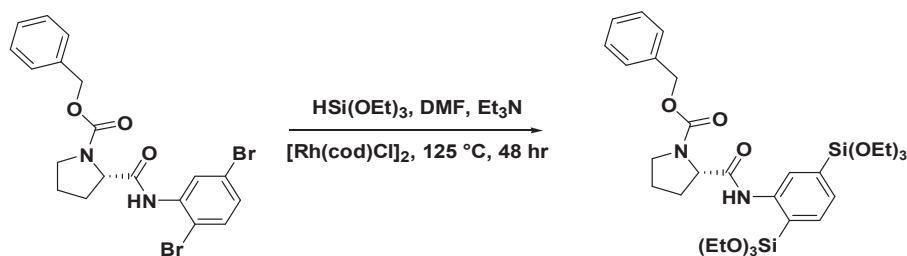


Figure 1. Synthesis of proline monomer

Notes:

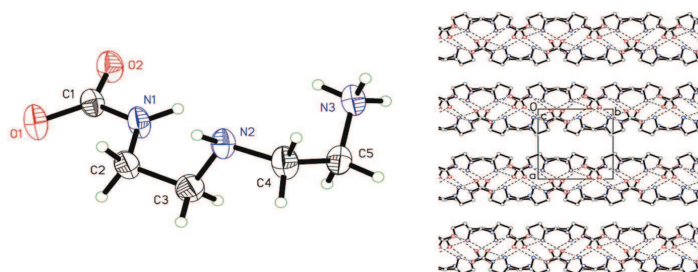
1A-4 Luke Murphy, Saint Mary's University

**Carbon Dioxide Capture with Amines in Non-Volatile Solvents
and the Effect of Sulfur Dioxide on the Absorbent**

Luke Murphy

Department of Chemistry, Saint Mary's University

Building on previous research, diethylenetriamine (DETA) was further studied in ionic liquids and polymeric solvents for its carbon dioxide capture capabilities. DETA reacts reversibly with CO₂ to form a zwitterionic adduct. The temperature at which CO₂ is released from the adduct was determined using both a titrimetric method and TGA. Both gave similar results, a release temperature in the range of 120-150°C. The adduct between DETA and CO₂ is a solid material which introduces transport, storage and regeneration complications. By preparing mixtures of DETA and other amines, stable liquid products were able to be obtained.



Crystal structure (left) and packing diagram (right) of the DETA:CO₂ adduct.

The effect of a common flue gas contaminant (SO₂) was investigated. It was found that in the presence of air, sulfur dioxide will react with DETA to form a sulfite salt in most cases, though this reactivity is slightly altered in an ionic liquid solvent. SO₂ also reacts with di-*n*-alkylamines to form bisulfate salts.

Notes:

1A-5 Alanna Durand, Saint Mary's University**Imidazolium Ionic Liquid Based Salen Derivatives for Use in Asymmetric Catalysis**

Durand, Alanna M.; Singer, Robert D.

Department of Chemistry, Saint Mary's University

Ionic liquids possess a variety of useful physical properties such as high polarity, low volatility and low flammability. They have been recognized as useful compounds, notably as alternative solvents in the field of green chemistry. Task specific ionic liquids, TSILs, result from the structural manipulation of ionic liquid cores. The addition of specific functionalities allows for the attainment of desired properties. The incorporation of imidazolium ionic cores into salen ligands has resulted in the formation of a TSIL designed to chelate metals for use in catalysis. These catalysts possess the desirable property of recyclability, as they can be entrained in a typical ionic liquid. Salen derivatives incorporating chiral diamines are well established for use in asymmetric catalysis. Recent work involving chiral salen ligand derivatives with appended ionic cores, their use in metal chelation and catalysis and future directions involving recyclability will be discussed.

Notes:

1B-1 Jean Gillis, Cape Breton University

An ab initio Study on the Competition of Hydrogen and Halogen Bonding in Hypohalous Acid (HOX, X=F, Cl, Br, I) Complexes

Jean Gillis and C. Dale Keefe

Department of Chemistry, Cape Breton University

Hypohalous acids (HOX, X = F, Cl, Br, or I) are reactive halogen species that play a role in reaction cycles involving ozone depletion. An interesting property of these acids is their potential to participate in non-covalent interactions such as hydrogen bonding and halogen bonding. The current study analyzes hydrogen bonding and halogen bonding interactions in systems with hypohalous acids (HOX, where X = F, Cl, Br, or I) that form complexes with one of the four following molecules at a given time: acetaldehyde, nitroformaldehyde, trifluoroacetaldehyde, and methyl formate. Geometry optimization and frequency calculations were performed for the HOX-acceptor systems using the MP2 level of theory and aug-cc-pVTZ basis set for all atoms except iodine, which was treated using the aug-cc-pVTZ-PP effective core potential (ECP). A topological analysis was completed using the Atoms in Molecules (AIM) and all complexes have either a hydrogen bond or halogen bond present. The molecular electrostatic potential (MEP) surfaces were also calculated. The calculations showed that the size of the σ -hole and therefore the strength of the halogen bond increases with the size of the halogen atom. The hydrogen bonded complexes were found to be more stable than the halogen bonded complexes for all systems, except those containing hypoiodous acid where the halogen bonded configuration was preferred. The substituent effects of electron withdrawing groups (NO₂, CF₃) and electron donating groups

Notes:

1B-2 Jane Ferguson, Saint Mary's University**An Improved Method for Extending the STO-NG Basis Sets
to be Applied to all Elements of the Periodic Table**

Jane Ferguson

Department of Chemistry, Saint Mary's University

Current computational chemistry research is limited to examining molecules which contain elements of the first five periods of the periodic table, as the majority of popular basis sets are only available for these elements. The STO-NG basis sets are simple yet effective as an economical method of obtaining initial geometries for calculations which will improve the convergence behaviour of subsequent computations. The development of a simple method for obtaining orbital exponents, expansion coefficients and residual errors for the STO-NG basis sets with $N = 1 - 6$ will allow for the extension of these basis sets to include the entirety of the periodic table. The existing method was simplified with the use of new functions for the evaluation of complicated least-squares integrals to improve the efficiency and reproducibility of the calculations. Gaussian expansions of Slater-type atomic orbitals were found by least-squares analysis using Microsoft Excel® with these simplified methods for all orbitals up to $7p$. All orbitals up to $5f$ were compared to the current accepted expansions. For the cases with $N > 3$ the errors obtained were usually larger than the expected values by an order of magnitude. In most cases for $N \leq 3$ the results were identical, indicating that the method works for these small expansions. Based on this conclusion, new expansions were found for the $6s$, $6p$, $6d$, $7s$, and $7p$ orbitals

Notes:

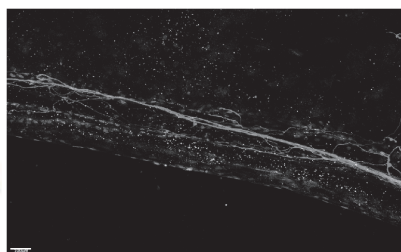
1B-3 Lucas Stewart, Memorial University

Artificial Tissue Scaffolds

Lucas Stewart, Dr. Erika F. Merschrod S.
Department of Chemistry, Memorial University

While standard organ donor implants have been common for some time, there is a significantly higher risk of implant rejection of donor organs over the use of artificial implants.¹ Hence, the ability to synthesize artificial matrices which provides favourable cellular environments is an essential step towards these artificial implants. Collagen matrices have shown promising results as a potential artificial scaffolds², however little work has been done in the area.

One potential factor affecting cellular response to collagen matrices is collagen fibril size. Fibril size can vary depending on the sample preparation method.³ Several collagen fibril samples were made via acid/base titration, varying the pH profile of each sample. The response of both adipocytes and neuronal cells to select collagen matrices were monitored, and compared to the cellular response of a collagen monomer solution. Atomic Force Microscopy (AFM) was used to analyze the topography and fibril size of the resulting collagen samples; in an attempt to correlate the cellular response to the physical properties of the collagen matrix.



1. Hassell Jr, J.R., Birk, D.E. *Exp. Eye. Res.* **2010**. 91. p. 326

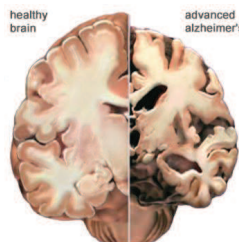
2. Gendon, R., Kumar, M.R., Paradis, H., Martin, D., Ho, N., Gardiner, D., Merschrod S., E.F., Poduska, K. *Macromol. Biosci.* **2012**, 12, p. 360

3. Li, Y., Asadi, A., Monroe, M.R., Douglas, E.P. *Mat. Sci. & Eng. C.* **2009**. 29. p. 1643

Notes:

1B-4 Osai Clarke, Saint Mary's University**Development of Novel Spectroscopic Methods for
In Situ Characterization of Amyloid Aggregate Formation**Osai Clarke, Christa Brosseau**Department of Chemistry, Saint Mary's University*

Some neurodegenerative diseases such as Alzheimer's are classified as protein aggregation disorders. While the exact cause of neuronal death in Alzheimer's disease is unknown, a leading theory referred to as the "amyloid pore hypothesis" theorises that misfolded protein aggregates, known as amyloids, form pores in cellular membranes that eventually result in loss of cellular homeostasis and neuronal death. This thesis research has explored two vibrational spectroscopic techniques, namely attenuated total internal reflection FTIR (ATR-FTIR) and electrochemical surface enhanced Raman spectroscopy (E-SERS) for the study of protein aggregation. Insulin was chosen as a model protein capable of forming amyloid aggregates. Insulin aggregates formed under conditions of elevated temperature, and were easily characterized using ATR-FTIR, albeit ex situ. Normal Raman spectroscopy of the amyloid aggregate exhibited intense fluorescence, and so E-SERS was explored as an alternate analysis tool. Weak surface interaction between insulin and the SERS substrate necessitated covalent linkage of the insulin peptide to the substrate surface via a cysteamine linker layer and EDC/NHS coupling. The amide I band of insulin, once linked to the surface was observable and can be used in future work aimed at in situ studies of protein aggregation under varying experimental conditions.



Notes:

1B-5 Christina LeGay, St. Francis Xavier University

New Tools for Organic Synthesis and Natural Product CharacterizationChristina LeGay, Laura Brothers, Nikolai Zollinger, Darren Derksen.*Department of Chemistry, Saint Francis Xavier University*

Polyketides and cycloalkanols provide the basis of numerous commonly used antibiotics and analgesics, such as erythromycin A and menthol, respectively. Current methods for synthesizing and characterizing these natural products have a number of disadvantages. One of the major challenges of synthesizing polyketides lies in their complex stereochemistry. In order to stereoselectively introduce the different polyketide subunits, efficient synthetic approaches rely heavily on auxiliary-based synthesis methods. Ideally, the method used to synthesize polyketide natural products would utilize catalysis to reduce the number of synthetic steps, decrease cost and improve the overall atom economy. Our approach to this problem is to identify a catalyst capable of asymmetric retro-aldol catalysis, thereby producing a single diastereoisomer from a racemic mixture. This method and the kinetic resolutions of cycloalkanols can be used for characterizing natural products. Kinetic resolutions using DMAP and chiral derivatives of DMAP have been found to be highly effective for the purification of secondary alcohols. They can also be tailored for characterizing natural products, by comparing the rates at which enantiomers react. This talk outlines our approach to developing these two methodologies, enhancing their substrate scopes and our preliminary results.

1. Vaishnav, P.; Demain, A. L. Unexpected applications of secondary metabolites. *Biotechnol. Adv.* **2010**, *29*, 223-229.
2. Luengo, J.; Konialian, A.; Holt, D. Studies on the chemistry of rapamycin: Novel transformations under Lewis-acid catalysis. *Tet. Lett.* **1993**, *34*, 991-994.
3. Rodriguez, M.; Zweifel, M. Trimethylamine N-oxide: A novel reagent for the promotion of the retro-aldol reaction of R106-1 (LY295337). *Tet. Lett.* **1996**, *37*, 4301-4304.
4. Fu, Gregory C. Asymmetric Catalysis with "Planar-Chiral" Derivatives of 4-(Dimethylamino)pyridine. *Acc. Chem. Res.* **2004**, *37*, 542-547.
5. Ruble, J. C.; Tweddell, J.; Fu, G. C. Kinetic Resolution of Aryl Alkyl Carbinols Catalyzed by a Planar-Chiral Derivative of DMAP: A New Benchmark for Non-Enzymatic Acylation. *J. Org. Chem.* **1998**, *63*, 2794-2795.

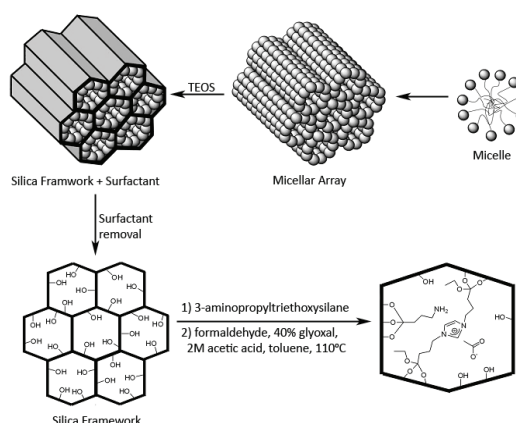
Notes:

2A-1 Chris MacLean, Cape Breton University

Building N-Heterocyclic Carbenes on the Surface of Ordered Materials

Chris MacLean and Dr. S. MacQuarrie
Department of Chemistry, Cape Breton University

In recent years, *N*-heterocyclic carbenes (NHCs) have gained much interest for their use as both ligands for organometallic complexes used in metal catalysis and as organic catalysts. NHC's are typically employed as homogeneous catalysts which, especially for organocatalysis, require a large catalyst loading resulting in difficult purifications, poor reusability and recovery of the catalyst. In today's air of environmentally favourable processes it is critical to develop greener alternatives; more efficient catalysts that are easily recyclable and recoverable. By incorporating the NHC onto highly porous ordered heterogeneous support the recovery and reusability of the catalyst are greatly increased. This catalyst will be designed to overcome some of the drawbacks of functionalizing materials through grafting or PMO formation. Incorporating click chemistry an NHC with an acetate counter ion can be constructed on the surface of a silica material. It will be anchored through multiple points to improve stability and reusability. This results in recoverable reusable NHC catalysts that can be used as ligands in organometallic complexes or as organic catalysts.



Notes:

2A-2 Raha Omran, Dalhousie University**The synthesis of an antigen against Lyme disease**

Raha Omran

Department of Chemistry, Dalhousie University

Lyme disease is a vector-borne infection caused by the tick transmitted spirochete agent, *Borrelia burgdorferi*. Currently, there is no human vaccine to prevent LD and the rapid expansion of LD has increased the need for an effective vaccine. A synthetic pathway has been formulated to one of the two identified glycolipid antigens, *BbGL1*, which is sufficiently active to make vaccines. This report describes the three first steps of the proposed synthetic pathway. NMR spectroscopy and ESI mass spectroscopy were used to characterize the compound. The first two steps of the synthetic sequence starting with D-galactose have been performed successfully. To ultimately synthesize cholesteryl 6-O-acyl- β -D-galactopyranoside (*BbGL1*), more work still has to be done.

Notes:

2A-3 Nicholas Randell, Memorial University

Structural and Magnetic Properties of [2x2] Self-Assembled Ln₄ grids

N.M Randell*, L.K Thompson, M.U. Anwar, L.N. Dawe

Department of Chemistry, Memorial University of Newfoundland

A number of [2X2] self-assembled lanthanide grids are reported (Ln = Dy, Gd). Ligand design, focusing on a series of ditopic carbo-hydrazones, has been successful in templating a series of tetranuclear square lanthanide complexes. The multidentate ligands (H₂L1, H₂L2) align in two perpendicular pairs, above and below the Ln₄ square plane, creating eight or nine-coordinate coordination environments; additional μ_4 -O²⁻, μ_2 -OH⁻, μ_2 -OCH₃⁻, and μ_2 -1,1-N₃⁻ ligands complete the coordination spheres of each metal center depending on the ligand environment. Complex **1** [Dy₄(L1)₄(μ_2 -1,1-N₃)₄(μ_4 -O)]¹ exhibits single molecule magnet behaviour with **2** independent relaxation processes at U_{eff} = 51 and 91 K in the absence of a magnetic field and U_{eff} = 270K in an optimized external magnetic field of 1600 Oe. Complex **2**, [Gd₄(L2)₄(μ_2 -OCH₃)₄], exhibits weak antiferromagnetic coupling consistent with spin-spin coupling of four isotropic Gd(III) metal centers arranged in a square grouping, with a calculated $J_{\text{Gd-Gd}}$ = -0.095 cm⁻¹.

Figure 1: Structural Representation of H₂L1 and H₂L2

1.M.U. Anwar, L.K. Thompson, L.N. Dawe, F. Habib and M. Murugesu, *Chem. Commun.*, 2012, Accepted Manuscript, DOI: 10.1039/C2CC17546K

Notes:

2A-4 Arthur Hendsbee, Saint Mary's University

Reactions of Symmetrical Dichalcogen Species With NHCs

Arthur Hendsbee, Dr. Jason Masuda

Department of Chemistry, Saint Mary's University

The bulky N-heterocyclic carbene (NHC), 1,3-bis(2,6-diisopropylphenyl)imidazolidin-2-ylidene (SIPr) is known to be more electrophilic when compared to other N-heterocyclic carbenes that are unsaturated and feature less steric crowding.[1]. In this study the reactivity of the sterically encumbered carbene species SIPr with symmetrical compounds containing chalcogen-chalcogen bonds is investigated. New reactivity is observed from this source of chalcogen and this reactivity is compared to reported reactions of NHC and chalcogens in their elemental form.[2],[3]

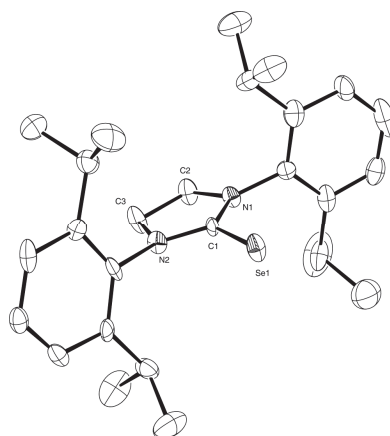


Figure 1: One of the products obtained from the reaction of SIPr with diphenyl diselenide.

[1] Sauers, R. R. *Tetrahedron Lett.* 1996, 37, 149-152

[2] Kuhn, N.; Al-Sheikh, A. *Coord. Chem. Rev.* 2005, 249, 829-857.

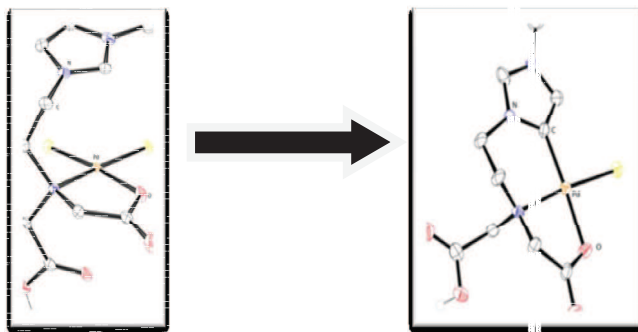
[3] Weiss, R.; Reichel, S. *Eur. J. Inorg. Chem.* 2000, 1935-1939.

Notes:

2A-5 Tyler Cuthbert, Saint Mary's University

Kinetic analysis of the formation of an abnormal N-heterocyclic carbene - palladium complex from a Task Specific Ionic LiquidCuthbert, T.; Gomez, A.T.; Singer, R.D.*Department of Chemistry, Saint Mary's University*

Synthesis of imidazolium based task specific ionic liquids for complexation with palladium metal has led to the formation of an abnormal N-heterocyclic carbene – palladium species. A second non-NHC palladium complex was isolated from the original reaction mixture and was shown to be a possible intermediate complex leading to the NHC-Pd species. Modification of the tether length between the imidazolium cation core and the chelating group of the ionic liquid leads to a different mode of chelation. Recent results outlining the kinetics of complex formation and the effect of tether length will be discussed.



Notes:

2B-1 Barbara Lynn Goodall, Saint Mary's University

An *ab Initio* Investigation of the Hydration of the d^0 Transition Metal Tetraoxo Complexes: CrO_4^{2-} , MnO_4^- , FeO_4

Barbara Lynn Goodall

Department of Chemistry, Saint Mary's University

The aqueous solution chemistry of simple oxometalates can be very complex and extremely important to understand experimentally and to describe computationally. The solvated oxometalate anion is considered to be surrounded by successive layers of the solvent water molecules creating a series of hydration shells, or spheres. This study is an examination of the first innermost hydration sphere of oxometalate species and the effect of the hydration sphere on the structure of the oxoanion. *ab Initio* calculations using HF, MP2, and B3LYP levels of theory and extended basis sets including polarization and diffuse functions, were systematically performed to calculate the optimized geometries and vibrational spectra of the anion-hydration sphere complex. The results of the calculations were compared to experimental values where possible. A correlation between hydration number and bond distance was routinely observed. Most frequently this relationship was the increase in bond distance between the anion and water molecules. In general, it was found that with increasing oxidation number of the central metal atom on the anion, the metal-to-oxygen bond distance decreased. This is attributed to an increase in the level of sigma interaction, and is supported by the predicted increase in corresponding vibrational energies of the tetrahedral point groups of CrO_4^{2-} , MnO_4^- , and FeO_4 .

Notes:

2B-2 Mary Tait, Cape Breton University

Entrapment of Phenylalanine Ammonia Lyase in Functionalized Periodic Mesoporous Materials

Mary Tait

MacQuarrie Research Group

Department of Chemistry, Cape Breton University

Infants born without the enzyme phenylalanine hydroxylase suffer from a serious genetic disorder called phenylketonuria (PKU), resulting in abnormal L-Phenylalanine metabolism. Phenylalanine hydroxylase catalyzes the conversion of L-Phenylalanine (L-Phe) to L-Tyrosine in the body. However, if there is no phenylalanine hydroxylase present L-Phe will build up in the body. In large concentrations, L-Phe is a neurotoxin and therefore, it can lead to brain damage before the age of one. **Phenylalanine ammonia lyase** (PAL) can be used to help reduce levels of L-Phe by converting it to a less toxic substance, trans-cinnamic acid. However, the development of enzymes as pharmaceuticals and biocatalysts is a significant challenge to researchers in this field. Before these catalytic processes are economically feasible enzymes must first be i) stabilized under a variety of conditions (varied pH and temperatures) and ii) easily recoverable and reusable. Enzymes can be stabilized by using metal ion stabilization, stabilization in glycerol and stabilization by immobilization. Immobilization also provides an approach to developing heterogeneous enzyme catalysts which can be easily recovered and reused. We have prepared a variety of **periodic mesoporous silicas**(PMS) and **hybrid periodic mesoporous organosilicas**(HPMO) to **entrap** PAL. PAL loaded materials with ultra large pores (23nm) show the highest enzyme activity and we have been able to recover and recycle these materials up to eight times!

Notes:

2B-3 Lauren Keyes, Saint Mary's University

Reactions of NacNac aluminum dihydride with benzophenone, benzaldehyde, phenols, and TEMPO-H

Lauren K. Keyes, Nick A. Giffin, Arthur D. Hendsbee, Amber D. Blair, Jason D. Masuda

Department of Chemistry, Saint Mary's University

The NacNac ligand system, $[(2,6\text{-iPr-C}_6\text{H}_3)\text{NC}(\text{CH}_3)_2\text{CH}]$, has been used extensively in the literature.¹ Part of its popularity is due to the favourable electronic and steric properties it possesses. In our current work, we are investigating the reactivity of the aluminum hydride species, NacNacAlH₂², with benzophenone, benzaldehyde and phenols with varying electronic and steric requirements. Parallel to this work we have isolated the reaction product of NacNacAlH₂ with anhydrous TEMPO-H³, a hydroxylamine with unique properties. The systems have been characterized by a variety of methods including NMR spectroscopy and single crystal X-ray diffraction.

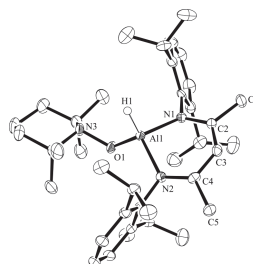


Figure 1: Reaction product of NacNacAlH₂ and TEMPO-H.

1. A SciFinder search of the NacNac ligand system revealed 580 references! (Date Accessed **2011-04-27**)
2. Cui, C.; Roesky, H. W.; Hao, H.; Schmidt, H.-G.; Noltemeyer, M. *Angew. Chem. Int. Ed.* **2000** 1815.
3. **Giffin, N.A.**; Makramalla, M.; **Hendsbee, A.D.**; Robertson, K.N.; Sherren, C.; Pye, C.C.; Masuda, J.D.*; Clyburne, J.A.C.* *Organic & Biomolecular Chemistry*, **2011**, 9, 3672-3680.

Notes:

2B-4 Scott Harroun, Saint Mary's University**Gold deposited by vapour deposition onto an array of polystyrene microspheres**

Scott Harroun

Department of Chemistry, Saint Mary's University

Spectroscopic and electrochemical characterisation of ionic liquids is key to understanding the physical properties of these important molecules. An isomeric series of 3-(alkoxycarbonyl)-1-methylpyridinium triflimide ionic liquids were analysed by electrochemical surface-enhanced Raman spectroscopy (E-SERS). It was determined that the isobutyl and *sec*-butyl isomers have the strongest interactions with the silver nanoparticle electrode at potentials below -1.6 V, whereas the interactions for the *tert*-butyl and *n*-butyl isomers were much weaker. In order to achieve uniform signals for SERS, a topologically uniform surface is required in order to generate a uniform array of SERS "hot-spots" which exhibit intense electromagnetic fields and form as a result of the localised surface plasmon resonance (LSPR). Several techniques were used to develop these surfaces, including electrochemical deposition and nanosphere lithography (NSL). It was found that galvanostatic electrodeposition of gold onto a screen printed electrode (SPE) brought about the greatest SERS for gold substrates. On the other hand, the best SERS enhancement for silver was achieved by Ag vapour deposition onto polystyrene microspheres that had been templated onto the SPE into an ordered array. These novel E-SERS substrates will be used for future research involving quantitative analysis of ionic liquids.

Notes:

3A-1 Kenson Ambrose, Saint Mary's University

Salen containing imidazolium based salts as ligands in cobalt complexes

Kenson Ambrose and Robert D. Singer
Department of Chemistry, Saint Mary's University

In the field of green chemistry, ionic liquids have been renowned for their useful physical properties such as high polarity, low flammability and low volatility. Careful introduction of functionality into ionic liquids has allowed them to be tuned to possess desired properties affording task specific ionic liquids, TSILs. TSILs developed in our research group have lead to salen ligands containing tethered imidazolium cations. These TSILs have made possible the preparation of cobalt (III) complexes capable of catalyzing oxidation reactions while being entrained in another ionic liquid as a solvent. Recent results involving successful recycling of such a salen cobalt complex in a catalytic application will be discussed.

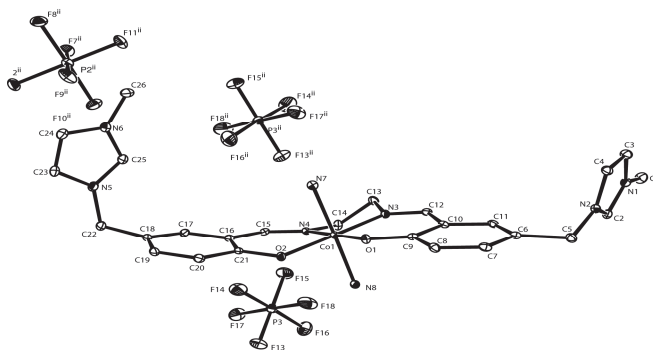


Figure 1: Molecular Structure of PF₆-IL-Salen-Co Complex

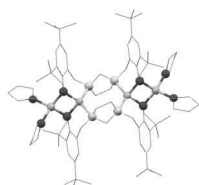
Notes:

3A-2 Marcus Drover, Memorial University

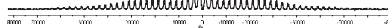
Structural, Catalytic and Spectroscopic Studies of Lithium and Bismuth Coordination Compounds

Marcus Drover, C.M. Schneider, N. Ikpo, L.N. Dawe and F.M. Kerton*
Department of Chemistry, Memorial University of Newfoundland

A series of dimeric, tetranuclear lithium diamine-bis(phenolate) complexes; $\{Li_2[O_2N_2]^{RRIm}\}_2 \cdot 4THF$ (**1**) and $\{Li_2[O_2N_2]^{RRPip}\}_2 \cdot 3THF$ (**2**) (R=tBu) were synthesized and examined using 7Li solution and solid-state NMR spectroscopy. Variable temperature 7Li NMR revealed that these tetramers are labile in solution, readily collapsing to afford two dimeric entities at high temperature. Additionally, 7Li MAS NMR provided pivotal information regarding lithium coordination environment including quadrupolar coupling (C_Q) and asymmetry (η_Q) constants. Reaction of $BiCl_3$ with complexes **1** or **2** in THF provided the desired diamine-bis(phenolate) bismuth chlorides, $[Bi[O_2N_2]^{RRIm}Cl]$ (**3**) and $[Bi[O_2N_2]^{RRPip}Cl]$ (**4**). In the presence of adventitious moisture, an oxo-bridged, tetrametallic cluster $[Bi_4(Cl)_3(\mu_2-Cl)(\mu_3-O)(O)_2\{[O_2N_2]^{RRPip}\}_2]$ (**5**) was also obtained. The definitive molecular structures of complexes **1**, **2** and **5** were provided by single-crystal X-ray diffraction. Additionally, complexes **1-5** were characterized by elemental analysis, MALDI-TOF MS and multinuclear NMR. Compounds **3-5** were probed at 14.1T using ^{209}Bi solid-state NMR incl. ultra frequency-stepped Hahn-echo and QCPMG measurements. Relaxation times, quadrupolar coupling (C_Q) and asymmetry (η_Q) constants were also extracted from ^{209}Bi SSNMR data. Finally, the reactivity of **1** was assessed in the ring-expansion polymerization of ϵ -caprolactone (ϵ -CL). Rates of polymerization were first order with respect to both monomer and initiator concentrations, and activation energies for the reactions were determined.



7Li MAS of **1** $n_r = 2.50$ kHz.



Notes:

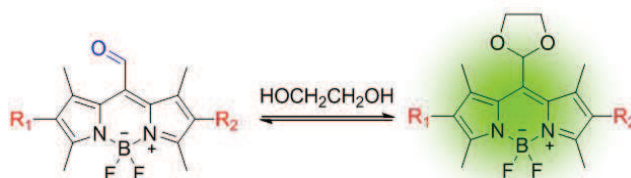
3A-3 Richard Lincoln, Acadia University

***meso*-Functionalized BODIPY Dyes:
Designing Fluorogenic Probes for Nucleophiles**

Richard Lincoln^a, Lana Greene^b, Katerina Krumova^b, and Dr. Gonzalo Cosa^{*b}

^a Department of Chemistry, Acadia University

^b Department of Chemistry, McGill University



A series of recently prepared *meso*-functionalized BODIPY dyes was studied for their possible application as fluorogenic probes for nucleophiles. The *meso*-formyl BODIPY dyes are non-emissive compared to their *meso*-acetoxy or hydroxymethyl counterparts, and thus can serve as fluorogenic off/on probes for nucleophilic attack. Preliminary kinetic studies are herein described where hemi-acetal or acetal formation is followed in real time in acetonitrile and liposomes in the presence of various alcohols and thioalcohols as substrates. It was found that electron-withdrawing groups increased the reactivity of the dyes and that the dyes were more sensitive to small nucleophiles. The photostability of the *meso*-acetoxymethyl BODIPY dyes was studied in the presence and absence of dissolved oxygen to provide insight on the mechanism of BODIPY photodecomposition. It was found that the dyes were more photostable in the absence of oxygen, and that the addition of cyano groups at the C2 and C6 positions drastically increased photostability. The *meso*-formyl dyes were further studied to explain their non-emissive behaviour and were found to be luminescent at 77 K in diethyl ether glass. In addition to the kinetic studies, the synthesis of a new series of α,β -unsaturated BODIPY aldehydes was pursued as possible sensors for Michael addition, but the reactions were unsuccessful.

Notes:

3A-4 Lauren Doyle, Dalhousie University

Synthesis and Reactivity of Late Metal Complexes Featuring Novel PSiN Mixed Donor Tridentate Ligands

Lauren Doyle, Adam Ruddy and Laura Turculet*
Department of Chemistry, Dalhousie University

The design of new ancillary ligands that have the ability to impose new bonding environments on a metal center is key to the development of transition metal complexes for applications in catalysis. Tridentate pincer ligands are a highly modular class of ancillary ligands, whose steric and electronic features are readily altered to achieve desired specifications. Such ligands have been utilized extensively to develop coordinatively and electronically unsaturated late transition metal complexes that can mediate challenging stoichiometric and catalytic transformations. In this context, unprecedented platinum group metal PSiN pincer complexes that feature a mixed neutral donor set have been reported and studies have shown that the amine donor arm is hemilabile. This hemilability is anticipated to render PSiN-ligated complexes responsive to the changing electronic and coordinative requirements at a metal center that arise during catalytic transformations, and may provide access to new and/or enhanced reactivity. In this regard, two novel PSiN ligands, ^tBu-PSiNQn and ^tBu-PSiNPy are proposed. These ligands feature quinolyl and pyridyl N-donors, respectively, and it is proposed that they will lead to the formation of metal complexes that demonstrate improved reactivity relative to the previously reported PSiN ligands that feature aniline and benzylamine N-donors. The synthesis of the [^tBu-PSiNPy]H pro-ligand will be described, as well as the formation of three group 10 transition metal complexes featuring this ligand: [^tBu-PSiNPy]NiBr, [^tBu-PSiNPy]PdCl and [^tBu-PSiNPy]PtCl (Figure 1). Progress towards the synthesis of [^tBu-PSiNQn]H will also be detailed.

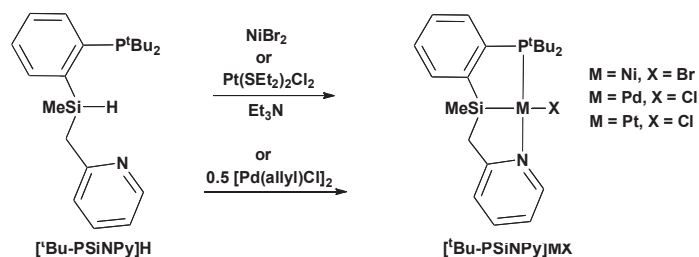


Figure 1. Synthesis of [^tBu-PSiNPy]MX (M = Ni, Pd and Pt; X = Br or Cl) complexes

Notes:

3A-5 Adam Brown, Cape Breton University**Synthesis and Characterization of Biomimetic Copper Complexes with N,S-Based Ligands**

Adam Brown and Dr. Matthias Bierenstiel
Department of Chemistry, Cape Breton University

A series of mononuclear and binuclear copper complexes were synthesized by the reaction of *N,S*-ligands with CuAc_2 , CuCl_2 and $\text{Cu}(\text{ClO}_4)_2$ in ethanol or acetonitrile solvent. The series of five *N,S*-ligands was based on the *ortho*-aminothiophenol motive with a thioether sulfur functional group in addition to either an anilinyll amine or an imine and a pyridine as nitrogenous functional groups. This ligand system was selected because the copper complex products are targeted as biomimetic models of the active sites of copper-dependent proteins. Synthesis of the blue coloured copper complexes was efficient at 50 °C and at room temperature. UV-vis spectra of copper complexes in DMF included new absorbances observed near 510 nm. Atomic absorption spectroscopy was used to determine the copper content of complexes, in which one mononuclear target complex was found to likely be binuclear, suggesting the binuclear complex is more favoured. Elemental analysis suggested a preference for binuclear complexes with CuAc_2 as the copper source and **1** as the ligand. Raman analysis of copper complexes was unsuccessful due to fluorescence of deeply coloured samples. IR spectra were collected in KBr medium and vibration assignment was complicated by overlapping bands.

Notes:

3B-1 Liam Whelan, Memorial University**Novel Sensing Substrates for Surface Enhanced Raman Spectroscopy (SERS)**

Liam Whelan

Department of Chemistry, Memorial University

Surface Enhanced Raman Spectroscopy (SERS), a surface technique discovered by Martin Fleischman in 1974, has shown some remarkable enhancements over traditional Raman spectroscopy. Signal enhancements as large as 10^{11} times greater than standard Raman have been reported, which implies the possibility of single molecule detection. This technique is particularly interesting, as it's possible to couple this with other emerging technologies such as Lab-on-A-Chip technology to detect trace amounts of analytes outside the lab setting. Previous work in the Merschrod group has been focused on developing Au/Cr based alloys on glass slide substrates to be used as a suitable surface for SERS studies. Four variations of this Au/Cr based film were tested, with varying degrees of enhancement observed. While this film does provide significant signal enhancement, it is not without issues. Namely, this alloy has shown to be fragile and prone to chipping. This has provided the group with motivation to investigate alternative metal alloys as potential SERS substrates. An analogous alloy – Ag/Cr – has been proposed on the basis of Ag's improved ductile strength compared to Au. Furthermore, it has been found that Ag has SERS enhancing capabilities of its own, which when coupled with Cr would ideally further improve the SERS enhancement observed.

Notes:

3B-2 Tiffany Wilcox, Cape Breton University**The use of infrared and Raman spectroscopy to identify impurities in acetaminophen**

Tiffany Wilcox and Dr. C. Dale Keefe

Department of Chemistry, Cape Breton University

Acetaminophen is a common and valuable non-steroidal, anti-inflammatory drug. It is classified as both an analgesic (pain reliever) and an antipyretic (fever reliever) and is used by a variety of patients including children, elderly and pregnant women. Impurities that exist in pharmaceuticals are unwanted chemicals that remain with the active pharmaceutical ingredients (APIs). The impurities can exist as starting materials, intermediates, by-products or residual solvents. Even small amounts of impurities can influence the efficiency and safety of the pharmaceutical drug. The identification of impurities as well as the amount present in the drug by regulatory authorities currently receives critical attention. The International Conference on Harmonization (ICH) has published guidelines on impurities in new drug substances, products, and residual solvents. They state that the maximum daily intake of impurities should be $\leq 2\text{g/day}$. Common organic impurities that are developed during the manufacturing process of acetaminophen are n-propionyl-p-aminophenol, 3-chloro-4-hydroxyacetanilide, 4'-hydroxyacetophenone, 4-hydroxyacetophenone oxime, 4'-chloroacetanilide, 4-acetoxyacetanilide, p-aminophenol and diacetyl p-aminophenol. High Performance Liquid Chromatography (HPLC) has been used to identify these impurities in acetaminophen. With HPLC, the sample preparation time can be long and tedious therefore run time can be extensive. Raman and Infrared (IR) spectroscopy are capable of identifying the functional groups present in the impurities and there is little to no sample preparation required for either technique. Because of this, Raman and IR techniques would be faster for impurity identification.

Raman and IR spectroscopy were used to identify p-aminophenol, 4'-hydroxyacetophenone and 4'-chloroacetanilide in acetaminophen. Samples of acetaminophen were spiked with each of the three impurities and infrared and Raman spectra were collected of the samples. Infrared spectra were collected using a Nicolet 6700 FT-IR spectrometer and Raman spectra were collected using a Nicolet NXR 9560 Raman spectrometer. Spectra from both the IR and Raman showed evidence of peaks that could represent the impurities, however after spectral analysis it was determined that IR cannot be used to identify impurities in acetaminophen due to complex spectra. However, Raman is capable of identifying only one out of the three impurities which were analyzed. A marker peak was determined for 4'-hydroxyacetophenone at 1075 cm^{-1} . Raman could not detect marker peaks for 4'-chloroacetanilide and p-aminophenol.

3B-3 Hannah Nickerson, Acadia University**Effect of Thin-Cavity Thickness on PM IRRAS Background of the Gold-Solution Interface**

Hannah A. Nickerson and Vlad Zamlynny*
Department of Chemistry, Acadia University

Polarization Modulation Infrared Reflection Absorption Spectroscopy (PM IRRAS) is a surface analytical technique that allows for the investigation of ultra-thin films of molecules adsorbed at a metal surface. The application of this technique to water-soluble surfactants, such as corrosion inhibitors, has proved particularly challenging due to the presence of molecules in the bulk analyte.

The application of PM IRRAS as a method for the investigation of corrosion inhibitors, benzotriazole (BTAH) and benzimidazole (BIA), at charged metal surfaces has been evaluated. PM IRRAS spectra have been simulated using the optical constants of these molecules in deuterated water (D_2O). The simulations predict that PM IRRAS investigations of BTAH and BIA at the electrolyte/gold surface shall be successful, in the region of the prominent 1450 cm^{-1} absorption band.

In the process of PM IRRAS simulations, it was discovered that the thin-cavity thickness (gap) of the PM IRRAS flow cell alters the appearance of the spectra background, which may result in difficulty when the baseline is subtracted during data processing, thus affecting the resulting spectra. A thin-cavity thickness of $3.0\text{ }\mu\text{m}$ was determined to provide the smoothest

Notes:

3B-4 Kelsey Aucoin, Cape Breton University**The Development of Analytical Methodology for the Analyses of Indian Sugar Mill Products, Byproducts, and Environmental Wastes**

Kelsey AuCoin

Department of Chemistry, Cape Breton University

There are 1.2 billion people living in India. It is difficult for the country to sustain a sufficient safe water supply. The scarcity of safe drinking water is a fundamental issue in India. Along with water contamination from human waste, a potential source of contamination is from the pesticides being sprayed on agricultural products. In fact, pesticides have been found in human breast milk. India is a large producer for many agricultural products such as rice, sugarcane and coconut. There are incentives from the government (such as subsidies for pesticides and fertilizers) to produce greater yields. This added bonus for high production can cause farmers to overspray, which leads to leaching of chemicals into soil and groundwater. The “if some is good, more is better” approach can be an unhealthy one. There has to be a limit put in place so that it is known when the pesticides are being sprayed in too great of an excess. If an analysis is used in the field to measure the level of pesticides in the soil, hopefully the amount sprayed will be reduced and water contamination will be decreased. If not for health, the incentive to save money may result in reduced pesticide use.

A fast analytical method for the separation of pesticides from Indian soil, water and sugarcane byproducts has been developed using GC-MS and GC-ECD with nano stationary phase column technology. In less than 4.5 minutes, rather than the current 45 minute analysis, an extract from soil can be separated using GC to detect some pesticides remaining from previous harvests down to the part-per-trillion level.

Notes:

4A-1 Ting-Yi Chou, Acadia University

Synthesis of Isoindolo[2,1-a]quinoline Derivatives via Inverse Demand Diels-Alder ReactionTing-Yi Chou,^a T. Stanley Cameron,^b Amitabh Jha^{*a}^a Department of Chemistry, Acadia University^b Department of Chemistry, Dalhousie University

Imino Diels-Alder reaction between electron-rich *N*-vinylpyrrolidone or *N*-vinylcaprolactam with *N*-aryl-3-hydroxy-isoindolinones in presence of boron trifluoride-etherate at room temperature resulted in formation of corresponding 5-(2-oxopyrrolidin-1-yl)-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-ones in moderate to good yields. *N*-aryl-3-hydroxy-isoindolinones were prepared by reducing corresponding phthalimide by sodium borohydride. The results obtained thus far will be discussed.

Notes:

4A-2 Julien Martin, University of New Brunswick**Conductive Paper as a Replacement Current Collector in Lithium Ion Batteries**

Julien Martin

Department of Chemistry, University of New Brunswick

Lithium-ion cells offer advantages in scalability, specific energy and energy density, and high voltage of operation. These attributes have made them highly suitable for secondary power applications ranging from miniature electronics to electric vehicles. Despite the rigorous work dedicated to improving lithium-ion cell systems, with many advances having been made in electrolyte and active material research, very little attention has been given to the inactive components used in the construction of a typical battery. Of particular interest are the current collectors, which act as direct contacts between the active materials in a cell and the external circuit. In this work, we use cellulose-based 3-dimensional conductive polymer composites as cheap substitutes for the typical 2-dimensional aluminum current collectors used in commercial batteries. Our aim is to improve the cost-effectiveness and specific capacities of the cells by using a lighter weight current collector with better contact with the active material.

Notes:

4A-3 Martin Sickinga, Acadia University**Characterization and Membrane Bioreactor Treatment of Oily Water Pollution**

M. C. Sickinga, A. J. Ghoshdastidar, J. Wang and A. Z. Tong*
Department of Chemistry, Acadia University

Water pollution is the discharge of contaminants into water at concentrations that can have adverse effects on human health, aquatic organisms and the environment. Oil pollution is one of the most common point and non-point source of water pollution, which mainly is present as an oil-water emulsion. Petroleum oil is a complex mixture of aliphatic and aromatic hydrocarbons, for example, n-alkanes, biomarkers and polycyclic aromatic hydrocarbons (PAHs). Chemical analysis of alkanes and biomarkers generates information of great importance to environmental forensic investigations. PAHs are among the most common petrogenic hydrocarbon pollutants. Many of these compounds have been confirmed or suspected to be carcinogenic, mutagenic and teratogenic in nature. High levels of exposure can be detrimental to human and animal health, which necessitates an environmentally friendly treatment method for these pollutants.

This research is divided into two phases. In Phase 1, oil-contaminated water, collected from the coastal Nova Scotia, will be characterized. Biomarkers, n-alkanes and PAHs will be extracted by solid phase extraction and analyzed by GC/MS. Fish and sediment samples will also be analyzed for these targets. In Phase 2, petrogenic hydrocarbons in water will be treated using membrane bioreactor technology to produce simpler, less toxic molecules. Hydrocarbons will be introduced to simulated wastewater and monitored using GC/MS analysis. Effluent water quality will be determined by spectrophotometric testing including chemical oxygen demand. Dissolved oxygen and pH will be optimized for the bacterial consortium. Our aim is to develop a method to decontaminate oil-laden water for safe discharge.

Notes:

4A-4 Crystal Sweeney, Acadia University**Sweating the small stuff: study of pesticides and primary metabolites excreted in human sweat**

Crystal L. Sweeney and Anthony Z. Tong*
Department of Chemistry, Acadia University

Prince Edward Island produces over 30% of Canada's total potato production annually. Correspondingly, pesticide use in PEI is substantial, with as many as 20 different pesticides applied to potato crops each season. Pesticides can leach into neighbouring wells and contaminate drinking water. Several of these pesticides are classified as "probable human carcinogens" by the U.S. Environmental Protection Agency. Cancer incidence was 10% higher in PEI males and 8% higher in PEI females than in Canada over the decade preceding 2006. We hypothesize that considerable concentrations of pesticides are excreted in sweat of exposed individuals. This excretion mechanism may be a vital means of eliminating carcinogenic pesticides that may otherwise accumulate in the body and lead to the development of cancers. Our objective is to collect sweat, during infrared sauna sessions, from a sample population in PEI and analyze samples by chromatography and mass spectrometry techniques for the following pesticides and their key metabolites: chlorothalonil, mancozeb, metiram, diquat, phorate, chlorpyrifos, glyphosate, methamidophos, dimethoate, linuron, S-metolachlor and thiophanate-methyl. These pesticides were selected based on top sales in PEI, known or suspected carcinogenic potential, acute toxicity and relative persistence in the environment. As we may find that perspiration of exposed individuals contains significant concentrations of pesticides, regular infrared sauna sessions may provide a therapeutic approach to remove harmful pesticides from the body. This purging of potentially carcinogenic chemicals offers a promising approach to cancer prevention.

Notes:

4B-1 Khushwant Bhullar, NS Agricultural College**Antioxidant, Antihypertensive, Anticancer and Anti-HIV Properties of Curcumin and its Analogues**

Khushwant Bhullar,^{*1} Amitabh Jha,² Dani Youssef^{2,3} and H.P. Vasantha Rupasinghe¹

¹Department of Environmental Sciences, Nova Scotia Agricultural College

²Department of Chemistry, Acadia University, ³Département des Science, Université Sainte Anne

Curcumin, derived from *Curcuma longa*, is a naturally occurring phenolic compound with numerous pharmacological properties. An assessment of antioxidant and selected *in vitro* biological activities of curcumin and its 15 structural analogues were conducted. Structural modification of curcumin significantly influenced the antioxidant (DPPH, ORAC, and FRAP), antihypertensive (angiotensin converting enzyme inhibition), anticancer (tyrosinase and HepG2 proliferation inhibition), and anti-HIV (human HIV-I protease inhibition) activities. Strong relation between the structure and evaluated activity revealed that compounds with specific functional groups and carbon skeleton had specific biological profile. Among the compounds assayed, (*E*)-2-(3,4-dimethoxybenzylidene)-5-((*E*)-3-(3,4-dimethoxyphenyl)acryloyl)cyclopentanone, (*E*)-2-(4-hydroxy-3-methoxybenzylidene)-5-((*E*)-3-(4-hydroxy-3-methoxyphenyl)acryloyl)-cyclopentanone and curcumin exhibited the strongest free radical scavenging and antioxidant capacity. Biological activities analyzed using specific concentrations of compounds showed that (*E*)-2-(4-hydroxy-3-methoxybenzylidene)-5-((*E*)-3-(4-hydroxy-3-methoxyphenyl)-acryloyl)-cyclopentanone was the most potent ACE inhibitor while (*E*)-2-(4-hydroxybenzylidene)-6-((*E*)-3-(4-hydroxyphenyl)acryloyl)cyclohexanone, (*E*)-2-(3,4-dimethoxybenzylidene)-6-((*E*)-3-(3,4-dimethoxyphenyl)acryloyl)cyclohexanone and (*E*)-2-(3,4-dimethoxybenzylidene)-5-((*E*)-3-(3,4-dimethoxyphenyl)acryloyl)cyclopentanone promised complete tyrosinase inhibition. *In vitro* study using human hepato-carcinoma cell line (HepG2), showed that (*E*)-2-(4-hydroxybenzylidene)-6-((*E*)-3-(4-hydroxyphenyl)acryloyl)cyclohexanone was the strongest inhibitor of cancer cell proliferation. Furthermore, (*E*)-2-(3,4-dimethoxybenzylidene)-6-((*E*)-3-(3,4-dimethoxyphenyl)acryloyl)cyclohexanone was also found to be strongest human HIV-1 protease inhibitor *in vitro* among the tested compounds.

Keywords: Curcumin, antioxidant, ORAC, DPPH, FRAP, tyrosinase, angiotensin converting enzyme, HIV

Notes:

4B-2 Jim Ghoshdastidar, Acadia University**Occurrence of Pharmaceuticals in the Cornwallis and Annapolis River Watersheds**

A.J. Ghoshdastidar, B. Crouse, and A.Z.Tong*
Department of Chemistry, Acadia University

Pharmaceuticals released into the environment through human excretion, improper disposal and agricultural runoff. Wastewater acts a common sink for these contaminants. As wastewater treatment plants (WWTPs) are not specifically designed to breakdown these drugs into inactive compounds, many pharmaceuticals are incompletely degraded before discharge into receiving waters. Chronic exposure to and potential bioaccumulation of pharmaceuticals can result in significant ecological and health effects. The synergistic effects from trace level contamination of multiple pharmaceuticals in ground and surface drinking water sources is an emerging concern for human health.

Samples were collected from eight WWTP effluents in the Cornwallis and Annapolis River watersheds, downstream from discharge sites, and the Mill Cove WWTP in Halifax. Target pharmaceuticals were extracted using Solid Phase Extraction (SPE) and four acidic pharmaceuticals and two neutral pharmaceuticals were analyzed using GC-MS. Method detection limits ranged from 7 ng/L for ibuprofen to 105 ng/L for cotinine. A further three acidic and six basic pharmaceuticals will be analyzed using LS-MS/MS.

Results from GC-MS analysis confirm pharmaceutical concentrations were highest in effluent from the MillCove WWTP ranging from 570 ng/L for cotinine to 17 mg/L for caffeine. Pharmaceutical occurrence in effluents and receiving waters in the Cornwallis River watershed were higher than the Annapolis River watershed. Salicylic acid was detected in each of the WWTP effluents sampled and sites downstream.

Notes:

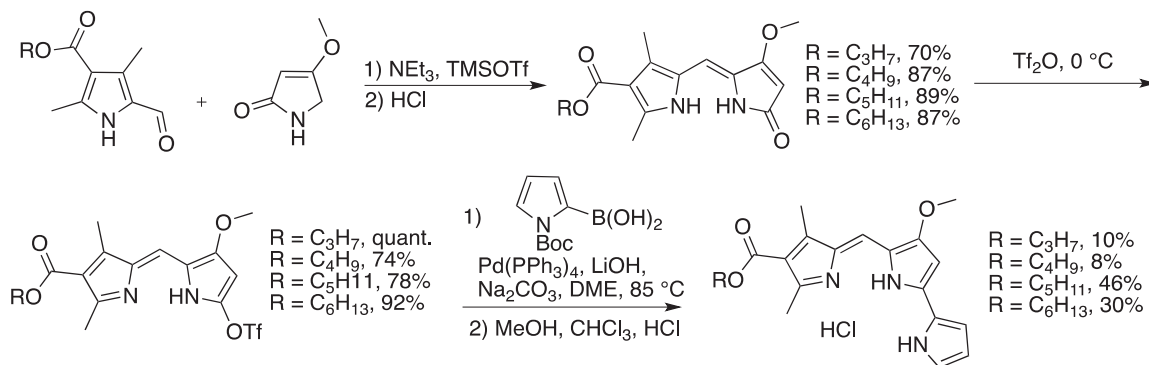
4B-3 Brandon Groves, Dalhousie University

Synthesis of Short-Chain Ester Prodigiosenes via a Concise Synthetic Pathway

Brandon R. Groves

Department of Chemistry, Dalhousie University

Prodigiosenes are a family of highly coloured tripyrrolic compounds isolated from the *Serratia* and *Streptomyces* genus of bacteria.¹ In addition to possessing an array of immunosuppressive activities, they also exhibit the capacity for the induction of apoptosis in malignant cells. Routes through which cell death is thought to occur include copper assisted cleavage of DNA,² protein phosphate cellular process inhibition,³ and cross-membrane H⁺/Cl⁻ ion transport.⁴ To explore the relationship between these desired activities, and the structure of the parent natural product prodigiosin, a method for the concise synthesis of prodigiosene derivatives has been developed (Figure 1).



Beginning from the corresponding 4-formyl pyrrole, prepared in-house, Makayama-type aldol condensation with 4-methoxy-3-pyrrolin-2-one produces the dipyrrole in high yields. Triflation of these compounds, and subsequent Suzuki coupling with *N*-BOC-2-pyrrole boronic acid produces the desired short-chain ester prodigiosenes in a concise and reliable manner.

- (1) Wrede, F.; Hettche, O. *Ber. Dtsch. Chem. Ges.* **1929**, 62, 2678.
- (2) Melvin, M. S.; Tomlinson, J. T.; Saluta, G. R.; Kucera, G. L.; Lindquist, N.; Manderville, R. A. *J. Am. Chem. Soc.* **2000**, 122, 6333.
- (3) Witney, F. R.; Failla, M. L.; Weinberg, E. D. *Appl. Environ. Microbiol.* **1977**, 33, 1042.
- (4) Seganish, J. L.; Davis, J. T. *Chem. Commun.* **2005**, 5781.

Notes:

Abstracts: Poster

P1 Alex Chase, Acadia University

Photogeneration of cycloalkyl and amino quinone methides

Alex Chase and Matthew Lukeman*

Department of Chemistry, Acadia University

Quinone methides are reactive intermediates of significant interest for a myriad of reasons. Firstly, they contain a benzylic carbon that is capable of reacting with both amino and nucleic acids. This has the potential to induce cell death, indicating possible therapeutic applications. Secondly, they are the primary intermediates upon irradiation of a wide range of recently developed photocages. Thirdly, particular quinone methides may be of importance in the light-controlled production of certain industrial chemicals. A more detailed understanding of the reactivity of these quinone methides will be invaluable as it determines their biological suitability. Despite the importance of the reactivity of these compounds, relatively little is known about the impact of varying the substitution patterns. The principle goal of this honours project is to evaluate the effect of disubstituting the benzylic position of quinone methides with cycloalkyl rings. We will also investigate a number of other structural variations including introducing acetals and amino substituents at the benzylic position. This will be achieved by irradiating the parent cycloalkylhydroxybenzyl alcohols, along with a host of other compounds, following their preparation from appropriate starting materials. The reaction products will be characterized through common analytical methods (IR, NMR, GC-MS), which will allow the reaction efficiencies to be measured. Additionally, the rates of reaction with biologically relevant molecules will be measured through nanosecond laser flash photolysis. The determination of these rate constants will aid the future rational design of quinone methide based phototherapeutic agents as well as providing insight into quinone methide based synthetic routes.

Notes:

P2 Emily Fraser, Acadia University

Free-Radical Scavenging Properties of Synthesized Fatty Acid Esters of Phloridzin and Isoquercitrin

Emily Fraser, Ziaullah, H.P. Vasantha Rupasinghe*

Department of Environmental Sciences, Nova Scotia Agricultural College

Flavonoids are known to have antioxidant properties *in vitro*, and have been linked to the prevention of various cancers and cardiovascular disease. Previous research suggests that increased lipophilicity of flavonoids can enhance the ability to incorporate them into more hydrophobic systems, as well as enhancing their bioavailability. To achieve this, hydrophobic groups, such as fatty acids, can be added to the flavonoid molecule through enzyme-catalyzed acylation. In the current study, twelve esters were synthesized by enzymatic acylation using the flavonoids phloridzin and isoquercitrin, long chain fatty acids as the acyl donor, and lipase from *Candida antarctica*, Novozym 435®, as the catalytic enzyme. The reaction scheme, using isoquercitrin as an example, is illustrated in Figure 1. The antioxidant properties of the synthesized esters were characterized by their free radical scavenging activity, by performing an assay using the free radical, 2,2-diphenyl-1-picrylhydrazyl (DPPH). The anti-radical activities of the esters were expressed by their IC₅₀ value, the concentration required to scavenge 50% of the DPPH free radical. All of the synthesized isoquercitrin esters had lower antioxidant capacity than the parent isoquercitrin, which was consistent with literature, and the phloridzin esters were very comparable antioxidants to the parent phloridzin. No correlation between either acyl donor chain length and IC₅₀ value or degree of unsaturation and IC₅₀ value were observed. Further study is re-

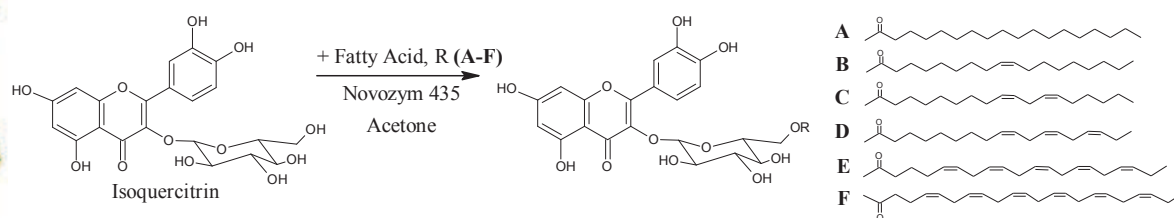


Figure 1. Reaction scheme of enzymatic acylation of isoquercitrin.

Notes:

Abstracts: Poster

P3 Julie Colpitts, Acadia University

Investigation of Activatable DNA Damaging Agents

Julie Colpitts and Sherri A. McFarland*

Department of Chemistry, Acadia University

The research to be presented will focus on DNA damage caused by several synthetic prodigiosenes and coordination complexes of Ru(II). Various forms of damage were mediated by the presence of light (of varying wavelengths and doses) or Cu(II). The goal of this research is to identify compounds that can be activated by some external trigger (such as light or copper) and only cause damage to DNA when “turned on”. Herein DNA damage is assessed by the proportions of Forms I, II and III plasmid DNA resulting when increasing concentrations of the compound is incubated with DNA with or without the trigger. The DNA damage was directly visualized and quantified on agarose gels stained with ethidium bromide and photographed under UV light. Findings may have important and exciting implications in human applications as activatable DNA damage leading to cell death shows promise for directed cancer therapies that may be less toxic than traditional chemotherapy.

Notes:

P4 Kimberly Hyson, Acadia University

***N,N*-Bound Phosphenium Cations: Synthesis and Reactivity with Carbon Dioxide and Oxidizing Reagents**

Kimberly D. Hyson and Bobby D. Ellis*
Department of Chemistry, Acadia University

Reducing atmospheric carbon dioxide levels is a major focus within the research community. Our research group has developed specific types of main group compounds, which include salts containing *N,N*-bound cyclic phosphenium cations, as possible sequestering agents for carbon dioxide. In addition, we have explored the reactivity of *N,N*-bound cyclic phosphonium cations with chalcogen-based oxidation reagents. The *N,N*-bound cyclic phosphenium cations showed signs of interaction with carbon dioxide, suggesting their potential applications for sequestering carbon dioxide. The *N,N*-bound cyclic phosphenium cations also showed reactivity toward trimethylamine *N*-oxide, a common oxygen atom transfer reagent. These phosphenium cations were developed by reactions between bulky diazabutadienes and their hydrogenated analogues with phosphorus tribromide to produce the desired phosphine halide precursor. Finally, the phosphenium cations were produced through halide abstraction with aluminum chloride. An *N,N*-bound acyclic phosphenium cation also showed coordination to a low valent tin complex. These acyclic phosphenium cations were developed in a similar manner to the *N,N*-bound cyclic phosphenium cations. The ligands synthesized were analyzed with ^1H NMR spectroscopy, while the phosphine halides and salts containing *N,N*-bound phosphenium cations were primarily characterized with ^{31}P $\{^1\text{H}\}$ NMR spectroscopy.

Notes:

P5 Tariq Sainuddin, Acadia University**Synthesis & Characterization of Polypyridyl Ruthenium complexes for Photodynamic Therapy**

Tariq Sainuddin and Sherri A. McFarland*
Department of Chemistry, Acadia University

Transition metal complexes have a significant role in medicinal chemistry especially in its application in cancer therapy. One such drug is Cisplatin which is used as an anticancer drug for ovarian and testicular cancer. Although platinum-based compounds are used for treating 50-70% of cancer patients, the main problem is its non-specificity and resulting toxicity due to its distribution throughout the body, and this can affect normal body cells. Research on other metal complexes has been carried out especially on metals like ruthenium, osmium and rhodium, and photoactivation of such complexes may provide a promising approach to cancer therapy called photodynamic therapy. However, many drawbacks exist regarding their solubility, a requirement for molecular oxygen to function, and the relatively short wavelengths of light required for their activation. Herein different derivatives of ruthenium complexes are synthesised and tested for their effectiveness as photobiological agents. The main area of focus will be on synthesis of ruthenium complex ligands which can impart both DNA binding and photocleavage properties. Complexes with a select group of ligands, based on the imidazo[4,5-f][1,10]phenanthroline scaffold with varying R-groups, will be presented. Synthesis and characterisation of derivatives of ruthenium compounds has been performed, and their DNA binding and photocleaving properties have been studied. In vitro DNA interactions have been compared to ex vivo photocytotoxicity and indicate that good in

Notes:

P6 Alexander Baker, Dalhousie University**Efficient synthesis of 4,4-difluoro-4-bora-3a,4a-diaza-s-indacenes (F-BODIPY's)**

Alexander Baker

Department of Chemistry, Dalhousie University

4,4-Difluoro-4-bora-3a,4a-diaza-s-indacenes (*F*-BODIPY's) are a popular research subject due to their bright fluorescent properties for use as biological markers, their protecting group ability and chemical robustness. The current method of synthesizing *F*-BODIPY's requires use of 9 equivalents of boron trifluoride diethyletherate ($\text{BF}_3 \cdot \text{OEt}_2$) and 6 equivalents of triethylamine (TEA) which is inefficient, costly and wasteful. Our work involves the development of a more efficient synthesis involving the use of only 1 equivalent of $\text{BF}_3 \cdot \text{OEt}_2$, using lab bench conditions giving *F*-BODIPY's in high yield for both small and large scale reactions.

Notes:

Abstracts: Poster

P7 Amber Blair, Saint Mary's University

Lewis Base Complexes of Magnesocene with Bulky β -Diketiminates

Amber D. Blair Art D. Hendsbee, Nick A. Giffin, Tom D. Rogers, Jason D. Masuda*

The Maritimes Centre for Green Chemistry and Saint Mary's University

One aspect of the research in the Masuda group is the investigation of new main group metal cyclopentadienyl complexes with a sterically encumbered beta-diketiminate ligand. We find the reaction of magnesocene with dipp-nacnac ($\text{CH}(\text{CMe})(2,6\text{-iPr}_2\text{C}_6\text{H}_3\text{N})_2$) proceeds smoothly in THF to give $\text{C}_{29}\text{H}_{44}\text{MgCp}(\text{THF})$. In efforts to change the Lewis base donor on the magnesium atom we have approached this through a number of methods including preparing coordination compounds of magnesocene with pyridine and 4-dimethylaminopyridine. Preliminary results of extending this chemistry to other Group 2 and Group 12 elements will also be discussed.

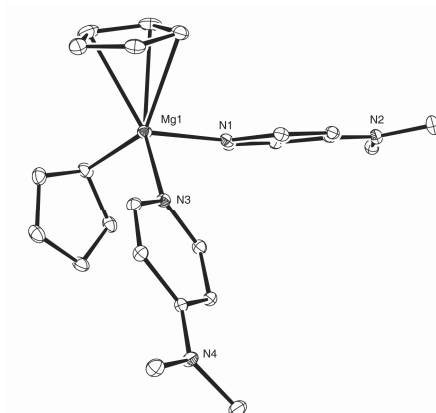


Figure 1. Reaction product of magnesocene and 4-dimethylaminopyridine

Notes:

P8 André Odjélé, Université de Moncton**The troublesome Tribbles; key kinase suspects in glioblastoma multiforme cases**

André Odjélé, Dean Ferguson and Pier Jr Morin.

Department of Chemistry and Biochemistry, Université de Moncton

Tribbles proteins are key regulators of multiple signaling pathways and their dysregulation has been linked to loss of cellular homeostasis and carcinogenesis. Following the results generated by microarray which focused on identifying differentially regulated kinase mRNAs in primary brain tumour samples, we reported an up-regulation of tribbles-1 (trb-1) and tribbles-2 (trb-2) transcripts in the most aggressive type of glioma: glioblastoma multiforme (GBM). GBMs are correlated with a 12-14 months patient survival and improving the current therapeutic approaches is essential. We next assessed trb-1 and trb-2 transcript levels in a panel of GBM cell lines by RT-PCR. Western blotting was also performed and revealed that selected cell lines did in fact strongly expressed Trb-1 protein. We next wish to differentially regulate Trb-1 expression in selected cellular models and measure the impact of varying tribbles levels on cancerous phenotypes. The goal of our research is to identify proteins that are most likely involved in driving gliomagenesis and GBM development. We thus hope that our findings will lead to the development of a pharmaceutical approach able to target these leads and to the elaboration of an improved therapeutic regimen for GBMs.

Notes:

P9 Andrew Long, Saint Mary's University

Investigation into the Thermally Mediated Rearrangement of Azulene into Naphthalene using Muon Spectroscopy

Andrew Long, Brett M. McCollum, Cory Pye, Jean-Claude Brodovitch, Paul W. Percival, and Jason A.C. Clyburne

Department of Chemistry and TRIUMF, Simon Fraser University, The Maritimes Centre for Green Chemistry, Department of Chemistry, Saint Mary's University

The thermally mediated rearrangement of the polar aromatic naphthalene to the nonpolar benzenoid naphthalene has interested both experimentalists and theoreticians for decades. [1] several groups have attempted to elucidate the mechanism of this rearrangement but questions still remain as to the exact pathway. [2,3] Currently accepted theory has postulated that two radical promoted mechanisms, the spiran mechanism and the methylene walk mechanism, both play an important role, but previous research using muon spectroscopy has suggested that the addition of a methylene or a hydrogen radical to a bridge head carbon, which both mechanisms, was highly unfavorable. To elucidate this problem muonium ($\text{Mu} = \square^+\text{e}^-$), a light "isotope" of hydrogen, was used to probe azulene. We have been able to detect and identify the products of the addition of Mu to azulene, based on the hyperfine coupling constants of the spin active species with the aid of computational models.

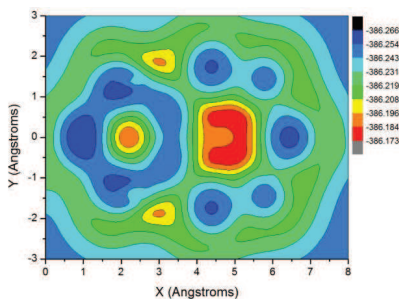


Figure: A PES of a proton 1.5Å above the surface of an azulene ring.

- [1] E. Heilbronner, P.A. Plattner, K. Wieland, *Experientia* **1947**, 3, 70-71.
- [2] R. W. Alder, G. Whittaker, *J. Am. Chem. Soc.* **1975**, 714.
- [3] R. W. Alder, et al., *J. Am. Chem. Soc.* **2003**, 125, 5375-5387.

Notes:

Abstracts: Poster

P10 Carole Hébert, Université de Moncton

Characterizing the role of C/EBP α in glioblastomas

Carole Hébert, André Odjélé and Pier Jr Morin.

Department of Chemistry and Biochemistry, Université de Moncton

Glioblastoma multiforme (GBM) is the most common aggressive brain cancer. With the current therapeutic approach, patients have a life expectancy of 12 to 14 months. A better understanding of the signaling pathways driving this malignancy is therefore essential to improve this outcome. Following the results generated by microarray which focused on identifying differentially regulated kinase mRNAs in primary brain tumor samples, we reported up-regulation of trib1, a member of the tribbles family of proteins. Tribbles proteins are key regulators of cellular signaling and their deregulation has been linked to loss of cellular homeostasis and carcinogenesis. The current project focuses on the C/EBP α transcription factor, a cell cycle regulatory protein whose transcript levels are known to be influenced by Trib1. We have successfully designed primers and measured C/EBP α transcript levels in a panel of GBM cell lines via RT-PCR. Several lines show low levels of C/EBP α transcripts. We next aim to measure C/EBP α protein levels via western blot in the same cellular models and assess if they correlate inversely with Trib1 levels. Overall, this project will further improve our understanding of the Trib1/C/EBP α signaling axis in glioblastoma development and progression.

Notes:

P11 Ngocnu Maithi, Université de Moncton**Transformations of sedimentary organic matter during the last 10 000 years**

Ngocnu Maithi, Guillaume St-Onge and Luc Tremblay
Department of Chemistry and Biochemistry, Université de Moncton

The goal of this work was to evaluate the diagenesis of organic matter (OM) and to estimate the bacterial contribution to OM. For these purposes, we measured amino acids (AA) and the bacterial biomarkers muramic acid (Mur) and D-enantiomers of AA (D-AA) in two long sediment cores (7-8 m) from the estuary and the gulf of St. Lawrence (Canada). Several layers of these sediments were dated. The deepest layers were deposited about 10 000 years ago. The result showed that the proportion of AA, the percentages of total organic carbon as AA (%C_{AA}) and of total nitrogen as AA (%N_{AA}) were higher in the gulf than in the estuary. This indicated a greater in situ production of OM in the gulf, including bacterial biomass revealed by higher Mur yields. In both sediment cores, the proportion of AA, %C_{AA}, %N_{AA}, AA:D-AA the ratio between aspartic acid (Asx), glutamic acid (Glx) and their non-protein degradation product, Asx:β-Ala and Glx:γ-Aba respectively, decreased with depth indicating that OM became increasingly degraded. However, the degradation index (DI), calculated from AA composition, revealed that new AA were produced in the sediments by benthic bacteria. The slight increase of the DI with depth suggested this indicator was not the best marker of bulk OM diagenetic status in these conditions. Based on biomarker yields, ~7 - 40% of C and 15-70% of N in the estuary and in the gulf were of bacterial origin.

Notes:

Abstracts: Poster

P12 Chris Keefe, Cape Breton University

Single File Diffusion in Orthosilicate Thin Films

Chris Keefe

Department of Chemistry, Cape Breton University

The diffusion of particles one after the other across a membrane or film is known as single file diffusion. The kinematics and dynamics of single file diffusion are poorly understood at best. Learning more about the physics involved in this action would lead to more reliable methods of creating porous catalysts and build upon mankind's understanding of nature at scales undetectable to the human eye. The goal of this research project is to carefully engineering orthosilicate thin films composed of highly ordered parallel pores after which carefully selected diffusive molecules will be used to experimentally develop a mathematical model representing the movement of particles diffusing in single file.

Notes:

P13 Colin Kelly, Saint Francis Xavier University

The Effect of Phenyl Ring Position on Hydrocarbon Chains of Potential Diruthenium Liquid Crystals

Colin Kelly

Department of Chemistry, Saint Francis Xavier University

Most liquid crystals today are organic in nature; however, they can often be synthesized using transition metals which offer unique chromophoric, magnetic, and electronic properties that organic liquid crystals often can't match. This project aimed to explore liquid crystals synthesized using a mixed-valent diruthenium (II, III) tetracarboxylate system. The literature has shown that by exchanging the carboxylates with fatty acids, it is possible to induce mesogenic properties. The main objective of this project was to synthesize, purify, and characterize mixed-valent diruthenium complexes bonded to hydrocarbon chains that contain a phenyl group with the focus on how the position of this phenyl group affects the stability and liquid crystal properties of these complexes.

This project saw the successful synthesis of three novel diruthenium (II,III) complexes. The complexes are $[\text{Ru}_2(\mu\text{-O}_2\text{CC}_6\text{H}_4(\text{CH}_2)_7\text{CH}_3)_4(\text{EtOH})(\text{H}_2\text{PO}_4)]$ (**III**), $[\text{Ru}_2(\mu\text{-O}_2\text{C}(\text{CH}_2)_7\text{C}_6\text{H}_5)_4(\text{EtOH})(\text{H}_2\text{PO}_4)]$ (**IV**) and $[\text{Ru}_2(\mu\text{-O}_2\text{C}(\text{CH}_2)_{11}(\text{C}_6\text{H}_5)(\text{EtOH})_2)\text{PF}_6]$ (**V**). Differential scanning calorimetry (DSC) and thermal polarizing optical microscopy (POM) confirmed that none of these complexes exhibited a liquid crystal phase. DSC results also suggest that having the phenyl ring position at the start of the fatty acid, so it will be directly adjacent to the diruthenium core, offered improved thermal stability to the complex as a whole.

An interesting aspect of the project was the unexpected hydrolysis of the PF_6^- counter-ion in the synthesis of (**III**) and (**IV**). The PF_6^- anion is exceptionally stable in solution; however, hydrolysis is known to occur under strongly acidic conditions with heating over long periods of time. This does not correspond to our reactions which take place at 78°C and very mildly acidic conditions. We believe it is possible that the ruthenium complex may have acted as a catalyst in this hydrolysis reaction.

Notes:

P14 Dean Ferguson, Université de Moncton

5-Lipoxygenase inhibitors: GBM's magic bullets?

Dean Ferguson¹, G. Lassalle-Claux¹, Suzette d'Eon¹, Miroslava Cuperlovic-Culf², Mohamed Touaibia¹, Pier Jr Morin¹

¹*Department of Chemistry and Biochemistry, Université de Moncton*

²*National Research Council of Canada, Institute for Information Technology*

Glioblastoma multiforme (GBMs) are grade IV astrocytomas. They are the most common and aggressive type of brain cancer. Median survival is 12-14 months and there is an urgent need to improve the current therapeutic approaches associated with GBMs. The current study focuses on a potential target in GBMs, the enzyme 5-Lipoxygenase (5-LO), which has been previously reported to be overexpressed and to promote cell proliferation in selected gliomas and other malignancies. 5-LO transcript and protein levels were initially measured in a panel of GBM cell lines via RT-PCR and Western blot, respectively. We next developed small molecule inhibitors derived from caffeic acid phenylethyl ester (CAPE), a molecule known to inhibit 5-LO activity, and tested this library of compounds in GBM cell lines which strongly expressed this enzyme. Two of these inhibitors were particularly cytotoxic towards the A172, Hs683 and U373 cell lines; MT30 and MT36. ¹H NMR metabolomics analysis was also used to further explore specific pathways changed after inhibitors treatment. These results provide the first glimpse of the importance of investigating the 5-LO enzyme and its signaling cascade as potential pharmacological targets to treat GBMs.

Notes:

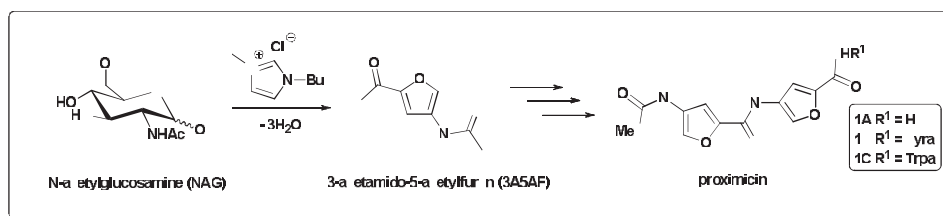
P15 Jennifer Murphy, Memorial University

Novel Process for the Direct Conversion of N-acetyl-D-glucosamine to 3-acetamido-5-acetylfuran Using Imidazolium Based Ionic Liquids

M.W. Drover, J.N. Murphy, K.W. Omari and F.M. Kerton*

Department of Chemistry, Memorial University

As of late, the transformation of biomass feedstocks has become an increasingly popular area of chemistry, seeking to mitigate global dependence on natural fuel sources. In particular, we have elucidated a novel pathway for the conversion of N-acetyl-D-glucosamine (NAG) to the aminofuran, 3-acetamido-5-acetylfuran (3A5AF). In particular, this moiety constitutes a simply achieved retron for the synthesis of proximicins, which show exceptional cytostatic activity toward human tumor cells. [1] We have studied the formation of 3A5AF using conventional and microwave heating to determine the effect of metal additive, solvent, temperature and time in order to achieve maximum yield and product selectivity. We have also shown, that use of two equivalents of boric acid; $B(OH)_3$ in 1-butyl-3-methylimidazolium chloride afforded the desired product in 60 % at 180 °C. High yields with $B(OH)_3$ and poor yields with organic base additives such as 1,4-diazabicyclo[2.2.2]octane and 1,8-diazabicyclo[5.4.0]undec-7-ene(16.5%) suggests the reaction was acid catalyzed. Also the anion of the 1-butyl-3-methylimidazolium based ionic liquid had an effect on the yield of 3A5AF. We have found that 1-butyl-3-methylimidazolium chloride affords the best results and larger anions such as bromide and acetate inhibit the production of the desired compound.



P16 Pierre Lyons, Université de Moncton

microRNAs: A “cool” family of ribonucleic acids

Pierre Lyons, Lynn Courteau and Pier Jr Morin.

Department of Chemistry and Biochemistry, Université de Moncton

Methods to preserve organs involve maintaining life at non-physiological temperatures. While our molecular understanding of the freezing process has improved the field of cryopreservation, much remains to be done to comprehend life in the cold and to translate this knowledge to known biomedical applications. Natural models of hypometabolism hold keys to our understanding of biochemical processes at play during freezing. Overwintering strategies employed by these models are decreased metabolic rate and, at the molecular level, significant down-regulation of energy-consuming processes. To gain new perspectives on freeze tolerance, we studied differential expression of members of a novel family of nucleic acids named the microRNAs (miRNAs) in the freeze tolerant fly *Eurosta solidaginis*. miRNAs are small ribonucleic acids capable of inhibiting the energy-consuming process of protein translation by silencing expression of selected transcripts. Our laboratory has identified a signature of cold-related miRNAs in control (+5 °C) and frozen (-15 °C) insects using microarray- and RT-PCR-based approaches. We report here for the first time amplification and expression of miR-210 in frozen *E. solidaginis*. This miRNA is particularly interesting as it is a downstream target of HIF-1, a transcription factor known to be overexpressed at low temperatures in *E. solidaginis*. Future studies will aim to further characterize the involvement of miR-210 and related miRNAs at low temperatures.

Notes:

P17 Reem Karaballi, Saint Mary's University

Development of a SERS-based Biosensor for Rapid Detection of Tuberculosis

Reem Karaballi, Christa L Brosseau
Department of Chemistry, Saint Mary's University

This project focuses on the development of a portable DNA-aptamer based biosensor that would aid in the diagnosis of a contagious disease known as tuberculosis. An important aspect of this project is to obtain a DNA signal, before using an aptamer that would detect certain biomarkers, by Electrochemical Surface Enhanced Raman Spectroscopy (E-SERS). This method was used to detect the signals of DNA bases, nucleotides, and an oligonucleotide. Screen printed electrodes modified with silver colloidal nanoparticles were immersed in the DNA base and nucleotide solutions. A voltage was applied varying from 0 to -0.1V. These experiments showed that DNA components are able to be detected using E-SERS.

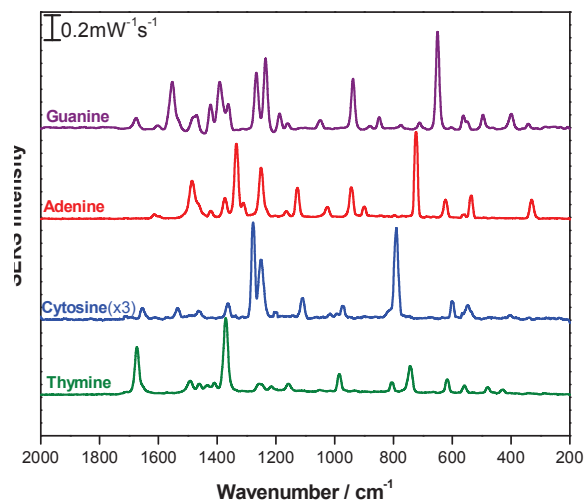


Figure 1. Normal Raman spectra of the four DNA bases

Notes:

P18 Zack Brown, Dalhousie University**Detection of Carbon Dioxide in Carbonated Beverages with Agar Based Indicator Gels**

Zack Brown

Department of Chemistry, Dalhousie University

With the rise in atmospheric carbon dioxide (CO₂) level, low cost detection and monitoring of CO₂ has a crucial importance in the area of gas sensors. In this short term study, a simple CO₂ detection device was created in the hopes the concept may be extrapolated in future studies, including those involving gas sensors. The CO₂ detection device was utilized in the context of determining whether or not a beer was fresh or flat. Using the bicarbonate equilibrium²,



an initial pH strip device was successfully built to detect the pH change from carbon dioxide dissolving in water. A more efficient water based agar phenolphthalein indicator gel was subsequently created and was found to successfully determine the distinction between a fresh beer and flat beer.

Suggested future studies include improving the sensitivity of the created gel, applying the gel's used to broader CO₂ detection issues, and creating gels that detect harmful gases (ex. carbon monoxide).

1)C. Cobianu, B. Serban, Honeywell Romania SRL, "Novel concepts for CO₂ detection by differential resonant nanosensing", Micro and Nanoengineering, 2010.

2)Seager, S. L., Slabaugh M. R. Organic and Biochemistry for Today. Brooks/Cole Cengage Learning, 7th ed. Belmont, 2011.

Notes:

Abstracts: Poster

P19 Erica Campbell, Cape Breton University

Measuring Vibrational intensities: Current Techniques and Examples

Erica Campbell, C. Dale Keefe

Department of Chemistry, Cape Breton University

A review of vibrational intensities, both the experimental measurement and the applications, is presented. Different experimental techniques of measuring the absolute infrared intensities and the physiochemical properties that can be determined from the vibrational intensities are discussed. Recent use of computational techniques to enhance the experimental measurements is presented, as well as recent studies. Current work on the absorption intensities of bromoform will be presented.

Notes:

P20 Zack O'Toole, Saint Francis Xavier University

Rheology Modification in Anionic/zwitterionic Surfactant Mixture by Non-aromatic Hydrotropic Salts: Monomeric and Dimeric inducers

Zachary O'Toole, Kulbir Singh,* Aleisha McLachlan, D. G. Marangoni
Department of Chemistry, St. Francis Xavier University

In this paper, we report induced micellar growth and rheology modification for mixtures of anionic (Sodium dodecylsulfate, SDS) and zwitterionic (N-alkylated Glycine Derivative, Empigen BB or EBB) surfactants. Two non-aromatic hydrotropic salt (Hexyltrimethylammonium Bromide, C6TAB and/or dibutylenebis-(dimethylbutylammonium bromide), 4-4-4) are used as novel additives for inducing the micellar growth in these systems. Photon correlation spectroscopy (PCS) and rheology measurements were employed to assess micellar growth and rheology modifications present upon addition of the non aromatic-hydrotropes to the micellar mixtures. In this study, both hydrotropic ions have been found to contribute to similar structural modifications in the mixed micelles of the anionic and zwitterionic surfactant; however, the extents of the rheology modification in solutions are found to be quite different when the gemini hydrotrope is employed versus the monomeric hydrotrope.

Notes:



