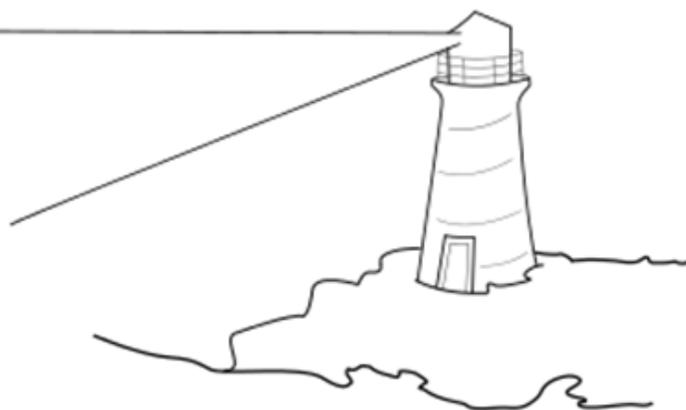
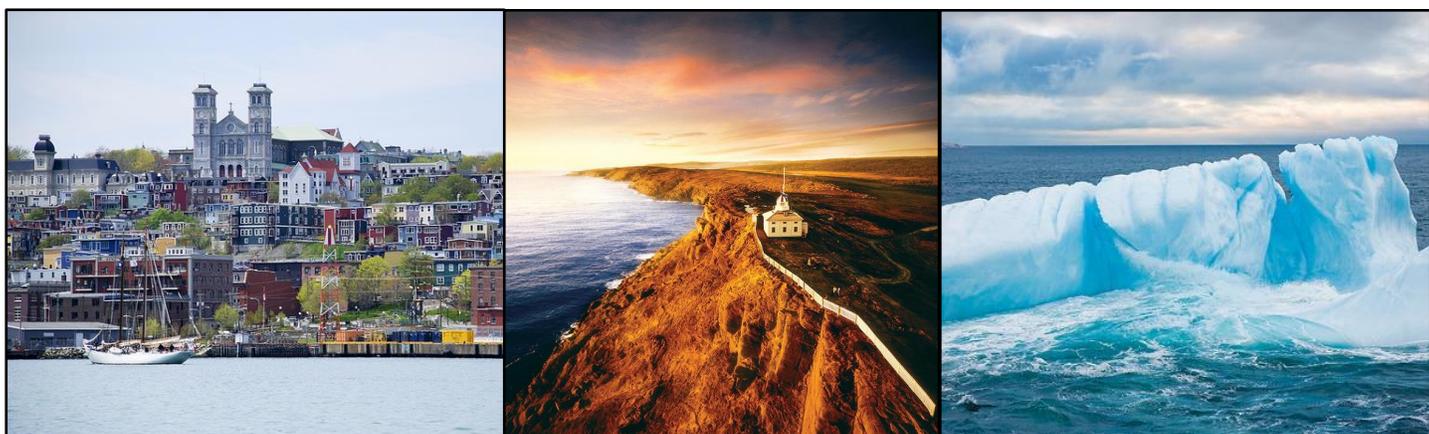

ChemCon 2013

Chemistry on the Edge



38th Annual Science Atlantic / CIC Student Chemistry Conference

May 21st - 23rd, 2013

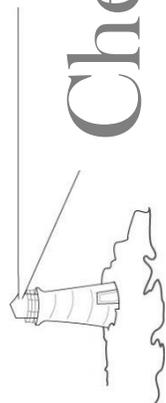


Program and Abstract Book

Science  Atlantic
connecting science education and research



Memorial University of Newfoundland
St. John's NL



ChemCon 2013

Chemistry on the Edge



Table of Contents

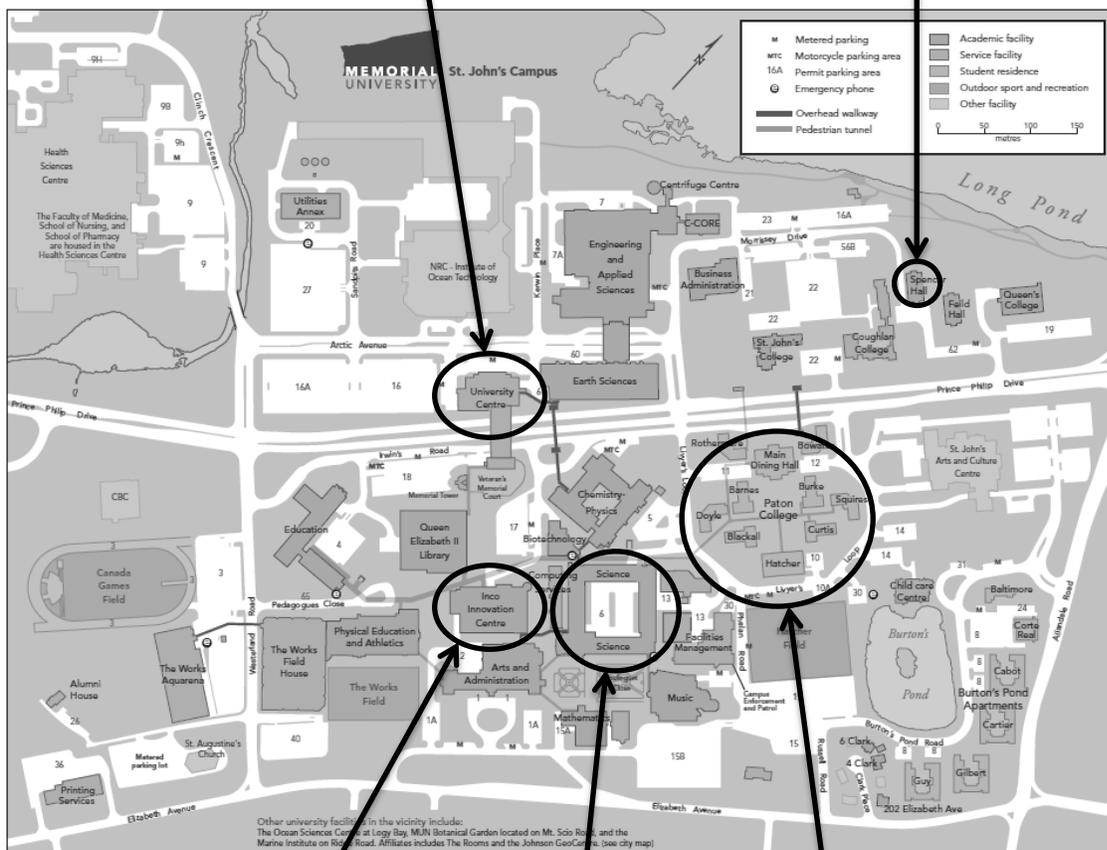
Campus Map	2
Map to Downtown	3
Restaurants	4
General Information	5
Message from the Conference Chair	6
Message from the Department Chair	7
Organizing Committee	8
Presenting Delegates	9
Keynote Speakers	11
Chalk Talks	13
Sponsors	14
Awards	15
Schedule of Events	16
Presentation Schedule	19
Abstracts: Oral	22
Abstracts: Posters	63



Campus Map

The University Center (Where you'll find the Breezeway!!)

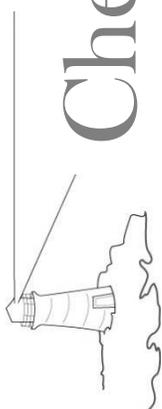
Bitters Restaurant and Lounge Location



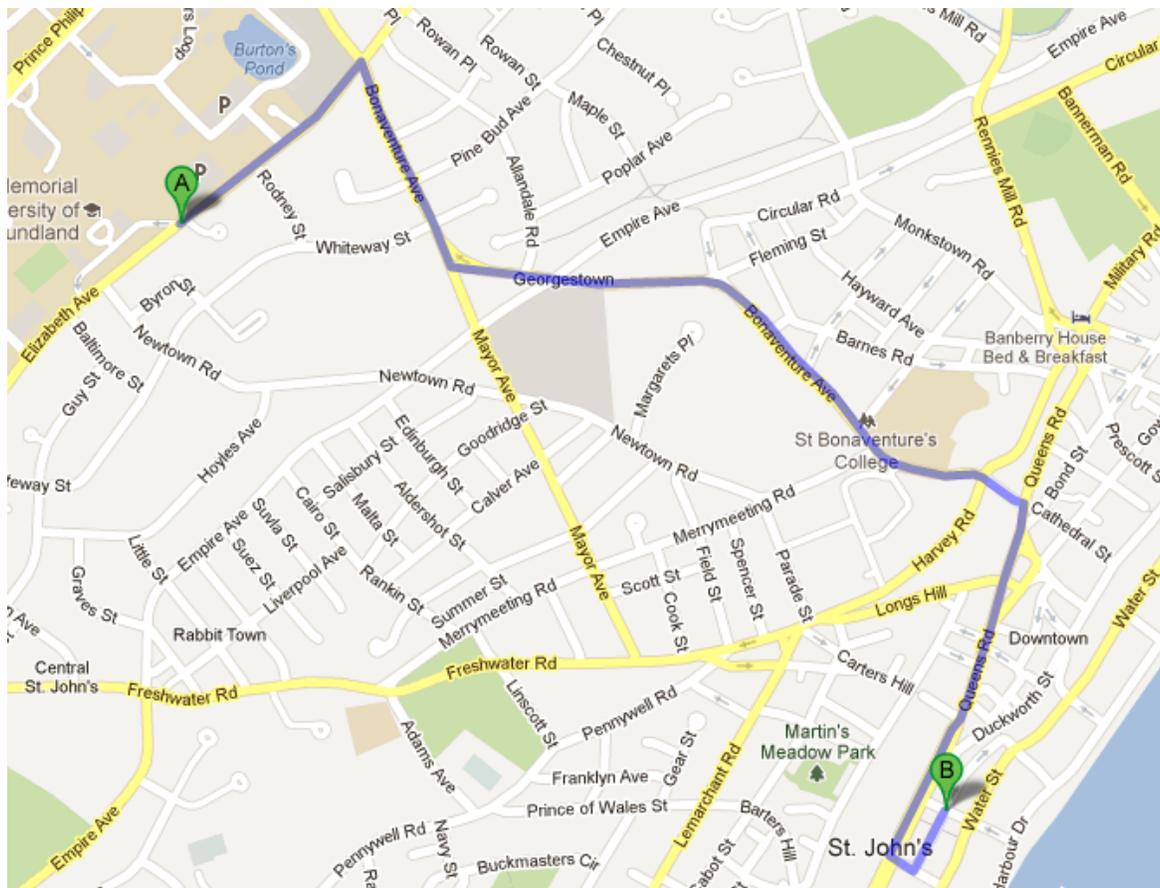
Bruneau Centre, previously INCO Innovation Center (location of May 22nd talks and poster fair)

Residence / Dining Hall

Science Building (location of May 23rd talks)

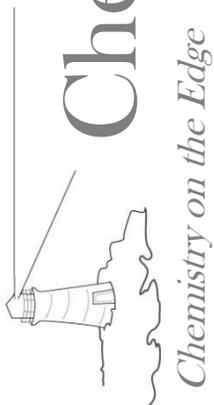


Map to Downtown



Directions from MUN:

- Leaving the school, turn left onto Elizabeth Avenue
- Turn right onto Bonaventure Avenue
- Turn left to stay on Bonaventure Avenue
- Continue onto Garrison Hill
- Turn right onto Queens Road
- Continue onto New Gower Street
- Turn left onto Queen Street
- Take first left onto George Street



Restaurants

Restaurants On Campus:

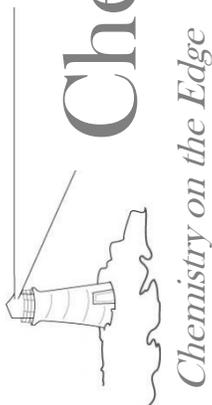
- University Center Food Court
 - Mrs. Vanelli's
 - Dairy Queen
 - Booster Juice
 - Mr. Sub
 - Treats
 - Extreme Pita
 - Just Fries
- Tim Horton's (located in the Aquarena)
- Bitters (see Campus Map)

Restaurants Near Campus:

- Subway
- Quintana's
- A&W
- Big Bite Pizza
- Pizza Hut
- Pasta Plus
- Pier 17
- East Side Mario's

Nearby Liquor Stores (NLC):

- Ropewalk Lane Location
- Elizabeth Avenue Location



General Information

Presentations

- Presentations will be split between the Bruneau Centre and the Science Building. Oral presentations and keynote talks will be held in Room IC2001 in the Bruneau Centre on May 21st-22nd, and in Room SN2109 in the Science Building on May 23rd. Poster presentations will take place in the Bruneau Centre lobby on May 22nd.
- In the case of oral presentations, presenters are allowed a total of 15 minutes – 12 minutes for the presentation and 3 minutes for questions. The schedule will be strictly followed. Presentations must be uploaded to the computer before each session.

Welcome Barbeque

- A free barbeque will be provided by Sobeys on May 21st at the Breezeway (located in the University Center). Come join us for food, fun, trivia, and prizes!

Newfie Night at the Breezeway

- This event is inspired by Newfoundland traditions and music. It will take place at the Breezeway from 7:00pm to 10:00pm, and will be followed by a tour of local establishments in downtown St. John's. We will leave as a group from the Breezeway (see Map to Downtown).

Banquet

- The cost of the banquet is \$35.00 for all participants. Transportation will be provided to the banquet venue, the Johnson GEO CENTRE, from the front of the Chemistry-Physics Building at 6:00pm and 6:45pm. Busses will be leaving the GEO CENTRE heading back to MUN at 10:00pm and again at 12:45am.

Bids for ChemCon 2014

- Bids can be made for ChemCon 2014 at the banquet on May 23rd. Computer and projector will be provided.



Message from the Conference Chairs

Welcome to ChemCon 2013

On behalf of the ChemCon 2013 planning committee it is our pleasure to welcome you all to Memorial University for the 38th Science Atlantic/CIC Chemistry Conference. Our department is honoured to host this conference for the first time since 2004. With one of the largest chemistry departments in Atlantic Canada, we encourage you to get to know our faculty and research facilities. Tours will be available. Additionally, St. John's is a fun city and we hope that you will be able to participate in the recreational and sight-seeing opportunities here.

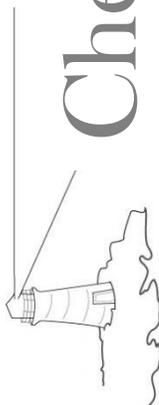


This annual conference is an important part of undergraduate development, as it allows undergraduate students the ability to share their research with their counterparts from Atlantic Canada, and gain a valuable life experience. The conference also allows chemists to hear addresses from keynote speakers from across the country. We are pleased to welcome as our keynote speakers, Canada Research Chair in Energy Conversion Dr. Curtis Berlinguette (UCalgary), and Dr. Jean-Philip Lumb (McGill), and we hope you enjoy their lectures.

We would like to thank our fellow committee members for their hard work and time spent planning for ChemCon 2013. A very sincere thanks also goes to Dr. Chris Flinn, our Faculty advisor, and Mary Flinn, who both kept us all on track.

Take advantage of the activities planned and enjoy chatting with your fellow chemists. We are thrilled to have you here and hope you enjoy this conference, and we wish you all the best during your stay in Newfoundland. If you want any tips for places to visit and things to do around St. John's, don't hesitate to ask us.

Landon Hiscock and Jennifer Murphy
Conference Chairs



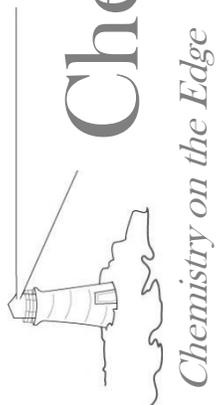
Message from the Department Head

As Head of the Department of Chemistry, it is my pleasure to extend greetings to the delegates of the 38th Annual Science Atlantic/CIC Chemistry Conference, Chemcon 2013. The faculty and students of the chemistry department are delighted to be your host for this event. The conference, being held at Memorial University for the first time since 2004, focuses primarily on undergraduate research in all areas of chemistry and provides a forum for undergraduate students from the universities of the four Atlantic Provinces to come together in a spirit of friendship and to share the results of their research endeavours. I have no doubts that this meeting of young minds and outstanding keynote speakers will further stimulate your interest in pursuing a career in research as well as stimulating new ideas and approaches to solving the research problems that interest you. While you are in the department, I invite you to take the opportunity to meet our faculty members and visit our research laboratories to learn more about the exciting research in progress here at Memorial.



I would like to formally thank the organizing committee, keynote speakers, sponsors, and all those who tirelessly work towards the success of this conference. On behalf of the faculty and staff of the Department of Chemistry at Memorial University, I wish you an enjoyable, memorable and successful ChemCon2013.

Peter Pickup
Professor & Head, Department of Chemistry, Memorial University



ChemCon 2013



Organizing Committee

Co-Chairs

Landon Hiscock
Jennifer Murphy

Faculty Advisor

Dr. Chris Flinn

Abstract Coordinator

Victoria Grandy

Events Coordinator

Liam Whelan

Food and Housing Coordinator

April Woods

Financial Coordinator

Kerry-Lynn Williams

Technical/Photography Coordinator

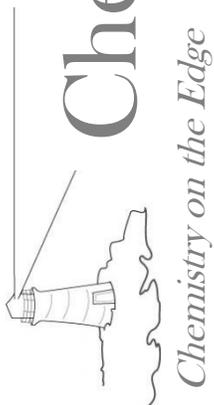
Teles Furlani

Secretary/Webmaster

Brandon Fancy

Volunteers

Jennifer Smith
Tiffany Tozer
Leif Hickey
Mary Flinn



Presenting Delegates

Acadia University

Alex Chase
Julie Colpitts
Amber Davidson
Emily Fraser
Robie Hennigar
Kimberly Hyson
Jakob Nickerson
Tariq Sainuddin
Eric Sampson
Martin Sickinga
Hilary Simon
Mat Stephenson
Crystal Sweeney
Lynsay Thurber
Hillary Wheeler
Stephen Wolfe
Julia Wright
Huimin Yin

Cape Breton University

Shawna Corcoran
Brittany MacDonald
Marybeth MacDonald
John MacInnis
Preston MacQueen
Alyssa Moss

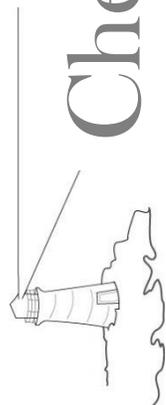
Karanbir Pahil

Dalhousie University

William Curry
Vinayak Mishra

Memorial University

Zaher Algharaibeh
Dalal Alhashmi
Jessica Besaw
Ashley Bungay
Kerri Burton
Hua Chen
Greg Curtis
Katalin Devaine
Robert Di Lorenzo
Stefana Egli
Ali Elkurtehi
Brandon Fancy
Shaheen Fatima
Teles Furlani
Brandon Furlong
Victoria Grandy
Iyad Hailat
Qing He
Landon Hiscock
Yasaman Jami



ChemCon 2013

Chemistry on the Edge



Presenting Delegates

Memorial University

Mohammad Javashi

Heidi Kavanagh

Yi Liu

Marc MacKinnon

Pasha Majidi

Maryam Moghaddam

Jennifer Murphy

Saleh Riahi

Kiran Sagar

Tim Strange

Kerry-Lynn Williams

April Woods

Chuan Xu

Muyi Xu

Saint Mary's University

Reem Karaballi

Chris Lavoie

Trevor McGrath

Ashley Robinson

Maraw Yasmin



Keynote Speakers

Dr. Curtis Berlinguette

Department of Chemistry, University of Calgary



*Director, Centre for Advanced Solar Materials
Fellow, Institute for Sustainable Energy, Environment &
Economy
Canada Research Chair in Energy Conversion
Alfred P. Sloan Fellow
Alberta Ingenuity New Faculty*

Dr. Curtis P. Berlinguette is an Associate Professor of Chemistry and Director of the Centre for Advanced Solar Materials at the University of Calgary. After graduating with a B.Sc. in 2000 from the University of Alberta, Dr. Berlinguette headed to Texas A&M University to pursue a Ph.D. in Inorganic Chemistry (Advisor: Prof. K. R. Dunbar) before doing two years of postdoctoral studies at Harvard University (Advisor: Prof. R. H. Holm). He then returned to his hometown in 2006 to lead an independent research program at the University of Calgary. Dr. Berlinguette leads a research program fully dedicated to solar energy conversion, which includes the design of novel nanoscale materials for advanced solar cells, and developing economically viable ways of storing solar electricity as high density fuels. Dr. Berlinguette holds five (provisional) patents, has authored over 40 scientific articles, holds a Canada Research Chair in Energy Conversion and an Alfred P. Sloan Research Fellowship and has co-founded the renewable fuels company, FireWater Fuel Corporation.

May 21st 2013 from 4:30-5:30 PM

Room IC2001



Keynote Speakers

Dr. Jean-Philip Lumb

Department of Chemistry, McGill University



Assistant Professor

Dr. Jean-Philip Lumb is an Assistant Professor of Chemistry at McGill University. After receiving his B.A. magna cum laude in 2002 from Cornell University, Dr. Lumb pursued a Ph.D. in Organic Chemistry at the University of California, Berkley (Advisor: Prof. D. Trauner) followed by a three-year postdoctoral study at Stanford University (Advisor: Prof. B. M. Trost). In 2011, Dr. Lumb was appointed an assistant professorship at McGill University where his research team actively pursues new strategies that address the challenge of chemical synthesis in the face of growing concerns over fossil fuel utilization. The scope of his research includes the development of cascade reactions that rapidly generate molecular complexity by maximizing atom economy and minimizing total step count and the diversification of chemical feedstocks, with an emphasis on the deoxygenation of polyol starting materials.

May 22nd 2013 from 4:30-5:30 PM
Room IC2001



Chalk Talks

May 23rd 2013 from 12:00pm-1:00pm



A Lexicon of Organic Transformations: Chemical, Professional and Personal

Dr. Graham Bodwell

Room SN2101

Solid State Characterizations: NMR and X-Ray Crystallography

Dr. Louise Dawe and Dr. Celine Schneider

Room SN2105



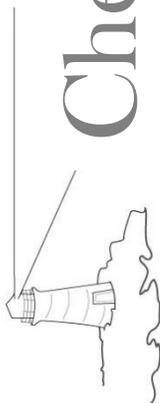
"Captain We're Sensing Something in the Water": Multi-Disciplinary Approaches to New Sensing Systems for Remote Detection of Environmental Contaminants



Dr. Erika Merschrod and Dr. Christina Bottaro

Room SN2018

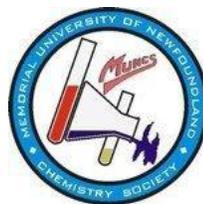




Sponsors

Platinum

- Memorial University of Newfoundland Chemistry Society
- Memorial University Department of Chemistry
- Memorial University Faculty of Science



Gold

- CIC Chemical Education Fund
- CIC Biological and Medicinal Chemistry Division
- Memorial University Student Union
- Wiley, Springer, and RSC Publishing Companies



Silver

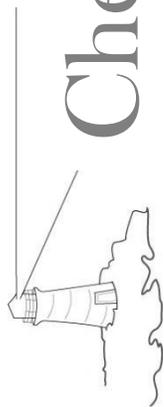
- CIC Newfoundland and Labrador Local Section
- CIC Surface Science Division
- CIC Organic Chemistry Division
- CIC Analytical Chemistry Division
- The City of St. John's, Newfoundland
- Canadian Society for Chemistry



Bronze

- CIC Physical, Theoretical, and Computational Chemistry Division
- CIC Inorganic Chemistry Division
- Memorial University Student Affairs Division





ChemCon 2013

Chemistry on the Edge



Awards

- CIC Award for the Best *Undergraduate* Oral Presentation in Physical, Theoretical, or Computational
- CIC Award for the Best *Undergraduate* Poster in Physical, Theoretical, or Computational
- CIC Award for the Best *Undergraduate* Oral Presentation in Biological/Medicinal
- CIC Award for the Best *Undergraduate* Poster in Biological/Medicinal
- CIC Award for the Best *Undergraduate* Oral Presentation in Materials Chemistry
- CIC Award for the Best *Undergraduate* Poster in Materials Chemistry
- CIC Award for the Best *Undergraduate* Oral Presentation in Organic Chemistry
- CIC Award for the Best *Undergraduate* Poster in Organic Chemistry
- CIC Award for the Best *Undergraduate* Oral Presentation in Analytical Chemistry
- CIC Award for the Best *Undergraduate* Poster in Analytical Chemistry
- CIC Award for the Best *Undergraduate* Oral Presentation in Inorganic Chemistry
- CIC Award for the 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
- Science Atlantic Science Communication Award
- ACEmat (former AIMMS) Award in Computational Modeling of Materials
- Hugh Anderson Memorial Award for the Best Overall Oral Presentation by an *Undergraduate*



Schedule of Events

Day 1: Tuesday, May 21st 2013

Bruneau Centre

12:00pm-3:45pm Registration and Check-in – Lobby

4:15pm-4:30pm Opening Remarks – IC2001

4:30pm-5:30pm Keynote Address by Dr. Curtis Berlinguette – IC2001

The Breezeway

5:30pm Welcome BBQ and Trivia

Day 2: Wednesday, May 22nd 2013

7:00am-8:15am Breakfast – Main Dining Hall

Bruneau Center

8:30am-10:30am Oral Presentation Session 1A – IC2001

10:30am-10:45am Nutrition Break – Lobby

10:45am-12:00pm Oral Presentation Session 1B – IC2001

12:00pm-12:50pm Lunch – Main Dining Hall

1:00pm-2:00pm Oral Presentation Session 1C – IC2001

2:00pm-3:00pm Keynote Address by Dr. Jean-Philip Lumb – IC2001

3:00pm Poster Setup – Lobby

3:30pm-5:30pm Poster Presentations – Lobby



Schedule of Events

The Breezeway

7:00pm-10:00pm Newfie Night at the Breezeway

10:00pm Tour of Local Establishments – Leave from the Breezeway

Day 3: Thursday, May 23rd 2013

7:30am-8:45am Breakfast – Main Dining Hall

Science Building

9:00am-10:30am Oral Presentation Session 2A – SN2109

10:30am-10:45am Nutrition Break – Lobby

10:45am-12:00pm Oral Presentation Session 2B – SN2109

12:00pm-1:00pm Box Lunch & Chalk Talks – Science Building (see Chalk Talks)

1:15pm-2:30pm Oral Presentation Session 2C – SN2109

2:30pm-2:45pm Nutrition Break – Lobby

2:45pm-4:00pm Oral Presentation Session 2D – SN2109

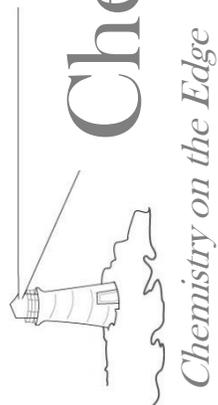
4:00pm-4:30pm Judges Meeting – C4002

4:30pm-5:30pm The Maritime Section of the CIC Meeting – C4002

5:30pm-6:30pm The Science Atlantic Chemistry Committee Meeting – C4002

6:00pm First Bus Leaves for Banquet from Front of Chemistry-Physics Building

6:45pm Last Bus Leaves for Banquet from Front of Chemistry-Physics Building



ChemCon 2013

Chemistry on the Edge



Schedule of Events

Johnson GEO CENTRE

6:30pm Cocktail Hour

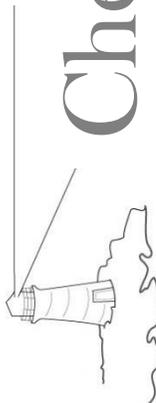
7:30pm Dinner Starts

8:30pm Awards Presentations

9:00pm Bid for ChemCon 2014

10:00pm First Bus / Start of Dance

12:45am Last Bus / End of Dance



Presentation Schedule

May 22nd 2013

Session 1A

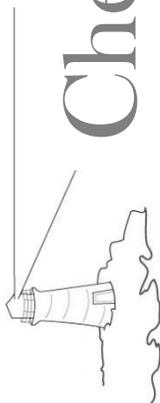
1A-1	8:30	Crystal Sweeney, Acadia University
1A-2	8:45	Ashley Bungay, MUN
1A-3	9:00	Preston MacQueen, CBU
1A-4	9:15	Vinayak Mishra, Dalhousie University
1A-5	9:30	Jessica Besaw, MUN
1A-6	9:45	Teles Furlani, MUN
1A-7	10:00	Julie Colpitts, Acadia University
1A-8	10:15	Trevor McGrath, SMU

Session 1B

1B-1	10:45	Landon Hiscock, MUN
1B-2	11:00	Robie Hennigar, Acadia University
1B-3	11:15	April Woods, MUN
1B-4	11:30	William Curry, Dalhousie University
1B-5	11:45	Hillary Wheeler, Acadia University

Session 1C

1C-1	1:00	Reem Karaballi, SMU
1C-2	1:15	Brandon Fancy, MUN
1C-3	1:30	Julia Wright, Acadia University
1C-4	1:45	Jennifer Murphy, MUN



Presentation Schedule

May 23rd 2013

Session 2A

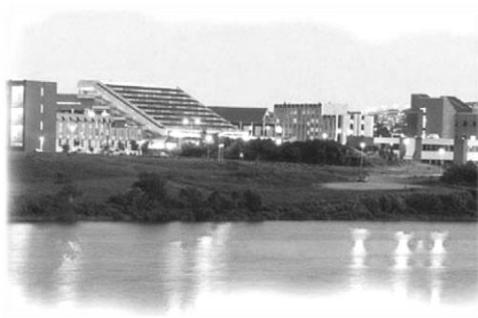
2A-1	9:00	Emily Fraser, Acadia University
2A-2	9:15	Ashley Robinson, SMU
2A-3	9:30	Mat Stephenson, Acadia University
2A-4	9:45	Chris Lavoie, SMU
2A-5	10:00	Brandon Furlong, MUN
2A-6	10:15	Alex Chase, Acadia University

Session 2B

2B-1	10:45	Tiffany Tozer, MUN
2B-2	11:00	Heidi Kavanagh, MUN
2B-3	11:15	Chuan Xu, MUN
2B-4	11:30	Tariq Sainuddin, Acadia University
2B-5	11:45	Shaheen Fatima, MUN

Session 2C

2C-1	1:15	Greg Curtis, MUN
2C-2	1:30	Maryam Moghaddam, MUN
2C-3	1:45	Martin Sichinga, Acadia University
2C-4	2:00	Muyi Xu, MUN
2C-5	2:15	Stefana Egli, MUN



Presentation Schedule

May 23rd 2013

Session 2D

2D-1	2:45	Pasha Majidi, MUN
2D-2	3:00	Robert Di Lorenzo, MUN
2D-3	3:15	Saleh Riahi, MUN
2D-4	3:30	Qing He, MUN
2D-5	3:45	Zaher Algharaibeh, MUN



Abstracts: Oral

1A-1 Crystal Sweeney, Acadia University

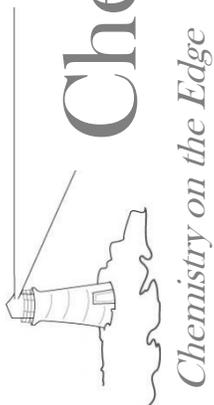
Sweating the Small Stuff: Study of Pesticides and Primary Metabolites Excreted in Human Sweat

C. Sweeney and Anthony Z. Tong

Undergraduate Student, Department of Chemistry, Acadia University

In regions of intense agriculture, pesticides can leach into neighbouring wells and contaminate drinking water. Several pesticides used in Prince Edward Island and Nova Scotia are classified as “probable human carcinogens” by the U.S. Environmental Protection Agency. It is hypothesized 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. The purpose of this research is to investigate the waste excretory function of eccrine sweat glands by quantifying pesticide concentrations in human sweat. The research objective is to analyze sweat samples, collected from sample populations in western PEI and Nova Scotia’s Annapolis Valley during infrared sauna sessions, using chromatography and mass spectrometry techniques. The analytical method will encompass the detection of 22 pesticides and key metabolites, including chlorothalonil, dimethoate and linuron. Target compounds were selected based on top sales in PEI and NS, known or suspected carcinogenic potential, acute toxicity and relative persistence in the environment. If 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 may offer a promising approach to cancer prevention.

Notes:



Abstracts: Oral

1A-2 Ashley Bungay, Memorial University

Human Impact on Drinking Water

Ashley Bungay and Erika F. Merschrod S.

Undergraduate Student, Department of Chemistry, Memorial University

Caffeine in drinking water is a way to tell if a water source has been contaminated by the population using this water. This can only be tested in areas of smaller populations where the water is not being recycled. Caffeine has a unique Raman fingerprint like all analytes in water. By taking samples on drinking water and obtaining the Raman spectra of said sample one can identify the presence (if any) of caffeine in the water. Also since caffeine is consumed it will have metabolites, products of caffeine being digested and metabolized. When looking of caffeine the main signal to look for is a strong peak at about 1698cm^{-1} . Other peaks to look for would be 3121cm^{-1} , 1605cm^{-1} , 1409cm^{-1} , 1333cm^{-1} , 555cm^{-1} . If some of these signals can be obtained in a spectrum even with other analytes in the sample one could conclude that the population has had an impact on the drinking water in the specific area of interest.

Notes:



Abstracts: Oral

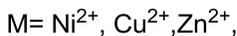
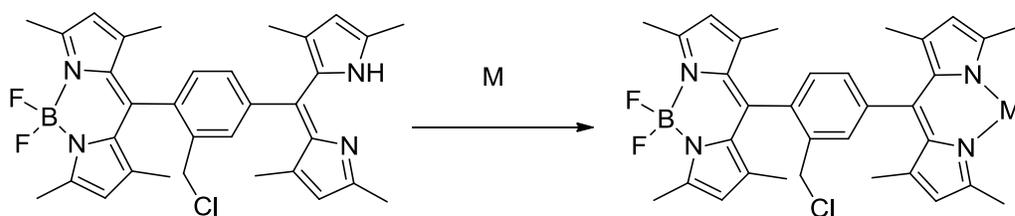
1A-3 Preston MacQueen, Cape Breton University

New BODIPY Mesoporous Materials for Fluorescence Devices

Preston MacQueen, Chuan Xu, Matthias Bierenstiel, and Stephanie MacQuarrie
 Undergraduate Student, Department of Chemistry, Cape Breton University

Transition metals impurities and pollutants are of growing concern in the environment. In order to gain information about metals and their interactions with their environments, the ability to qualitatively and quantitatively test for the presence, or absence, of metals independently of their environments is required. A solution is to sense metals with fluorescent dyes. Fluorescent Boron-dipyrromethene's (BODIPY's) have become popular in recent years in the field of metal sensing. The fluorescence of a metal, complexed to a BODIPY molecule, is proportional to its concentration. As chemical metal sensors BODIPY's combined with appropriate chelator groups present a versatile method of metal sensing in a variety of environments. BODIPY metal sensors can be improved upon by anchoring them into periodic mesoporous organo-silicas (PMO's). The ability of sensing metals in the solid phase is beneficial because the fluorescent material can be easily recovered from solution and reused.

The focus of the study is to prepare a BODIPY compound and study its complexation ability. The BODIPY ligand will be prepared in such a way that it can later be incorporated into a periodic mesoporous organo-silicate lending its optical properties to a solid phase material.





Abstracts: Oral

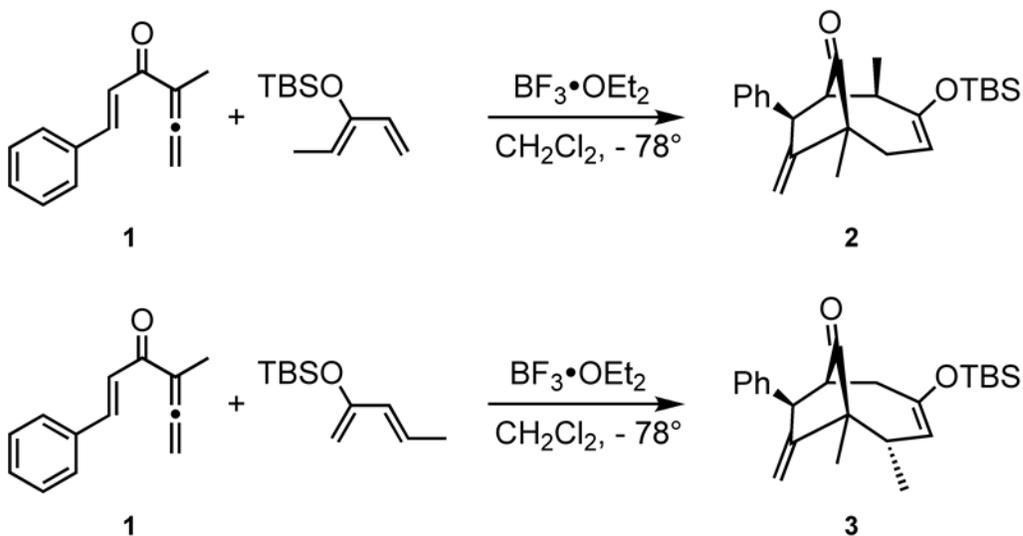
1A-4 Vinayak Mishra, Dalhousie University

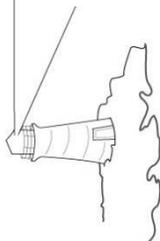
Nazarov Reactions Intercepted by (4+3)-Cyclization with Oxygen-substituted Dienes

Vinayak Mishra, Francois M. LeFort, and D. Jean Burnell

Undergraduate Student, Department of Chemistry, Dalhousie University

Allenyl vinyl ketones, such as (E)-4-methyl-1-phenylhexa-1,4,5-trien-3-one (**1**), are excellent substrates for tandem Nazarov reactions-with-further cyclizations because their oxyallyl cationic intermediates of the Nazarov reactions are longer lived than those of simple divinyl ketones. Previous studies using alkyl-substituted dienes as reactants in this “interrupted” mode of Nazarov reaction has allowed the preparation of a host of products arising from (4+3)- and (3+2)-cyclizations. In this study, tert-butyl dimethylsilyloxy-substituted dienes were employed as reactants to trap the intermediate oxyallyl cation forming two new carbon-carbon bonds in one highly regioselective (4+3)-cyclization step. The stereoselectivity of the tandem Nazarov-(4+3)-cycloaddition is dependent on the relative positions of the substituents to the oxygen of the diene. β -Substituted dienes give products arising from an “extended” transition state (**2**), whereas α -substituted dienes give products arising from a “compact” transition state (**3**). The mechanistic implications of these observations will be discussed.





Abstracts: Oral

1A-5 Jessica Besaw, Memorial University

Atoms and Bonds in Molecules: A Radial Density Analogue to the Quantum Theory of Atoms in Molecules

J. E. Besaw, R. A. Poirier, and P. L. Warburton

Undergraduate Student, Department of Chemistry, Memorial University

Richard Bader's quantum theory of atoms in molecules partitions molecules into their atomic contributions according to zero flux surfaces in electron density. A consequence of this partitioning scheme is that 'real atoms do not overlap'. A promising alternative that enables the division of molecules into atomic and bonding regions is weighted radial density. This concept stems from the radial distribution function of atoms which exhibits shell structure. The shell structure of atoms in molecules based on radial density will be compared to the Bader-Gillespie model of shells. The radial density model has the potential to provide a more realistic description of atoms and bonds in molecules.

Notes:



Abstracts: Oral

1A-6 Teles Furlani, Memorial University

Optimization and Evaluation of Thin-Film Molecularly Imprinted Polymers for the Analysis of Cotinine in Human Fluids

Teles C. Furlani, Adam G. Beaton, and Christina S. Bottaro

Undergraduate Student, Department of Chemistry, Memorial University

Molecularly imprinted polymers (MIPs) are porous materials with a selective binding site for a target compound. The analyte and the MIP interact by non-covalent interactions (e.g. H-bonding, pi-pi stacking). Our group has been working on MIPs in thin film format for direct analysis by desorption electrospray ionization – mass spectrometry (DESI-MS), and for applications in sensors. In advance of installation of the DESI-MS, all optimization experiments have been followed using GC-MS on extracts. Optimization has been completed on MIPs for the analysis of cotinine, the primary metabolite of nicotine, which is used as a biomarker for active and passive smokers. In this study, the pre-polymerization solution was optimized to obtain a ratio between the template, functional monomer, cross-linker, and porogen to maximize the amount of cotinine taken up by the polymer. Previous studies had lengthy template removal procedures; therefore, work was done to reduce the amount of time spent on removal. Residual template left in the MIP can lead to template bleeding, one of the most common problems with MIPs. Work has been done to correct this using a pseudo-template with a similar structure to cotinine, namely myosmine. Results of the optimization, as well as tests of the optimal MIPs on saliva and urine spiked with cotinine will be presented.

Notes:



Abstracts: Oral

1A-7 Julie Colpitts, Acadia University

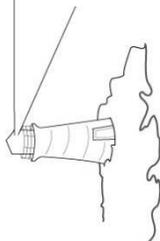
Biological Evaluation of Coordination Complexes as Photosensitizers for Photodynamic Therapy

J. Colpitts¹ and S. McFarland^{1,2}

Undergraduate Student, ¹Department of Biology and ²Department of Chemistry, Acadia University

Due to the limitations of current cancer treatments, research is underway to develop nontoxic chemotherapeutic agents which can be activated to “turn on” their cytotoxic effects. One such approach, photodynamic therapy (PDT), uses light to activate the therapeutic agent, or photosensitizer (PS). Widespread use of PDT is limited by drawbacks that characterize current clinical PSs; consequently, there is ongoing interest in designing new PSs with better properties. Metal-based coordination complexes are of particular interest, and represent one such class. To assess the effectiveness of these metal-based PSs as potential agents for PDT, a series of relatively simple biological experiments was performed. A variety of techniques was used to evaluate the intricacies of each PS, including the presence of DNA binding, light-induced DNA damage, as well as cytotoxicity and photocytotoxicity of each compound in two cancer cell lines. A new technique to determine the mechanism of action (necrosis vs. apoptosis) of cell death was employed to assess its value as a potential screening procedure for PSs, and although it was informative, it was deemed impractical as a screening method. Results were used to judge which compounds should be further developed through the resource-intensive process of *in vivo* biological evaluation, leading eventually to human clinical trials. Several compounds deemed successful by *in vitro* experimentation have now been used in a PDT model in mice with varying degrees of success. As *in vitro* results do not necessarily predict *in vivo* activity, these results have been extremely important to improving methodology in our lab.

Notes:



Abstracts: Oral

1A-8 Trevor McGrath, Saint Mary's University

Kinetic and Computational Study of Palladium Complexation with an Ethylamine Diacetic Acid Substituted Imidazolium Hexafluorophosphate Salt

Trevor A. McGrath, Tyler Cuthbert, Robert D. Singer, and Cory C. Pye
Undergraduate Student, Department of Chemistry, Saint Mary's University

The synthesis of an imidazolium based task specific ionic liquid (TSIL) designed for complexation with palladium has led to an abnormal C4 metallated species. Formation of the C4 metallated species was found to proceed through a non-NHC palladium intermediate complex. The kinetics of the conversion from the non-NHC intermediate to the NHC species were studied via VT-NMR spectroscopy. The experimentally determined activation energy was then used to direct a computational study in an attempt to elucidate a mechanism of the conversion from the non-NHC to the NHC species.

Notes:



Abstracts: Oral

1B-1 Landon Hiscock, Memorial University

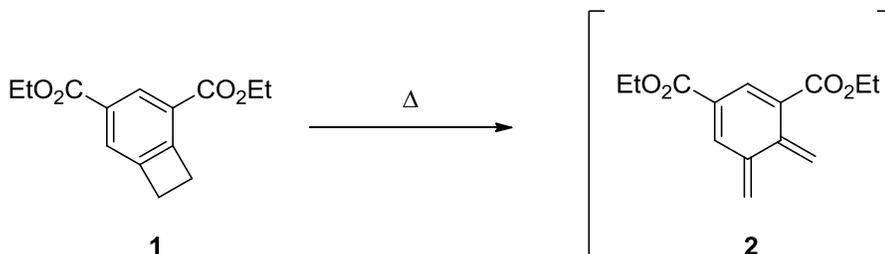
Synthesis of Benzocyclobutene-3,5-dicarboxylic Acid Diethyl Ester and its Attempted Use as an *o*-Xylylene Precursor

L. K. Hiscock and G. J. Bodwell

Undergraduate Student, Department of Chemistry, Memorial University

The ability to control the outcome of a reaction is an essential factor in the usefulness thereof. For a Diels-Alder (DA) type reaction, the regiochemistry of the cycloadduct is highly important, and through electronic biasing of the diene and dienophile, this can be controlled. Likewise in inverse electron demand Diels-Alder reactions (IEDDA), the regiochemistry can be controlled in a predictable manner. Often, this is done by placing electron-withdrawing or electron-donating groups at the 1,3-positions of the diene.^[1]

o-Xylylene is an extremely reactive diene, which would be expected to impart little regioselectivity to DA or IEDDA reactions due to its very high reactivity. To date, very little work has been published on the regioselectivity of these reactions. A common precursor to *o*-xylylenes is benzocyclobutenes, which can undergo a thermally allowed, electrocyclic reaction to afford the *o*-xylylene.^[2] The purpose of this study is to synthesize an electron-deficient benzocyclobutene (1), and utilize it as a source of *o*-xylylene 2 in IEDDA reactions to determine whether some control over regiochemistry can be imparted due to electronic bias. Additionally, the effect of electron-withdrawing substituents on the temperature of ring-opening for the benzocyclobutene compound will be discussed.



[1] Danishefky, S.; Kitahara, T. J. Am. Chem. Soc. 1974, 96, 7807-7808.

[2] Mehta, G. Tetrahedron 2001, 57, 626-654.



Abstracts: Oral

1B-2 Robie Hennigar, Acadia University

Photophysical Investigation of Coordination Complexes for Application in Photodynamic Therapy

R. Hennigar

Undergraduate Student, Department of Chemistry, Acadia University

Photodynamic therapy (PDT) is a mechanism for destroying unwanted cells that has been used clinically to treat cancer as well as age-related macular degeneration. PDT is unique in that it employs a relatively nontoxic drug that becomes active upon irradiation with light. Light absorption produces an excited state of the photosensitizer (PS) that is capable of participating in energy or electron transfer to create reactive species, such as cytotoxic singlet oxygen. Thus, PDT is inherently targeted by virtue of localized light delivery to only cancerous tissue saturated with PS. PDT can be optimized for a specific cancer through judicious choice of the PS, the light dose, and the protocol. Our laboratory combines approaches from biology, chemistry, and physics in order to create and improve photodynamic compounds (PDCs) derived from metal-containing coordination complexes. My research has focused on linking the effectiveness of the PDCs in cancer cells with the photophysical properties of the compound. By outlining the photophysical and photochemical properties of a given PDC, I am able to offer insight to the chemists on how to further optimize the compound for a specific photobiological application, thereby removing a lot of guess work. Using spectroscopic techniques we study the singlet oxygen generating capabilities, photostability, absorption characteristics, and emission properties of the compounds, and use this information to create a model of how the PDC operates in vitro and in vivo. Our efforts have resulted in several highly effective PDCs, including one of the first known stable near-IR PDCs.

Notes:



Abstracts: Oral

1B-3 April Woods, Memorial University

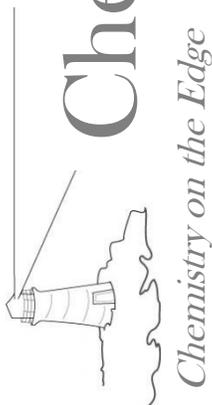
Thin-Film Molecularly Imprinted Polymers for the Detection of Caffeine in Surface Water

April Woods

Undergraduate Student, Department of Chemistry, Memorial University

With an increasing global population and trends towards urbanization, evaluation of the impact of our activities on the environment is of great importance. To do this, selected compounds can be used as markers for anthropogenic contamination. Due our prolific consumption of caffeinated beverages, pharmaceuticals and foods, and its remarkable, stability and persistence in the environment, caffeine is an ideal candidate for a marker of anthropogenic contamination. However, low detection limits are need for analysis of caffeine at environmentally-relevant concentrations, where contaminated surface waters often only have caffeine at low part-per-billion concentrations. Therefore, preconcentration is a necessary step for most analytical methods, and molecularly imprinted polymers (MIPs) are ideal for this endeavor. MIPs are solid sorbents that can be designed for selective uptake of target analytes, based on molecular recognition similar to that seem with enzymes. In this work, the optimization of the pre-polymer components and synthesis of MIPs is carried out to determine the most robust material with best selectivity and uptake performance. The optimal system used a template/monomer /cross-linker ratio of 1:4:8 and a ratio of pre-polymer components to porogen (solvent) of 1:2. This performance of this system was tested on caffeine-spiked and unspiked raw stream water, with detection by LC-MS As this MIP system effectively took-up caffeine from the spiked surface water sample, it is suitable for its intended purpose. No caffeine was detected in the unspiked surface water, indicating there is none present or it is below the limit of quantification of 0.11 ppm.

Notes:



Abstracts: Oral

1B-4 William Curry, Dalhousie University

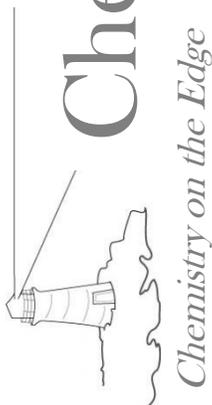
Antihypertensive Properties in Vitro of Phytochemicals in Haskap Berries

William L. Curry and H. P. Vasantha Rupasinghe

*Undergraduate Student, Department of Environmental Sciences, Faculty of Agriculture,
Dalhousie University*

Hypertension, which is caused by many factors, can lead to cardiovascular diseases such as stroke and acute myocardial infarction. Hypertension is mainly due to overstimulation of the Renin-angiotensin aldosterone system (RAAS) because of poor diet, age, obesity, genetics, smoking, alcohol consumption, life style and their combinations. Angiotensin-converting enzyme (ACE) is one of the key enzymes of RAAS. The main objective of this study was to determine the ability of phytochemical-rich extracts prepared from two haskap (*Lonicera caerulea* L.) cultivars to inhibit ACE activity in vitro in comparison with three other fruit extracts (cranberry, blueberry and blackcurrant). In addition, total phenolic (TP) and total flavonoid (TF) content of the extracts were analyzed. Data were analyzed using SAS for mean separation by Tukeys's method at P-value of 0.05. The results showed that percentage ACE inhibition was significantly different among type of berry and concentration of extract. Blackcurrant extracts being the most effective at most concentrations (99.7% inhibition at the two highest concentrations). There was a significant difference among type of berry for the amount of TP and TF within them. Blackcurrant had the greatest amount of TP within the berries (74.6 ± 0.63 μM galic acid equivalents/g fresh weight (FW)). The 'Tundra' haskap had the highest amount of TF (15.5 ± 0.16 μM quercetin equivalents/g FW). This suggests that some phytochemicals such as polyphenols in the extract might have a better ability to inhibit ACE in vitro. Further studies need to be conducted to identify these unique polyphenol constituents of these berries.

Notes:



Abstracts: Oral

1B-5 Hillary Wheeler, Acadia University

Development of an Atom Economical Method for Phosphenium Cation Synthesis

Hillary C. Wheeler and Bobby D. Ellis

Undergraduate Student, Department of Chemistry, Acadia University

N,C-bound dibromophosphine compounds were produced through the reaction of an aryl Grignard reagent with PBr_3 (Aryl substituent = Tripp = triisopropylphenyl / TerMes = 2,6-*bis*(2,4,6-trimethylphenyl)phenyl) and was characterized through ^{31}P NMR spectroscopy. Through a reaction with diisopropylamine, an *N,C*-bound monobromophosphine was formed which was also characterized by ^{31}P NMR spectroscopy. An attempt was made to produce phosphenium cations from these synthesized monobromophosphine compounds through halide abstraction by Lewis acidic Al_2Cl_6 to remove the remaining bromide anion, leaving a phosphorus(III) cationic centre still containing an aryl and amido substituents and a AlCl_3Br^- counter ion. The synthetic steps, including production of an aryl Grignard reagent, organolithium reagent, C-P bond formation, and amination, were successful until the halide abstraction in which a ^{31}P NMR peak was not observed at the expected chemical shift range of approximately 500 ppm. This multiple unexpected NMR peaks were indicative of moisture contamination of the reaction mixture.

Notes:



Abstracts: Oral

1C-1 Reem Karaballi, Saint Mary's University

Development of a SERS-based Aptasensor for Rapid Detection of Human Disease

Reem Karaballi, Andrew Nel, Jonathan Blackburn, and Christa L. Brosseau

Undergraduate Student, Department of Chemistry, Saint Mary's University

This project focuses on the development of a portable DNA-aptamer based aptasensor that would aid in the diagnosis of the highly contagious disease 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 0.0 to -1.0V. These experiments showed that DNA components can be detected using E-SERS. Several molecules were tested as possible choices for back-filling, in order to prevent surface denaturation of the DNA and to prevent non-specific binding. Signal was detected for the aptamer (referred to as probe 1). Hybridization studies between probe 1 and its complimentary sequence, target 1, were successful. These results indicate that a SERS-based aptasensor has great potential in the field of rapid diagnostics.

Notes:

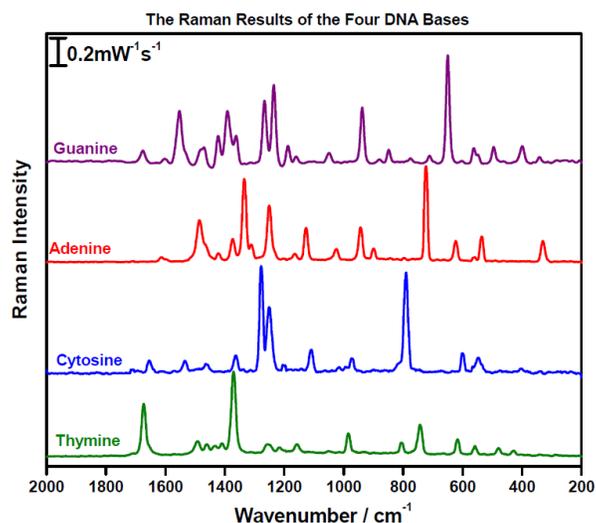


Figure 1. Normal Raman spectra of the four DNA bases.



Abstracts: Oral

1C-2 Brandon Fancy, Memorial University

Application of Ionic Liquids for Matrix-Assisted Laser Desorption Ionization Mass Spectrometry

Brandon Fancy and Christina Bottaro

Undergraduate Student, Department of Chemistry, Memorial University

Since their introduction, ionic liquids (ILs) have been lauded for their versatility as solvents, and for catalytic properties. More recently, use of ILs has been extended into the realm of matrix-assisted laser desorption ionization (MALDI) mass spectrometry (MS), where ionic liquid matrices (ILMs) have emerged as a new class tunable matrices that are suitable alternatives to traditional crystalline matrices. Many ILMs are based on the combination of equimolar amounts of a traditional crystalline MALDI matrix, such as β -cyano-4-hydroxycinnamic acid (CHCA) or 2,5-dihydroxybenzoic acid (DHB), with a suitable organic base. The resulting mixtures of anions and cations show many desirable features unique to ILs including exceptionally low vapour pressures, a range of viscosities, low melting points, etc., combined with the ability of a solid matrix to absorb the laser energy and promote desorption and ionization. Unlike crystalline matrices that lead to the inhomogeneous and irregular dispersion of an analyte, the most important benefit of ILMs is a noteworthy increase in sample homogeneity; providing better spot-to-spot and shot-to-shot reproducibility.

Several ILMs based on the combination of CHCA and DHB with a range of organic bases (1-methylimidazole, triethylamine, isoquinoline, acridine, or tributylamine) were synthesized and their suitability for detection and quantitation of caffeine, diclofenac, thiamine, and 2,4-dichloroacetic acid by MALDI-MS was evaluated. Two types of sample preparation were tested for each ILM with all analytes, and performance was evaluated on the basis of analyte signal strength and extent of spectral noise. In instances where promising results were seen, preliminary work was carried out to determine linearity of response necessary for quantitative analysis. In several instances ILM gave substantially fewer and less intense matrix peaks compared to their solid matrix counterparts.



Abstracts: Oral

1C-3 Julia Wright, Acadia University

Biological Activity of Extracts from *Polygonum Cuspidatum*

Julia Wright¹ and Sherri McFarland^{1,2}

Undergraduate Student, ¹Department of Biology and ²Department of Chemistry, Acadia University

Polygonum cuspidatum, more commonly known as Japanese knotweed, is an invasive species located throughout Nova Scotia. Although Japanese knotweed is viewed as an encroaching weed to the common gardener, it is of great scientific interest due to its phytochemical content. Japanese knotweed contains a variety of stilbenes and anthraquinones, including resveratrol and emodin, respectively. These phytochemicals display diverse biological properties, ranging from antioxidant to anti-inflammatory to anticancer activity. In fact, resveratrol has been implicated in a phenomenon known as the “French Paradox”, which correlates the low incidence of coronary artery disease in the French population to their consumption of red wine (of which resveratrol is a component). Emodin is currently being investigated in relation to Type 2 diabetes and for its ability to act as a neuroprotective agent. My research involves developing a proprietary method for producing Japanese knotweed extracts enriched in resveratrol or emodin, which give rise to interesting in vitro biological activity. These results will be discussed in my oral presentation.

Notes:



Abstracts: Oral

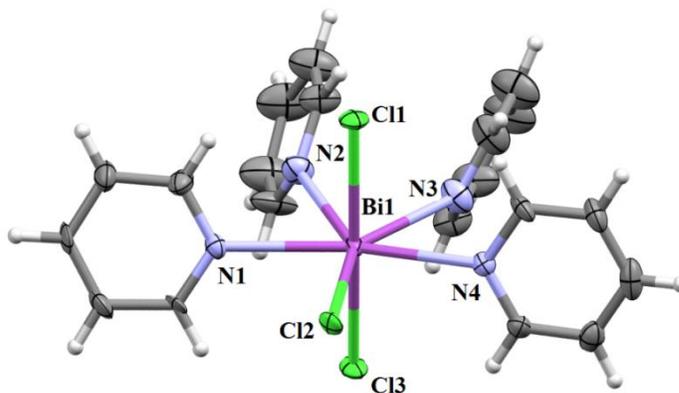
1C-4 Jennifer Murphy, Memorial University

Solving Novel Bismuth Complex Structures by Single Crystal X-ray Diffraction: Two Polymorphs of $\text{BiCl}_3 \cdot 4\text{py}$

J. N. Murphy, L. N. Dawe, and F. M. Kerton

Undergraduate Student, Department of Chemistry, Memorial University

Two polymorphs of $\text{BiCl}_3 \cdot 4\text{py}$ were synthesized of which crystals suitable for X-ray diffraction were grown. One polymorph, complex **C1** has a $Z'=1$ and the other polymorph, complex **C2** has a $Z'=4$. Complex **C1** has intra and intermolecular π - π stacking, complex **C2** shows no π - π interactions. There are eight solvent pyridine molecules in the lattice of complex **C2**, however, there is no pyridine solvent in the lattice of **C1**. The refinement of single crystal X-ray diffraction structures was completed using, modern, open-source, free crystallographic programs. The structures were solved using direct methods by SHELX through Olex2 software.



Notes:



Abstracts: Oral

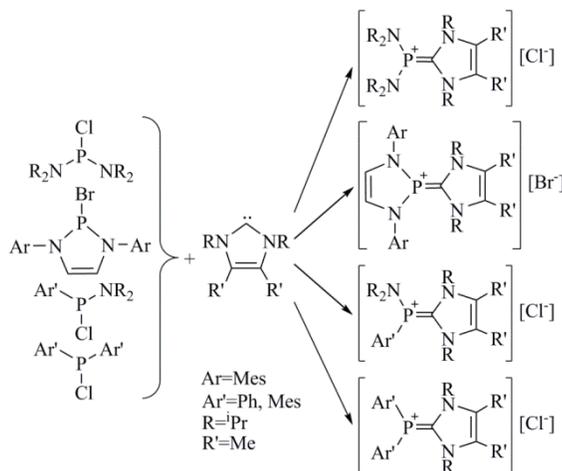
2A-1 Emily Fraser, Acadia University

Towards the Synthesis of Heavy Main Group Compounds with Asymmetric Double Bonds

E. Fraser and B. Ellis*

Undergraduate Student, Department of Chemistry, Acadia University

The multistep synthesis of asymmetric double bonds between heavy main group species is often a time-consuming process, as preassembled precursor molecules undergo base-promoted dehydrohalogenation to form the desired double bonds. A more general method to synthesize heavy main group asymmetric double bonds would be advantageous. In the current study, several N,N-bound halophosphine precursors and subsequent phosphonium cations were synthesized and characterized by ^{31}P NMR spectroscopy. N,C-bound and C,C-bound halophosphines were also synthesized and characterized. These compounds were then treated with an N-heterocyclic carbene in THF, in an attempt to form a compound with a heteronuclear double bond between phosphorus and carbon. All reactions with the carbene produced a colourless precipitate, in a filtrate which ranged in colour from yellow to red. The reactions with the carbene and the C,C-bound halophosphines showed the most potential in the formation of a compound with phosphorus-carbon bonds, as the $^{31}\text{P}\{1\text{H}\}$ NMR chemical shifts of the colourless precipitates appeared from -30 ppm to -50 ppm, which is consistent with reported values for related species, and were similar to values as predicted by DFT calculations. The reactions with the carbene and phosphonium cations were found to be least successful in forming P-C bonds, as the ^{31}P NMR chemical shifts of the filtrate suggested that the counter anion had been attacked by the carbene, regenerating the halophosphine precursors.





Abstracts: Oral

2A-2 Ashley Robinson, Saint Mary's University

Electrochemical-Surface Enhanced Raman Spectroscopy (E-SERS) of Uric Acid: A Potential Rapid Diagnostic Method for Early Preeclampsia Detection

Ashley Megan Robinson

Undergraduate Student, Department of Chemistry, Saint Mary's University

Preeclampsia, a hypertensive disorder that can occur during pregnancy and a leading cause of maternal death worldwide, can be characterized by an increase in uric acid in urine and plasma. This work presents the preliminary steps toward the development of a rapid tool for early diagnosis of preeclampsia, by detection of uric acid in urine using electrochemical surface-enhanced Raman spectroscopy (E-SERS). Uric acid samples were characterized using UV spectroscopy, cyclic voltammetry, Raman spectroscopy and E-SERS. It was found that E-SERS was capable of easily detecting uric acid at concentrations $< 1\text{mM}$ in urine stimulant. This demonstrates promise as a rapid point-of-care diagnostic tool for early onset preeclampsia in developing nation settings, as neither costly enzymes nor bulky equipment were required.

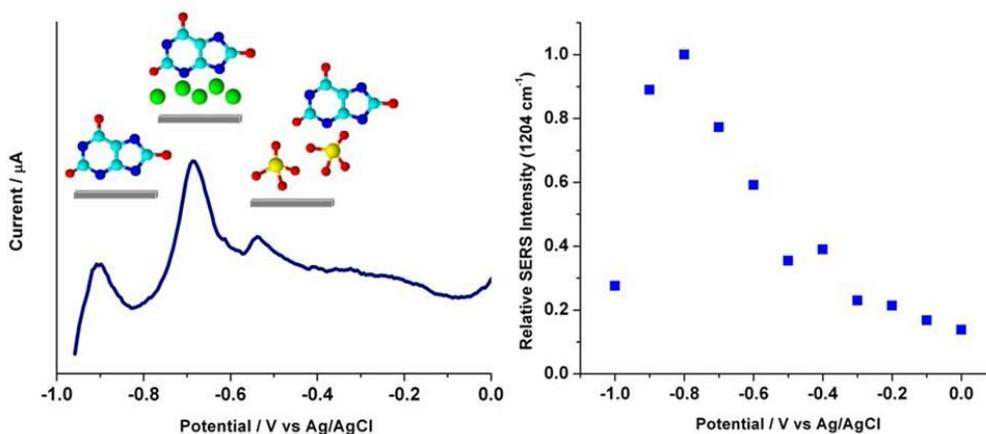
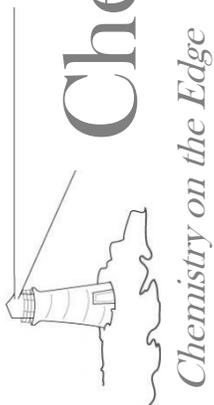


Figure 1. (a) CV signal of uric acid on the silver nanoparticle surface in the presence of chloride and citrate and (b) relative SERS intensity of the 1204 cm^{-1} band in the uric acid SERS signal against the applied potential.



Abstracts: Oral

2A-3 Mat Stephenson, Acadia University

Photophysical Investigation of DNA-intercalating Coordination Complexes as Photosensitizers for Photodynamic Therapy

Mat Stephenson and Sherri McFarland

Undergraduate Student, Department of Chemistry, Acadia University

Photodynamic therapy (PDT) has been used in the clinical treatment of several diseases, including certain cancers. PDT operates on the premise that the absorption of light by a photosensitizer (PS) promotes the PS to an excited state where it can participate in electron or energy transfer, producing reactive species (e.g. cytotoxic singlet oxygen) that destroy unwanted cells. Localized light delivery to targeted cells that contain the PS offers a minimally invasive form of treatment. PDT can be optimized for a specific disease by altering the PS, light dose/wavelength, and the treatment protocol. Our laboratory group develops inorganic PSs for PDT, evaluating their effectiveness against cancer cells growing in culture and probing their excited state properties using spectroscopic methods. My research involves the determination of (i) photostability, (ii) absorption and emission characteristics, and (iii) singlet oxygen yields of these PSs. The spectroscopic information obtained is used to construct a photophysical profile of a given PS that explains the photobiological events that are triggered by these compounds when they absorb light. My input is very important to the design of new PSs in our laboratory group.

Notes:



Abstracts: Oral

2A-4 Chris Lavoie, Saint Mary's University

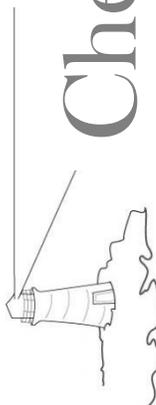
The Synthesis of Task Specific Ionic Liquids for Asymmetric Catalysis

Chris Mark Lavoie, Christine Prudhoe, and Robert D. Singer

Undergraduate Student, Department of Chemistry, St. Mary's University

Salen ligands and their corresponding complexes are well known in the field of asymmetric catalysis due to their success in stereoselective reactions. A method that easily allows for recycling of the catalyst without degradation of catalytic activity would make them more industrially viable. The generation of a Task Specific Ionic Liquid (TSIL) by attaching tributylphosphonium moieties to Jacobsen's ligand could promote the entrainment of the catalyst in an ionic liquid (IL). This would potentially create a recyclable system where the desired product can be extracted, leaving the IL/catalyst layer behind ready for reuse. The racemic and asymmetric versions of the ligand, 5,5'-(1E,1'E)-(cyclohexane-1,2-diylbis(azan-1-yl-1-ylidene))bis(methan-1-yl-1-ylidene)bis(3-tert-butyl-4-hydroxy-5,1-phenylene)bis(methylene)bis(tributylphosphonium) hexafluorophosphate, as well as their respective copper complexes were successfully synthesized and characterized. These were applied to aziridinations of styrene, using tosyliminophenyl iodine (PhINTs) as a nitrene source, in both acetonitrile and three different ILs. Acetonitrile generated yields of up to 88%, however no product was extracted from 1-butyl-3-methylimidazolium hexafluorophosphate, tetradecyl(trihexyl)phosphonium hexafluorophosphate and chloride.

Notes:



Abstracts: Oral

2A-5 Brandon Furlong, Memorial University

An Introduction to Raman Spectroscopy

Brandon Furlong

Undergraduate Student, Department of Chemistry, Memorial University

Raman spectroscopy is very useful in determining information such as the types of molecules present, and the structure of inorganic solids. One disadvantage of Raman spectroscopy is low signal. Surface Enhanced Raman Spectroscopy (SERS) is the amplification of Raman signals by several orders of magnitude due to the electromagnetic interaction of light with metals. The main metals used to make SERS films are the Noble Metals (gold, silver and copper). They are primarily used in SERS because found within the visible range of light, which is the common range of wavelengths use for Raman excitation. In this talk, I will discuss the advantages and disadvantages of these metals, as well as some real world applications of SERS. I will also compare plastic and glass as substrates for SERS films in sensing devices.

Notes:



Abstracts: Oral

2A-6 Alex Chase, Acadia University

Substituent Effects on the Reaction Rates of Photogenerated Quinone Methide: Applications in the Development of Novel Photolabile Protecting Groups

Alex Chase and Dr. Matthew Lukeman

Undergraduate Student, Department of Chemistry, Acadia University

The synthesis, isolation, purification, and photochemical study of two target compounds was successfully achieved. The first compound synthesized was 2-(1-hydroxycyclohexyl)phenol 69, designed to generate a cyclohexyl-fused quinone methide (QM) upon photolysis. 69 was synthesized via a one-pot reaction sequence on 2-bromophenol. Attempts to synthesize 70 and 71 via this route, however, were unsuccessful. Following purification, the photoreactions of 69 proceeded smoothly in aqueous methanol and acetonitrile. The expected QM was generated efficiently with a quantum yield of ~ 0.5 . It was then observed directly via laser flash photolysis (LFP) and displayed absorbance maxima at 290 and 400 nm with lifetimes of ~ 0.9 ms in aqueous acetonitrile and ~ 0.5 ms in aqueous methanol.

The second compound synthesized was the cyclic acetal of the photolabile protecting group 2-naphthol (78). This was designed to release 1,3-propanediol upon irradiation in hopes of future release of polyhydroxyl compounds, such as carbohydrates. This synthesis involved a three-step procedure followed by column chromatography. The photoproducts were analyzed by ^1H NMR, UV-Vis, and GC-MS. Photolysis of 78 in aqueous methanol afforded the clean release of the caged diol without undesired by-products as indicated by the GC-MS data and the clean isosbestic points in the UV-Vis spectra. Quantum yield studies indicated that photorelease proceeded with $\sim 10\%$ efficiency. Furthermore, the caging process proceeded cleanly at room temperature with good isolated yields ($>80\%$). 78 was also studied with LFP and a transient intermediate was detected with an absorbance maximum of 310 nm and a lifetime of 12.5 ms in aqueous acetonitrile.



Abstracts: Oral

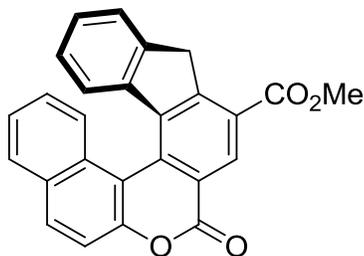
2B-1 Tiffany Tozer, Memorial University

The Synthesis of Heterohelicenes Using Inverse Electron Demand Diels-Alder Chemistry

Tiffany Tozer and Graham J. Bodwell*

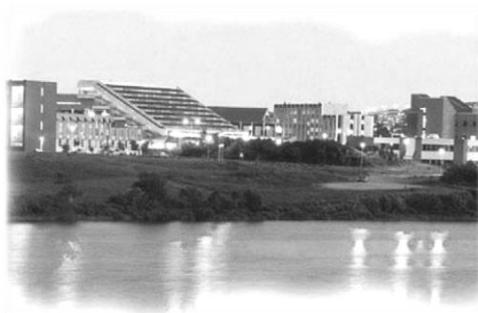
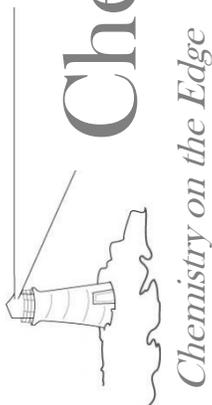
Undergraduate Student, Department of Chemistry, Memorial University

Heterohelicenes are chiral helically shaped aromatic compounds that possess interesting properties due to their unique structure. In this work, heterohelicenes were produced via a domino reaction consisting of Knoevenagel condensation, transesterification, inverse electron demand Diels-Alder cycloaddition, 1,2-elimination, and transfer hydrogenation. The key reaction of this process, hallmark chemistry of the Bodwell group, is the IEDDA reaction which involving a dienophile, an enamine with an electron donating group, and a diene with electron withdrawing groups in the 1 and 3 positions. This methodology was previously used by our group in the synthesis of 6H-dibenzo[*b,d*]pyran-6-ones^[1]. This reaction can be performed in two manners: by using enamines generated *in situ* or by using preformed enamines. Both of these techniques were employed in a series of reactions to synthesize and examine the properties of some five and six ring heterohelicenes.



[1] Pottie, I. R.; Nandaluru, P. R.; Benoit, W. L.; Miller, D. O.; Dawe, L. N.; Bodwell, G. J. *J. Org. Chem.* 2011, 76, 9015.

Notes:



Abstracts: Oral

2B-2 Heidi Kavanagh, Memorial University

Carbon Substrate Utilization by Microbial Methanogens at Active Sites of Serpentinization: Tablelands Ophiolite, Newfoundland and Cedars Complex, California

Heidi Kavanagh and Penny L. Morrill

Graduate Student, Department of Earth Sciences, Memorial University

The goal of this study was to determine if there was a potential for active microbial production of methane in ultra-basic reducing springs at two sites of present-day serpentinization, the Tablelands, NL and The Cedars, CA. The Tablelands in Gros Morne National Park, Newfoundland, is an ophiolite thought to have been obducted during the closing of the Iapetus Ocean several hundred million years ago. The Cedars in California is a section of a peridotite body that was obducted as part of the Franciscan Subduction Complex and is also part of California's Coast Ranges. These sites are relatively barren due to their lack of usual nutrients, low levels of calcium, high concentration of magnesium and toxic amounts of heavy metals. They contain the extreme environment of active serpentinization, low-temperature oxidation and hydrolization of ultramafic rocks into serpentine, with anoxic conditions that include elevated pH, dissolved H_2 and low redox potential (Eh) values. Serpentinization provides an environment amenable to the abiogenic and biogenic production of CH_4 . Serpentinization is suspected to have occurred on Mars, which is why the Tablelands and The Cedars are considered Mars analogue sites.

In the laboratory ^{13}C labeled substrate experiments were performed to determine if microbial methanogens were present and what carbon source(s) they may use. ^{13}C -labeled organic acids (formate, acetate and propionate) and bicarbonate were added to water and sediment collected from the most basic and reducing spring. The ^{13}C labeled acetate experiment showed the methyl carbon produced CH_4 and the carboxyl carbon produced CO_2 at both sites. This study demonstrated that heterotrophic microbial methanogens are present in the ultra-basic springs and, if acetate is present, they may produce microbial methane using an acetotrophic metabolic pathway.



Abstracts: Oral

2B-3 Chuan Xu, Memorial University

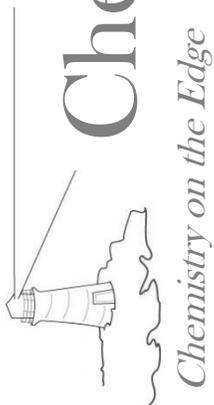
Mechanical Properties of Atomic Force Microscope Cantilever

Chuan Xu

Graduate Student, Department of Chemistry, Memorial University

Atomic force microscopy (AFM) is widely used in materials characterization. In an AFM, a sharp tip is brought to the sample surface and the interaction between them is recorded to generate AFM images and force curves. The tip-sample interaction is determined by the detection of a cantilever to which the tip is attached. Hence the AFM image and force curve quality greatly depend on the cantilever mechanical properties (e.g. resonant frequency and spring constant). A better understanding of the cantilever mechanical properties is beneficial for AFM data interpretation. The ability to predict these mechanical properties is essential for AFM cantilever design, fabrication. Finite element and analytical methods were applied to determine the AFM cantilever mechanical properties. The results are consistent with the experimental data.

Notes:



Abstracts: Oral

2B-4 Tariq Sainuddin, Acadia University

Development of Inorganic Photosensitizers for Photodynamic Therapy

T. Sainuddin and S. A. McFarland

Graduate Student, Department of Chemistry, Acadia University

Metal complexes play a significant role in cancer therapy, specifically metals like platinum (e.g., cisplatin and carboplatin), whereby alteration of DNA secondary structure leads to cell death. Such approaches in cancer therapy, while arguably successful in treating many primary cancers, often lead to debilitating side effects and sometimes secondary cancers due to the high systemic toxicity of the drug. An alternate strategy for using metal-based drugs in cancer therapy employs a nontoxic drug, called a photosensitizer (PS), which can be activated with light to destroy tumours. This approach is called photodynamic therapy (PDT), and current PS for PDT are derived from organic compounds that require molecular oxygen to function. Herein we explore the use of metal-based compounds as agents for PDT by evaluating the photosensitizing abilities of a number of constructs against human leukemia cells growing in culture. Metal complexes offer a number of distinct advantages over their organic counterparts, including: long-wavelength absorption with high extinction coefficients, Type I and Type II photosensitization mechanisms, water solubility, synthetic ease and tunability, and others. Particular emphasis will be placed on a comparison of mononuclear and dinuclear PSs in an effort to obtain larger absorption cross-sections and higher photoreactivity in the multimetallic systems, and these results will be discussed in the context of PDT.

Notes:



Abstracts: Oral

2B-5 Shaheen Fatima, Memorial University

Predicting and Understanding Non-Linear Optical (NLO) Properties in Organic Molecules

Shaheen Fatima, Muyi Xu, and Erika Merschrod

Graduate Student, Department of Chemistry, Memorial University

The materials with large NLO properties are useful in telecommunications, optical switching and data processing. In designing and developing nonlinear optical materials, labor, facilities and time are needed, which sometime hampered by uncertain results. A Computational approach of designing and predicting properties of materials have been proved very effective in saving time and energy. In last two decades quantum mechanical techniques have proved very useful in improving the hyperpolarizabilities via rational designing of the NLO systems. We have developed several design principles to enhance NLO properties of π -conjugated organic systems, through variations within the π -conjugated systems and through the addition of Donor-Acceptor (D-A) groups. More generally, we have identified simple predictors for strong NLO response, developing geometric structure and NLO properties relationships that could be used to synthesize organic opto-electronics materials with large β and γ values.

Notes:



Abstracts: Oral

2C-1 Greg Curtis, Memorial University

Task-Specific Ionic Liquids for CO₂ Utilization

Greg Curtis

Graduate Student, Department of Chemistry, Memorial University

As the petroleum energy industry begins the shift to cleaner burning natural gas in various forms (shale gas, bio-gas & FT-synthesis gas) there is more need than ever to utilize CO₂ emissions. The development of recyclable catalytic materials for transformations of CO₂ is important in this regard, especially if the principles of green chemistry are employed in their preparation. Such catalysts could find use in polycarbonate synthesis and cyclic carbonate production for lithium-ion battery electrolytes.

The research I am carrying out involves the conversion of amino-carbohydrates in water into a more functionalized intermediate compound. I am currently attempting to use this as a reagent with amino acids for the production of organic task-specific ionic liquids. At the same time, I am preparing a chitosan-derived mesoporous carbon material to be used with the ionic liquid to give a supported ionic liquid catalyst. The catalyst will then be employed for cyclization-dehydration reactions involving CO₂ and glycerol for the production of glycerol carbonate.

Notes:



Abstracts: Oral

2C-2 Maryam Moghaddam, Memorial University

IRMPD Spectroscopic Study of Solvated $[\text{Na}(\text{AlaGly})]^+$, $[\text{Na}(\text{GlyAla})]^+$, $[\text{Ca}(\text{AlaGly-H})]^+$ and $[\text{Ca}(\text{GlyAla-H})]^+$ Complexes in the Gas Phase

Maryam B. Moghaddam and Travis D. Fridgen

Graduate Student, Department of Chemistry, Memorial University

Metal ions play important roles in biological function of proteins. Amino acids and peptides are the building blocks of proteins. So in order to understand the detailed activities of proteins, it is necessary to first study their smaller components, amino acids and peptides as well as their complexes with metal ions. In this study, the structures of $[\text{Na}(\text{GlyAla})(\text{H}_2\text{O})]^+$ and $[\text{Ca}(\text{GlyAla-H})(\text{H}_2\text{O})_n]^+$, ($n = 1, 2, \text{ or } 3$) solvated ion-molecule complexes (as well as the AlaGly isomers) were investigated using infrared multiple photon dissociation (IRMPD) spectroscopy and computational methods. IRMPD results and electronic calculations showed that in all clusters, a water molecule was directly bound to the metal ion. The spectra for all $[\text{Ca}(\text{GlyAla-H})(\text{H}_2\text{O})_n]^+$ complexes were absent of the carboxylic acid O-H stretch whereas for $[\text{Na}(\text{AlaGly})(\text{H}_2\text{O})]^+$ a band appeared which corresponds to carboxylic O-H stretching region. A strong band between 3300 and 3400 cm^{-1} related to the amide N-H stretch was observed to be significantly red-shifted compared to a normal amide N-H stretch, indicative of hydrogen bonding. The hydrogen-bonded amide N-H stretching feature showed a blue-shift upon addition of each water in Ca^{2+} clusters.

Notes:



Abstracts: Oral

2C-3 Martin Sichinga, Acadia University

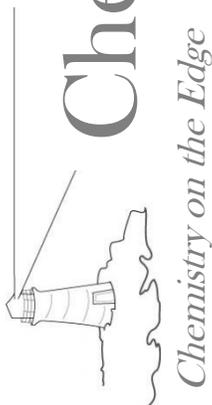
Aerobic Biotreatment of Oil-laden Water Using Integrated Membrane Bioreactor Technology

Martin C. Sichinga, Avik J. Ghoshdastidar, and Anthony Z. Tong*
Graduate Student, Department of Chemistry, Acadia University

Oil pollution is one of the most common point and non-point sources of water pollution, and it is mainly present as an oil-water emulsion, which cannot effectively be treated by a conventional gravity separator. Petroleum oil is a complex mixture of aliphatic and aromatic hydrocarbons, including n-alkanes and polycyclic aromatic hydrocarbons (PAHs). 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 focuses on the treatment of petrogenic hydrocarbons in water using membrane bioreactor (MBR) technology. Petroleum hydrocarbons are biologically degraded to simpler, less toxic inorganics and microbial biomass followed by membrane filtration with nano-sized pores. Industrial oily wastewater with mixed fractions of hydrocarbons was collected and continuously treated for 85 days. MBR effluent samples were analyzed daily for various hydrocarbons using gas chromatography–mass spectrometry (GC-MS). Other important water quality parameters such as dissolved oxygen, pH and bacterial population were also closely monitored. An effective treatment method was developed in this research to decontaminate oil-laden water for safe discharge or reuse.

Notes:



Abstracts: Oral

2C-4 Muyi Xu, Memorial University

Molecular Dynamic Simulation of Mica Structure

Muyi Xu and Erika Merschrod

Graduate Student, Department of Chemistry, Memorial University

Mica has a layered silicate sheet structure and is widely used as a substrate for imaging biological samples. Experimentally we have observed protein alignment on the mica surface in register with underlying crystal directions. In particular, we apply molecular dynamics (MD) calculations to investigate whether the mica substrate affects ordering of the ions in fluid or environmental water. Our calculations show that ion arrangements on the mica surface play an important role in water pattern formation.

In this way, the nano-scale crystallographic reconstruction of the mica surface might be able to translate into a micro-scale pattern for protein alignment. For future runs, protein (peptide) will replace water molecules and add into the system of interests. Ions and protein reorganization will be checked to match experiment results.

Notes: _____



Abstracts: Oral

2C-5 Stefana Egli, Memorial University

Novel Molecularly Imprinted Polymeric Films for Highly Sensitive and Selective Detection of Polycyclic Aromatic Hydrocarbons in Aqueous Environments

Stefana N. Egli and Christina S. Bottaro

Graduate Student, Department of Chemistry, Memorial University

In a quest for new, more efficient sampling and monitoring techniques for aquatic pollutants associated with oil and gas production, we developed new molecularly imprinted polymers (MIPs) in thin-film format for analysis of low concentrations of polycyclic aromatic hydrocarbons (PAHs) in water. Since this is a large class of compounds, the analytes studied were PAHs with ring numbers ranging from two to four; these were chosen to represent a range of commonly occurring and abundant PAHs. Optimization of the polymerization process to achieve better selectivity and optimal phase separation was carried out resulting in novel MIPs using toluene as a pseudo-template, 4-vinyl pyridine as functional monomer, ethylene glycol dimethacrylate as cross-linker, 2,2-dimethoxy-2-phenylacetophenone as initiator. Binding assays showed a superior selectivity of the novel MIPs over the non-imprinted materials and linearity for both types of materials over a 10-100 $\mu\text{g L}^{-1}$ concentration range. In the method, the MIP was used for uptake of PAHs from aqueous solution; the bound PAHs were extracted into a small amount of organic solvent, and analyzed by GC-MS in selected ion monitoring (SIM) mode. Sensitivity down to 18 ng L^{-1} for naphthalene was achieved. We found that other non PAH compound could interfere to a certain extent in the uptake of PAHs, however uptake in real waste water samples was possible. The performance characteristics of these materials suggest that this system could be integrated into a microfluidic device for use in on-site monitoring approaches.

Notes:



Abstracts: Oral

2D-1 Pasha Majidi, Memorial University

Oxidation of Ethanol Under Potential Scanning

Pasha Majidi and Peter G. Pickup

Graduate Student, Department of Chemistry, Memorial University

The electrochemical oxidation of ethanol is currently considerable as a good and new energy source. Moreover, this electrochemical reaction can be used as an alternative fuel for fuel cells. The CO_2 is the major product of the complete ethanol oxidation.

In this work a carbon dioxide monitor has been used to measure the amount of CO_2 produced from the oxidation of ethanol in a direct ethanol fuel cell. During the oxidation of ethanol, adsorbed CO accumulates on the surface of the Pt (anode) electrode. Linear sweep and cyclic voltammetry in combination with the CO_2 monitor can be used to investigate its oxidation CO_2 . The periodic oxidation of adsorbed CO increases the CO_2 yield and so can increase the efficiency of the direct ethanol fuel cell.

Linear sweep experiments – As seen in fig. 1, curve a, is Stripping of CO from the anode by a linear sweep while monitoring CO_2 concentration in the fuel cell exhaust resulted in only a transient production of CO_2 , even when the potential was held at the upper limit of +0.9V for an extended period. This procedure leads to oxidation of adsorbed CO to CO_2 , but negligible sustained ethanol oxidation.

Cyclic voltammetry experiments – In contrast, it has been found that with cycling voltammetry, the CO_2 produced increased significantly and was sustained for the duration of the potential cycling period (Fig. 1, curve b). Thus CO that is stripped from anode at high potential by ethanol adsorption and partial oxidation.

Additional results obtained over a range of temperature and with a variety of anode catalyst will be presented.

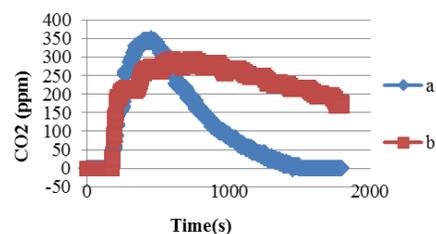


Figure 1. CO_2 (ppm) vs. Time (s) curve for (a) linear sweep experiment (b) cyclic voltammetry experiment in a direct ethanol fuel cell with 0.1M ethanol in anode and N_2 at cathode.

[1] A. Ghuman and P.G. Pickup, *Journal of Power Source*, 2008, **179**, 280-285.

[2] R.M. Moghaddam, P.G. Pickup, *Electrochemistry Commun.*, 2011, **13**, 707-706.

[3] S. Rousseau, C. Coutanceau, C. Lamy, J. M. Leger, *Journal of Power Source*, 2006, **158**, 18-24.



Abstracts: Oral

2D-2 Robert Di Lorenzo, Memorial University

Method Development for the Analysis of PFAs in Atmospheric Particulate Matter by GC-MS

Robert Di Lorenzo and Cora Young

Graduate Student, Department of Chemistry, Memorial University

Perfluorinated acids (PFAs), more specifically perfluorinated carboxylic acids (PFCAs) and perfluorinated sulfonic acids (PFSAs) are common analytes for environmental study due to their potential health effects, propensity for bioaccumulation, chemical persistence and ubiquitous presence in biological and environmental matrices. Not only are certain congeners of PFAs of industrial relevance, they are also degradation products of a suite of industrially produced fluorinated surfactants and polymers. Arctic contamination of PFAs is of particular concern, since their primary mode of transport has yet to be confirmed. Although oceanic transport of PFAs and gas phase transport of volatile PFA precursors has been investigated, the role of atmospheric particulate matter on the global dissemination of PFAs is unknown.

Traditionally, PFAs are quantified in various matrices by liquid chromatography (LC) coupled to tandem mass spectrometry (MS/MS) but these analyses usually require extensive sample preparation and clean-up. We will describe recent efforts to develop a simple yet rigorous analytical method for the part-per-billion level quantification of PFAs in atmospheric particulate matter by gas chromatography–mass spectrometry (GC-MS). This is achieved through the optimization of a simple liquid-liquid extraction followed by benzyl esterification of the native PFAs before injection onto the GC column. This method not only allows for rigorous and sensitive quantification of PFAs, but allows for the simultaneous analyses of the relevant volatile PFA precursors. Preliminary results and analytical verification will be discussed.

Notes:



Abstracts: Oral

2D-3 Saleh Riahi, Memorial University

Study of the Dynamics and Structure of H₂S

Saleh Riahi and Christopher N. Rowley

Graduate Student, Department of Chemistry, Memorial University

Hydrogen sulfide (H₂S) is one of the most important contaminants in crude oil and natural gas due to its corrosivity and toxicity. Molecular dynamics is a powerful tool for developing new chemical processes to manage H₂S, providing data that are difficult to obtain experimentally. Existing non-polarizable models are ineffective for some properties, such as the molecular dipole moment, dielectric constant, and hydration free energy. These errors reflect the neglect of induced electronic polarization in these models, which is problematic in highly polarizable molecules like H₂S. We have developed a polarizable force field for H₂S based on the Drude model. This model was designed to be analogous to the SWM4-NDP water model, with 3 charged atomic centers, a charged lone pair site on < HSH bisector, and a charged Drude particle harmonically tethered to the S atom. We parameterized this model to reproduce the bulk density, enthalpy of vaporization, and dielectric constant of liquid H₂S at 212 K and 1 atm. This model is in very good agreement with the experimental density, enthalpy of vaporization shear viscosity, and diffusion coefficient over the temperature range of 212-298 K. The radial distribution function calculated using this model is in good agreement with those determined using neutron diffraction and *ab initio* molecular dynamics. These calculations confirm that hydrogen bonding is transient and the liquid behaves as a simple, hard-sphere-like fluid rather than an associated liquid like its chemical analogue, water.

Notes:



Abstracts: Oral

2D-4 Qing He, Memorial University

Synthesis of Cyclic Carbonates from CO₂ and Epoxides with Cobalt(II) Deep Eutectic Solvent

Qing He and Francesca M. Kerton

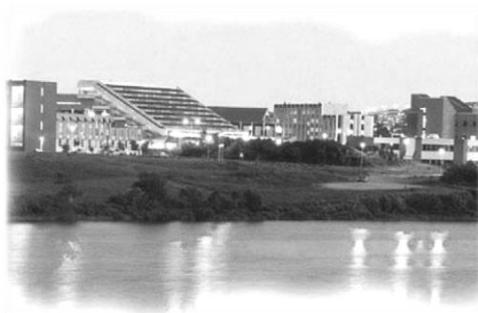
Graduate Student, Department of Chemistry, Memorial University

Utilization of carbon dioxide as a cheap, widely available and non-toxic feedstock for chemical production is currently an important area of research.^[1] A deep eutectic solvent (DES) formed by choline chloride (ChCl) and cobalt chloride hexahydrate is an effective catalyst for the coupling reaction of CO₂ with epoxides. A DES is a type of ionic liquid, which has a low melting point near room temperature.^[2] It is easily prepared, air/moisture insensitive and environmentally benign. Physical properties of the DES depend on the ratio of the two components from which it is prepared. Thermal characteristics (TGA and DSC data) of the DES will be presented. The DES catalyzes the coupling reaction of CO₂ with epoxides under mild (e.g. 10 bar and 100 °C) and solvent-free conditions. ¹H NMR spectra and GC-MS confirmed product formation, high reaction selectivity and good yields. The effects of reaction parameters like temperature, CO₂ pressure, reaction time and DES of different ratios will be presented.

[1] North, M.; Pasquale, R.; Young, C.; *Green Chem.*, 2010, 12, 1514.

[2] Abbott, A. P.; Barron, J. C.; Ryder, K. S.; and Wilson, D. *Chem. Eur. J.*, 2007, 13, 6495.

Notes:



Abstracts: Oral

2D-5 Zaher Algharaibeh, Memorial University

Charge Trapping in Poly(1-amino-anthraquinone) Films

Zaher Algharaibeh

Graduate Student, Department of Chemistry, Memorial University

Electroactive polymers containing anthraquinone functionality [1–4] are of interest in diverse fields, ranging from oxygen reduction [5–8] to charge storage in batteries [9,10] and supercapacitors [11–14]. Poly(1-amino-anthraquinone) films were prepared by potentiodynamic electrochemical polymerization of 1-amino-9,10-anthraquinone in 6 M $\text{H}_2\text{SO}_4(\text{aq})$. Cyclic voltammetry of these films in a monomer-free 6 M $\text{H}_2\text{SO}_4(\text{aq})$ have shown unusual electrochemical behaviour of anthraquinone. The reduction peak of anthraquinone was observed at the expected formal potential (i.e. -0.1 V vs. SCE) while the oxidation peak was unexpectedly shifted to much higher potentials (i.e. 0.36 V vs. SCE) even at 5 mV s^{-1} . This trapping of the quinone in its reduced state can be explained by an increase in the resistance of the film as the poly-aniline backbone is reduced as indicated by impedance spectroscopy.

Notes:



Abstracts: Posters

P1 Dalal Alhashmi, Memorial University

Synthesis and Characterization of Cobalt Amine-bis(phenolate) Complexes and Their Catalytic Activity in Polymerization

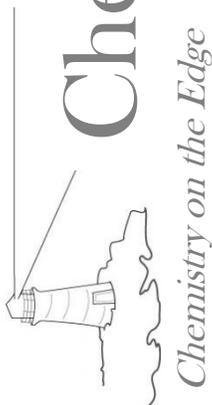
Dalal Alhashmi and Francesca M. Kerton*

Graduate Student, Department of Chemistry, Memorial University

The use of CO₂ as an ideal, renewable, abundant, cheap feedstock has received much attention within the scientific community. CO₂ may offer alternative routes to industrially useful organic compounds that are normally derived from fossil fuel resources. Considerable interest has focused on the coupling reaction between CO₂ and epoxides to form cyclic carbonates or polycarbonates. Transition metal complexes supported by tetradentate amine-bis(phenolate) ligands have recently been used in catalyst systems for the conversion of CO₂ because they offer greater flexibility in their steric and electronic characteristics. In terms of cobalt chemistry, cobalt complexes of salen ligands have been used to copolymerize CO₂ with epoxides and their performance exhibits high activity and selectivity for this chemical fixation to produce polycarbonates. Monometallic Co(II)/(III) complexes of tripodal amine-bis(phenolate) ligands have been effective in the coupling of CO₂ with propylene oxide under neat reaction conditions.^[1] My research involves the characterization of bimetallic cobalt complexes, based on tetradentate amine-bis(phenolate) ligands, using MALDI-TOF mass spectrometry, NMR and X-ray diffraction and exploring their catalytic activity towards the reaction of CO₂ and epoxides.

[1] L. N. Saunders, N. Ikpo, C. F. Patten, U. K. Das, L. N. Dawe, C. M. Kozak, F.M. Kerton, *Catalysis communications*, 2012, 18, 165.

Notes:



Abstracts: Posters

P2 Kerri Burton, Memorial University

Optimizing Pre-Polymerization Composition for PAH MIPs

Kerri Burton and Christina Bottaro

Graduate Student, Department of Chemistry, Memorial University

Many potentially harmful compounds can be released into the environment from nearby industrial facilities. Polycyclic aromatic hydrocarbons (PAHs) are organic compounds with two or more fused aromatic rings, and may serve as a reasonable proxy for many such substances. They are produced from the incomplete combustion of organic fuels such as oil, coal, and tar, and many are known carcinogens, mutagens, and teratogens. The purpose of this study was to optimize the composition of molecularly imprinted polymers (MIPs) to selectively uptake specific analytes from an aqueous mixture, and analyze the extracts by GC-MS. Thin-film MIPs were produced using toluene as the template, 4-vinyl pyridine as the monomer, and ethylene glycol dimethacrylate as the crosslinker. The compounds examined in this study were naphthalene, phenanthrene, fluorene, and pyrene, all of which can be taken up using the toluene template. This poster will present and compare the results of different polymer compositions on the selective uptake of PAHs. Potential applications for this method include monitoring contaminants in the water around oil rigs and mining effluent ponds, and it may one day be incorporated into microfluidic devices for faster and more efficient online analysis.

Notes:



Abstracts: Posters

P3 Hua Chen, Memorial University

Synthesis of Cr Complexes of Amine-bis(phenolate) Ligands for Polymerization Catalysis

Hua Chen and Christopher M. Kozak*

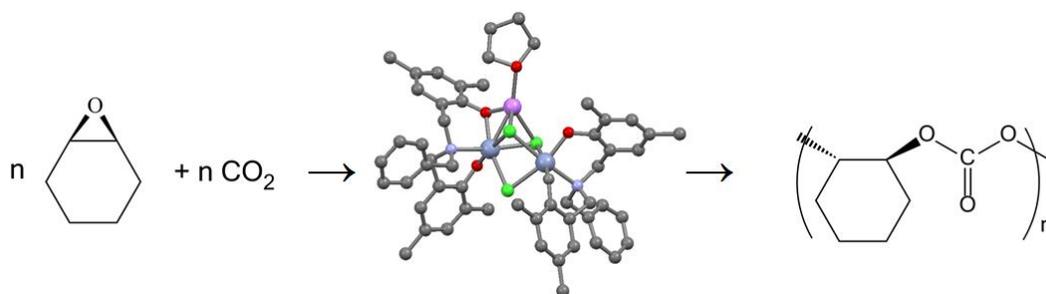
Graduate Student, Department of Chemistry, Memorial University

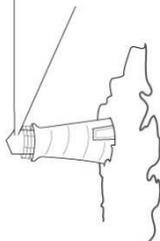
Amine-bis(phenolate)-donor ligands are an important class of potentially tetradentate and tridentate ligands capable of coordinating to a variety of metals.

These ligands are versatile in that they may be easily modified both sterically and electronically by changing the nature of the pendant donor group as well as the substituents on the phenol fragment.

Cr(III) complexes of related salen ligands have been extensively studied as polymerization catalysts and shown excellent activity towards CO₂/epoxide copolymerization. (Darensbourg D.J. *Inorg Chem.* **2004**, *43*, 1831-1833) Therefore, we sought to prepare highly active Cr(III) catalysts for synthesis of polycarbonates.

The synthesis and characterization of new amine-bis(phenolate) chromium(III) complexes and their activity as catalyst for the copolymerization of CO₂ with epoxides to give polycarbonates will be presented.





Abstracts: Posters

P4 Shawna Corcoran, Cape Breton University

Controlled Grafting of N-Heterocyclic Carbene Monomers within the Pore Walls of Large Pore Silica-Based Materials

Shawna Corcoran and Stephanie MacQuarrie*

Undergraduate Student, Department of Chemistry, Cape Breton University

Recently N-heterocyclic carbenes have been used in organocatalytic reactions, however they cannot be adopted for industrial purposes yet as unacceptably high catalyst loadings are required for reasonable reaction rates. These high catalyst loadings lead ultimately to more expensive, environmentally harmful processes that require large amounts of solvents for purification and separation of the final products. There is extensive need for heterogeneous, large pore (2-50nm) materials composed of organic catalysts for use as greener alternative organocatalysts. This research project is directed towards the synthesis of these materials specifically through the preparation and comprehensive characterization of highly organized functionalized mesoporous (2-50nm) materials composed of N-heterocyclic carbene (NHC) skeletons. The advantages of such functionalized materials are their reusability as heterogeneous catalysts, thermal and chemical stability and simple synthesis by a modular approach. The mesoporous organic-inorganic hybrid materials (PMOs) that are prepared result in improved diffusion and enantioselectivity during catalysis. By controlling the placement of the functional catalysts, to be mainly on the surfaces and not buried inside the walls of the materials we should see very high catalytic activity. In addition to testing these novel materials for catalytic activity, recent literature suggests that they may also be useful materials for carbon dioxide capture; therefore we are also investigating their absorption properties.

Notes:



Abstracts: Posters

P5 Amber Davidson, Acadia University

Development of an Online Kinetic Partial Extraction Method for Geochemical Exploration

A. Davidson

Undergraduate Student, Department of Chemistry, Acadia University

Partial extractions have been proposed to detect surface anomalies associated with buried mineral deposits. Partial extraction methods primarily leach metal ions that are weakly bound to soil particles, which may accumulate from vertical migration of metals from buried mineralization. However, many commercial partial extractions rely on proprietary methods in which the chemistry is not known. An online kinetic partial extraction method has been developed and tested on soil samples collected from Latties Brook, Nova Scotia. Fe, Ni, Zn, Cu, Pb, As, and U were monitored at 35 s intervals during the extraction by Inductively Coupled Plasma – Mass Spectrometry. Arsenic was measured in dynamic reaction cell mode using oxygen as a reaction gas. The pH and redox conditions were also measured during each extraction to monitor the digestion conditions. Redox conditions were monitored by measuring the $\text{Fe}(\text{OH})_3(\text{am})\text{-Fe}^{2+}$ couple which is likely the dominant iron mineral in the samples in this study. Two distinct patterns were observed from the partial extractions: 1) a rapid rise and fall in metal concentration which results in a maximum at approximately 10 min. and 2) a slightly slower increase in concentration that gradually levels off. A plot of the maximum concentration from each kinetic extraction was found to give much higher geochemical contrasts than possible by conventional batch extractions.

Notes:



Abstracts: Posters

P6 Katalin Devaine, Memorial University

Chromium(III) Amine-bis(phenolate) Complexes as Catalysts in the Copolymerization of CO₂ and Cyclohexene-oxide

Katalin Devaine P. and Christopher M. Kozak*

Graduate Student, Department of Chemistry, Memorial University

Chromium complexes utilized as catalysts for the coupling of CO₂ and epoxides have been widely studied recently. Specifically, chromium complexes with amine-bis(phenolate) ligands have been investigated in details in our group. Four different chromium(III) amine-bis(phenolate) complexes have been synthesized and characterized as prospective catalysts. The catalytic activity of the complexes have been investigated in the copolymerization of CO₂ and cyclohexene oxide. The synthesis and structure of the complexes as well as preliminary copolymerization results will be presented.

Aliphatic polycarbonates have become an attractive class of polymers due to their desirable properties, including high transparency, heat resistance, durability as well as potential biodegradability. The preparation of these classes of polymers from cheap and abundant ubiquitous feedstocks such as carbon dioxide (CO₂) is economically and environmentally appealing. Chromium compounds supported by salen (diimine-bis(phenolate)) ligands have been shown by others to be very active for the catalysis of CO₂/epoxide copolymerization (Darensbourg, *Adv Polym Sci.*, 2012, 245, 1) We are, therefore interested in assessing the reactivity of chromium in CO₂/epoxides copolymerization. Chromium(III) complexes supported by amine-bis(phenolate) ligands have been synthesized, structurally characterized and their reactivity explored. We sought to study the related, but structurally and electronically different, chromium (III) complexes of amine-bis(phenolate) ligands (see figure) as catalysts for this reaction. The synthesis and, structural characterization of the complexes as well as the preliminary CO₂/cyclohexene oxide copolymerization results will be presented.

Notes:



Abstracts: Posters

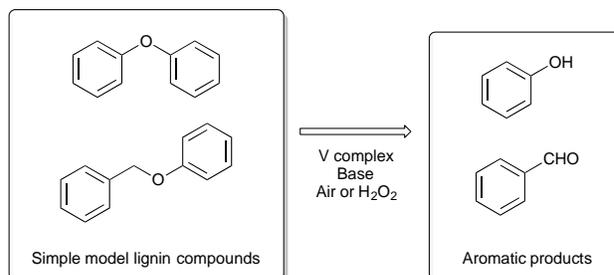
P7 Ali Elkurtehi, Memorial University

Oxidation Reactions Catalyzed by Vanadium Complexes of Amine-bis(phenolate) Ligands

Ali Elkurtehi and Francesca M. Kerton*

Graduate Student, Department of Chemistry, Memorial University

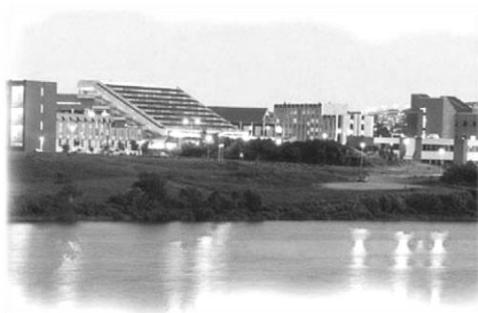
Lignin, a natural polymer composed of methoxy-substituted phenolic subunits, is an integral constituent of non-food biomass and potential source of valuable aromatic compounds. If suitable conversion chemistry is developed to break lignin down in a selective fashion it could potentially serve as a renewable chemical feedstock for chemicals or fuels. Vanadium compounds supported by *N,O*-containing ligands have been shown by others to be very active for the catalysis of C–O and C–C bond cleavage reactions in lignin model compounds.^{[1],[2]} Related oxovanadium complexes with amine-bis(phenolate) ligands possessing different steric, geometric and electronic parameters were prepared by us as possible catalysts for this reaction. The synthesis and structural characterization of the complexes as well as their initial catalysis for oxidation of 4-methoxybenzyl alcohol, diphenyl ether, benzyl phenyl ether and model lignin compounds results will be presented.



[1] Son, S.; Toste, F.D. *Angew. Chem. Int. Ed.* 2010, 49, 3791-3794.

[2] Hanson, S. K.; Baker, R. T.; Gordon, J. C.; Scott, B. L.; Thorn, D. L. *Inorg. Chem.* 2010, 49, 5611-5618.

Notes:



Abstracts: Posters

P8 Victoria Grandy, Memorial University

Vibrational Density of States of Glassy Silica Systems via Molecular Dynamics Simulations

Victoria R. Grandy, Kristin Poduska, and Ivan Saika-Voivod
Undergraduate Student, Department of Physics, Memorial University

In this study, vibrational properties of silica-based materials are correlated with details of chemical and structural disorder, with glassy silica serving as a reference system. Molecular dynamics computer simulations are carried out on glassy silica, using GROMACS software, to track changes in the vibrational density of states (VDOS) – calculations related to vibrational modes also observed in infrared spectra – as well as in the radial distribution function, a more direct measure of structure. Several impurities are studied: sodium, aluminum, phosphorus, and hydroxide. The addition of such atoms to the glassy silica system result in observable and correlated changes to the calculated VDOS. Modes observed in the VDOS are correlated with modes in real silica systems, and it is shown that each impurity type affects the system differently. Coupled with pair correlation and coordination number analysis, changes in peak intensity and shape are inferred based on the vibrational modes of the system. Because of this relation, it is plausible that Gaussian peak analysis of the VDOS could allow for more precise understanding of how different types of impurities affect each mode separately, and subsequently give predictive power to the simulations. These simulations may be used to decipher and predict the modes, and hence related IR spectra, of real glassy and crystalline silicate materials, such as siliceous phytoliths found in archaeological sites. This may then be used in determining material composition.

Notes:



Abstracts: Posters

P9 Iyad Hailat, Memorial University

Identification of Steryl Esters in Margarine and Corn Kernels Using ESI-MS/MS and ESI-MS/MS/MS Ion Trap-Mass Spectrometry

Iyad A. Hailat, Christopher C. Parrish, and Robert J. Helleur

Graduate Student, Department of Chemistry, Memorial University

Steryl esters play an important role in the inhibition of intestinal cholesterol absorption and in other biochemical processes and their direct analysis by MS would be very useful. We demonstrate here a new approach for steryl ester identification using ESI-MS/MS and ESI-MSMS/MS ion trap mass spectrometry sterols and other lipids were extracted from samples using hexane and the steryl esters separated from other lipids using solid phase extraction cartridge (strata NH₂). The steryl ester fraction was found to elute with hexane: diethyl ether (98:2, v/v).

The steryl esters were dissolved in chloroform: methanol (2:1) followed by addition ammonium acetate at a final concentration of 20 mM. They were detected as ammoniated adducts [M+NH₄]⁺. Many of steryl ester isomers were identified using ESI-MS/MS by the facile ester cleavage and observation of both the sterol hydrocarbon and fatty acid ions. The order of abundance in steryl esters in margarine was found to be: 18:0 β-sitosteryl, 18:1 β-sitosteryl, 18:0 campesteryl, and 18:1 stigmasteryl. In corn: 18:1 β-sitosteryl and 18:1 stigmasteryl. For final confirmation of the structure of the sterol, ESI-MS/MS/MS was carried out where the fragmentation patterns of the steryl precursor ions were similar to those from free sterol standards.

For example, the following ion was selected for tandem MS structural elucidation of 18:0 β-sitosteryl ester.

ESI-MS	ESI-MS/MS	ESI-MS/MS/MS
698.6 (18:0 β-sitosteryl ester)	698.6 → 397.4(β-sitosterol)	397.4 → fragments similar to β-sitosterol standard

Our method was successfully used for identification of steryl esters extracted from margarine and corn kernels.



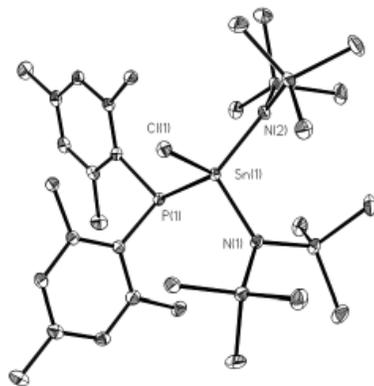
Abstracts: Posters

P10 Kimberly Hyson, Acadia University

The Study of Asymmetric Heavy Main Group Multiple Bonds With Phosphenium Cation Precursors and Tin(II)

Kimberly D. Hyson, Paul A. Gray, Emily C. Fraser, Jason D. Masuda, and Bobby D. Ellis*
Undergraduate Student, Department of Chemistry, Acadia University

Compounds containing multiple bonds between heavier main group elements continue to exhibit interesting and new properties. While symmetric heavy multiple bonds are relatively easy to synthesize through the reduction of appropriate precursors, general routes to asymmetric multiple bonds continue to be synthetically challenging. Our research group has been developing methodologies for asymmetric heavy multiple bond synthesis by employing reactive phosphenium cations and precursors with divalent Group 14 compounds: *N*-heterocyclic carbenes (:CR_2) and stannylenes (:SnR_2). The phosphorus-carbene products resulted in Lewis acid-Lewis base adducts, while the phosphorus-stannylene products yielded a different structural arrangement of a stannylphosphine, $\text{Ar}_2\text{P-SnClR}_2$. The products have been characterised with ^1H , $^{13}\text{C}\{^1\text{H}\}$ and $^{31}\text{P}\{^1\text{H}\}$ NMR spectroscopy; one of the stannylphosphines produced was further characterised with X-ray crystallography.



Notes:



Abstracts: Posters

P11 Yasaman Jami, Memorial University

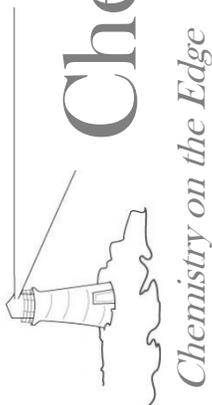
Irreversible Enzyme Inhibitors

Yasaman Jami

Graduate Student, Department of Chemistry, Memorial University

Many drug molecules are enzyme inhibitors, so their discovery and improvement is an important part of research in biochemistry and pharmacology. These molecules can bind either reversibly or irreversibly. Many irreversible inhibitors act through a Michael addition reactions of an electrophile to the thiol moiety of a cysteine side chain. The efficiency of these drugs is influenced by the rate and reversibility of these reactions. Four electrophiles were studied computationally; cinnamaldehyde, methyl cinnamate, cinnamitrile, and (E)-Methyl 2-cyano-3-phenylacrylate. A reaction was modeled between these molecules and the deprotonated thiolate, which serves as a model nucleophile. The thermodynamic reversibility of this nucleophilic reaction on $\alpha\beta$ -unsaturated carbons can be predicted by scanning the potential energy surface (PES) where bond breaking and forming occurs. Different density functional theory (DFT) and wave function methods showed a variety of PESs. In order to rationalize these observations, we looked at the charge distribution during the scan and the composition of molecular orbitals during the formation of the carbanion using natural bond orbital theory. Electron affinities of the thiolates were calculated in an attempt to rationalize the deviation in the result of Hartree Fock method compared to DFT methods. Finally, the effect of solvent effects on the reaction energy were calculated using implicit solvation methods.

Notes:



Abstracts: Posters

P12 Mohammad Javashi, Memorial University

Formic Acid Oxidation at Polyaniline Supported Pt Nanoparticles

Mohammad Javashi and Peter G. Pickup

Graduate Student, Department of Chemistry, Memorial University

The electrocatalytic activity of platinum toward oxidation of formic acid has been widely studied during recent years, in part because of its importance to the development of formic acid fuel cells. It has been shown that using conducting polymers (CPs) as catalyst supports has a considerable positive impact on the activity.

The present work is aimed at comparing the catalytic activity of Pt nanoparticles in the presence and absence of various polyaniline derivatives as catalyst supports. Chronopotentiometry has been used to polymerize the various aniline-derivatives on the surface of glassy carbon (GC) electrodes. The Pt nanoparticles were then drop-coated onto both bare and CP coated GC electrodes. To investigate the electrocatalytic activity of the catalysts, cyclic voltammetry (CV) was used. Results have shown enhanced catalytic activity towards formic acid oxidation for GC/Polyaniline-Pt electrodes compared to GC/Pt. Methyl and trifluoromethyl substituents on the polyaniline decrease its effect.

Notes:



Abstracts: Posters

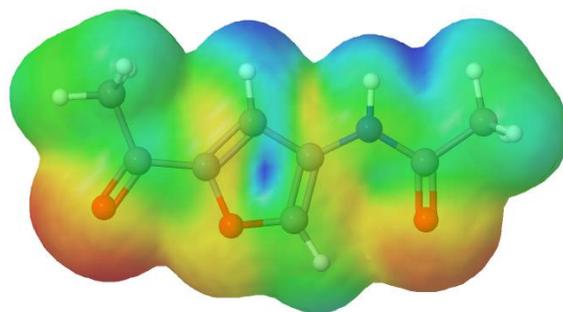
P13 Yi Liu, Memorial University

The Synthesis of 3-Acetamido-5-acetylfuran from N-Acetyl-D-glucosamine Using Ionic Liquids

Yi Liu and Francesca M. Kerton*

Graduate Student, Department of Chemistry, Memorial University

Chitin can be obtained from the shells of crustaceans (i.e. shellfish waste), and is the most abundant biopolymer in the ocean. N-acetyl-D-glucosamine (NAG), a sugar, is the monomer of chitin. Controlled dehydration of NAG can generate a new compound, 3-acetamido-5-acetylfuran (3A5AF).^[1] This is the first nitrogen-containing product obtained from the dehydration of a hexose in solution, and we hope that it can act as a platform chemical for a series of substances. We are interested in the synthesis of 3A5AF from NAG using ionic liquids. The first one we used was [Bmim]Cl, and since this initial study we have tried some acidic ionic liquids, such as [Bmim][HSO₄] and [Bmim-SO₃H][HSO₄]. The function of additives (NaCl and B(OH)₃), and extracting solvents (EtOAc, 2,5-Me-THF) has also been tested. The reaction was conducted under different conditions, and results were compared for improvement of the yield. In addition, some properties of 3A5AF were also explored through computational studies. The pK_a value of 3A5AF is 14.75 according to calculations, and this result will be checked through lab experiments. The electrostatic potential of the molecule (see below), as well as the frontier molecular orbitals, were also computed.



Electrostatic potential of 3A5AF
(Red area: electron rich; blue area: electron poor)

[1] Omari *et al.*, *ChemSusChem*, **2012**, *5*, 1767-72; Drover *et al.*, *RSC Advances*, **2012**, *2*, 4642-4643.



Abstracts: Posters

P14 Brittany MacDonald, Cape Breton University

Application of Microwave Irradiation for the Enhancement and Desulphurization of Heavy Crude Oils

Brittany MacDonald

Undergraduate Student, Department of Chemistry, Cape Breton University

Microwave energy is becoming the most diverse form of energy transfer and has been used in the petroleum industry for inspecting coiled tubing and line pipe, measuring multiphase flow, and the mobilization of asphaltic crude oil. Though its implications in petroleum applications are yet to be fully understood, the non-thermal aspects of energy transfer between microwaves and other forms of matter are always visible in processes where microwave energy is used to cause a chemical or physical change in the irradiated material. In Canada, efforts have been intensified to develop microwave irradiation technology for in-situ enhanced oil recovery of the country's large deposits of bitumen and heavy oil. Of the estimated 30 billion barrels of heavy oil in place, about 26 billion barrels are considered unrecoverable using the current technology. The microwave technology improved recovery by 20 percent with no discharge of greenhouse gas into the environment. The new technology employs specific frequency microwaves targeted into the formation containing heavy hydrocarbons to initiate conversion of the hydrocarbon into synthetic crude. Results thus far showed strong indications for the microwave technology to be employed not only for hydrocarbon extractions but also for in-situ upgrading and field upgrading of heavy oil and bitumen desulphurization of crude oil, and future upgrading of coal and oil shale. As much as 80 percent desulphurization of heavy oil has been obtained with microwave irradiation. Overall, the microwave technology presents the best alternative, economically and environmentally, to the existing technologies for enhanced oil recovery operations and processing.

Notes:



Abstracts: Posters

P15 Marybeth MacDonald, Cape Breton University

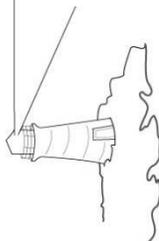
Rhodotorula glutinis Phenylalanine Ammonia Lyase Enzyme Catalyzed Synthesis of the Methyl Ester of p-Hydroxycinnamic Acid

Marybeth MacDonald

Undergraduate Student, Department of Chemistry, Cape Breton University

The hypothesis that *Rhodotorula glutinis* phenylalanine/tyrosine ammonia lyase (PAL/TAL) enzyme can be successfully used in the transformation of L-tyrosine methyl ester (L-TM) to the methyl ester of *para* hydroxycinnamic acid (p-HCAM) was tested. Formation of p-HCAM was followed by spectrophotometric determination at 315 nm. The following conditions were optimized for maximal transformation of L-TM to p-HCAM: pH (8.5), temperature (37 °C), incubation time (60 min), speed of agitation (50 rpm), enzyme concentration (0.08 μM), and substrate concentration (1.0 mM). The product (p-HCAM) of the reaction of PAL/TAL with L-TM was analyzed using reversed-phase ultra high performance liquid chromatography (UPLC) coupled with electrospray ionization mass spectrometry (UPLC-ESI-MS) and nuclear magnetic resonance (NMR) spectroscopy. The ultra-violet (UV) spectrophotometric assays, and the UPLC-MS chromatograms and mass spectra of PAL/TAL reaction product and authentic p-HCAM demonstrated the feasibility of carrying out PAL/TAL catalyzed biotransformation of L-TM to p-HCAM.

Notes:



Abstracts: Posters

P16 John MacInnis, Cape Breton University

Evaluation of Novel 6% Cyanopropylphenyl 94% Dimethylpolysiloxane and NSPPAH GC Columns for Analysis of Volatile Organic Compounds Using GC and GC-MS

Krishnat P. Naikwadi, Allen J. Britten, John J. MacInnis, and Kelsey D. AuCoin
Undergraduate Student, Department of Chemistry, Cape Breton University

Development and applications of new 6% Cyanopropylphenyl 94% Dimethylpolysiloxane, a mid-polarity nano stationary phase GC column (NSP-624), 5% Phenyl 95% dimethylpolysiloxane (NSP-5) and NSP-PAH columns were evaluated for analysis of volatile organic compounds specified in various USEPA methods. Lower thermal stability is a limiting factor for the use of cyanopropyl-substituted columns, which results in longer run times. In the current investigation a 6% Cyanopropylphenyl 94% Dimethylpolysiloxane stationary phase in the nano form is developed (designated as NSP-624), which is stable up to 320°C. The highly phenylated NSP-PAH column was evaluated for EU, USEPA, and Environment Canada priority PAH.

Notes:



Abstracts: Posters

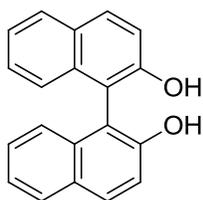
P17 Marc Mackinnon, Memorial University

BIPOL: Pyrene Goes on an Unexpected Journey

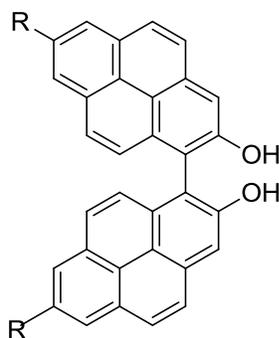
M. R. MacKinnon and G. J. Bodwell

Graduate Student, Department of Chemistry, Memorial University

1,1'-Bi-2-naphthol (BINOL) (**1**) and its derivatives are ubiquitous in asymmetric catalysis. Not only are BINOL and its derivatives extensively used as chiral ligands in a broad range of asymmetric catalytic reactions, but they have also found frequent application as enantioselective fluorescent sensors, despite BINOL's low quantum yield (0.02). Pyrene is a polycyclic aromatic hydrocarbon that is prized for its photophysical properties and has been incorporated as a fluorescent probe in numerous systems. However, no marriage of the axially chiral BINOL with the unique photophysical properties of pyrene has been reported in the literature. The synthesis and resolution of this new compound, 1,1'-bi-2-pyrenol (**2**), will be discussed along with its properties.



1



2

R = H, *t*-butyl

Notes:



Abstracts: Posters

P18 Alyssa Moss, Cape Breton University

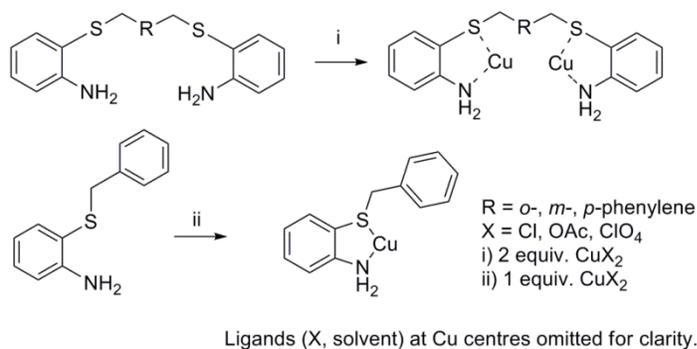
Synthesis and Characterization of Mono- and Binuclear Copper Complexes with Multidentate N,S- Ligands

Alyssa Moss

Undergraduate Student, Department of Chemistry, Cape Breton University

An important class of Cu containing monooxygenases is the heterodomain of peptidylglycine alpha-amidating monooxygenase (PAM) and peptidylglycine alpha-hydroxylating monooxygenase (PHM). PAM is the only known enzyme involved in the biosynthesis of α -amidated peptide hormones – an essential class of hormones for mammals, insects and cnidarians (jelly fish); α -amidated peptide hormones are also reported to be autocrine growth factors for small cell lung cancer. Both PHM and its sister-enzyme dopamine beta monooxygenase (DbM) are essential for neuroendocrine function. Although PHM and DbM share only 27% sequence homology, the active site architecture is similar with respect to the ligand environments of each Cu domain and their respective spacing (10.6 Å). In addition, both enzymes utilize a Cu-superoxo nucleophile to cleave the C-H bond of each substrate resulting in stereospecific hydroxylation, S for PHM and R for DbM, respectively.

We synthesized a series of mono- and binuclear copper complexes as biomimetic models for type-II Cu enzyme domains with histidine- and methionine coordination (scheme 1). Complexes were synthesized in variety of solvents (acetonitrile, MeOH, EtOH) and various copper salts (CuCl₂, Cu(OAc)₂ and Cu(ClO₄)₂) and N,S-ligands containing the ortho-aminothiophenol motif.



Scheme 1



Abstracts: Posters

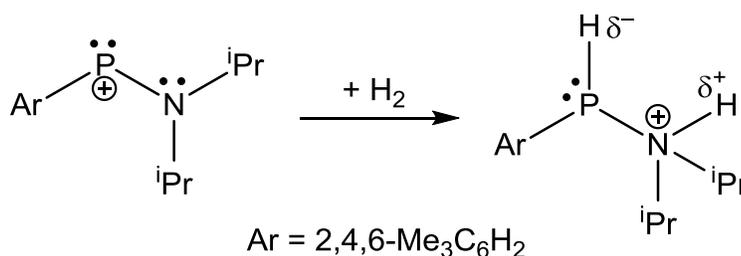
P19 Jakob Nickerson, Acadia University

New Green Reducing Agents: Hydrogenated Phosphenium Cations

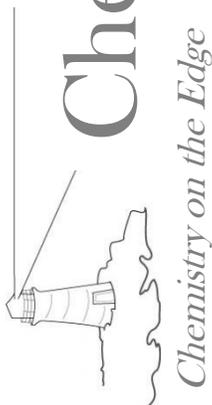
Jakob Nickerson

Undergraduate Student, Department of Chemistry, Acadia University

Phosphenium cations are isoelectronic with carbenes; both species are dicoordinate, with a lone pair of electrons and an empty orbital. Phosphenium cations, like carbenes, are typically stabilised by sigma-withdrawing and pi-donating substituents (*e.g.*, NR₂, OR, SR). Bis(amido) phosphenium cations, P(NR₂)₂⁺, are stabilised such that they do not react with hydrogen gas, however, when one of the amido substituents is exchanged with an aryl substituent hydrogenation occurs. Whereas the analogous *N,C*-bonded carbenes add both hydrogen centres to the divalent carbon, *N,C*-bonded phosphenium cations add hydrogen across the P–N bond resulting in products with both hydric and protic hydrogen centres. Application of this hydrogenated product as a reducing agent for polar multiple bonds is investigated.



Notes:



Abstracts: Posters

P20 Karanbir Pahil, Cape Breton University

Optical Constants and Vibrational Intensities of Trichloromethane

K. S. Pahil

Undergraduate Student, Department of Chemistry, Cape Breton University

Infrared and Raman spectra have been collected and analyzed for both liquid chloroform and liquid chloroform-d. The imaginary polarizability (IP) spectra, under the Lorentz local field model, have been calculated from the experimental infrared spectra and curve fit to separate intensities. The curve fit and vibrational assignment of chloroform and chloroform-d are presented as well as previous assignments of chloroform. A total of 293 peaks are required to fit the experimental imaginary molar polarizability spectrum of chloroform with CDHO bands while 166 peaks are required to fit the experimental imaginary molar polarizability spectrum of chloroform-d with CDHO bands. The R^2 -values of both fits are very close to 1, indicating a near perfect fit. The areas under the fitted spectra of chloroform and chloroform-d are 0.2% and 0.3% larger than the area under the experimental spectra, respectively. The non-polarized, parallel polarized and perpendicular polarized Raman spectra of chloroform were fit with 32, 44 and 39 peaks, respectively. Computational *ab initio* calculations were performed to create theoretical chloroform and chloroform-d spectra, which aided in assigning vibrations in the experimental spectrum. The dipole moment derivatives with respect to normal, symmetry and internal coordinates are also presented.

Notes:



Abstracts: Posters

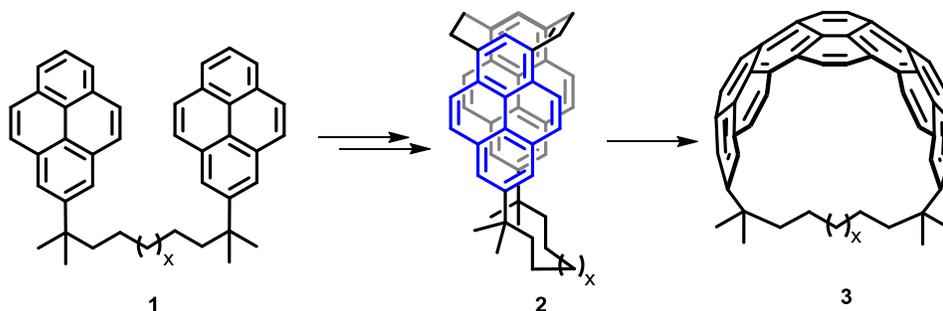
P21 Kiran Sagar, Memorial University

Synthesis and Fluorescence Properties of a Series of 1,1,*n*,*n*-Tetramethyl[*n*](2,11)teropyrenophanes

Kiran Sagar U. and Graham J. Bodwell*

Graduate Student, Department of Chemistry, Memorial University

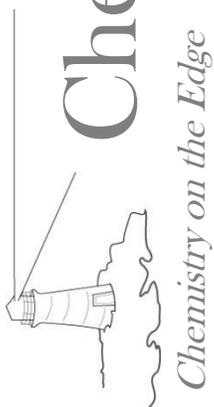
The chemistry of nonplanar aromatics draws considerable attention due to its synthetic and theoretical interest in the field of fullerene and carbon nanotube chemistry. Due to their optical properties, these compounds may find various applications in materials chemistry. One way of distorting an aromatic system from its normal planar geometry is to introduce a bridge between nonadjacent positions, i.e. to incorporate it into a cyclophane. For the past two decades the Bodwell group has reported the synthesis of various pyrenophanes^[1] and, more recently, a cyclophane with a much larger nonplanar aromatic system, 1,1,8,8-tetramethyl[8](2,11)teropyrenophane **3** ($x = 2$).^[2] The higher and lower homologues of this cyclophanes have now been synthesized using a common approach. The synthetic route utilizes McMurry and Wurtz-type couplings to install the two-carbon bridges in cyclophanemono-ene **2** and a valence isomerization/dehydrogenation (VID)^[3] reaction to generate the nonplanar teropyrene system.



[1] Bodwell, G. J.; Miller, D. O.; Vermeij, R. J. *Org. Lett.* 2001, 3, 2093-2096; Zhang, B.; Manning, G. P.; Dobrowolski, M. A.; Cyranski, M. K.; Bodwell, G. J. *Org. Lett.* 2008, 10, 273-276.

[2] Merner, B. L.; Dawe, L. N.; Bodwell, G. J. *Angew. Chem. Int. Ed.* 2009, 48, 5487-5491.

[3] Mitchell, R. H.; Boekelheide, V. J. *Am. Chem. Soc.* 1970, 92, 3510-3512.



Abstracts: Posters

P22 Eric Sampson, Acadia University

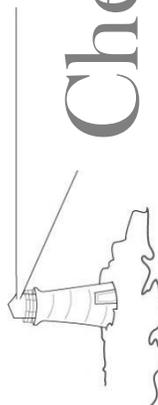
Synthesis of Coordination Complexes for Photodynamic Therapy

Eric Sampson and Sherri A. McFarland

Undergraduate Student, Department of Chemistry, Acadia University

Photodynamic therapy (PDT) has been used clinically to treat cancer by destroying unwanted cells. This form of therapy uniquely employs a drug of low toxicity that only becomes toxic upon activation with light, allowing spatial and temporal selectivity through the judicious choice of irradiation conditions. Current PDT methods employ organic compounds whereby cell damage is inflicted indirectly via singlet oxygen generation by excited triplet states. Organic photosensitizers, therefore, rely on the presence of oxygen and do not function in hypoxic environments. This inability to function at low oxygen tension and their marginal extinction coefficients for red light warrant the development of better PDT agents. Herein we will report efforts aimed at developing inorganic photosensitizers for PDT. These have certain advantages over organic photosensitizers such as the potential for oxygen independent activity and absorption of red and NIR light. Synthetic processes will be discussed, and *in vitro* photobiological results will be highlighted.

Notes:



Abstracts: Posters

P23 Hilary Simon, Acadia University

Synthesis of Photoremovable Protecting Groups for Diols

Hilary Simon, Alex Chase, and Matthew Lukeman

Undergraduate Student, Department of Chemistry, Acadia University

2-Naphthols substituted with leaving groups at the 3-position have been shown to be capable of releasing a variety of biologically relevant substrates when irradiated with light in the UVA region. These reactions generate a naphthoquinone methide intermediate, which can be detected and characterized by laser flash photolysis. We have recently used this chromophore to 'cage' 1,3-propane diol, which is a simple diol that is representative of more complex diols such as carbohydrates. Exposure with UVA light leads to the smooth release of the free diol and the corresponding formyl-naphthol, which is detected by ^1H NMR spectroscopy and GCMS. We have detected the naphthoquinone methide intermediate and investigated its kinetics, and based on this we believe that the diol release takes place within tens of milliseconds. We are actively pursuing other related molecules.

Notes:



Abstracts: Posters

P24 Tim Strange, Memorial University

Excited State Dynamics Between Chloroquine and Ga(III)(PPIX)OMe

Tim Strange

Graduate Student, Department of Chemistry, Memorial University

The antimalarial properties of chloroquine (CQ) have been known for some time; elucidating the exact mechanism by which the activity takes place has provided quite a challenge.^[1] Recent work by Dodd et al. at the University of McGill has yielded information about the structural basis for the activity.^[2] Using gallium (III) protoporphyrin IX ([Ga(III)(PPIX)OMe]) as a NMR active substitute iron heme, a crystal structure was obtained depicting the structural interaction between the drug (chloroquine) and target molecule ([Ga(III)(PPIX)OMe]). Photophysical investigations of the same compounds at similar concentrations have provided insight into the solution structure between chloroquine and [Ga(III)(PPIX)OMe] adducts. The results of detailed excited state measurements will be presented and discussed in light of current theories for rapid energy transfer.

[1] <http://www.cdc.gov/malaria/about/history/#chloroquine>

[2] Dodd et al., Manuscript

Notes:



Abstracts: Posters

P25 Lynsay Thurber, Acadia University

Towards an Improved Passive In-Situ Sampler for Studying Trace Elements in Fresh Waters

Lynsay Thurber and John Murimboh

Undergraduate Student, Department of Chemistry, Acadia University

Diffusive gradients in thin films (DGT), an *in-situ* passive sampling technique, was developed and tested for measuring the bioavailability of trace metals in the aquatic environment. DGT is comprised of a three-layer system: filter membrane, diffusive layer, and a metal binding phase. Metals diffuse through the filter and diffusive layer to the binding layer which serves as a metal sink, creating a steady-state concentration gradient that forms the basis for measuring labile metal concentrations in solution. The sensitivity and reproducibility of DGTs were tested using a binding phase containing Chelex 100 resin embedded with polyacrylamide hydrogel and 3M Empore chelating extraction disk embedded with 90% imidodiacetate functionalized polystyrene divinylbenzene interwoven in a Teflon polytetrafluoroethylene (PTFE) support. DGTs were employed in four different bodies of fresh water to measure the bioavailability of Cu, Ni, Zn, Pb, and Cd. After a fixed length of time, the samples were extracted and the concentrations of various trace elements were measured using an ICP-MS.

Notes:



Abstracts: Posters

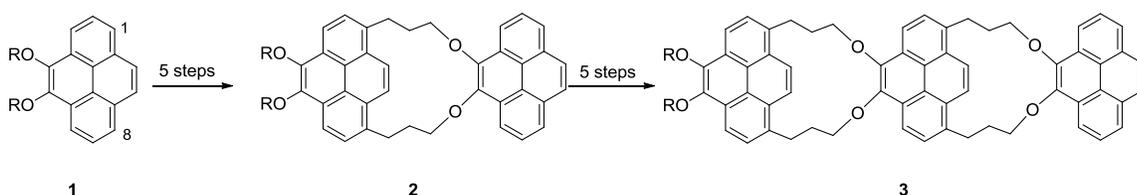
P26 Kerry-Lynn Williams, Memorial University

One Link at a Time: An Iterative Synthetic Route Towards Pyrenophane Chains

Kerry-Lynn M. Williams and Graham J. Bodwell*

Graduate Student, Department of Chemistry, Memorial University

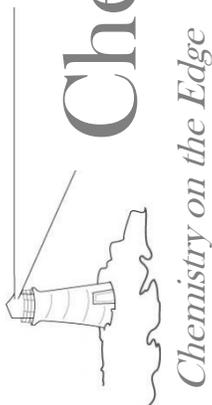
The use of pyrene as a building block for molecules with applications in optoelectronic devices is becoming increasingly important.[1] In this regard, the development of methodology that provides convenient and highly regioselective access to functionalized pyrenes will facilitate progress in this area. For example, our group recently showed that the placement of alkoxy groups at the 4 and 5 positions on pyrene (*e.g.* **1**) both activates the pyrene system towards electrophilic substitution and effectively hinders the 3 and 6 positions.[2] This methodology has been used in the synthesis of (1,8-pyrenylene)-ethynylene macrocycles[1] and is now at the heart of an iterative 5 step strategy aimed at the synthesis of oligomeric pyrenophanes **2**, **3** and beyond. Details of the synthesis and properties of these pyrenophane chains will be presented.



[1] Figueira-Duarte, T. M.; Müllen, K. *Chem. Rev.*, **2011**, *111* (11), 7260–7314.

[2] Venkataramana, G.; Dongare, P.; Dawe, L. N.; Thompson, D. W.; Zhao, Y.; Bodwell, G. J. *Org. Lett.*, **2011**, *13* (9), 2240–2243.

Notes:



Abstracts: Posters

P27 Stephen Wolfe, Acadia University

Synthesis of *m*-Nitrophenylacetate Photoremovable Protecting Groups

S. Wolfe and M. Lukeman

Undergraduate Student, Department of Chemistry, Acadia University

Photoremovable protecting groups, or PPGs, are compounds that can release a biologically active molecule when irradiated with light. We have developed a new type of PPG that undergoes photodecarboxylation to produce a carbanion intermediate when irradiated with light. This carbanion then undergoes β -elimination to release the protected molecule in its anionic form. This type of PPG offers many advantages, including good aqueous solubility, high reaction efficiency, and very fast kinetics (sub-nanosecond). One such PPG that we have been working on recently involves the photodecarboxylation of a substituted *meta*-nitrophenylacetic acid, which we have shown can efficiently release halide ions when irradiated in water. We are currently working at releasing substrates that have greater biological relevance, such as carboxylic acids and alcohols. In this presentation, we will present our recent progresses toward this goal.

Notes:



Abstracts: Posters

P28 Marwa Yasmin, Saint Mary's University

'Fab-Chips': Metal-Coated Fibers as Potential Substrates for Surface Enhanced Raman Spectroscopy

Marwa Yasmin and Christa L. Brosseau

Undergraduate Student, Department of Chemistry, Saint Mary's University

The 'Fab-Chips' project focuses on the development of metal-coated fabric based lab-on-a-chip device for rapid and portable diagnostic application. For instance, the 'fab-chips' may contain embedded microfluidics, which can detect disease biomarkers at point-of-care testing, or in military applications to monitor exposure to explosive residues and chemical warfare agents, or detecting environmental pollutants. The use of metal coating on fiber makes such chip a potential substrate for detection using surface-enhanced Raman scattering (SERS). An important aspect of this project is to optimize the SERS signals/activity of the "fab-chips" using wet chemical etching. For this purpose, different types of metal-coated fibers such as silver-electroplated copper fiber wrapped on silk were roughened by cyclic voltammetry (CV) in different solutions of 0.1 M silver nitrate, sulfuric acid and potassium chloride solution as well as by incubating fibers in silver nanoparticle (AgNP) solution for AgNP deposition. The roughened fibers were then incubated in 4, 4'-bipyridine solution and SERS spectra for 4, 4'-bipyridine detection were collected using roughened fibers as SERS substrate. Images of roughened fiber surface obtained by scanning electron microscope (SEM) is used for further surface morphology analysis. These experiments suggest that optimization of SERS activity of metal-coated fiber roughened by AgNP deposition is a promising method.

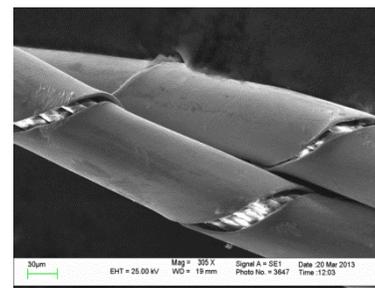
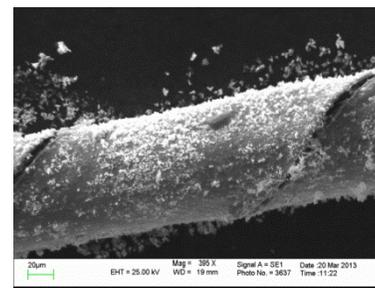
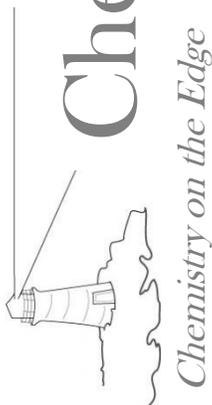


Figure 1. Top – SEM image of an untreated metal-coated fiber surface. Bottom – SEM image of a roughened metal-coated fiber surface showing silver nanoparticles (AgNPs)



Abstracts: Posters

P29 Huimin Yin, Acadia University

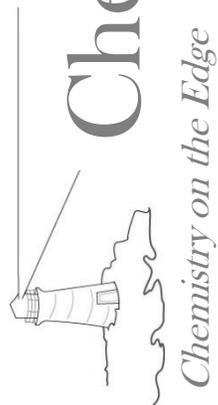
Development of In Vitro Screening Methods for Anticancer Agents

Huimin Yin and Sherri A. McFarland

Graduate Student, Department of Chemistry, Acadia University

Photodynamic therapy (PDT) is regarded as a new weapon to treat cancer, which uses light to activate otherwise nontoxic drugs. High systemic toxicity is one of the drawbacks associated with conventional chemotherapy, and PDT offers the opportunity to destroy cancer without debilitating side-effects. Current PDT approaches utilize a drug, called a photosensitizer (PS), red light, and oxygen to destroy unwanted cells, but significant effort is aimed at developing new PSs that function in the absence of oxygen and can be activated with NIR light. Unfortunately, it is difficult to compare a new PS to established clinical agents or to agents in the literature owing to the large number of variables associated with in vitro PDT evaluation. In order to ascertain whether a PS can act as a PDT agent and to compare a given agent with other agents, in vitro assays must be developed that standardize parameters such as: (i) pre-PDT incubation time, (ii) light dose (wavelength and time), (iii) light source (continuous or pulsed lasers, LEDs, lamps, etc.), (iv) post-PDT incubation time (v) cell viability determination (method and time), and (v) average number of replicates for each cancer cell type of interest. In this presentation, an in-house, standardized method for evaluating new PS for PDT will be discussed, and several examples from synthetic drug design and natural products chemistry will be used to illustrate the advantages and disadvantages of the methodology.

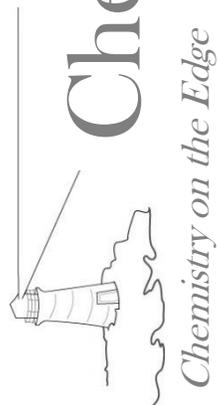
Notes:



ChemCon 2013



Notes



ChemCon 2013



Notes
